NONLOCAL FINITE ELEMENT SOLUTIONS FOR STEADY STATE UNSATURATED FLOW IN BOUNDED RANDOMLY HETEROGENEOUS POROUS MEDIA USING THE KIRCHHOFF TRANSFORMATION

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DEDICATION

To

My parents Qiuju Zhu & Shaoliang Lu

My wife Xiaoxi Wu

And

My children Megan & Helen

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ABSTRACT

We consider steady state unsaturated flow in bounded randomly heterogeneous soils under influence of random forcing terms. Our purpose is to predict pressure heads and fluxes and evaluate uncertainties associated with these predictions, without resorting to Monte Carlo simulation, upscaling or linearization of the constitutive relationship between unsaturated hydraulic conductivity and pressure head. Following *Tartakovsky et al.* [1999], by assuming that the Gardner model is valid and treating the corresponding exponent α as a random constant, the steady-state unsaturated flow equations can be linearized by means of the Kirchhoff transformation. This allows us develop exact integro-differential equations for the conditional first and second moments of transformed pressure head and flux. The conditional first moments are unbiased predictions of the transformed pressure head and flux, and the conditional second moments provide the variance and covariance associated with these predictions. The moment equations are exact, but they cannot be solved without closure approximations. We developed their recursive closure approximations through expansion in powers of σ_Y and σ_β, the standard deviations of $Y = \ln K_s$ and $\beta = \ln\alpha$, respectively, where K_s is saturated hydraulic conductivity. Finally, we solve these recursive conditional moment equations to second-order in σ_Y and σ_β, as well as second-order in standard deviations of forcing terms by finite element methods. Computational examples for unsaturated flow in a vertical plane, subject to deterministic forcing terms including a point source, show an excellent agreement between our nonlocal solutions and the Monte Carlo solution of the original

stochastic equations using finite elements on the same grid, even for strongly heterogeneous soils.

CHAPTER 1
INTRODUCTION

1.1 SCALE ISSUES AND SPATIAL HETEROGENEITY

Geological materials are ubiquitously heterogeneous. Even within a given soil type, the hydraulic properties may vary significantly in space [*Warrick and Nielsen*, 1980]. As a result, soil properties that enter as input parameters to water flow and solute transport equations may exhibit spatial variability or heterogeneity. Hydraulic properties exhibit spatial variations on various scales: in the laboratory due to variations in pore size and pore geometry; in the field due to soil stratification; and on a regional scale due to large-scale geological variability. Theories of flow and solute transport through porous media are typically based on, and supported by, laboratory experiments. Therefore, we encounter a scale problem when applying these theories to field situations in which heterogeneities appear on a larger scale. Two approaches have been used to address this issue in a vadose zone context: a system approach and a physically-based approach. In the system approach, the vadose zone is treated as a black box whose governing principle is determined by the relationship between available input and output records [*Jury et al.*, 1986]. The physically-based approach relies on the upscaling of laboratory experimental results to various field scales of interest.

At the pore-scale, fluid flow is governed by the Navier-Stokes equation. However, it is neither practical nor necessary to describe flow in all individual pores of the medium mathematically; in practice, one is interested mainly in average (macroscopic) descriptions of flow over volumes of the medium that allow measurement of phenomenological parameters and system states. Details of flow on scales smaller than such support volumes are ignored. Phenomenological parameters and states measured or defined on support volumes are associated with a mathematical point at the center of the volume and considered as functions of space, defined over a continuum of such points.

Heterogeneity depends on the size of the support volume. Soil properties measured on a small support scale may exhibit rapid (high frequency) and large (high amplitude) spatial variations. In a statistically homogeneous medium, these variations decrease in amplitude and frequency as the support volume increases. In such a medium, it may sometimes be useful to speak of a Representative Elementary Volume (REV) at which the variations are smooth enough to disregard their statistical character. In general, however, natural soils and rocks tend to be statistically non-homogeneous and the concept of a REV loses its utility. Even in statistically homogeneous media, REVs are often difficult to define and may differ (sometimes substantially) from the support volumes of available data. We will therefore base our discussion on the idea that data are available on a given support scale which is not necessarily an REV, and that the flow equations must describe phenomena on the same scale so as to be compatible with the data.

A rigorous analysis of water flow and solute transport in partially saturated media should consider the simultaneous movements of water and air. Often, the movement of air can be ignored when one is interested mainly in the flow of water. Our interest centers on steady state water flow in a variably saturated soil that is governed by

$$\nabla \cdot \left[K(\boldsymbol{x},\psi) \nabla \left(\psi(\boldsymbol{x}) + x_3 \right) \right] = 0 \qquad \boldsymbol{x} \in \Omega \tag{1-1}$$

The unsaturated hydraulic conductivity $K(\boldsymbol{x}, \psi)$ in (1-1) varies with location and the pressure head ψ (or, equivalently, water content or saturation). Mathematical formulae [*Brooks and Corey*, 1966; *Mualem*, 1976; *van Genuchten*, 1980] are typically employed to describe its dependence on pressure head or water content. One popular formula is the exponential model of *Gardner* [1958],

$$K(\psi) = K_S \exp(\alpha\psi) \tag{1-2}$$

where K_s is saturated hydraulic conductivity and α is a pore-size distribution parameter. Gardner's model often fails to reproduce adequately measured relationships between K and ψ over the entire range of saturations [*Russo*, 1988]. *Zhang et al.* [1998] developed and compared one-dimensional flow solutions for gravity-dominated flow in second-order stationary media using Brooks-Corey and Gardner-Russo models. They found that the two models yield significantly different mean head and mean effective water content at extreme values of saturation (dry and wet), but rather similar values at intermediate saturations. They also found that the Brooks-Corey model has certain advantages over the Gardner-Russo model. The Gardner model is nevertheless appealing due to its relative simplicity, which has made it a favorite among analysts of unsaturated flow in randomly heterogeneous soils.

In addition to its simplicity, the main reason for adopting Gardner's model in this dissertation is that it allows one to preserve constitutive nonlinearity when one uses the Kirchhoff transformation to solve a stochastic version of (1-1). For this, one must define α as a space-independent random constant. *Tartakovsky et al.* [1999] justified this assumption on the basis of published data concerning the spatial variability α. Treating α as a random constant allowed them to develop exact conditional first and second moment equations for stochastic steady state unsaturated flow, which have integro-differential forms similar to those developed for steady state saturated flow by *Neuman and Orr* [1993a,b], *Neuman et al.* [1996], and *Guadagnini and Neuman* [1997, 1998, 1999a,b]. Upon imposing a limitation on the variability of α, they were able to solve these stochastic moment equations analytically with the aid of the Kirchhoff transformation. The following several paragraphs regarding the variability of α are mainly based on *Tartakovsky et al.* [1999].

Whereas many studies have been done about the spatial variability of K_s [for example, *Byers and Stephens*, 1983; *Sudicky*, 1986], relatively few studies have concerned themselves with the spatial statistics of α [*Reynolds and Elrick*, 1985; *Greenholtz et al.*, 1988; *White and Sully*, 1987, 1992; *Unlü et al.* , 1990; *Russo and Bouton*, 1992; *Ragab and Cooper*, 1993a, b; *Russo et al.*, 1997]. Unlike K_s that can be measured directly, the soil parameter α can be determined only by indirect methods. These include least square analyses of measured unsaturated hydraulic conductivity [*Russo* 1983, 1984a; *Unlü et al* ., 1990] or water retention [*Wierenga et al.*, 1991], sorptivity measurements [*White and Sully*, 1992], and inversion of infiltration measurements [*Russo and Bouton*, 1992]. All these studies find both K_s and α to be log-normally distributed except *Unlü et al.* [1990] who found α to be approximately normal. *White and Sully* [1992] attributed the lognormality of both K_s and α to the dependence of both parameters on the internal pore structure of the soil.

Values of α appear to depend strongly on soil texture and vegetation. *White and Sully* [1987] found α to range from 0.05cm^{-1} for clay to 0.71cm^{-1} for gravely loam fine sand; *Ragab and Cooper* [1993a, b] reported ranges of 0.15 - 1.34cm^{-1} for grassland, 0.36-0.37cm^{-1} for woodland, and 0.28 - 0.89cm^{-1} for arable land. The variance of lnα can be either large or small relative to that of lnK_s, depending on the study. *Unlü et al.* [1990] reported variances of lnα in the range 0.045-0.112, compared to a range of 0.391-0.960 for the variance of lnK_s. *Russo et al.* [1997] found the variance of lnα to be on the order of 0.425, compared to 1.242 for lnK_s. According to *Russo and Bouton* [1992] and *White and Sully* [1992], the variances of lnα and lnK_s are of similar orders. *Ragab and Cooper* [1993a, b] found the variance of lnα to exceed that of lnK_s. Both the latter authors and *Russo* [1992] reported large coefficients of variation for lnα.

There is no agreement on the correlation scales of lnK_s and lnα, and cross-correlation between these two parameters. *Russo and Bouton* [1992] reported that the estimated correlation scales of lnα in both vertical and horizontal directions were approximately 3 times smaller than the respective correlation scales of K_s. The lnα data of *Unlü et al* . [1990] exhibit a larger spatial auto-correlation scale than that of lnK_s. *Ragab and Cooper* [1993a,b] found a lack of cross-correlation between lnα and lnK_s in all three soil types they have investigated. *Russo and Bouton* [1992] reported weak cross-correlation ($\rho \approx 0.3$) between lnK_s and lnα, and treated them as independent (and thus uncorrelated) random functions based on experimental evidence due to *Russo* [1983, 1984]. They ascribed such lack of cross-correlation to the fact that, in field soils, K_s is controlled by structural (macro) voids, while α is controlled by the entire continuum of pore sizes. Weak cross-correlation was reported also for the Las Cruces trench site [*Wierenga* et al. 1991]. On the other hand, *Russo et al.* [1997] found lnα and lnK_s data to exhibit a moderate correlation coefficient of 0.68, while *Unlü et al* . [1990] reported a correlation coefficient as high as 0.80.

Considering the above findings, *Tartakovsky et al.* [1999] felt comfortable treating both K_s and α as being log-normally distributed. They also felt comfortable disregarding cross-correlations between K_s and α, and their logarithms, as these correlations are week in the majority of soils examined to date. The same approach is adopted in this study.

1.2 STOCHASTIC ANALYSIS

The characterization of heterogeneity requires information about the hydraulic properties of the porous medium. As the medium cannot be sampled exhaustively, the available data must be analyzed statistically. That is, the spatial variation of hydraulic properties is characterized by their joint probability distributions and/or statistical moments, as inferred from available measurements. Hydraulic conductivities are usually reported to be univariate lognormal [*Bakr*, 1976; *de Marsily*, 1986; *Sudicky*, 1986, *Jensen et al.*, 1987]. Based on this assumption, *Freeze* [1975] treated hydraulic conductivity as a spatially uncorrelated random variable and analyzed uncertainty in groundwater flow by numerical Monte Carlo simulation. Although hydraulic conductivity varies significantly in space, its variation is not entirely random, but correlated in space [*Bakr*, 1976; *Byers and Stephens*, 1983; *Hoeksema and Kitanidis*, 1984; *Russo and Bouton*, 1992]. This suggests that hydraulic conductivity must be treated as a random field rather than a single random variable.

1.2.1 Monte Carlo Simulation

The most intuitive way to analyze spatial variability stochastically is via (conditional) Monte Carlo simulation. The principle of Monte Carlo simulation is straightforward. One treats hydraulic conductivity as a correlated random field whose statistical properties (typically mean, variance and correlation scales) can be inferred from its measured values at different points in space, on a given support scale. Since values at other points are unknown, they are generated at random so that the generated random field honors (corresponds to, within a prescribed margin of error) the measured data. Each randomly generated realization of the hydraulic conductivity field is used to solve the flow equations numerically in a deterministic manner. Each realization thus yields a random flow solution, conditioned on the measured hydraulic conductivity data. A statistical analysis of many such random solutions provides (among others) their (conditional) mean, variance and covariance. The mean provides an optimum unbiased prediction of flow in the soil under uncertainty (due to unknown spatial variability of the hydraulic conductivity), and the variance-covariance provides a measure of the corresponding predictive uncertainty.

During the past two decades, Monte Carlo simulation has been widely used to investigate the effect of heterogeneity on flow in groundwater systems [for example, *Smith and Schwartz*, 1980, 1981a,b; *Ababou et al.*, 1989; *Tompson and Gelhar,* 1990]. For flow in the vadose zone, many researchers [such as *Bresler and Dagan*, 1981; *Dagan and Bresler*, 1979; *Ünlü et al.*, 1990; *Russo and Dagan*, 1991; and *Destouni and Cvetkovic*, 1991] have used Monte Carlo simulation to examine the effect of areal variability on flow and/or solute movement. *Hopman et al.* [1988] used Monte Carlo simulation to examine the effect of heterogeneity on multi-dimensional flow regimes. *Eaton and McCord* [1994] used Monte Carlo simulation to determine effective hydraulic conductivity in two-dimensional porous media, and to verify the moisture-dependent anisotropy concept. Because of numerical difficulties, most of the above studies have relied on relatively few Monte Carlo simulations [*Ünlü* et al., 1990; *Russo and Dagan*, 1991; *Polmann et al.*, 1991; *Tseng and Jury*, 1993; *Russo et al;* 1994; *Roth*, 1995]. As a result, the corresponding sample statistics may not be representative. Because of nonlinearity of the unsaturated Richards flow equation, numerical methods must rely on iterative schemes and a large number of iterations are required for the solution. In addition, Monte Carlo simulation requires a relatively dense grid to resolve high frequency variations of random fields. As a result, solving the Richards equation in a Monte Carlo mode is computationally expensive, even though computational time may be reduced by using a first-order perturbation solution as an initial guess for the numerical solution [*Harter and Yeh,* 1993]. Monte Carlo simulation of flow in the vadose zone is further hindered by the fact that numerical iterative schemes do not guarantee convergence of the solution during a given simulation, especially when the medium is highly heterogeneous. Furthermore, to obtain meaningful statistics from Monte Carlo simulations, one has to perform a large number of simulations. The number of simulations required for obtaining meaningful results increases with heterogeneity. More importantly, there are no reliable criteria to assess convergence of the method.

Based on the above discussion, there is a need to develop alternative approaches for solving stochastic unsaturated flow problems.

1.2.2 Alternative Approaches

One alternative to Monte Carlo simulation is to solve the stochastic flow and transport equation analytically by approximation, which usually consists of perturbation and linearization [*Yeh et al.*, 1985a-c; *Mantoglou and Gelhar*, 1987a-c; *Russo*, 1993]. By employing the Gardner's model, *Yeh et al.* [1983a-c] analyzed analytically the effect of variability of hydraulic conductivity and the pore size distribution parameter on unsaturated flow in an unbounded domain under a unit mean hydraulic gradient. Their analysis was based on a spectral solution of a perturbation approximation for the stochastic flow equation. Analytical expressions were derived that describe the variance of pressure head, flux and effective hydraulic conductivity as functions of statistical properties of the porous medium and the mean flow characteristics (such as mean hydraulic gradient). One important finding was that the effective hydraulic conductivity in stratified soil formations is anisotropic. *Mantoglou and Gelhar* [1987a,b] extended the analysis of *Yeh et al.* [1985a-c] to transient flow in an unbounded domain and found significant hysteresis in pressure head variance, unsaturated hydraulic conductivity and moisture capacity. Certain assumptions have been made by *Yeh et al.* [1983a-c] and *Mantoglou and Gelhar* [1987a,b], which limit the applicability of their models to specific cases. Both assumed that hydraulic properties are spatially homogeneous. While this assumption may be satisfactory in many situations, it is by no means always applicable.

In many cases, adoption of this assumption may be due to mathematical convenience rather than an accurate representation of the actual field conditions. For example, *Rajaram and McLaughlin* [1990] studied the hydraulic conductivity data from the Columbus Air Force Base and proposed methods for estimating large scale trends; *Rehfeldt et al.* [1992] examined the hydraulic conductivity at the same Columbus Air Force Base site and found that the conductivity field can be associated with a third-order polynomial trend. More importantly, both *Yeh et al.* [1983a-c] and *Mantoglou and Gelhar* [1987a,b] ignored the product of conditional perturbation terms in their mean flow equations, which does not yield the conditional mean head and thus their solutions are biased, unless the product of conditional perturbation terms is zero. The product terms will be zero if and only if all the values of the hydraulic conductivity field are known exactly, otherwise, it is non-zero and its magnitude comparing to the other terms in mean equations is unknown. *Mantoglou* [1992] further extended their models to a finite flow domain and nonstationality of the soil properties and flow characteristics, but again, the expected values of perturbation products of higher order have been neglected. Thus this methodology requires small fluctuations. Based on a small-perturbation approximation, *Indelman et al.* [1993a,b], without invoking the unit mean hydraulic gradient assumption developed a similar analytical model for bounded flow domain that allows the head field to be nonstationary. More recently, *Zhang* [1997] investigated, to first order in σ_Y^2, the combined effect of boundaries and nonstationarity due to a trend in log conductivity on the statistics of the head field and derived general equations governing the statistical moments of hydraulic head for steady state unsaturated flow. The results have been extended to transient unsaturated flow [*Zhang*, 1999].

Another alternative is to use traditional deterministic models, i.e., simply replacing the parameters in standard deterministic models by their (conditional) mean values. Since system outputs are generally nonlinear in the controlling parameters, results from this approach are generally different from the conditional mean outputs of Monte Carlo simulations. As shown later, such deterministic outputs would generally be biased and therefore less than optimal. To render these models less biased, there has been an intensive search in the literature for effective or equivalent parameters that could be used to replace their suboptimal counterparts. The search has focused on a method called upscaling which is the process of transferring information from a scale of actual heterogeneity to that of computational elements which are used to solve the stochastic equations numerically. Upscaling has been conducted numerically based on empirical equivalence criteria. More rigorous theoretical criteria of equivalence have been proposed for saturated hydraulic conductivity by *Indelman and Dagan* [1993a,b] and *Indelman* [1993] who established necessary and sufficient conditions to be satisfied by upscaling, but these are not easy to implement in practice.

A major conceptual difficulty with upscaling is that it postulates a local relationship between (conditional) mean driving force and flux (Darcy's law) when in fact this relationship is generally nonlocal [*Neuman and Orr,* 1993; *Neuman et al.,* 1996; *Tartakovsky and Neuman,* 1998a, b]. Even where localization is possible, the constitutive equations satisfied by conditional mean predictors may be fundamentally different from those satisfied by their random counterparts [*Neuman et al.,* 1998]. Another conceptual difficulty with traditional upscaling, according to *Neuman* [1997], is that it requires a priori definition of a numerical grid even though there are no firm theoretical guidelines for its selection. Hence it is necessary to continue developing alternative ways of predicting flow and transport deterministically in a manner consistent with (conditional) stochastic theory.

Still another deterministic alternative to Monte Carlo simulation is to write a system of partial differential equations satisfied approximately by the first two ensemble moments of hydraulic head, then solve them numerically. Since mean functions are usually smoother than their random counterpart, especially when sparse conditional points are available, a coarse grid can be employed.

Exact conditional moment equations for steady state flow in saturated media have been developed by *Neuman and Orr* [1993] and *Neuman et al.* [1996], for transient flow in saturated media by *Tartakovsky and Neuman* [1997, 1998a, b], for advective transport by *Neuman* [1993], for advective-dispersive transport by *Zhang and Neuman* [1996]. All these conditional moment equations are integro-differential and include nonlocal parameters that depend on more than one point in space and/or time. *Guadagnini and Neuman* [1997, 1998, 1999a-b] developed recursive approximations of these conditional moment equations for steady state saturated flow, which are similar to those for transient flow by *Tartakovsky and Neuman* [1997, 1998a, b], and showed how to solve these approximations numerically.

Exact conditional moment equations for steady state flow in unsaturated media have been developed by *Tartakovsky et al.* [1999]. They presented a deterministic alternative to (conditional) Monte Carlo simulation which allows predicting steady state unsaturated flow under uncertainty, and assess the latter by means of conditional second moments, without having to generate random fields or variables, without upscaling and without linearizing the constitutive characteristics of the soil. It should be noted that virtually all previously published moment analyses of unsaturated flow, whether analytical [*Andersson and Shapiro,* 1983; *Yeh et al.,* 1985a, b; *Mantoglou and Gelhar,* 1987a-c; *Yeh,* 1989; *Mantoglou,* 1992; *Russo,* 1995; *Zhang et al.,* 1998] or numerical [*Zhang and Winter,* 1998], have found it necessary to rely on perturbation approximations of soil constitutive relations.

Tartakovsky et al. [1999] have demonstrated that when the scaling parameter of pressure head is a random variable independent of location, the steady state unsaturated flow equation can be linearized by means of the Kirchhoff transformation for gravity-free flow. Linearization is also possible in the presence of gravity when hydraulic conductivity varies exponentially with pressure head according to the exponential model of *Gardner* [1958]. This allowed *Tartakovsky et al.* [1999] to develop exact conditional first and second moment equations for unsaturated flow which are nonlocal (integro-differential) and therefore non-Darcian. The authors solved their equations analytically by perturbation for unconditional vertical infiltration. Their solution treats α as a nonrandom constant and is otherwise valid to second order in the standard deviation, σ_Y, of natural log saturated hydraulic conductivity, $Y = \ln K_s$.

1.3 SCOPE OF THIS STUDY

In this study we extend the conditional moment theory of *Tartakovsky et al.* [1999] to include uncertainties in α and all driving forces (sources and boundary conditions) during steady state unsaturated flow in a randomly heterogeneous soil. By means of Kirchhoff transformation, we transform the original nonlinear Richards equation into a linear equation, and formulate exact nonlocal conditional first and second moment equations for the transformed variable and the flux $\boldsymbol{q}$ (Chapter 2). These equations are nonlocal and not closed. Following *Guadagnini and Neuman* [1997, 1998, 1999a-b], in Chapter 3, we derive perturbation approximations for these equations, valid to second order in σ_Y, σ_β, standard deviations of $Y=\ln K_s$ and $\beta= \ln\alpha$, respectively, and to second order in the standard deviations of driving forces. Based on these approximations, in Chapter 4, we develop a finite element algorithm for two-dimensional flow in the vertical plane with deterministic driving forces when Y and β are mutually uncorrelated. Once we solved for the mean transformed variable and its related (cross-)covariances, we then are able to find the mean and variance of the original variable, pressure head (Chapter 5). We show some computational results for $\sigma_\beta = 0$ in the presence of a point source, and compare them with those of (un)conditional Monte Carlo simulations in Chapter 6. Finally, the conclusions can be found in Chapter 7. Lengthy mathematical derivations have been relegated to Appendices A-D.

CHAPTER 2

EXACT CONDITIONAL MOMENT EQUATIONS FOR STEADY UNSATURATED STATE FLOW IN BOUNDED RANDOMLY HETEROGENEOUS POROUS MEDIA

2.1 INTRODUCTION

We describe steady state unsaturated flow by means of Darcy's law

$$\boldsymbol{q}(\boldsymbol{x}) = -K(\boldsymbol{x},\psi)\,\nabla\left[\psi(\boldsymbol{x}) + g x_3\right] \qquad \boldsymbol{x}\in\Omega \tag{2-1}$$

and the continuity equation

$$-\nabla\cdot\boldsymbol{q}(\boldsymbol{x}) + f(\boldsymbol{x}) = 0 \qquad \boldsymbol{x}\in\Omega \tag{2-2}$$

subject to the boundary conditions

$$\psi(\boldsymbol{x}) = \Psi(\boldsymbol{x}) \qquad \boldsymbol{x}\in\Gamma_D \tag{2-3}$$

$$-\boldsymbol{q}(\boldsymbol{x})\cdot\boldsymbol{n}(\boldsymbol{x}) = Q(\boldsymbol{x}) \qquad \boldsymbol{x}\in\Gamma_N \tag{2-4}$$

Here the Darcian flux $\boldsymbol{q}$ (LT^{-1}), the unsaturated hydraulic conductivity K (LT^{-1}) and the pressure head gradient $\nabla\psi(\boldsymbol{x})$ are representative of a bulk support volume ω centered about a point $\boldsymbol{x}=(x_1, x_2, x_3)^T$, such that ω is small compared to the flow domain Ω but is sufficiently large for equations (2-1) - (2-4) to be locally valid [*Neuman and Orr*, 1993a; *Tartakovsky et al.*, 1999]. The volume ω does not need to be a REV in the traditional sense [*Bear*, 1972]. The only requirement is that all quantities in (2-1)-(2-4) are measurable at the support scale ω inside the domain Ω and on its boundary Γ, which is the union of Dirichlet boundary Γ_D and Neumann boundary Γ_N. The term $f(\boldsymbol{x})$ is a random source/sink, $\Psi(\boldsymbol{x})$ is a randomly prescribed pressure head on Γ_D, $Q(\boldsymbol{x})$ is a randomly prescribed flux into Ω across Γ_N, $\boldsymbol{n}(\boldsymbol{x})=(n_1, n_2, n_3)^T$ is a unit outward normal to the boundary Γ, and g is 1 for flow with gravity and 0 for gravity-free flow. We assume that $f(\boldsymbol{x})$, $\Psi(\boldsymbol{x})$ and $Q(\boldsymbol{x})$ are random and prescribed in a statistically independent manner at the scale ω.

Substituting (2-1) into (2-2) gives

$$\nabla \cdot \left[K(\boldsymbol{x},\psi) \nabla \left(\psi(\boldsymbol{x}) + g x_3 \right) \right] + f(\boldsymbol{x}) = 0 \qquad \boldsymbol{x} \in \Omega \tag{2-5}$$

It is assumed in this work that unsaturated hydraulic conductivity $K(\boldsymbol{x}, \psi)$ satisfies

$$K(\boldsymbol{x},\psi) = K_s(x) K_r(\boldsymbol{x},\psi) \tag{2-6}$$

and the exponential model [*Gardner*, 1958]:

$$K_r(\boldsymbol{x},\psi) = e^{\alpha(\boldsymbol{x})\psi(\boldsymbol{x})} \tag{2-7}$$

where $K_s(\boldsymbol{x})$ and $K_r(\boldsymbol{x},\psi)$ are saturated and relative unsaturated hydraulic conductivity, respectively, and α is the reciprocal of the macroscopic capillary length scale [*Raats*, 1976]. As argued in Chapter 1, we take α to be space-independent, which allows us to define the Kirchhoff transformation [*Tartarkovsky et al.*, 1999]

$$\Phi(\boldsymbol{x}) = \int_{-\infty}^{\psi(\boldsymbol{x})} K_r(\xi)\, d\xi = \int_{-\infty}^{\psi(\boldsymbol{x})} e^{\alpha\xi} d\xi = \frac{1}{\alpha} e^{\alpha\psi(\boldsymbol{x})} \tag{2-8}$$

The latter transforms (2-5) and boundary conditions (2-3) and (2-4), respectively, into

$$\nabla\cdot\left[K_s(x)\left(\nabla\Phi(x)+g\alpha\Phi(x)e_3\right)\right]+f(x)=0 \qquad x\in\Omega \tag{2-9}$$

$$\Phi(x)=H(x),\quad H(x)=\frac{1}{\alpha}e^{\alpha\Psi(x)} \qquad x\in\Gamma_D \tag{2-10}$$

$$n(x)\cdot\left[K_s(x)\left(\nabla\Phi(x)+g\alpha\Phi(x)e_3\right)\right]=Q(x) \qquad x\in\Gamma_N \tag{2-11}$$

where $e_3=(0, 0, 1)^T$ and T denotes transpose.

2.2 EXACT CONDITIONAL MEAN EQUATIONS

2.2.1 Exact Mean Equations for the Transformed Variable Φ(x)

We treat saturated hydraulic conductivity as a random field and separate it into an ensemble mean $\langle K_s(x)\rangle$ and a zero mean perturbation.

$$K_s(x)=\langle K_s(x)\rangle+K_s'(x) \qquad \langle K_s'(x)\rangle\equiv 0 \tag{2-12}$$

The mean saturated hydraulic conductivity represents a relatively smooth unbiased estimate of the unknown random function $K_s(x)$. It may be estimated using standard geostatistical methods, such as kriging, which produce unbiased estimates that honor measurements and provide uncertainty measures for these estimates. Here we assume that the saturated hydraulic conductivity field is conditioned at some measurement points, which means that the field may not be statistically homogeneous. By the same token, we define the conditional ensemble means $\langle\Phi(x)\rangle$ and $\langle\alpha\rangle$, and the corresponding perturbation terms $\Phi'(x)$ and α' as

$$\Phi(x)=\langle\Phi(x)\rangle+\Phi'(x) \qquad \langle\Phi'(x)\rangle\equiv 0 \tag{2-13}$$

$$\alpha = \langle \alpha \rangle + \alpha' \qquad \langle \alpha' \rangle \equiv 0 \tag{2-14}$$

Substituting (2-12)-(2-14) into (2-9), (2-10), and (2-11), and taking their ensemble mean, yields the exact conditional mean equation for the Kirchhoff-transformed variable $\Phi(\boldsymbol{x})$

$$\begin{cases} \nabla \cdot \left[\langle K_s(\boldsymbol{x}) \rangle \nabla \langle \Phi(\boldsymbol{x}) \rangle - \boldsymbol{r}(\boldsymbol{x}) + g\left(\langle \alpha \rangle \langle K_s(\boldsymbol{x}) \rangle \langle \Phi(\boldsymbol{x}) \rangle + \langle \alpha \rangle R_{K\Phi}(\boldsymbol{x}) \right.\right. & \\ \quad \left.\left. + \langle K_s(\boldsymbol{x}) \rangle R_{\alpha\Phi}(\boldsymbol{x}) + R_{\alpha K\Phi}(\boldsymbol{x}) \right) \boldsymbol{e}_3 \right] + \langle f(\boldsymbol{x}) \rangle = 0 & \boldsymbol{x} \in \Omega \\ \langle \Phi(\boldsymbol{x}) \rangle = \langle H(\boldsymbol{x}) \rangle & \boldsymbol{x} \in \Gamma_D \\ \boldsymbol{n}(\boldsymbol{x}) \cdot \left[\langle K_s(\boldsymbol{x}) \rangle \nabla \langle \Phi(\boldsymbol{x}) \rangle - \boldsymbol{r}(\boldsymbol{x}) + g\left(\langle \alpha \rangle \langle K_s(\boldsymbol{x}) \rangle \langle \Phi(\boldsymbol{x}) \rangle + \langle \alpha \rangle R_{K\Phi}(\boldsymbol{x}) \right.\right. & \\ \quad \left.\left. + \langle K_s(\boldsymbol{x}) \rangle R_{\alpha\Phi}(\boldsymbol{x}) + R_{\alpha K\Phi}(\boldsymbol{x}) \right) \boldsymbol{e}_3 \right] = \langle Q(\boldsymbol{x}) \rangle & \boldsymbol{x} \in \Gamma_N \end{cases} \tag{2-15}$$

Here $\langle H(\boldsymbol{x}) \rangle$ is ensemble mean of Φ on the Dirichlet boundary, $\langle f(\boldsymbol{x}) \rangle$ is ensemble mean of the source/sink term, and $\langle Q(\boldsymbol{x}) \rangle$ is ensemble mean of prescribed flux along the Neumann boundary. The other terms in (2-15) are defined as

$$\begin{aligned} \boldsymbol{r}(\boldsymbol{x}) &= -\langle K_s'(\boldsymbol{x}) \nabla \Phi'(\boldsymbol{x}) \rangle \\ R_{K\Phi}(\boldsymbol{x}) &= \langle K_s'(\boldsymbol{x}) \Phi'(\boldsymbol{x}) \rangle \\ R_{\alpha\Phi}(\boldsymbol{x}) &= \langle \alpha' \Phi'(\boldsymbol{x}) \rangle \\ R_{\alpha K\Phi}(\boldsymbol{x}) &= \langle \alpha' K'(\boldsymbol{x}) \Phi'(\boldsymbol{x}) \rangle \end{aligned} \tag{2-16}$$

2.2.2 Perturbation Equations for $\Phi(\boldsymbol{x})$

To solve (2-15), we need to evaluate the terms in (2-16), which requires formulating an expression for $\Phi'(\boldsymbol{x})$. Substituting (2-12)-(2-14) into (2-8), (2-9) and (2-10), and subtracting mean flow equation (2-15) yields implicit equations for $\Phi'(\boldsymbol{x})$,

$$\begin{cases} \nabla \cdot F(x) + f'(x) = 0 & x \in \Omega \\ \Phi'(x) = H'(x) & x \in \Gamma_D \\ n(x) \cdot F(x) = Q'(x) & x \in \Gamma_N \\ F(x) = K_s(x)\ \nabla\Phi'(x) + K_s'(x)\ \nabla\langle\Phi(x)\rangle + r(x) + g\left(\alpha K_s(x)\Phi'(x) + \alpha' K_s(x)\langle\Phi(x)\rangle\right. & \\ \qquad \left. + \langle\alpha\rangle K_s'(x)\langle\Phi(x)\rangle - \langle\alpha\rangle R_{K\Phi}(x) - \langle K_s(x)\rangle R_{\alpha\Phi}(x) - R_{\alpha K\Phi}(x)\right) e_3 & \end{cases} \tag{2-17}$$

where H' is a perturbation of H on the Dirichlet boundary, Q' is a perturbation of prescribed flux along the Neumann boundary, and f' is a perturbation of the sink/source term. To obtain an explicit expression for $\Phi'(\boldsymbol{x})$, we introduce an auxiliary function $G(\boldsymbol{y},\boldsymbol{x})$ that satisfies

$$\begin{cases} \nabla_y \cdot \left[K_s(y)\nabla_y G(y,x)\right] - g\alpha e_3^T K_s(y)\nabla_y G(y,x) + \delta(x-y) = 0 & x, y \in \Omega \\ G(y,x) = 0 & x \in \Omega,\quad y \in \Gamma_D \\ \nabla_y G(y,x) \cdot n(y) = 0 & x \in \Omega,\quad y \in \Gamma_N \end{cases} \tag{2-18}$$

where δ is the Dirac delta. Unlike the symmetric Green's function presented in *Guadagnini and Neuman* [1999a] for saturated flow, here G is non-symmetric. Rewriting (2-17) in terms of $\boldsymbol{y}$, multiplying by G, integrating with respect to $\boldsymbol{y}$ over Ω, and applying Green's first identity yields an explicit expression for $\Phi'(\boldsymbol{x})$

$$\begin{aligned} \Phi'(x) = &-\int_\Omega \nabla_y^T\ G(y,x)\Big[K_s'(y)\ \nabla\langle\Phi(y)\rangle + r(y) + g\left(\alpha' K_s(y)\langle\Phi(y)\rangle + \langle\alpha\rangle K_s'(y)\langle\Phi(y)\rangle\right. \\ &\qquad \left. - \langle\alpha\rangle R_{K\Phi}(y) - \langle K_s(y)\rangle R_{\alpha\Phi}(y) - R_{\alpha K\Phi}(y)\right) e_3\Big] d\Omega \\ &+ \int_\Omega f'(y)\ G(y,x)\ d\Omega \\ &+ \int_{\Gamma_N} G(y,x) Q'(y)\ d\Gamma \\ &- \int_{\Gamma_D} H'(y) K_s(y)\ \nabla_y G(y,x) \cdot n(y)\ d\Gamma \end{aligned} \tag{2-19}$$

This allows us to develop explicit integral expressions for all four terms in (2-16),

$$
\begin{aligned}
\boldsymbol{r}(\boldsymbol{x}) &= -\left\langle K_s'(\boldsymbol{x})\nabla\Phi'(\boldsymbol{x})\right\rangle \\
&= \int_\Omega \left\langle K_s'(\boldsymbol{x})\nabla_x\nabla_z^T G(\boldsymbol{z},\boldsymbol{x})K_s'(\boldsymbol{z})\right\rangle\left[\nabla\left\langle\Phi(\boldsymbol{z})\right\rangle + g\left\langle\alpha\right\rangle\left\langle\Phi(\boldsymbol{z})\right\rangle \boldsymbol{e}_3\right]\mathrm{d}\Omega \\
&\quad + \int_\Omega \left\langle K_s'(\boldsymbol{x})\nabla_x\nabla_z^T G(\boldsymbol{z},\boldsymbol{x})\right\rangle \boldsymbol{r}(\boldsymbol{z})\mathrm{d}\Omega \\
&\quad + \mathrm{g}\int_\Omega \left\langle \alpha' K_s'(\boldsymbol{x})\nabla_x\nabla_z^T G(\boldsymbol{z},\boldsymbol{x})\, K_s(\boldsymbol{z})\right\rangle\left\langle\Phi(\boldsymbol{z})\right\rangle \boldsymbol{e}_3\mathrm{d}\Omega \\
&\quad - g\int_\Omega \left\langle K_s'(\boldsymbol{x})\nabla_x\nabla_z^T G(\boldsymbol{z},\boldsymbol{x})\right\rangle\left(\left\langle\alpha\right\rangle R_{K\Phi}(\boldsymbol{z}) + \left\langle K_s(\boldsymbol{z})\right\rangle R_{\alpha\Phi}(\boldsymbol{z}) + R_{\alpha K\Phi}(\boldsymbol{z})\right)\boldsymbol{e}_3\mathrm{d}\Omega \\
&\quad + \int_{\Gamma_D} \left\langle K_s'(\boldsymbol{x})H'(\boldsymbol{z})\nabla_x\nabla_z^T G(\boldsymbol{z},\boldsymbol{x})K_s(\boldsymbol{z})\right\rangle \boldsymbol{n}(\boldsymbol{z})d\Gamma
\end{aligned}
\tag{2-20}
$$

$$
\begin{aligned}
R_{K\Phi}(\boldsymbol{x}) &= \left\langle K_s'(\boldsymbol{x})\Phi'(\boldsymbol{x})\right\rangle \\
&= -\int_\Omega \left\langle K_s'(\boldsymbol{x})\nabla_z^T G(\boldsymbol{z},\boldsymbol{x})K_s'(\boldsymbol{z})\right\rangle\left[\nabla\left\langle\Phi(\boldsymbol{z})\right\rangle + g\left\langle\alpha\right\rangle\left\langle\Phi(\boldsymbol{z})\right\rangle \boldsymbol{e}_3\right]\mathrm{d}\Omega \\
&\quad - \int_\Omega \left\langle K_s'(\boldsymbol{x})\nabla_z^T G(\boldsymbol{z},\boldsymbol{x})\right\rangle \boldsymbol{r}(\boldsymbol{z})\mathrm{d}\Omega \\
&\quad - \mathrm{g}\int_\Omega \left\langle \alpha' K_s'(\boldsymbol{x})\nabla_z^T G(\boldsymbol{z},\boldsymbol{x})K_s(\boldsymbol{z})\right\rangle\left\langle\Phi(\boldsymbol{z})\right\rangle \boldsymbol{e}_3\mathrm{d}\Omega \\
&\quad + g\int_\Omega \left\langle K_s'(\boldsymbol{x})\nabla_z^T G(\boldsymbol{z},\boldsymbol{x})\right\rangle\left(\left\langle\alpha\right\rangle R_{K\Phi}(\boldsymbol{z}) + \left\langle K_s(\boldsymbol{z})\right\rangle R_{\alpha\Phi}(\boldsymbol{z}) + R_{\alpha K\Phi}(\boldsymbol{z})\right)\boldsymbol{e}_3\mathrm{d}\Omega \\
&\quad - \int_{\Gamma_D} \left\langle K_s'(\boldsymbol{x})H'(\boldsymbol{z})\nabla_z^T G(\boldsymbol{z},\boldsymbol{x})K_s(\boldsymbol{z})\right\rangle \boldsymbol{n}(\boldsymbol{z})d\Gamma
\end{aligned}
\tag{2-21}
$$

$$
\begin{aligned}
R_{\alpha\Phi}(\boldsymbol{x}) &= \left\langle \alpha'\Phi'(\boldsymbol{x})\right\rangle \\
&= -\int_\Omega \left\langle \alpha'\nabla_z^T G(\boldsymbol{z},\boldsymbol{x})K_s'(\boldsymbol{z})\right\rangle\left[\nabla\left\langle\Phi(\boldsymbol{z})\right\rangle + g\left\langle\alpha\right\rangle\left\langle\Phi(\boldsymbol{z})\right\rangle \boldsymbol{e}_3\right]\mathrm{d}\Omega \\
&\quad - \int_\Omega \left\langle \alpha'\nabla_z^T G(\boldsymbol{z},\boldsymbol{x})\right\rangle \boldsymbol{r}(\boldsymbol{z})\mathrm{d}\Omega \\
&\quad - \mathrm{g}\int_\Omega \left\langle \alpha'^2\nabla_z^T G(\boldsymbol{z},\boldsymbol{x})K_s(\boldsymbol{z})\right\rangle\left\langle\Phi(\boldsymbol{z})\right\rangle \boldsymbol{e}_3\mathrm{d}\Omega \\
&\quad + g\int_\Omega \left\langle \alpha'\,\nabla_z^T G(\boldsymbol{z},\boldsymbol{x})\right\rangle\left(\left\langle\alpha\right\rangle R_{K\Phi}(\boldsymbol{z}) + \left\langle K_s(\boldsymbol{z})\right\rangle R_{\alpha\Phi}(\boldsymbol{z}) + R_{\alpha K\Phi}(\boldsymbol{z})\right)\boldsymbol{e}_3\mathrm{d}\Omega \\
&\quad - \int_{\Gamma_D} \left\langle \alpha' H'(\boldsymbol{z})\nabla_z^T G(\boldsymbol{z},\boldsymbol{x})K_s(\boldsymbol{z})\right\rangle \boldsymbol{n}(\boldsymbol{z})d\Gamma
\end{aligned}
\tag{2-22}
$$

$$
\begin{aligned}
R_{\alpha K\Phi}(\boldsymbol{x}) &= \left\langle \alpha' K_s'(\boldsymbol{x})\;\Phi'(\boldsymbol{x})\right\rangle \\
&= -\int_\Omega \left\langle \alpha' K_s'(\boldsymbol{x})\nabla_z^T G(\boldsymbol{z},\boldsymbol{x})K_s'(\boldsymbol{z})\right\rangle\left[\nabla\left\langle\Phi(\boldsymbol{z})\right\rangle + g\left\langle\alpha\right\rangle\left\langle\Phi(\boldsymbol{z})\right\rangle \boldsymbol{e}_3\right]\mathrm{d}\Omega \\
&\quad - \int_\Omega \left\langle \alpha' K_s'(\boldsymbol{x})\nabla_z^T G(\boldsymbol{z},\boldsymbol{x})\right\rangle \boldsymbol{r}(\boldsymbol{z})\mathrm{d}\Omega \\
&\quad - \mathrm{g}\int_\Omega \left\langle \alpha'^2 K_s'(\boldsymbol{x})\nabla_z^T G(\boldsymbol{z},\boldsymbol{x})\, K_s(\boldsymbol{z})\right\rangle\left\langle\Phi(\boldsymbol{z})\right\rangle \boldsymbol{e}_3\mathrm{d}\Omega \\
&\quad + g\int_\Omega \left\langle \alpha' K_s'(\boldsymbol{x})\nabla_z^T G(\boldsymbol{z},\boldsymbol{x})\right\rangle\left(\left\langle\alpha\right\rangle R_{K\Phi}(\boldsymbol{z}) + \left\langle K_s(\boldsymbol{z})\right\rangle R_{\alpha\Phi}(\boldsymbol{z}) + R_{\alpha K\Phi}(\boldsymbol{z})\right)\boldsymbol{e}_3\mathrm{d}\Omega \\
&\quad - \int_{\Gamma_D} \left\langle \alpha' K_s'(\boldsymbol{x})H'(\boldsymbol{z})\nabla_z^T G(\boldsymbol{z},\boldsymbol{x})K_s(\boldsymbol{z})\right\rangle \boldsymbol{n}(\boldsymbol{z})d\Gamma
\end{aligned}
\tag{2-23}
$$

The integrals over Γ_N and those containing f' are zero because α', K'_s and G are independent of Q' and f'. The integrals over Γ_D remain because both H' and G depend on α'. The derivation of other terms can be found in Appendix D.

We mention in passing that equations (18) and (19) of *Tartakovsky et al.* [1999] for $\boldsymbol{r}$, $R_{K\Phi}$ and $R_{\alpha\Phi}$, which correspond to our equations (2-20) - (2-22), do not include integrals over the Dirichlet boundary. Even in the special case where Ψ is deterministic, the Kirchhoff-transformed variable H on this boundary is not deterministic unless α is also deterministic. It follows that (18) - (19) of the above authors should include integrals over the Dirichlet boundary whenever either ψ or α is random. However, as we show in Appendix D, these integrals vanish to second order in σ_Y, and so the corresponding approximations (33) and (34) of *Tartakovsky et al.* [1999] are still valid because both α and the prescribed pressure head were assumed to be deterministic in their analysis.

2.2.3 Mean Expression for $\boldsymbol{q}(\boldsymbol{x})$

Using (2-6) and (2-7), we can rewrite equation (2-1) in terms of $\Phi(\boldsymbol{x})$ as

$$\boldsymbol{q}(\boldsymbol{x}) = -K_s(\boldsymbol{x})[\nabla\Phi(\boldsymbol{x}) + g\alpha\Phi(\boldsymbol{x})\,\boldsymbol{e}_3] \tag{2-24}$$

Writing $\boldsymbol{q}(\boldsymbol{x}) = \langle \boldsymbol{q}(\boldsymbol{x})\rangle + \boldsymbol{q}'(\boldsymbol{x})$, substituting (2-12)-(2-14) into (2-24), and taking ensemble mean, we obtain an exact expression for the conditional mean flux $\langle \boldsymbol{q}(\boldsymbol{x})\rangle$,

$$\begin{aligned}\langle \boldsymbol{q}(\boldsymbol{x})\rangle = &-\langle K_s(\boldsymbol{x})\rangle\left[\nabla\langle\Phi(\boldsymbol{x})\rangle + g\langle K_s(\boldsymbol{x})\rangle\left(\langle\alpha\rangle\langle\Phi(\boldsymbol{x})\rangle + R_{\alpha\Phi}(\boldsymbol{x})\right)\boldsymbol{e}_3\right] \\ &+\boldsymbol{r}(\boldsymbol{x}) - g\left(\langle\alpha\rangle R_{K\Phi}(\boldsymbol{x}) + R_{\alpha K\Phi}(\boldsymbol{x})\right)\boldsymbol{e}_3\end{aligned} \tag{2-25}$$

where $\boldsymbol{r}(\boldsymbol{x})$, $R_{\alpha\Phi}(\boldsymbol{x})$, $R_{K\Phi}(\boldsymbol{x})$, and $R_{\alpha K\Phi}(\boldsymbol{x})$ are defined in (2-20)-(2-23).

2.2.4 Perturbation Expression for $q(x)$

In order to evaluate the covariance of flux, which is required for stochastic analysis of solute transport, we need to have an expression for the flux perturbation $q'(x)$. Subtracting (2-25) from (2-24) and using (2-12)-(2-14) yields

$$\begin{aligned} q'(x) = &-\langle K_s(x)\rangle\left(\nabla\Phi'(x) + g\left(\langle\alpha\rangle\Phi'(x) + \alpha'\Phi(x)\right)e_3\right) - K_s'(x)\left(\nabla\Phi(x) + g\alpha\Phi(x)e_3\right) \\ &- r(x) + g\left(\langle\alpha\rangle R_{K\Phi}(x) + \langle K_s(x)\rangle R_{\alpha\Phi}(x) + R_{\alpha K\Phi}(x)\right)e_3 \end{aligned} \tag{2-26}$$

2.3 EXACT CONDITIONAL SECOND MOMENT EQUATIONS

2.3.1 Covariance of the Kirchhoff-Transformed Variable

An equation for the covariance function $C_\Phi(x, y)$ of Φ can be obtained upon multiplying (2-17) by $\Phi'(y)$ and taking conditional ensemble mean,

$$\begin{cases} \nabla_x \cdot F(x,y) + \langle f'(x)\Phi'(y)\rangle = 0 & x\in\Omega, y\in\Omega \\ C_\Phi(x,y) = \langle H'(x)\Phi'(y)\rangle & x\in\Gamma_D, y\in\Omega \\ n(x)\cdot F(x,y) = \langle Q'(x)\Phi'(y)\rangle & x\in\Gamma_N, y\in\Omega \\ F(x,y) = \langle K_s(x)\rangle\nabla_x C_\Phi(x,y) + \langle K_s'(x)\Phi'(y)\nabla\Phi'(x)\rangle + \langle K_s'(x)\Phi'(y)\rangle\nabla\langle\Phi(x)\rangle & \\ \qquad + g\left(\langle\alpha\rangle\langle K_s(x)\rangle C_\Phi(x,y) + \langle\alpha\rangle\langle K_s'(x)\Phi'(x)\Phi'(y)\rangle + \langle\alpha' K_s'(x)\Phi'(x)\Phi'(y)\rangle\right. & \\ \qquad + \langle K_s(x)\rangle\langle\alpha'\Phi'(x)\Phi'(y)\rangle + \langle K_s(x)\rangle R_{\alpha\Phi}(y)\langle\Phi(x)\rangle + C_{\alpha K\Phi}(x,y)\langle\Phi(x)\rangle & \\ \qquad \left. + \langle\alpha\rangle C_{K\Phi}(x,y)\langle\Phi(x)\rangle\right)e_3 & \end{cases} \tag{2-27}$$

Here the cross-covariance functions $\langle f'(x)\Phi'(y)\rangle$ and $\langle Q'(x)\Phi'(y)\rangle$ can be evaluated using the explicit expression for $\Phi'(x)$ in (2-19). Expressing the latter in terms of y, multiplying by $f'(x)$ and $Q'(x)$, respectively, and taking conditional ensemble mean gives

$$\langle f'(x)\Phi'(y)\rangle = \int_{\Omega} \langle f'(x)f'(z)\rangle\langle G(z,y)\rangle d\Omega$$
$$\langle Q'(x)\Phi'(y)\rangle = \int_{\Gamma_N} \langle Q'(x)Q'(z)\rangle\langle G(z,y)\rangle d\Gamma \qquad (2\text{-}28)$$

The term $\langle H'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle$ cannot be formulated in this way, because $H'(\boldsymbol{x})$ depends on α and through it on other terms, such as $G(\boldsymbol{y}, \boldsymbol{x})$. However, we obtain it by expressing $H'(\boldsymbol{x})$ explicitly, multiplying by $\Phi'(\boldsymbol{y})$, and taking conditional ensemble mean, as shown in (A-13) of Appendex A.

Again, the implicit equation and boundary conditions for the conditional covariance C_Φ in (A7)-(A9) of *Tartakovsky et al.* [1999] need to be modified. Instead of a homogeneous boundary condition on the Dirichlet boundary, one should write $C_\Phi(\boldsymbol{x},\boldsymbol{y})=\langle H'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle$. Their second order results are correct, as we show in Appendix D.

Equation (2-25) shows that to solve for $C_\Phi(\boldsymbol{x}, \boldsymbol{y})$, one needs to evaluate terms such as $\langle K_s'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle$ and $\langle \alpha' K_s'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle$, which in turn involve evaluating still other terms. Equations for all these terms can be derived upon multiplying (2-17) or (2-19) by the appropriate quantities and taking their conditional ensemble means (see Appendix D)

2.3.2 Flux Covariance Tensor $C_{qq}(\boldsymbol{x},\boldsymbol{y})$

The covariance tensor of the flux $C_{qq}(\boldsymbol{x},\boldsymbol{y})$ can be obtained upon multiplying $\boldsymbol{q}'(\boldsymbol{x})$ in (2-26) by its transpose in terms of $\boldsymbol{y}$, and taking conditional ensemble mean,

$$
\begin{aligned}
C_{qq}(\boldsymbol{x},\boldsymbol{y}) &= \left\langle q'(\boldsymbol{x})\, q'^{T}(\boldsymbol{y})\right\rangle \\
&= \left\langle \boldsymbol{K}_s(\boldsymbol{x})\right\rangle \nabla_x \nabla_y^T C_\Phi(\boldsymbol{x},\boldsymbol{y}) \left\langle \boldsymbol{K}_s(\boldsymbol{y})\right\rangle + g\left\langle\alpha\right\rangle \left\langle \boldsymbol{K}_s(\boldsymbol{x})\right\rangle \nabla_x C_\Phi(\boldsymbol{x},\boldsymbol{y})\, e_3^T \left\langle \boldsymbol{K}_s(\boldsymbol{y})\right\rangle \\
&+ g\left\langle \boldsymbol{K}_s(\boldsymbol{x})\right\rangle \left(\nabla R_{\alpha\Phi}(\boldsymbol{x})\left\langle\Phi(\boldsymbol{y})\right\rangle + \nabla_x \left\langle \alpha'\Phi'(x)\Phi'(y)\right\rangle\right) e_3^T \left\langle \boldsymbol{K}_s(\boldsymbol{y})\right\rangle \\
&+ \left\langle \boldsymbol{K}_s(\boldsymbol{x})\right\rangle \left\langle \nabla\Phi'(x)\nabla^T \left\langle\Phi(\boldsymbol{y})\right\rangle \boldsymbol{K}_s'(\boldsymbol{y})\right\rangle + \left\langle \boldsymbol{K}_s(\boldsymbol{x})\right\rangle \left\langle \nabla_x\Phi'(\boldsymbol{x})\nabla_y^T\Phi'(\boldsymbol{y})\boldsymbol{K}_s'(\boldsymbol{y})\right\rangle \\
&+ g\left\langle\alpha\right\rangle \left\langle \boldsymbol{K}_s(\boldsymbol{x})\right\rangle \left(\left\langle \nabla\Phi'(\boldsymbol{x})\, e_3^T \boldsymbol{K}_s'(\boldsymbol{y})\right\rangle \left\langle\Phi(\boldsymbol{y})\right\rangle + \left\langle \nabla\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\, e_3^T \boldsymbol{K}_s'(\boldsymbol{y})\right\rangle\right) \\
&+ g\left\langle \boldsymbol{K}_s(\boldsymbol{x})\right\rangle \left\langle \alpha'\nabla\Phi'(\boldsymbol{x})\, e_3^T \boldsymbol{K}_s'(\boldsymbol{y})\right\rangle \left\langle\Phi(\boldsymbol{y})\right\rangle + g\left\langle \boldsymbol{K}_s(\boldsymbol{x})\right\rangle \left\langle \alpha'\nabla_x\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\, e_3^T \boldsymbol{K}_s'(\boldsymbol{y})\right\rangle \\
&+ g\left\langle\alpha\right\rangle \left\langle \boldsymbol{K}_s(\boldsymbol{x})\right\rangle e_3 \nabla_y^T C_\Phi(\boldsymbol{x},\boldsymbol{y}) \left\langle \boldsymbol{K}_s(\boldsymbol{y})\right\rangle + g\left\langle\alpha\right\rangle^2 \left\langle \boldsymbol{K}_s(\boldsymbol{x})\right\rangle C_\Phi(\boldsymbol{x},\boldsymbol{y})\, \boldsymbol{E}_3 \left\langle \boldsymbol{K}_s(\boldsymbol{y})\right\rangle \\
&+ g\left\langle\alpha\right\rangle \left\langle \boldsymbol{K}_s(\boldsymbol{x})\right\rangle \boldsymbol{E}_3 \left(R_{\alpha\Phi}(\boldsymbol{x})\left\langle \boldsymbol{K}_s(\boldsymbol{y})\right\rangle \left\langle\Phi(\boldsymbol{y})\right\rangle + \left\langle \alpha'\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle \left\langle \boldsymbol{K}_s(\boldsymbol{y})\right\rangle\right) \\
&+ g\left\langle\alpha\right\rangle \left\langle \boldsymbol{K}_s(\boldsymbol{x})\right\rangle e_3 \left(\nabla^T \left\langle\Phi(\boldsymbol{y})\right\rangle C_{K\Phi}(y,x) + \left\langle \Phi'(\boldsymbol{x})\nabla_y^T\Phi'(\boldsymbol{y})\boldsymbol{K}_s'(\boldsymbol{y})\right\rangle\right) \\
&+ g\left\langle\alpha\right\rangle^2 \left\langle \boldsymbol{K}_s(\boldsymbol{x})\right\rangle \boldsymbol{E}_3 \left(\left\langle\Phi(\boldsymbol{y})\right\rangle C_{K\Phi}(y,x) + \left\langle \Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\boldsymbol{K}_s'(\boldsymbol{y})\right\rangle\right) \\
&+ 2g\left\langle\alpha\right\rangle \left\langle \boldsymbol{K}_s(\boldsymbol{x})\right\rangle \boldsymbol{E}_3 \left(\left\langle \alpha'\,\Phi'(\boldsymbol{x})\boldsymbol{K}_s'(\boldsymbol{y})\right\rangle \left\langle\Phi(\boldsymbol{y})\right\rangle + \left\langle \alpha'\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\,\boldsymbol{K}_s'(\boldsymbol{y})\right\rangle\right) \\
&+ g\left\langle \boldsymbol{K}_s(\boldsymbol{x})\right\rangle \left\langle\Phi(\boldsymbol{x})\right\rangle \left(e_3\nabla_y^T R_{\alpha\Phi}(\boldsymbol{y}) + \left\langle\alpha\right\rangle \boldsymbol{E}_3 R_{\alpha\Phi}(\boldsymbol{y})\right) \left\langle \boldsymbol{K}_s(\boldsymbol{y})\right\rangle \\
&+ g\left\langle \boldsymbol{K}_s(\boldsymbol{x})\right\rangle \left\langle\Phi(\boldsymbol{x})\right\rangle \boldsymbol{E}_3 \left(\left\langle \alpha'^2\right\rangle \left\langle\Phi(\boldsymbol{y})\right\rangle + \left\langle \alpha'^2\Phi'(\boldsymbol{y})\right\rangle\right) \left\langle \boldsymbol{K}_s(\boldsymbol{y})\right\rangle \\
&+ g\left\langle \boldsymbol{K}_s(\boldsymbol{x})\right\rangle \left\langle\Phi(\boldsymbol{x})\right\rangle e_3 \left\langle \alpha'\nabla^T\;\Phi'(\boldsymbol{y})\;\boldsymbol{K}_s'(\boldsymbol{y})\right\rangle \\
&+ g\left\langle \boldsymbol{K}_s(\boldsymbol{x})\right\rangle \left\langle\Phi(\boldsymbol{x})\right\rangle \boldsymbol{E}_3 \left(\left\langle\alpha\right\rangle \left\langle \alpha'\,\Phi'(\boldsymbol{y})\,\boldsymbol{K}_s'(\boldsymbol{y})\right\rangle + \left\langle \alpha'^2\Phi'(\boldsymbol{y})\boldsymbol{K}_s'(\boldsymbol{y})\right\rangle\right) \\
&+ g\left\langle \boldsymbol{K}_s(\boldsymbol{x})\right\rangle \left(e_3\nabla_y^T \left\langle \alpha'\,\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle + \boldsymbol{E}_3 \left\langle\alpha\right\rangle \left\langle \alpha'\,\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle\right) \left\langle \boldsymbol{K}_s(\boldsymbol{y})\right\rangle \\
&+ g\left\langle \boldsymbol{K}_s(\boldsymbol{x})\right\rangle \boldsymbol{E}_3 \left(\left\langle\Phi(\boldsymbol{y})\right\rangle \left\langle \alpha'^2\Phi'(x)\right\rangle + \left\langle \alpha'^2\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle\right) \left\langle \boldsymbol{K}_s(\boldsymbol{y})\right\rangle \\
&+ g\left\langle \boldsymbol{K}_s(\boldsymbol{x})\right\rangle e_3 \left(\nabla^T \left\langle\Phi(\boldsymbol{y})\right\rangle \left\langle \alpha'\Phi'(\boldsymbol{x})\;\boldsymbol{K}_s'(\boldsymbol{y})\right\rangle + \left\langle \alpha'\Phi'(\boldsymbol{x})\;\boldsymbol{K}_s'(\boldsymbol{y})\nabla_y^T\Phi'(\boldsymbol{y})\right\rangle\right) \\
&+ g\left\langle \boldsymbol{K}_s(\boldsymbol{x})\right\rangle \boldsymbol{E}_3 \left(\left\langle \alpha'^2\Phi'(x)\boldsymbol{K}_s'(\boldsymbol{y})\right\rangle \left\langle\Phi(\boldsymbol{y})\right\rangle + \left\langle \alpha'^2\Phi'(x)\Phi'(\boldsymbol{y})\boldsymbol{K}_s'(\boldsymbol{y})\right\rangle\right) \\
&+ \left(\left\langle \boldsymbol{K}_s'(\boldsymbol{x})\nabla_x\Phi'(\boldsymbol{x})\nabla_y^T\;\Phi'(\boldsymbol{y})\right\rangle + \left\langle \boldsymbol{K}_s'(\boldsymbol{x})\nabla\left\langle\Phi(\boldsymbol{x})\right\rangle \nabla_y^T\;\Phi'(\boldsymbol{y})\right\rangle\right) \left\langle \boldsymbol{K}_s(\boldsymbol{y})\right\rangle \\
&+ g\left\langle\alpha\right\rangle \left(C_{K\Phi}(\boldsymbol{x},\boldsymbol{y})\nabla\left\langle\Phi(\boldsymbol{x})\right\rangle + \left\langle \boldsymbol{K}_s'(\boldsymbol{x})\nabla_x\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle\right) e_3^T \left\langle \boldsymbol{K}_s(\boldsymbol{y})\right\rangle \\
&+ \mathrm{g}\left\langle \alpha'\boldsymbol{K}_s'(\boldsymbol{x})\nabla\Phi'(\boldsymbol{x})\right\rangle\; e_3^T \left\langle \boldsymbol{K}_s(\boldsymbol{y})\right\rangle \left\langle\Phi(\boldsymbol{y})\right\rangle \\
&+ g\left(\left\langle \alpha'\boldsymbol{K}_s'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle \nabla\left\langle\Phi(\boldsymbol{x})\right\rangle + \left\langle \alpha'\boldsymbol{K}_s'(x)\nabla_x\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle\right) e_3^T \left\langle \boldsymbol{K}_s(\boldsymbol{y})\right\rangle \\
&+ \left\langle \boldsymbol{K}_s'(\boldsymbol{x})\nabla\left\langle\Phi(\boldsymbol{x})\right\rangle \nabla^T \left\langle\Phi(\boldsymbol{y})\right\rangle \boldsymbol{K}_s'(\boldsymbol{y})\right\rangle + \left\langle \boldsymbol{K}_s'(\boldsymbol{x})\nabla\left\langle\Phi(\boldsymbol{x})\right\rangle \nabla_y^T\Phi'(\boldsymbol{y})\boldsymbol{K}_s'(\boldsymbol{y})\right\rangle \\
&+ \left\langle \boldsymbol{K}_s'(\boldsymbol{x})\nabla_x\Phi'(\boldsymbol{x})\nabla^T \left\langle\Phi(\boldsymbol{y})\right\rangle \boldsymbol{K}_s'(\boldsymbol{y})\right\rangle + \left\langle \boldsymbol{K}_s'(\boldsymbol{x})\nabla_x\Phi'(\boldsymbol{x})\nabla_y^T\Phi'(\boldsymbol{y})\boldsymbol{K}_s'(\boldsymbol{y})\right\rangle \\
&+ g\left\langle\alpha\right\rangle \left(\left\langle \boldsymbol{K}_s'(\boldsymbol{x})\nabla\left\langle\Phi(\boldsymbol{x})\right\rangle e_3^T \boldsymbol{K}_s'(\boldsymbol{y})\right\rangle + \left\langle \boldsymbol{K}_s'(\boldsymbol{x})\nabla_x\Phi'(\boldsymbol{x})\; e_3^T \boldsymbol{K}_s'(\boldsymbol{y})\right\rangle\right) \left\langle\Phi(\boldsymbol{y})\right\rangle
\end{aligned}
$$

$$\begin{aligned}
&+ g\langle\alpha\rangle\Big(\Big\langle \boldsymbol{K}_s'(\boldsymbol{x})\nabla\langle\Phi(\boldsymbol{x})\rangle\Phi'(\boldsymbol{y})\, e_3^T \boldsymbol{K}_s'(\boldsymbol{y})\Big\rangle + \Big\langle \boldsymbol{K}_s'(\boldsymbol{x})\nabla_x\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\, e_3^T \boldsymbol{K}_s'(\boldsymbol{y})\Big\rangle\Big)\\
&+ g\Big(\Big\langle \alpha'\boldsymbol{K}_s'(\boldsymbol{x})\nabla\langle\Phi(\boldsymbol{x})\rangle\, e_3^T \boldsymbol{K}_s'(\boldsymbol{y})\Big\rangle + \Big\langle \alpha'\boldsymbol{K}_s'(\boldsymbol{x})\nabla_x\Phi'(\boldsymbol{x})\, e_3^T \boldsymbol{K}_s'(\boldsymbol{y})\Big\rangle\Big)\langle\Phi(\boldsymbol{y})\rangle\\
&+ g\Big(\Big\langle \alpha'\boldsymbol{K}_s'(\boldsymbol{x})\nabla\langle\Phi(\boldsymbol{x})\rangle\, \Phi'(\boldsymbol{y}) e_3^T \boldsymbol{K}_s'(\boldsymbol{y})\Big\rangle + \Big\langle \alpha'\boldsymbol{K}_s'(\boldsymbol{x})\nabla_x\Phi'(\boldsymbol{x})\, \Phi'(\boldsymbol{y}) e_3^T \boldsymbol{K}_s'(\boldsymbol{y})\Big\rangle\Big)\\
&+ g\langle\alpha\rangle\Big(\langle\Phi(\boldsymbol{x})\rangle\Big\langle \boldsymbol{K}_s'(\boldsymbol{x}) e_3\nabla_y^T\Phi'(\boldsymbol{y})\Big\rangle + \Big\langle \boldsymbol{K}_s'(\boldsymbol{x})\Phi'(\boldsymbol{x}) e_3\nabla_y^T\Phi'(\boldsymbol{y})\Big\rangle\Big)\langle\boldsymbol{K}_s(\boldsymbol{y})\rangle\\
&+ g\Big(\langle\Phi(\boldsymbol{x})\rangle\Big\langle \alpha'\boldsymbol{K}_s'(\boldsymbol{x}) e_3\nabla_y^T\Phi'(\boldsymbol{y})\Big\rangle + \Big\langle \alpha'\Phi'(\boldsymbol{x})\boldsymbol{K}_s'(\boldsymbol{x}) e_3\nabla_y^T\Phi'(\boldsymbol{y})\Big\rangle\Big)\langle\boldsymbol{K}_s(\boldsymbol{y})\rangle\\
&+ g\langle\alpha\rangle^2\Big(\langle\Phi(\boldsymbol{x})\rangle C_{K\Phi}(\boldsymbol{x},\boldsymbol{y}) + \Big\langle \boldsymbol{K}_s'(x)\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Big\rangle\Big)\boldsymbol{E}_3\langle\boldsymbol{K}_s(\boldsymbol{y})\rangle\\
&+ g\Big(\langle\alpha\rangle\Big\langle \alpha'\Phi'(\boldsymbol{x})\boldsymbol{K}_s'(\boldsymbol{x})\Big\rangle + \Big\langle \alpha'^2\Phi'(\boldsymbol{x})\boldsymbol{K}_s'(\boldsymbol{x})\Big\rangle\Big)\boldsymbol{E}_3\langle\boldsymbol{K}_s(\boldsymbol{y})\rangle\langle\Phi(\boldsymbol{y})\rangle\\
&+ 2g\langle\alpha\rangle\Big(\langle\Phi(\boldsymbol{x})\rangle\Big\langle \alpha'\boldsymbol{K}_s'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Big\rangle + \Big\langle \alpha'\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\boldsymbol{K}_s'(\boldsymbol{x})\Big\rangle\Big)\boldsymbol{E}_3\langle\boldsymbol{K}_s(\boldsymbol{y})\rangle\\
&+ g\Big(\langle\Phi(\boldsymbol{x})\rangle\Big\langle \alpha'^2\boldsymbol{K}_s'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Big\rangle + \Big\langle \alpha'^2\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\boldsymbol{K}_s'(\boldsymbol{x})\Big\rangle\Big)\boldsymbol{E}_3\langle\boldsymbol{K}_s(\boldsymbol{y})\rangle\\
&+ g\langle\alpha\rangle\langle\Phi(\boldsymbol{x})\rangle\Big(\Big\langle \boldsymbol{K}_s'(\boldsymbol{x}) e_3\nabla^T\langle\Phi(\boldsymbol{y})\rangle\boldsymbol{K}_s'(\boldsymbol{y})\Big\rangle + \Big\langle \boldsymbol{K}_s'(\boldsymbol{x}) e_3\nabla_y^T\Phi'(\boldsymbol{y})\boldsymbol{K}_s'(\boldsymbol{y})\Big\rangle\Big)\\
&+ g\langle\alpha\rangle\Big(\Big\langle \boldsymbol{K}_s'(\boldsymbol{x})\Phi'(\boldsymbol{x}) e_3\nabla^T\langle\Phi(\boldsymbol{y})\rangle\boldsymbol{K}_s'(\boldsymbol{y})\Big\rangle + \Big\langle \boldsymbol{K}_s'(\boldsymbol{x})\Phi'(\boldsymbol{x}) e_3\nabla_y^T\Phi'(\boldsymbol{y})\boldsymbol{K}_s'(\boldsymbol{y})\Big\rangle\Big)\\
&+ g\langle\Phi(\boldsymbol{x})\rangle\Big(\Big\langle \alpha'\boldsymbol{K}_s'(\boldsymbol{x}) e_3\nabla^T\langle\Phi(\boldsymbol{y})\rangle\boldsymbol{K}_s'(\boldsymbol{y})\Big\rangle + \Big\langle \alpha'\boldsymbol{K}_s'(\boldsymbol{x}) e_3\nabla_y^T\Phi'(\boldsymbol{y})\boldsymbol{K}_s'(\boldsymbol{y})\Big\rangle\Big)\\
&+ g\Big(\Big\langle \alpha'\boldsymbol{K}_s'(\boldsymbol{x})\Phi'(\boldsymbol{x}) e_3\nabla^T\langle\Phi(\boldsymbol{y})\rangle\boldsymbol{K}_s'(\boldsymbol{y})\Big\rangle + \Big\langle \alpha'\boldsymbol{K}_s'(\boldsymbol{x})\Phi'(\boldsymbol{x}) e_3\nabla_y^T\Phi'(y)\boldsymbol{K}_s'(\boldsymbol{y})\Big\rangle\Big)\\
&+ g\langle\alpha\rangle^2\langle\Phi(\boldsymbol{x})\rangle\Big(\Big\langle \boldsymbol{K}_s'(\boldsymbol{x})\boldsymbol{E}_3\boldsymbol{K}_s'(\boldsymbol{y})\Big\rangle\langle\Phi(\boldsymbol{y})\rangle + \Big\langle \boldsymbol{K}_s'(\boldsymbol{x})\boldsymbol{E}_3\Phi'(y)\boldsymbol{K}_s'(\boldsymbol{y})\Big\rangle\Big)\\
&+ g\langle\alpha\rangle^2\Big(\Big\langle \Phi'(\boldsymbol{x})\boldsymbol{K}_s'(\boldsymbol{x})\boldsymbol{E}_3\boldsymbol{K}_s'(\boldsymbol{y})\Big\rangle\langle\Phi(\boldsymbol{y})\rangle + \Big\langle \Phi'(\boldsymbol{x})\boldsymbol{K}_s'(\boldsymbol{x})\boldsymbol{E}_3\Phi'(\boldsymbol{y})\boldsymbol{K}_s'(\boldsymbol{y})\Big\rangle\Big)\\
&+ 2g\langle\alpha\rangle\langle\Phi(\boldsymbol{x})\rangle\Big(\Big\langle \alpha'\boldsymbol{K}_s'(\boldsymbol{x})\boldsymbol{E}_3\boldsymbol{K}_s'(\boldsymbol{y})\Big\rangle\langle\Phi(\boldsymbol{y})\rangle + \Big\langle \alpha'\boldsymbol{K}_s'(\boldsymbol{x})\boldsymbol{E}_3\Phi'(\boldsymbol{y})\boldsymbol{K}_s'(\boldsymbol{y})\Big\rangle\Big)\\
&+ 2g\langle\alpha\rangle\Big(\Big\langle \alpha'\Phi'(\boldsymbol{x})\boldsymbol{K}_s'(\boldsymbol{x})\boldsymbol{E}_3\boldsymbol{K}_s'(\boldsymbol{y})\Big\rangle\langle\Phi(\boldsymbol{y})\rangle + \Big\langle \alpha'\Phi'(\boldsymbol{x})\boldsymbol{K}_s'(\boldsymbol{x})\boldsymbol{E}_3\Phi'(y)\boldsymbol{K}_s'(\boldsymbol{y})\Big\rangle\Big)\\
&+ g\langle\Phi(\boldsymbol{x})\rangle\Big(\Big\langle \alpha'^2\boldsymbol{K}_s'(\boldsymbol{x})\boldsymbol{E}_3\boldsymbol{K}_s'(\boldsymbol{y})\Big\rangle\langle\Phi(\boldsymbol{y})\rangle + \Big\langle \alpha'^2\boldsymbol{K}_s'(\boldsymbol{x})\boldsymbol{E}_3\Phi'(\boldsymbol{y})\boldsymbol{K}_s'(\boldsymbol{y})\Big\rangle\Big)\\
&+ g\Big(\Big\langle \alpha'^2\Phi'(\boldsymbol{x})\boldsymbol{K}_s'(\boldsymbol{x})\boldsymbol{E}_3\boldsymbol{K}_s'(\boldsymbol{y})\Big\rangle\langle\Phi(\boldsymbol{y})\rangle + \Big\langle \alpha'^2\Phi'(\boldsymbol{x})\boldsymbol{K}_s'(\boldsymbol{x})\boldsymbol{E}_3\Phi'(\boldsymbol{y})\boldsymbol{K}_s'(\boldsymbol{y})\Big\rangle\Big)
\end{aligned} \tag{2-29}$$

where $\boldsymbol{E}_3$ is a 3x3 matrix with '1' where the third row and third column intersect, and '0' everywhere else.

2.3.3 Cross-Covariance of Log Hydraulic Conductivity and Flux

Sometimes we may be interested to see how changes in hydraulic conductivity at one location affect the flow field. Expressing (2-26) in terms of $\boldsymbol{y}$, multiplying it by $Y'(\boldsymbol{x})$, and taking conditional mean yields

$$\begin{aligned}C_{Yq}(\boldsymbol{x},\boldsymbol{y}) &= \langle Y'(\boldsymbol{x})\boldsymbol{q}'(\boldsymbol{y})\rangle \\ &= -\langle K_s(\boldsymbol{y})\rangle\langle Y'(\boldsymbol{x})\nabla\Phi'(\boldsymbol{y})\rangle - \langle Y'(\boldsymbol{x})K_s'(\boldsymbol{y})\rangle\nabla\langle\Phi(\boldsymbol{y})\rangle - \langle Y'(\boldsymbol{x})K_s'(\boldsymbol{y})\nabla\Phi'(\boldsymbol{y})\rangle \\ &\quad - g\big[\langle\alpha\rangle\langle K_s(\boldsymbol{y})\rangle\langle Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle + \langle\alpha\rangle\langle Y'(\boldsymbol{x})K_s'(\boldsymbol{y})\rangle\langle\Phi(\boldsymbol{y})\rangle \\ &\qquad + \langle\alpha\rangle\langle Y'(\boldsymbol{x})K_s'(\boldsymbol{y})\Phi'(\boldsymbol{y})\rangle + \langle K_s(\boldsymbol{y})\rangle\langle\alpha'Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle + \langle\alpha'Y'(\boldsymbol{x})K_s'(\boldsymbol{y})\Phi'(\boldsymbol{y})\rangle\big]\boldsymbol{e}_3\end{aligned} \tag{2-30}$$

2.3.4 Cross-Covariance of ln α and Flux

Uncertainty in α may affect the flow field. Expressing (2-26) in terms of $\boldsymbol{y}$, multiplying it by β' (a perturbation of lnα) and taking conditional mean leads to

$$\begin{aligned}C_{\beta q}(\boldsymbol{y}) &= \langle\beta'\boldsymbol{q}'(\boldsymbol{y})\rangle \\ &= -\langle K_s(\boldsymbol{y})\rangle\nabla C_{\beta\Phi}(\boldsymbol{y}) - \langle\beta'K_s'(\boldsymbol{y})\nabla\Phi'(\boldsymbol{y})\rangle \\ &\quad - g\big[\langle\alpha\rangle\langle K_s(\boldsymbol{y})\rangle R_{\beta\Phi}(\boldsymbol{y})\langle K_s(\boldsymbol{y})\rangle\langle\alpha'\beta'\rangle\langle\Phi(\boldsymbol{y})\rangle \\ &\qquad + \langle\alpha\rangle\langle\beta'K_s'(\boldsymbol{y})\Phi'(\boldsymbol{y})\rangle + \langle K_s(\boldsymbol{y})\rangle\langle\alpha'\beta'\,\Phi'(\boldsymbol{y})\rangle + \langle\alpha'\beta'K_s'(\boldsymbol{y})\Phi'(\boldsymbol{y})\rangle\big]\,\boldsymbol{e}_3\end{aligned} \tag{2-31}$$

2.4 LOCALIZATION OF CONDITIONAL MEAN FLOW EQUATIONS

To solve the mean flow equation (2-15), we need to evaluate (2-20)-(2-23), i.e., $\boldsymbol{r}$, $R_{K\Phi}$ $R_{\alpha\Phi}$, and $R_{\alpha K\Phi}$, which are nonlocal (depending on more than one point in space). To evaluate these terms, one would need to use either high-resolution conditional Monte Carlo simulation or some type of closure approximation. As in the case of saturated flow [*Neuman and Orr*, 1993; *Guadagnini and Neuman*, 1999a], following *Tartakovsky et al.* [1999], the conditional mean $\langle K_s(\boldsymbol{x})\rangle$, the best available unbiased estimate of random function $K_s(\boldsymbol{x})$, does not represent an effective saturated hydraulic conductivity in the deterministic formulation of the stochastic unsaturated flow problem, due to the nonlocal nature of $\boldsymbol{r}$, $R_{K\Phi}$ $R_{\alpha\Phi}$, and $R_{\alpha K\Phi}$. Such an effective hydraulic conductivity does not exist, unless these terms can be localized. From (2-20)-(2-23) it turns out that the mean flow equation (2-15) can be localized only if

$$\langle \Phi(\boldsymbol{x}) \rangle = const. \tag{2-32}$$

which implies that ψ = constant in the flow domain, i.e., the mean flow is strictly due to gravity.

CHAPTER 3

RECURSIVE CONDITIONAL MOMENT APPROXIMATIONS FOR STEADY STATE UNSATURATED FLOW

3.1 INTRODUCTION

Although the moment equations presented in Chapter 2 are exact, they contain unknown mixed moments of the random auxiliary function G and are therefore not workable. To evaluate them, one would need to use either high-resolution conditional Monte Carlo simulation or some type of closure approximation. In this study, following *Gaudagnini and Neuman* [1999] and *Tartakovsky et al.* [1999], we use perturbation analysis to obtain recusive approximations for our moment equations. Specifically, we start by expanding all moments into infinte power series in terms of σ_Y and σ_β, the standard deviations of $Y = \ln K_s$ and $\beta = \ln\alpha$, respectively. We then equate terms of same order in σ_Y and σ_β on both sides of moment equations to obtain a set of recursive equations, in which higher-order terms can be solved once lower-order terms have been evaluated. Theoretically, we can evaluate any moment of interest to an arbotrary order in this manner. We derive in this chapter equations for mean and covariance functions to second order. Many of the mathematical details are relegated to Appendix C.

In the following analysis, we assume that it is possible to write

$$
\begin{aligned}
K_s(\boldsymbol{x}) &= e^{Y(\boldsymbol{x})} = e^{\langle Y(\boldsymbol{x})\rangle + Y'(\boldsymbol{x})} = K_G(\boldsymbol{x}) \sum_{\mathrm{n}=0}^{\infty} \frac{[Y'(\boldsymbol{x})]^n}{\mathrm{n}!} \\
\langle K_s(\boldsymbol{x})\rangle &= \langle e^{Y(\boldsymbol{x})}\rangle = \langle e^{\langle Y(\boldsymbol{x})\rangle + Y'(\boldsymbol{x})}\rangle = K_G(\boldsymbol{x}) \sum_{\mathrm{n}=0}^{\infty} \frac{\langle [Y'(\boldsymbol{x})]^n\rangle}{\mathrm{n}!} \\
K_s'(\boldsymbol{x}) &= K_s(\boldsymbol{x}) - \langle K_s(\boldsymbol{x})\rangle = K_G(\boldsymbol{x}) \sum_{\mathrm{n}=0}^{\infty} \frac{[Y'(\boldsymbol{x})]^n - \langle [Y'(\boldsymbol{x})]^n\rangle}{\mathrm{n}!}
\end{aligned}
\tag{3-1}
$$

and

$$
\begin{aligned}
\alpha &= e^{\beta} = e^{\langle\beta\rangle + \beta'} = \alpha_G \sum_{\mathrm{m}=0}^{\infty} \frac{\beta'^m}{\mathrm{m}!} \\
\langle\alpha\rangle &= \langle e^{\beta}\rangle = \langle e^{<\beta>+\beta'}\rangle = \alpha_G \sum_{\mathrm{m}=0}^{\infty} \frac{\langle\beta'^m\rangle}{\mathrm{m}!} \\
\alpha' &= \alpha - \langle\alpha\rangle = \alpha_G \sum_{\mathrm{m}=0}^{\infty} \frac{\beta'^m - \langle\beta'^m\rangle}{\mathrm{m}!}
\end{aligned}
\tag{3-2}
$$

where $Y(\boldsymbol{x})$ and $Y'(\boldsymbol{x})$ are the natural logarithm of saturated hydraulic conductivity and its perturbation, respectively, $K_G(\boldsymbol{x})$ is the geometric mean of the saturated hydraulic conductivity, β is the logarithm of the reciprocal of the macroscopic capillary length scale α and β' is its pertubation, and $\alpha_G = e^{\langle\beta\rangle}$ is the geometric mean of α.

To solve conditional mean and second-order moment equations approximately, we expand all related quantities, such as $\langle\Phi(\boldsymbol{x})\rangle$, $\langle \boldsymbol{q}(\boldsymbol{x})\rangle$, $\boldsymbol{r}(\boldsymbol{x})$, $R_{K\Phi}(\boldsymbol{x})$, $R_{\alpha\Phi}(\boldsymbol{x})$, $R_{\alpha K\Phi}(\boldsymbol{x})$, and $G(\boldsymbol{y}, \boldsymbol{x})$, in powers of σ_Y and σ_β, for example,

$$
\langle\Phi(\boldsymbol{x})\rangle = \sum_{n,m=0}^{\infty} \langle \Phi^{(n,m)}(\boldsymbol{x})\rangle \tag{3-3}
$$

where n and m designates terms that contain only σ_Y to n^{th} power and σ_β to m^{th} power. The expansion is not guaranteed to be valid for strongly heterogeneous soils with $\sigma_Y \geq 1$ and $\sigma_\beta \geq 1$. As we shall see, it actually works well for relatively large values of σ_Y as long as σ_β remains small. In the case of random driving forces, (3-3) should include powers of standard deviations of these forces. For simplicity, we suppressed the superscripts of these powers but derived equations that are second-order accurate in their standard deviations, unless stated otherwise.

3.2 RECURSIVE EQUATIONS FOR MEAN Φ AND FLUX

3.2.1 Recursive Equations for $\langle \Phi^{(n,m)}(x) \rangle$

Using (3-1) -(3-3), (2-15) can be written as

$$
\begin{aligned}
&\nabla \cdot \Big[\langle K_s(x) \rangle \, \nabla \langle \Phi(x) \rangle - r(x) + g \, \big(\langle \alpha \rangle \langle K_s(x) \rangle \langle \Phi(x) \rangle \\
&\qquad + \langle \alpha \rangle R_{K\Phi}(x) + \langle K_s(x) \rangle R_{\alpha\Phi}(x) + R_{\alpha K\Phi}(x) \big) e_3 \Big] + \langle f(x) \rangle \\
&= \nabla \cdot \Bigg[K_G(x) \sum_{n=0}^{\infty} \frac{\langle Y'^n(x) \rangle}{n!} \sum_{n,m=0}^{\infty} \nabla \langle \Phi^{(n,m)}(x) \rangle - \sum_{n,m=0}^{\infty} r^{(n,m)}(x) \\
&\qquad + g \Bigg(\alpha_G \sum_{n=0}^{\infty} \frac{\langle \beta'^n \rangle}{n!} K_G(x) \sum_{n=0}^{\infty} \frac{\langle Y'^n(x) \rangle}{n!} \sum_{n,m=0}^{\infty} \langle \Phi^{(n,m)}(x) \rangle + \alpha_G \sum_{n=0}^{\infty} \frac{\langle \beta'^n \rangle}{n!} \sum_{n,m=0}^{\infty} R_{K\Phi}^{(n,m)}(x) \\
&\qquad + K_G(x) \sum_{n=0}^{\infty} \frac{\langle Y'^n(x) \rangle}{n!} \sum_{n,m=0}^{\infty} R_{\alpha\Phi}^{(n,m)}(x) + \sum_{n,m=0}^{\infty} R_{\alpha K\Phi}^{(n,m)}(x) \Bigg) e_3 \Bigg] + \langle f(x) \rangle \\
&= \sum_{n,m=0}^{\infty} \Bigg\{ \nabla \cdot \Bigg[K_G(x) \sum_{k=0}^{n} \frac{\langle Y'^k(x) \rangle}{k!} \nabla \langle \Phi^{(n-k,m)}(x) \rangle - r^{(n,m)}(x) \\
&\qquad + g \Bigg(\alpha_G K_G(x) \sum_{k=0}^{n} \frac{\langle Y'^k(x) \rangle}{k!} \sum_{p=0}^{m} \frac{\langle \beta'^p \rangle}{p!} \langle \Phi^{(n-k,m-p)}(x) \rangle + \alpha_G \sum_{p=0}^{m} \frac{\langle \beta'^p \rangle}{p!} R_{K\Phi}^{(n,m-p)}(x) \\
&\qquad + K_G(x) \sum_{k=0}^{n} \frac{\langle Y'^k(x) \rangle}{k!} R_{\alpha\Phi}^{(n-k,m)}(x) + R_{\alpha K\Phi}^{(n,m)}(x) \Bigg) e_3 \Bigg] \Bigg\} + \langle f(x) \rangle = 0 \qquad x \in \Omega
\end{aligned}
\tag{3-4}
$$

subject to the boundary conditions

$$
\sum_{n,m=0}^{\infty} \langle \Phi(x) \rangle^{(n,m)} = \langle H(x) \rangle^{(n,m)} \qquad x \in \Gamma_D \tag{3-5}
$$

$$\sum_{n,m=0}^{\infty}\left\{ \boldsymbol{n}(\boldsymbol{x})\cdot\left[K_G(\boldsymbol{x})\sum_{k=0}^{n}\frac{\langle Y'^k(\boldsymbol{x})\rangle}{k!}\nabla\langle\Phi^{(n-k,m)}(\boldsymbol{x})\rangle-\boldsymbol{r}^{(n,m)}(\boldsymbol{x})\right.\right.$$
$$+g\left(\alpha_G K_G(\boldsymbol{x})\sum_{k=0}^{n}\frac{\langle Y'^k(\boldsymbol{x})\rangle}{k!}\sum_{p=0}^{m}\frac{\langle\beta'^p\rangle}{p!}\langle\Phi^{(n-k,m-p)}(\boldsymbol{x})\rangle+\alpha_G\sum_{p=0}^{m}\frac{\langle\beta'^p\rangle}{p!}R_{K\Phi}^{(n,m-p)}(\boldsymbol{x})\right. \tag{3-6}$$
$$\left.\left.\left.+K_G(\boldsymbol{x})\sum_{k=0}^{n}\frac{\langle Y'^k(\boldsymbol{x})\rangle}{k!}R_{\alpha\Phi}^{(n-k,m)}(\boldsymbol{x})+R_{\alpha K\Phi}^{(n,m)}(\boldsymbol{x})\right)\boldsymbol{e}_3\right]\right\}=\langle Q(\boldsymbol{x})\rangle \qquad \boldsymbol{x}\in\Gamma_N$$

where $\langle f(\boldsymbol{x})\rangle$ is the ensemble mean of the source/sink term, $\langle H(\boldsymbol{x})\rangle = \langle e^{\alpha\Psi(\boldsymbol{x})}/\alpha\rangle$ is the ensemble mean of the Kirchhoff-transformed variable specified on the Dirichlet boundary, and $\langle Q(\boldsymbol{x})\rangle$ is the ensemble mean flux normal to the Neuman boundary. Ensemble means $\langle f\rangle$ and $\langle Q\rangle$ in (3-6) are not expanded in powers of σ_Y and σ_β as we take them to be statistically independent. Although the pressure head and its auto-covariance, prescibed on the Dirichlet boundary, are also independent of Y and β, the transformed variable $H(\boldsymbol{x})$ on this boundary does depend on β, and therefore its mean must be evaluated. The mean is given to various orders of approximations by (see Appendix A)

$$\langle H^{(0,0)}(\boldsymbol{x})\rangle=\frac{e^{\alpha_G\langle\Psi(\boldsymbol{x})\rangle}}{\alpha_G}\left(1+\frac{1}{2}\alpha_G^2\sigma_\Psi^2(\boldsymbol{x})\right)$$
$$\langle H^{(0,2)}(\boldsymbol{x})\rangle=\frac{\sigma_\beta^2}{2}\frac{e^{\alpha_G\langle\Psi(\boldsymbol{x})\rangle}}{\alpha_G}\left[1-\alpha_G\langle\Psi(\boldsymbol{x})\rangle\left(1-\alpha_G\langle\Psi(\boldsymbol{x})\rangle\right)+\frac{1}{2}\alpha_G^2\left(1+\alpha_G\langle\Psi(\boldsymbol{x})\rangle\right)^2\sigma_\Psi^2(\boldsymbol{x})\right] \tag{3-7}$$

where $\sigma_\beta^2 = \langle\beta'^2\rangle$ is the variance of β. For a deterministic Dirichlet boundary condition, $\sigma_\Psi^2(\boldsymbol{x}) \equiv 0$ and (3-7) simplifies to

$$\langle H^{(0,0)}(\boldsymbol{x})\rangle=\frac{1}{\alpha_G}e^{\alpha_G\langle\Psi(\boldsymbol{x})\rangle}$$
$$\langle H^{(0,2)}(\boldsymbol{x})\rangle=\frac{\sigma_\beta^2}{2}\frac{e^{\alpha_G\langle\Psi(\boldsymbol{x})\rangle}}{\alpha_G}\left[1-\alpha_G\langle\Psi(\boldsymbol{x})\rangle\left(1-\alpha_G\langle\Psi(\boldsymbol{x})\rangle\right)\right] \tag{3-8}$$

Equating these with same order terms on both sides of (3-4)-(3-5) gives the following recursive equations for $\langle\Phi(\boldsymbol{x})\rangle$ to second order in σ_Y and σ_β,

$\langle\Phi^{(0,0)}(x)\rangle$:

$$\begin{cases} \nabla\cdot\left[K_G(\boldsymbol{x})\left(\nabla\left\langle\Phi^{(0,0)}(\boldsymbol{x})\right\rangle+g\alpha_G\left\langle\Phi^{(0,0)}(\boldsymbol{x})\right\rangle e_3\right)\right]+\left\langle f(\boldsymbol{x})\right\rangle=0 & \boldsymbol{x}\in\Omega \\ \left\langle\Phi^{(0,0)}(\boldsymbol{x})\right\rangle=\left\langle H^{(0,0)}(\boldsymbol{x})\right\rangle & \boldsymbol{x}\in\Gamma_D \\ \boldsymbol{n}(\boldsymbol{x})\cdot\left[K_G(\boldsymbol{x})\left(\nabla\left\langle\Phi^{(0,0)}(\boldsymbol{x})\right\rangle+g\alpha_G\left\langle\Phi^{(0,0)}(\boldsymbol{x})\right\rangle e_3\right)\right]=\left\langle Q(\boldsymbol{x})\right\rangle & \boldsymbol{x}\in\Gamma_N \end{cases} \tag{3-9}$$

$\langle\Phi^{(0,1)}(x)\rangle$:

$$\begin{cases} \nabla\cdot\left[K_G(\boldsymbol{x})\left(\nabla\left\langle\Phi^{(0,1)}(\boldsymbol{x})\right\rangle+g\alpha_G\left\langle\Phi^{(0,1)}(\boldsymbol{x})\right\rangle e_3\right)\right]=0 & \boldsymbol{x}\in\Omega \\ \left\langle\Phi^{(0,1)}(\boldsymbol{x})\right\rangle=0 & \boldsymbol{x}\in\Gamma_D \\ \boldsymbol{n}(\boldsymbol{x})\cdot\left[K_G(\boldsymbol{x})\left(\nabla\left\langle\Phi^{(0,1)}(\boldsymbol{x})\right\rangle+g\alpha_G\left\langle\Phi^{(0,1)}(\boldsymbol{x})\right\rangle e_3\right)\right]=0 & \boldsymbol{x}\in\Gamma_N \end{cases} \tag{3-10}$$

which has the solution

$$\left\langle\Phi^{(0,1)}(\boldsymbol{x})\right\rangle=0 \qquad \boldsymbol{x}\in\Omega \tag{3-11}$$

$\langle\Phi^{(0,2)}(x)\rangle$:

$$\begin{cases} \nabla\cdot\left[K_G(\boldsymbol{x})\nabla\left\langle\Phi^{(0,2)}(\boldsymbol{x})\right\rangle+gK_G(\boldsymbol{x})\left(\alpha_G\left\langle\Phi^{(0,2)}(\boldsymbol{x})\right\rangle+\frac{\sigma_\beta^2}{2}\alpha_G\left\langle\Phi^{(0,0)}(\boldsymbol{x})\right\rangle+R_{\alpha\Phi}^{(0,2)}(\boldsymbol{x})\right)e_3\right]=0 & \boldsymbol{x}\in\Omega \\ \left\langle\Phi^{(0,2)}(\boldsymbol{x})\right\rangle=\left\langle H^{(0,2)}(\boldsymbol{x})\right\rangle & \boldsymbol{x}\in\Gamma_D \\ \boldsymbol{n}(\boldsymbol{x})\cdot\left[K_G(\boldsymbol{x})\nabla\left\langle\Phi^{(0,2)}(\boldsymbol{x})\right\rangle+gK_G(\boldsymbol{x})\left(\alpha_G\left\langle\Phi^{(0,2)}(\boldsymbol{x})\right\rangle+\frac{\sigma_\beta^2}{2}\alpha_G\left\langle\Phi^{(0,0)}(\boldsymbol{x})\right\rangle+R_{\alpha\Phi}^{(0,2)}(\boldsymbol{x})\right)e_3\right]=0 & \boldsymbol{x}\in\Gamma_N \end{cases} \tag{3-12}$$

where $\langle H^{(0,2)}\rangle$ is defined in (3-8) and $R_{\alpha\Phi}^{(0,2)}$ is given by (see (C-11) of Appendix C)

$$R_{\alpha\Phi}^{(0,2)}(\boldsymbol{x}) = -g\alpha_G^2\sigma_\beta^2\int_\Omega \nabla_y^T G^{(0,0)}(\boldsymbol{y},\boldsymbol{x})\, K_G(\boldsymbol{y})\left\langle \Phi^{(0,0)}(\boldsymbol{y})\right\rangle \boldsymbol{e}_3 d\Omega \\ -\int_{\Gamma_D}\left\langle \alpha' H'(\boldsymbol{y})\nabla_y^T G(\boldsymbol{y},\boldsymbol{x}) K_s(\boldsymbol{y})\right\rangle^{(0,2)} \boldsymbol{n}(\boldsymbol{y})d\Gamma \tag{3-13}$$

$\langle\Phi^{(1,0)}(x)\rangle$:

$$\begin{cases} \nabla\cdot\left[K_G(\boldsymbol{x})\left(\nabla\left\langle\Phi^{(1,0)}(\boldsymbol{x})\right\rangle + g\alpha_G\left\langle\Phi^{(1,0)}(\boldsymbol{x})\right\rangle\boldsymbol{e}_3\right)\right]=0 & \boldsymbol{x}\in\Omega \\ \left\langle\Phi^{(1,0)}(\boldsymbol{x})\right\rangle = 0 & \boldsymbol{x}\in\Gamma_D \\ \boldsymbol{n}(\boldsymbol{x})\cdot\left[K_G(\boldsymbol{x})\left(\nabla\left\langle\Phi^{(1,0)}(\boldsymbol{x})\right\rangle + g\alpha_G\left\langle\Phi^{(1,0)}(\boldsymbol{x})\right\rangle\boldsymbol{e}_3\right)\right]=0 & \boldsymbol{x}\in\Gamma_N \end{cases} \tag{3-14}$$

which has the solution

$$\left\langle\Phi^{(1,0)}(\boldsymbol{x})\right\rangle = 0 \qquad \boldsymbol{x}\in\Omega \tag{3-15}$$

$\langle\Phi^{(1,1)}(x)\rangle$:

$$\begin{cases} \nabla\cdot\left[K_G(\boldsymbol{x})\left(\nabla\left\langle\Phi^{(1,1)}(\boldsymbol{x})\right\rangle + g\alpha_G\left\langle\Phi^{(1,1)}(\boldsymbol{x})\right\rangle\boldsymbol{e}_3\right)\right]=0 & \boldsymbol{x}\in\Omega \\ \left\langle\Phi^{(1,1)}(\boldsymbol{x})\right\rangle = 0 & \boldsymbol{x}\in\Gamma_D \\ \boldsymbol{n}(\boldsymbol{x})\cdot\left[K_G(\boldsymbol{x})\left(\nabla\left\langle\Phi^{(1,1)}(\boldsymbol{x})\right\rangle + g\alpha_G\left\langle\Phi^{(1,1)}(\boldsymbol{x})\right\rangle\boldsymbol{e}_3\right)\right]=0 & \boldsymbol{x}\in\Gamma_N \end{cases} \tag{3-16}$$

which has the solution

$$\left\langle\Phi^{(1,1)}(\boldsymbol{x})\right\rangle = 0 \qquad \boldsymbol{x}\in\Omega \tag{3-17}$$

$\langle\Phi^{(2,0)}(x)\rangle$:

$$
\begin{cases}
\nabla\cdot\Big[K_G(x)\Big(\nabla\big\langle\Phi^{(2,0)}(x)\big\rangle+0.5\sigma_Y^2(x)\nabla\big\langle\Phi^{(2,0)}(x)\big\rangle\Big)-r^{(2,0)}(x) & \\
\quad +g\Big(\alpha_G K_G(x)\Big(\big\langle\Phi^{(2,0)}(x)\big\rangle+0.5\sigma_Y^2(x)\nabla\big\langle\Phi^{(0,0)}(x)\big\rangle\Big)+\alpha_G R_{K\Phi}^{(2,0)}(x)\Big)e_3\Big]=0 & x\in\Omega \\
\big\langle\Phi^{(2,0)}(x)\big\rangle=0 & x\in\Gamma_{\mathrm{D}} \\
n(x)\cdot\Big[K_G(x)\Big(\nabla\big\langle\Phi^{(2,0)}(x)\big\rangle+0.5\sigma_Y^2(x)\nabla\big\langle\Phi^{(2,0)}(x)\big\rangle\Big)-r^{(2,0)}(x) & \\
\quad +g\Big(\alpha_G K_G(x)\Big(\big\langle\Phi^{(2,0)}(x)\big\rangle+0.5\sigma_Y^2(x)\nabla\big\langle\Phi^{(0,0)}(x)\big\rangle\Big)+\alpha_G R_{K\Phi}^{(2,0)}(x)\Big)e_3\Big]=0 & x\in\Gamma_{\mathrm{N}}
\end{cases}
\tag{3-18}
$$

where $\sigma_Y^2(x)=\langle Y'^2(x)\rangle$ is the conditional variance of the natural logarithm of the saturated hydraulic conductivity at point x in the flow domain, and $\boldsymbol{r}^{(2,0)}(x)=\boldsymbol{R}^{(2,0)}(x,x)$ and $R_{K\Phi}^{(2,0)}(x)=C_{K\Phi}^{(2,0)}(x,x)$ are given by (Appendix C)

$$
\begin{aligned}
\boldsymbol{r}^{(2,0)}(x)=\boldsymbol{R}^{(2,0)}(x,x)&=-\big\langle K_s'(x)\nabla\Phi'(x)\big\rangle^{(2,0)}\\
&=K_G(x)\int_\Omega C_Y(x,z)\nabla_x\nabla_z^T\big\langle G^{(0,0)}(z,x)\big\rangle K_G(z)\ \Big[\nabla\big\langle\Phi^{(0,0)}(z)\big\rangle+g\alpha_{\mathrm{G}}\big\langle\Phi^{(0,0)}(z)\big\rangle e_3\Big]d\Omega
\end{aligned}
\tag{3-19}
$$

$$
\begin{aligned}
R_{K\Phi}^{(2,0)}(x)=C_{K\Phi}^{(2,0)}(x,x)&=\big\langle K_s'(x)\Phi'(x)\big\rangle\\
&=-K_G(x)\int_\Omega C_Y(x,z)\nabla_z^T\big\langle G^{(0,0)}(z,x)\big\rangle K_G(z)\ \Big[\nabla\big\langle\Phi^{(0,0)}(z)\big\rangle+g\alpha_{\mathrm{G}}\big\langle\Phi^{(0,0)}(z)\big\rangle e_3\Big]d\Omega
\end{aligned}
\tag{3-20}
$$

$\langle\Phi^{(2,1)}(x)\rangle$:

$$
\begin{cases}
\nabla\cdot\Big[K_G(x)\Big(\nabla\big\langle\Phi^{(2,1)}(x)\big\rangle+g\alpha_G\big\langle\Phi^{(2,1)}(x)\big\rangle e_3\Big)\Big]=0 & x\in\Omega \\
\big\langle\Phi^{(2,1)}(x)\big\rangle=0 & x\in\Gamma_D \\
n(x)\cdot\Big[K_G(x)\Big(\nabla\big\langle\Phi^{(2,1)}(x)\big\rangle+g\alpha_G\big\langle\Phi^{(2,1)}(x)\big\rangle e_3\Big)\Big]=0 & x\in\Gamma_N
\end{cases}
\tag{3-21}
$$

which yields

$$
\big\langle\Phi^{(2,1)}(x)\big\rangle=0 \qquad x\in\Omega \tag{3-22}
$$

$\langle\Phi^{(2,2)}(x)\rangle$:

$$\begin{cases}\nabla\cdot F(x)=0 & x\in\Omega\\ \left\langle\Phi^{(2,2)}(x)\right\rangle=0 & x\in\Gamma_D\\ n(x)\cdot F(x)=0 & x\in\Gamma_N\\ F(x)=\Bigg[K_G(x)\left(\nabla\left\langle\Phi^{(2,2)}(x)\right\rangle+\frac{\sigma_Y^2(x)}{2}\nabla\left\langle\Phi^{(0,2)}(x)\right\rangle\right)-r^{(2,2)}(x) & \\ \quad+g\Bigg(\alpha_G K_G(x)\left(\left\langle\Phi^{(2,2)}(x)\right\rangle+\frac{\sigma_\beta^2}{2}\left\langle\Phi^{(2,0)}(x)\right\rangle+\frac{\sigma_Y^2(x)}{2}\left\langle\Phi^{(0,2)}(x)\right\rangle+\frac{\sigma_\beta^2\sigma_Y^2(x)}{4}\left\langle\Phi^{(0,0)}(x)\right\rangle\right) & \\ \quad+\alpha_G\left(R_{K\Phi}^{(2,2)}(x)+\frac{\sigma_\beta^2}{2}R_{K\Phi}^{(2,0)}(x)\right)+K_G(x)\left(R_{\alpha\Phi}^{(2,2)}(x)+\frac{\sigma_Y^2(x)}{2}R_{\alpha\Phi}^{(0,2)}(x)\right)+R_{\alpha K\Phi}^{(2,2)}(x)\Bigg)e_3\Bigg] & \end{cases} \tag{3-23}$$

where the following terms are evaluated in Appendix C,

$$\begin{aligned}R_{\alpha\Phi}^{(2,2)}(x)=&-\alpha_G\int_\Omega\left\langle Y'(y)\beta'\nabla_y^TG^{(1,1)}(y,x)\right\rangle K_G(y)\left(\nabla\left\langle\Phi^{(0,0)}(y)\right\rangle+g\alpha_G\left\langle\Phi^{(0,0)}(y)\right\rangle e_3\right)d\Omega\\ &-\alpha_G\int_\Omega\left\langle\beta'\nabla_y^TG^{(0,1)}(y,x)\right\rangle r^{(2,0)}(y)d\Omega\\ &-g\,\alpha_G^2\sigma_\beta^2\int_\Omega\Big[\left(0.5\sigma_Y^2(y)\nabla_y^TG^{(0,0)}(y,x)+\left\langle Y'(y)\nabla_y^TG^{(1,0)}(y,x)\right\rangle\right)\left\langle\Phi^{(0,0)}(y)\right\rangle\\ &\qquad+\nabla_y^T\left\langle G^{(2,0)}(y,x)\right\rangle\left\langle\Phi^{(0,0)}(y)\right\rangle+\nabla_y^TG^{(0,0)}(y,x)\left\langle\Phi^{(2,0)}(y)\right\rangle\Big]K_G(y)e_3d\Omega\\ &-g\alpha_G^2\int_\Omega\left\langle\beta'\nabla_y^TG^{(0,1)}(y,x)\right\rangle R_{K\Phi}^{(2,0)}(y)\,e_3d\Omega\\ &-\int_{\Gamma_D}\left\langle\alpha'H'(y)\nabla_y^TG(y,x)K_s(y)\right\rangle^{(2,2)}n(y)d\Gamma\end{aligned} \tag{3-24}$$

$$\begin{aligned}r^{(2,2)}(x)=R^{(2,2)}(x,x)=&\left\langle K_s'(x)\nabla\Phi'(x)\right\rangle^{(2,2)}\\ =&-K_G(x)\int_\Omega C_Y(x,z)\nabla_x\nabla_z^T\left\langle G^{(0,2)}(z,x)\right\rangle K_G(z)\left[\nabla\left\langle\Phi^{(0,0)}(z)\right\rangle+g\,\alpha_G\left\langle\Phi^{(0,0)}(z)\right\rangle e_3\right]d\Omega\\ &-K_G(x)\int_\Omega C_Y(x,z)\nabla_x\nabla_z^TG^{(0,0)}(z,x)K_G(z)\left[\nabla\left\langle\Phi^{(0,2)}(z)\right\rangle+g\,\alpha_G\left(\left\langle\Phi^{(0,2)}(z)\right\rangle+\frac{\sigma_\beta^2}{2}\left\langle\Phi^{(0,0)}(z)\right\rangle\right)e_3\right]d\Omega\\ &-g\,\alpha_GK_G(x)\int_\Omega\left[C_Y(x,z)\left\langle\beta'\nabla_x\nabla_z^TG^{(0,1)}(z,x)\right\rangle+\left\langle\beta'Y'(x)\nabla_x\nabla_z^TG^{(1,1)}(z,x)\right\rangle\right]K_G(z)\left\langle\Phi^{(0,0)}(z)\right\rangle e_3d\Omega\\ &+gK_G(x)\int_\Omega\left\langle Y'(x)\nabla_x\nabla_z^TG^{(1,0)}(z,x)\right\rangle K_G(z)\,R_{\alpha\Phi}^{(0,2)}(z)d\Omega\\ &-K_G(x)\int_{\Gamma_D}\left\langle Y'(x)H'(z)\nabla_x\nabla_z^TG(z,x)K_s(z)\right\rangle^{(2,2)}n(z)d\Gamma\end{aligned} \tag{3-25}$$

$$
\begin{aligned}
R_{K\Phi}^{(2,2)}(x) &= C_{K\Phi}^{(2,2)}(x,x) = \left\langle K_s'(x)\Phi'(x)\right\rangle^{(2,2)} \\
&= -K_G(x)\int_\Omega C_Y(x,z)\ \nabla_z^T\left\langle G^{(0,2)}(z,x)\right\rangle K_G(z)\ \left[\nabla\left\langle\Phi^{(0,0)}(z)\right\rangle + g\alpha_G\left\langle\Phi^{(0,0)}(z)\right\rangle e_3\right]d\Omega \\
&\quad - K_G(x)\int_\Omega C_Y(x,z)\nabla_z^T\left\langle G^{(0,0)}(z,x)\right\rangle K_G(z)\left[\nabla\left\langle\Phi^{(0,2)}(z)\right\rangle + g\alpha_G\left(\left\langle\Phi^{(0,2)}(z)\right\rangle + \frac{\sigma_\beta^2}{2}\left\langle\Phi^{(0,0)}(z)\right\rangle\right)e_3\right]d\Omega \\
&\quad - g\,\alpha_G K_G(x)\int_\Omega\left[C_Y(x,z)\ \left\langle\beta'\nabla_z^T G^{(0,1)}(z,x)\right\rangle + \left\langle\beta' Y'(x)\nabla_z^T G^{(1,1)}(z,x)\right\rangle\right]K_G(z)\left\langle\Phi^{(0,0)}(z)\right\rangle e_3 d\Omega \\
&\quad + gK_G(x)\int_\Omega\left\langle Y'(x)\ \nabla_z^T G^{(1,0)}(z,x)\right\rangle K_G(z)\ R_{\alpha\Phi}^{(0,2)}(z)d\Omega \\
&\quad - K_G(x)\int_{\Gamma_D}\left\langle Y'(x)H'(z)\nabla_z^T G(z,x)K_s(z)\right\rangle^{(2,2)}\ n(z)d\Gamma
\end{aligned}
\tag{3-26}
$$

$$
\begin{aligned}
R_{\alpha K\Phi}^{(2,2)}(x) &= C_{\alpha K\Phi}^{(2,2)}(x,x) = \left\langle\alpha' K_s'(x)\Phi'(x)\right\rangle^{(2,2)} \\
&= -\alpha_G K_G(x)\int_\Omega C_Y(x,z)\left\langle\beta'\nabla_z^T G^{(0,1)}(z,x)\right\rangle K_G(z)\left[\nabla\left\langle\Phi^{(0,0)}(z)\right\rangle + g\alpha_G\left\langle\Phi^{(0,0)}(z)\right\rangle e_3\right]d\Omega \\
&\quad - g\,\alpha_G^2\sigma_\beta^2 K_G(x)\int_\Omega\left\langle Y'(z)\nabla_z^T G^{(1,0)}(z,x)\right\rangle K_G(z)\left\langle\Phi^{(0,0)}(z)\right\rangle\ e_3 d\Omega \\
&\quad - K_G(x)\int_{\Gamma_D}\left\langle\alpha' Y'(x)H'(z)\nabla_z^T G(z,x)K_s(z)\right\rangle n(z)d\Gamma
\end{aligned}
\tag{3-27}
$$

The above derivation shows that we need to solve only for $\langle\Phi^{(0,0)}\rangle$, $\langle\Phi^{(0,2)}\rangle$, $\langle\Phi^{(2,0)}\rangle$, and $\langle\Phi^{(2,2)}\rangle$, while all first-order terms are zero.

3.2.2 Recursive Approximations for Conditional Mean Flux

Expressing $\langle \boldsymbol{q}(\boldsymbol{x})\rangle$ in (2-25) in powers of σ_Y and σ_β gives

$$
\begin{aligned}
\sum_{n,m=0}^{\infty}\left\langle q^{(n,m)}(x)\right\rangle = \sum_{n,m=0}^{\infty}\Bigg\{ &-K_G(x)\Bigg(\sum_{k=0}^{n}\frac{\left\langle Y'^k(x)\right\rangle}{k!}\nabla\left\langle\Phi^{(n-k,m)}(x)\right\rangle \\
&+ g\ \alpha_G\sum_{k=0}^{n}\sum_{p=0}^{m}\frac{\left\langle Y'^k(x)\right\rangle}{k!}\frac{\left\langle\beta'^p\right\rangle}{p!}\left\langle\Phi^{(n-k,m-p)}(x)\right\rangle e_3 + g\sum_{k=0}^{n}\frac{\left\langle Y'^k(x)\right\rangle}{k!}R_{\alpha\Phi}^{(n-k,m)}(x)e_3\Bigg) \\
&+ r^{(n,m)}(x) - g\left(\alpha_G\sum_{p=0}^{m}\frac{\left\langle\beta'^p\right\rangle}{p!}R_{K\Phi}^{(n,m-p)}(x) + R_{\alpha K\Phi}^{(n,m)}(x)\right)e_3\Bigg\} \qquad x\in\Omega
\end{aligned}
\tag{3-28}
$$

Comparing terms of same order on both sides, we obtain to second order

$$\left\langle q^{(0,0)}(x)\right\rangle = -K_G(x)\left(\nabla\left\langle \Phi^{(0,0)}(x)\right\rangle + g\alpha_G\left\langle \Phi^{(0,0)}(x)\right\rangle e_3\right) \qquad x\in\Omega \tag{3-29}$$

$$\begin{aligned}\left\langle q^{(2,0)}(x)\right\rangle = -K_G(x)\Bigg[&\nabla\left\langle \Phi^{(2,0)}(x)\right\rangle + \frac{\sigma_Y^2(x)}{2}\nabla\left\langle \Phi^{(0,0)}(x)\right\rangle \\ &+g\alpha_G\left(\left\langle \Phi^{(2,0)}(x)\right\rangle + \frac{\sigma_Y^2(x)}{2}\left\langle \Phi^{(0,0)}(x)\right\rangle\right)e_3\Bigg] + r^{(2,0)}(x) - g\alpha_G R_{K\Phi}^{(2,0)}(x)e_3 \quad x\in\Omega\end{aligned} \tag{3-30}$$

$$\left\langle q^{(0,2)}(x)\right\rangle = -K_G(x)\left[\nabla\left\langle \Phi^{(0,2)}(x)\right\rangle + g\alpha_G\left(\left\langle \Phi^{(0,2)}(x)\right\rangle + \frac{\sigma_\beta^2}{2}\left\langle \Phi^{(0,0)}(x)\right\rangle\right)e_3 + gR_{\alpha\Phi}^{(0,2)}(x)\, e_3\right] \tag{3-31}$$

$$\begin{aligned}\left\langle q^{(2,2)}(x)\right\rangle = -K_G(x)\Bigg[&\nabla\left\langle \Phi^{(2,2)}(x)\right\rangle + \frac{\sigma_Y^2(x)}{2}\nabla\left\langle \Phi^{(0,2)}(x)\right\rangle \\ &+ g\alpha_G\left(\left\langle \Phi^{(2,2)}(x)\right\rangle + \frac{\sigma_\beta^2}{2}\left\langle \Phi^{(2,0)}(x)\right\rangle + \frac{\sigma_Y^2(x)}{2}\left\langle \Phi^{(0,2)}(x)\right\rangle + \frac{\sigma_\beta^2\sigma_Y^2(x)}{4}\left\langle \Phi^{(0,0)}(x)\right\rangle\right)e_3 \\ &+ g\left(R_{\alpha\Phi}^{(2,2)}(x) + \frac{\sigma_Y^2(x)}{2}R_{\alpha\Phi}^{(0,2)}(x)\right)e_3\Bigg] \\ &+r^{(2,2)}(x) - g\left[\alpha_G\left(R_{K\Phi}^{(2,2)}(x) + \frac{\sigma_\beta^2}{2}R_{K\Phi}^{(2,0)}(x)\right) + R_{\alpha K\Phi}^{(2,2)}(x)\right]e_3\end{aligned} \tag{3-32}$$

All first-order terms are zero, hence the total flux to second order is

$$q^{[2,2]}(x) = q^{(0,0)}(x) + q^{(0,2)}(x) + q^{(2,0)}(x) + q^{(2,2)}(x) \tag{3-33}$$

3.3 RECURSIVE CONDITIONAL SECOND MOMENT APPROXIMATIONS

3.3.1 Recursive Equations for $C_\Phi(x,y)$

Expanding moments of quantities in (2-27) in powers of σ_Y and σ_β gives, for any integer $m \geq 0$,

$$\left\{\begin{array}{ll}
\nabla_x \cdot \left\{ K_G(\boldsymbol{x}) \sum_{k=0}^{n} \frac{\langle Y'^k(\boldsymbol{x})\rangle}{k!} \nabla_x C_{\Phi}^{(n-k,m)}(\boldsymbol{x},\boldsymbol{y}) + \sum_{k=0}^{n}\sum_{l=0}^{m} C_{K\Phi}^{(k,l)}(\boldsymbol{x},\boldsymbol{y}) \nabla \langle \Phi^{(n-k,m-l)}(\boldsymbol{x})\rangle + \langle K_s'(\boldsymbol{x})\Phi'(\boldsymbol{y})\nabla\Phi'(\boldsymbol{x})\rangle^{(n,m)} \right. & \\
\quad + \mathrm{g}\left[\alpha_G K_G(\boldsymbol{x}) \sum_{k=0}^{n}\sum_{p=0}^{m} \frac{\langle \beta'^p\rangle}{p!}\frac{\langle Y'^k(\boldsymbol{x})\rangle}{k!} C_{\Phi}^{(n-k,m-p)}(\boldsymbol{x},\boldsymbol{y}) + \alpha_G \sum_{p=0}^{m} \frac{\langle \beta'^p\rangle}{p!} C_{\Phi}^{(n-k,m-p)}(\boldsymbol{x},\boldsymbol{y}) \langle K_s'(\boldsymbol{x})\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle^{(n,m-p)} \right. & \\
\quad + K_G(\boldsymbol{x}) \sum_{k=0}^{n} \frac{\langle Y'^k(\boldsymbol{x})\rangle}{k!} \langle \alpha'\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle^{(n,m-p)} + \langle \alpha' K_s'(\boldsymbol{x})\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle^{(n,m)} & \\
\quad + K_G(\boldsymbol{x}) \sum_{p=0}^{m}\sum_{u+v+w=0}^{n} \frac{\langle Y'^u(\boldsymbol{x})\rangle}{u!} \langle \Phi^{(v,p)}(\boldsymbol{x})\rangle C_{\alpha\Phi}^{(w,m-p)}(\boldsymbol{y}) + \sum_{p=0}^{m}\sum_{k=0}^{n} \langle \Phi^{(k,p)}(\boldsymbol{x})\rangle \langle \alpha' K_s'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle^{(n-k,m-p)} & \\
\quad \left.\left. + \alpha_G \sum_{k=0}^{n}\sum_{u+v+w=0}^{n} \frac{\langle \beta'^u\rangle}{u!} \langle \Phi^{(k,v)}(\boldsymbol{x})\rangle C_{K\Phi}^{(n-k,w)}(\boldsymbol{x},\boldsymbol{y}) \right] e_3 \right\} + \langle f'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle^{(n,m)} = 0 & \boldsymbol{x},\boldsymbol{y}\in\Omega \\
C_{\Phi}^{(n,m)}(\boldsymbol{x},\boldsymbol{y}) = \langle H'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle^{(n,m)} & \boldsymbol{y}\in\Omega,\ \boldsymbol{x}\in\Gamma_D \\
\boldsymbol{n}(\boldsymbol{x})\cdot\{*\} = \langle Q'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle^{(n,m)} & \boldsymbol{y}\in\Omega,\ \boldsymbol{x}\in\Gamma_N
\end{array}\right. \tag{3-34}$$

where cross-moments $\langle f'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle^{(n,m)}$ and $\langle Q'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle^{(n,m)}$ can be derived from (2-28),

$$\begin{aligned}
\langle f'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle^{(n,m)} &= C_{f\Phi}^{(n,m)}(\boldsymbol{x},\boldsymbol{y}) = \int_{\Omega} C_f(\boldsymbol{x},\boldsymbol{z}) \langle G^{(n,m)}(\boldsymbol{z},\boldsymbol{y})\rangle d\Omega \\
\langle Q'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle^{(n,m)} &= C_{Q\Phi}^{(n,m)}(\boldsymbol{x},\boldsymbol{y}) = \int_{\Gamma_N} C_Q(\boldsymbol{x},\boldsymbol{z}) \langle G^{(n,m)}(\boldsymbol{z},\boldsymbol{y})\rangle d\Gamma
\end{aligned} \tag{3-35}$$

$C_f(\boldsymbol{x},\boldsymbol{z})$ and $C_Q(\boldsymbol{x},\boldsymbol{z})$ being auto-covariances of the source/sink term and prescribed boundary flux, respectively. The terms $\langle H'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle^{(n,m)}$ are evaluated up to second order in (A-26)-(A-29) of Appendix A. Collecting terms with same power of σ_Y and σ_β, one derives equtions for C_Φ to second order,

$$\left\{\begin{array}{ll}
\nabla_x \cdot \left[K_G(\boldsymbol{x})\ \nabla_x C_{\Phi}^{(0,0)}(\boldsymbol{x},\boldsymbol{y}) + \mathrm{g}\ \alpha_G K_G(\boldsymbol{x})\ C_{\Phi}^{(0,0)}(\boldsymbol{x},\boldsymbol{y}) e_3 \right] + C_{f\Phi}^{(0,0)}(\boldsymbol{x},\boldsymbol{y}) = 0 & \boldsymbol{x},\boldsymbol{y}\in\Omega \\
C_{\Phi}^{(0,0)}(\boldsymbol{x},\boldsymbol{y}) = C_{H\Phi}^{(0,0)}(\boldsymbol{x},\boldsymbol{y}) & \boldsymbol{y}\in\Omega,\ \boldsymbol{x}\in\Gamma_D \\
\boldsymbol{n}(\boldsymbol{x})\cdot\left[K_G(\boldsymbol{x})\ \nabla_x C_{\Phi}^{(0,0)}(\boldsymbol{x},\boldsymbol{y}) + \mathrm{g}\ \alpha_G K_G(\boldsymbol{x})\ C_{\Phi}^{(0,0)}(\boldsymbol{x},\boldsymbol{y}) e_3 \right] = C_{Q\Phi}^{(0,0)}(\boldsymbol{x},\boldsymbol{y}) & \boldsymbol{y}\in\Omega,\ \boldsymbol{x}\in\Gamma_N
\end{array}\right. \tag{3-36}$$

where $\langle f'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle^{(0,0)}$ and $\langle Q'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle^{(0,0)}$ can be obtained from (3-35),

$$\langle f'(x)\Phi'(y)\rangle^{(0,0)} = C_{f\Phi}^{(0,0)}(x,y) = \int_{\Omega} C_f(x,z)\langle G^{(0,0)}(z,y)\rangle d\Omega$$
$$\langle Q'(x)\Phi'(y)\rangle^{(0,0)} = C_{Q\Phi}^{(0,0)}(x,y) = \int_{\Gamma_N} C_Q(x,z)\langle G^{(0,0)}(z,y)\rangle d\Gamma \quad (3\text{-}37)$$

and $\langle H'(x)\Phi'(y)\rangle^{(0,0)}$ is derived in (A-26) of Appendix A,

$$\langle H'(x)\Phi'(y)\rangle^{(0,0)} = -e^{\alpha_G\langle\Psi(x)\rangle}\int_{\Gamma_D} e^{\alpha_G\langle\Psi(z)\rangle} C_\Psi(x,z) K_G(z)\nabla_z G^{(0,0)}(z,y)\cdot n(z) d\Gamma \quad (3\text{-}38)$$

The auto-covariance $C_\Phi^{(0,0)}(x,y)$ is zero only if all driving forces are deterministic, i.e., $C_f(x,z) = C_Q(x,z) = C_\Psi(x,z) = 0$, for all x and z. Equations for $C_\Phi(x,y)$ up to second order in σ_Y and σ_β are

$$\begin{cases} \nabla_x \cdot F(x,y) + C_{f\Phi}^{(2,0)}(x,y) = 0 & x,y\in\Omega \\ C_\Phi^{(2,0)}(x,y) = C_{H\Phi}^{(2,0)}(x,y) & y\in\Omega,\ x\in\Gamma_D \\ n(x)\cdot F(x,y) = C_{Q\Phi}^{(2,0)}(x,y) & y\in\Omega,\ x\in\Gamma_N \\ F(x,y) = \Big[K_G(x)\,\nabla_x C_\Phi^{(2,0)}(x,y) + C_{K\Phi}^{(2,0)}(x,y)\,\nabla\langle\Phi^{(0,0)}(x)\rangle & \\ \qquad + \mathrm{g}\,\alpha_G\Big(K_G(x)\,C_\Phi^{(2,0)}(x,y) + C_{K\Phi}^{(2,0)}(x,y)\langle\Phi^{(0,0)}(x)\rangle\Big)\,e_3\Big] & \end{cases} \quad (3\text{-}39)$$

$$\begin{cases} \nabla_x \cdot F(x,y) + C_{f\Phi}^{(0,2)}(x,y) = 0 & x,y\in\Omega \\ C_\Phi^{(0,2)}(x,y) = C_{H\Phi}^{(0,2)}(x,y) & y\in\Omega,\ x\in\Gamma_D \\ n(x)\cdot F(x,y) = C_{Q\Phi}^{(0,2)}(x,y) & y\in\Omega,\ x\in\Gamma_N \\ F(x,y) = K_G(x)\nabla_x C_\Phi^{(0,2)}(x,y) + \mathrm{g}\,K_G(x)\Big(\alpha_G C_\Phi^{(0,2)}(x,y) + R_{\alpha\Phi}^{(0,2)}(y)\langle\Phi^{(0,0)}(x)\rangle\Big)e_3 & \end{cases} \quad (3\text{-}40)$$

and

$$\begin{cases}\nabla_x \cdot F(x,y) + C_{f\Phi}^{(2,2)}(x,y) = 0 & x,y\in\Omega \\ C_{\Phi}^{(2,2)}(x,y) = C_{H\Phi}^{(2,2)}(x,y) & y\in\Omega,\ x\in\Gamma_D \\ n(x)\cdot F(x,y) = C_{Q\Phi}^{(2,2)}(x,y) & y\in\Omega,\ x\in\Gamma_N \\ F(x,y) = K_G(x)\,\nabla_x C_{\Phi}^{(2,2)}(x,y) + \dfrac{\sigma_Y^2(x)}{2}K_G(x)\nabla_x C_{\Phi}^{(0,2)}(x,y) + \left\langle K_s'(x)\Phi'(y)\nabla\Phi'(x)\right\rangle^{(2,2)} \\ \quad + C_{K\Phi}^{(2,0)}(x,y)\,\nabla\left\langle \Phi^{(0,2)}(x)\right\rangle + C_{K\Phi}^{(2,2)}(x,y)\,\nabla\left\langle\Phi^{(0,0)}(x)\right\rangle \\ \quad + g\left[\alpha_G K_G(x)\left(C_{\Phi}^{(2,2)}(x,y) + \dfrac{\sigma_Y^2(x)}{2}C_{\Phi}^{(0,2)}(x,y) + \dfrac{\sigma_\beta^2}{2}C_{\Phi}^{(2,0)}(x,y)\right)\right. \\ \quad + \alpha_G\left(\left\langle K_s'(x)\Phi'(x)\Phi'(y)\right\rangle^{(2,2)} + \dfrac{\sigma_\beta^2}{2}\left\langle K_s'(x)\Phi'(x)\Phi'(y)\right\rangle^{(2,0)}\right) \\ \quad + K_G(x)\left(\left\langle \alpha'\Phi'(x)\Phi'(y)\right\rangle^{(2,2)} + \dfrac{\sigma_Y^2(x)}{2}\left\langle\alpha'\Phi'(x)\Phi'(y)\right\rangle^{(0,2)}\right) \\ \quad + \left\langle \alpha' K_s'(x)\Phi'(x)\Phi'(y)\right\rangle^{(2,2)} \\ \quad + K_G(x)\left(\dfrac{\sigma_Y^2(x)}{2}\left\langle\Phi^{(0,0)}(x)\right\rangle R_{\alpha\Phi}^{(0,2)}(y) + \left\langle\Phi^{(2,0)}(x)\right\rangle R_{\alpha\Phi}^{(0,2)}(y) + \left\langle\Phi^{(0,0)}(x)\right\rangle R_{\alpha\Phi}^{(2,2)}(y)\right) \\ \quad + \alpha_G\left(\dfrac{\sigma_\beta^2}{2}\left\langle\Phi^{(0,0)}(x)\right\rangle C_{K\Phi}^{(2,0)}(x,y) + \left\langle\Phi^{(0,2)}(x)\right\rangle C_{K\Phi}^{(2,0)}(x,y) + \left\langle\Phi^{(0,0)}(x)\right\rangle C_{K\Phi}^{(2,2)}(x,y)\right) \\ \quad \left. + C_{\alpha K\Phi}^{(2,2)}(x,y)\left\langle\Phi^{(0,0)}(x)\right\rangle\right] e_3 \end{cases} \tag{3-41}$$

where $C_{H\Phi}^{(0,2)}(\boldsymbol{x}, \boldsymbol{y})$ and $C_{H\Phi}^{(2,2)}(\boldsymbol{x}, \boldsymbol{y})$ are given by (A-24)-(A-27) of Appendix A, and all other terms have been evaluated in Appendix C.

3.3.2 Recursive Approximations for $C_q(x, y)$

Expanding (2-29) in powers of σ_Y and σ_β, we obtained approximations for the covariance tensor of flux, $\boldsymbol{C_{qq}(x,y)} = \langle \boldsymbol{q}'(\boldsymbol{x})\boldsymbol{q}'^{T}(\boldsymbol{y})\rangle$, to second order in σ_Y and σ_β,

$$\begin{aligned} C_q^{(0,0)}(x,y) &= \left\langle q'(x)q'^T(y)\right\rangle^{(0,0)} \\ &= K_G(x)\left[\nabla_x\nabla_y^T C_{\Phi}^{(0,0)}(x,y) + g\alpha_G\left(\nabla_x C_{\Phi}^{(0,0)}(x,y)\, e_3^T + e_3\nabla_y^T C_{\Phi}^{(0,0)}(x,y) + \alpha_G C_{\Phi}^{(0,0)}(x,y)\, E_3\right)\right]K_G(y) \end{aligned} \tag{3-42}$$

$$
\begin{aligned}
\boldsymbol{C}_q^{(2,0)}(\boldsymbol{x},\boldsymbol{y}) &= \left\langle \boldsymbol{q}'(x)\boldsymbol{q}'^T(y)\right\rangle^{(2,0)} \\
&= K_G(\boldsymbol{x})\Big[\nabla_x\nabla_y^T C_\Phi^{(2,0)}(\boldsymbol{x},\boldsymbol{y}) + \nabla_x C_{Y\Phi}^{(2,0)}(\boldsymbol{y},\boldsymbol{x})\nabla_y^T\left\langle\Phi^{(0,0)}(\boldsymbol{y})\right\rangle \\
&\qquad + \nabla_y C_{Y\Phi}^{(2,0)}(\boldsymbol{x},\boldsymbol{y})\nabla_x^T\left\langle\Phi^{(0,0)}(\boldsymbol{x})\right\rangle + C_Y(\boldsymbol{x},\boldsymbol{y})\nabla_x\left\langle\Phi^{(0,0)}(\boldsymbol{x})\right\rangle\nabla_y^T\left\langle\Phi^{(0,0)}(\boldsymbol{y})\right\rangle\Big]K_G(\boldsymbol{y}) \\
&\quad + \mathrm{g}\alpha_G K_G(\boldsymbol{x})\Big[\nabla_x C_\Phi^{(2,0)}(\boldsymbol{x},\boldsymbol{y}) + \nabla_x C_{Y\Phi}^{(2,0)}(\boldsymbol{y},\boldsymbol{x})\left\langle\Phi^{(0,0)}(\boldsymbol{y})\right\rangle \\
&\qquad + C_{Y\Phi}^{(2,0)}(\boldsymbol{x},\boldsymbol{y})\nabla_x\left\langle\Phi^{(0,0)}(\boldsymbol{x})\right\rangle + C_Y(\boldsymbol{x},\boldsymbol{y})\nabla_x\left\langle\Phi^{(0,0)}(\boldsymbol{x})\right\rangle\left\langle\Phi^{(0,0)}(\boldsymbol{y})\right\rangle\Big]\, e_3^T K_G(\boldsymbol{y}) \\
&\quad + \mathrm{g}\alpha_G e_3 K_G(\boldsymbol{x})\Big[\nabla_y^T C_\Phi^{(2,0)}(\boldsymbol{x},\boldsymbol{y}) + C_{Y\Phi}^{(2,0)}(\boldsymbol{y},\boldsymbol{x})\nabla_y^T\left\langle\Phi^{(0,0)}(\boldsymbol{y})\right\rangle \\
&\qquad + \nabla_y^T C_{Y\Phi}^{(2,0)}(\boldsymbol{x},\boldsymbol{y})\left\langle\Phi^{(0,0)}(\boldsymbol{x})\right\rangle + C_Y(\boldsymbol{x},\boldsymbol{y})\left\langle\Phi^{(0,0)}(\boldsymbol{x})\right\rangle\nabla_y^T\left\langle\Phi^{(0,0)}(\boldsymbol{y})\right\rangle\Big]K_G(\boldsymbol{y}) \\
&\quad + \mathrm{g}\alpha_G^2 K_G(\boldsymbol{x})\Big[C_\Phi^{(2,0)}(\boldsymbol{x},\boldsymbol{y}) + C_{Y\Phi}^{(2,0)}(\boldsymbol{y},\boldsymbol{x})\left\langle\Phi^{(0,0)}(\boldsymbol{y})\right\rangle \\
&\qquad + C_{Y\Phi}^{(2,0)}(\boldsymbol{x},\boldsymbol{y})\left\langle\Phi^{(0,0)}(\boldsymbol{x})\right\rangle + C_Y(\boldsymbol{x},\boldsymbol{y})\left\langle\Phi^{(0,0)}(\boldsymbol{x})\right\rangle\left\langle\Phi^{(0,0)}(\boldsymbol{y})\right\rangle\Big]\boldsymbol{E}_3 K_G(\boldsymbol{y})
\end{aligned}
\tag{3-43}
$$

$$
\begin{aligned}
\boldsymbol{C}_q^{(0,2)}(\boldsymbol{x},\boldsymbol{y}) &= \left\langle \boldsymbol{q}'(x)\boldsymbol{q}'^T(y)\right\rangle^{(0,2)} \\
&= K_G(\boldsymbol{x})\nabla_x\nabla_y^T C_\Phi^{(0,2)}(\boldsymbol{x},\boldsymbol{y})K_G(\boldsymbol{y}) \\
&\quad + \mathrm{g}K_G(\boldsymbol{x})\Big[\alpha_G\nabla_x C_\Phi^{(0,2)}(\boldsymbol{x},\boldsymbol{y})\, e_3^T + \alpha_G e_3\nabla_y^T C_\Phi^{(0,2)}(\boldsymbol{x},\boldsymbol{y}) + \alpha_G^2 C_\Phi^{(0,2)}(\boldsymbol{x},\boldsymbol{y})\,\boldsymbol{E}_3 \\
&\qquad + \nabla_x R_{\alpha\Phi}^{(0,2)}(\boldsymbol{x})\, e_3^T\left\langle\Phi^{(0,0)}(\boldsymbol{y})\right\rangle + e_3\nabla_y^T R_{\alpha\Phi}^{(0,2)}(\boldsymbol{y})\left\langle\Phi^{(0,0)}(\boldsymbol{x})\right\rangle \\
&\qquad + \alpha_G\left(R_{\alpha\Phi}^{(0,2)}(\boldsymbol{x})\left\langle\Phi^{(0,0)}(\boldsymbol{y})\right\rangle + R_{\alpha\Phi}^{(0,2)}(\boldsymbol{y})\left\langle\Phi^{(0,0)}(\boldsymbol{x})\right\rangle\right)\boldsymbol{E}_3 \\
&\qquad + \alpha_G^2\sigma_\beta^2\left\langle\Phi^{(0,0)}(\boldsymbol{x})\right\rangle\left\langle\Phi^{(0,0)}(\boldsymbol{y})\right\rangle\boldsymbol{E}_3\Big]K_G(\boldsymbol{y})
\end{aligned}
\tag{3-44}
$$

$$
\boldsymbol{C}_{\mathrm{q}}^{(2,2)}(\boldsymbol{x},\boldsymbol{y}) = \left\langle \boldsymbol{q}'(x)\boldsymbol{q}'^{\mathrm{T}}(y)\right\rangle^{(2,2)} = \mathrm{U}(\boldsymbol{x},\boldsymbol{y}) + \mathrm{V}(\boldsymbol{x},\boldsymbol{y}) + \mathrm{V}^{\mathrm{T}}(\boldsymbol{y},\boldsymbol{x}) \tag{3-45}
$$

where U and V are defined as

$$
\begin{aligned}
&U(\boldsymbol{x},\boldsymbol{y}) = \\
&= K_G(\boldsymbol{x})\Big[\nabla_x \nabla_y^T C_\Phi^{(2,2)}(\boldsymbol{x},\boldsymbol{y}) + \frac{1}{2}\big(\sigma_Y^2(x)+\sigma_Y^2(y)\big)\nabla_x\nabla_y^T C_\Phi^{(0,2)}(\boldsymbol{x},\boldsymbol{y}) + \nabla_x\left\langle \Phi^{(0,0)}(x)\right\rangle \left\langle Y'(\boldsymbol{x})Y'(\boldsymbol{y})\nabla_y^T \Phi'(\boldsymbol{y})\right\rangle^{(2,2)} \\
&\qquad + \left\langle Y'(\boldsymbol{x})Y'(\boldsymbol{y})\nabla_{\boldsymbol{x}}^T\Phi'(\boldsymbol{x})\right\rangle^{(2,2)} \nabla_y^T \left\langle \Phi^{(0,0)}(\boldsymbol{y})\right\rangle + \left\langle Y'(\boldsymbol{x})Y'(\boldsymbol{y})\nabla_{\boldsymbol{x}}^T\Phi'(\boldsymbol{x})\nabla_y^T\Phi'(\boldsymbol{y})\right\rangle^{(2,2)} \\
&\qquad + C_Y(\boldsymbol{x},\boldsymbol{y})\Big(\nabla_x\left\langle \Phi^{(0,2)}(\boldsymbol{x})\right\rangle \nabla_y^T\left\langle \Phi^{(0,0)}(\boldsymbol{y})\right\rangle + \nabla_x\left\langle \Phi^{(0,0)}(\boldsymbol{x})\right\rangle \nabla_y^T\left\langle \Phi^{(0,2)}(\boldsymbol{y})\right\rangle\Big)\Big] K_G(\boldsymbol{y}) \\
&\quad + g K_G(\boldsymbol{x})\Big[\alpha_G^2\, C_\Phi^{(2,2)}(\boldsymbol{x},\boldsymbol{y}) + \frac{1}{2}\big(\sigma_Y^2(x)+\sigma_Y^2(y)\big) C_\Phi^{(0,2)}(\boldsymbol{x},\boldsymbol{y}) + \sigma_\beta^2 C_\Phi^{(2,0)}(\boldsymbol{x},\boldsymbol{y}) \\
&\qquad + \alpha_G\left(R_{\alpha\Phi}^{(2,2)}(\boldsymbol{x})\left\langle \Phi^{(0,0)}(\boldsymbol{y})\right\rangle + R_{\alpha\Phi}^{(0,2)}(\boldsymbol{x})\left(\left\langle \Phi^{(2,0)}(\boldsymbol{y})\right\rangle + \frac{1}{2}\big(\sigma_Y^2(x)+\sigma_Y^2(y)\big)\left\langle \Phi^{(0,0)}(\boldsymbol{y})\right\rangle \right)\right) \\
&\qquad + \alpha_G\left(R_{\alpha\Phi}^{(2,2)}(\boldsymbol{y})\left\langle \Phi^{(0,0)}(\boldsymbol{x})\right\rangle + R_{\alpha\Phi}^{(0,2)}(\boldsymbol{y})\left(\left\langle \Phi^{(2,0)}(\boldsymbol{x})\right\rangle + \frac{1}{2}\big(\sigma_Y^2(x)+\sigma_Y^2(y)\big)\left\langle \Phi^{(0,0)}(\boldsymbol{x})\right\rangle \right)\right) \\
&\qquad + \alpha_G^2\sigma_\beta^2\Big(\left\langle \Phi^{(2,0)}(\boldsymbol{x})\right\rangle\left\langle \Phi^{(0,0)}(\boldsymbol{y})\right\rangle + \left\langle \Phi^{(0,0)}(\boldsymbol{x})\right\rangle\left\langle \Phi^{(2,0)}(\boldsymbol{y})\right\rangle \\
&\qquad\qquad + \frac{1}{2}\big(\sigma_Y^2(x)+\sigma_Y^2(y)\big)\left\langle \Phi^{(0,0)}(\boldsymbol{x})\right\rangle\left\langle \Phi^{(0,0)}(\boldsymbol{y})\right\rangle\Big) \\
&\qquad + \left\langle \alpha'^2\Phi'(\boldsymbol{y})\right\rangle^{(2,2)}\left\langle \Phi^{(0,0)}(\boldsymbol{x})\right\rangle + \left\langle \alpha'^2\Phi'(\boldsymbol{x})\right\rangle^{(2,2)}\left\langle \Phi^{(0,0)}(\boldsymbol{y})\right\rangle \\
&\qquad + 2\alpha_G\left\langle \alpha'\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle^{(2,2)} + \left\langle \alpha'^2\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle^{(2,2)} \\
&\qquad + \alpha_G^2 C_Y(\boldsymbol{x},\boldsymbol{y})\Big(2\sigma_\beta^2\left\langle \Phi^{(0,0)}(\boldsymbol{x})\right\rangle\left\langle \Phi^{(0,0)}(\boldsymbol{y})\right\rangle + \left\langle \Phi^{(0,2)}(\boldsymbol{x})\right\rangle\left\langle \Phi^{(0,0)}(\boldsymbol{y})\right\rangle + \left\langle \Phi^{(0,0)}(\boldsymbol{x})\right\rangle\left\langle \Phi^{(0,2)}(\boldsymbol{y})\right\rangle\Big) \\
&\qquad + \alpha_G^2\left\langle Y'(\boldsymbol{x})Y'(\boldsymbol{y})\,\Phi'(\boldsymbol{x})\right\rangle^{(2,2)}\left\langle \Phi^{(0,0)}(\boldsymbol{y})\right\rangle + \alpha_G^2\left\langle Y'(\boldsymbol{x})Y'(\boldsymbol{y})\,\Phi'(\boldsymbol{y})\right\rangle^{(2,2)}\left\langle \Phi^{(0,0)}(\boldsymbol{x})\right\rangle \\
&\qquad + 2\alpha_G\left\langle \alpha' Y'(\boldsymbol{x})Y'(\boldsymbol{y})\Phi'(\boldsymbol{y})\right\rangle^{(2,2)}\left\langle \Phi^{(0,0)}(\boldsymbol{x})\right\rangle + 2\alpha_G\left\langle \alpha' Y'(\boldsymbol{x})Y'(\boldsymbol{y})\Phi'(\boldsymbol{x})\right\rangle^{(2,2)}\left\langle \Phi^{(0,0)}(\boldsymbol{y})\right\rangle \\
&\qquad + \alpha_G^2\left\langle Y'(\boldsymbol{x})Y'(\boldsymbol{y})\,\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle^{(2,2)}\Big] \boldsymbol{E}_3 K_G(\boldsymbol{y})
\end{aligned}
\tag{3-46}
$$

$$
\begin{aligned}
V(\boldsymbol{x},\boldsymbol{y}) = \mathrm{g}K_G(\boldsymbol{x})\boldsymbol{E}_3\Big[&\alpha_G^2\Big(C_{K\Phi}^{(2,2)}(\boldsymbol{y},\boldsymbol{x})\big\langle\Phi^{(0,0)}(\boldsymbol{y})\big\rangle + C_{K\Phi}^{(2,0)}(\boldsymbol{y},\boldsymbol{x})\Big(\big\langle\Phi^{(0,2)}(\boldsymbol{y})\big\rangle + \sigma_\beta^2\big\langle\Phi^{(0,0)}(\boldsymbol{y})\big\rangle\Big)\Big)\\
&+\alpha_G^2\big\langle K_s'(\boldsymbol{y})\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\big\rangle^{(2,2)} + \alpha_G\big\langle\Phi^{(0,0)}(\boldsymbol{x})\big\rangle\big\langle\alpha' K_s'(\boldsymbol{y})\Phi'(\boldsymbol{y})\big\rangle^{(2,2)}\\
&+2\alpha_G\big\langle\Phi^{(0,0)}(\boldsymbol{y})\big\rangle\big\langle\alpha' K'(\boldsymbol{y})\Phi'(\boldsymbol{x})\big\rangle^{(2,2)} + 2\alpha_G\big\langle\alpha' K_s'(\boldsymbol{y})\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\big\rangle^{(2,2)}\\
&+\big\langle\Phi^{(0,0)}(\boldsymbol{x})\big\rangle\big\langle\alpha'^2 K_s'(\boldsymbol{y})\Phi'(\boldsymbol{y})\big\rangle^{(2,2)} + \big\langle\Phi^{(0,0)}(\boldsymbol{y})\big\rangle\big\langle\alpha'^2 K_s'(\boldsymbol{y})\Phi'(\boldsymbol{x})\big\rangle^{(2,2)}\Big]\\
+\mathrm{g}K_G(\boldsymbol{x})\,\boldsymbol{e}_3\Big[&\alpha_G\Big(\nabla_y^T C_\Phi^{(2,2)}(\boldsymbol{x},\boldsymbol{y}) + \frac{1}{2}\big(\sigma_Y^2(\boldsymbol{x})+\sigma_Y^2(\boldsymbol{y})\big)\nabla_y^T C_\Phi^{(0,2)}(\boldsymbol{x},\boldsymbol{y}) + \frac{1}{2}\sigma_\beta^2\nabla_y^T C_\Phi^{(2,0)}(\boldsymbol{x},\boldsymbol{y})\Big)\\
&+\nabla_y^T R_{\alpha\Phi}^{(2,2)}(\boldsymbol{y})\big\langle\Phi^{(0,0)}(\boldsymbol{x})\big\rangle + \nabla_y^T R_{\alpha\Phi}^{(0,2)}(\boldsymbol{y})\Big(\big\langle\Phi^{(2,0)}(\boldsymbol{x})\big\rangle + \frac{1}{2}\big(\sigma_Y^2(\boldsymbol{x})+\sigma_Y^2(\boldsymbol{y})\big)\big\langle\Phi^{(0,0)}(\boldsymbol{x})\big\rangle\Big)\\
&+\alpha_G C_Y(\boldsymbol{x},\boldsymbol{y})\Big(\big\langle\Phi^{(0,2)}(\boldsymbol{x})\big\rangle\nabla_y^T\big\langle\Phi^{(0,0)}(\boldsymbol{y})\big\rangle + \big\langle\Phi^{(0,0)}(\boldsymbol{x})\big\rangle\nabla_y^T\big\langle\Phi^{(0,2)}(\boldsymbol{y})\big\rangle\\
&\qquad+\frac{1}{2}\sigma_\beta^2\big\langle\Phi^{(0,0)}(\boldsymbol{x})\big\rangle\nabla_y^T\big\langle\Phi^{(0,0)}(\boldsymbol{y})\big\rangle\Big)\\
&+\big\langle\alpha'\Phi'(\boldsymbol{x})\nabla_y^T\Phi'(\boldsymbol{y})\big\rangle^{(2,2)} + \big\langle\alpha' Y'(\boldsymbol{x})Y'(\boldsymbol{y})\Phi'(\boldsymbol{x})\big\rangle^{(2,2)}\nabla_y^T\big\langle\Phi^{(0,0)}(\boldsymbol{y})\big\rangle\\
&+\alpha_G\big\langle Y'(\boldsymbol{x})Y'(\boldsymbol{y})\Phi'(\boldsymbol{x})\big\rangle^{(2,2)}\nabla_y^T\big\langle\Phi^{(0,0)}(\boldsymbol{y})\big\rangle + \big\langle\alpha' Y'(\boldsymbol{x})Y'(\boldsymbol{y})\nabla_y^T\Phi'(\boldsymbol{y})\big\rangle^{(2,2)}\big\langle\Phi^{(0,0)}(\boldsymbol{x})\big\rangle\\
&+\alpha_G\big\langle Y'(\boldsymbol{x})Y'(\boldsymbol{y})\nabla_y^T\Phi'(\boldsymbol{y})\big\rangle^{(2,2)}\big\langle\Phi^{(0,0)}(\boldsymbol{x})\big\rangle + \alpha_G\big\langle Y'(\boldsymbol{x})Y'(\boldsymbol{y})\Phi'(\boldsymbol{x})\nabla_y^T\Phi'(\boldsymbol{y})\big\rangle^{(2,2)}\\
&+\big\langle\alpha' Y'(\boldsymbol{x})\Phi'(\boldsymbol{x})\nabla_y^T\Phi'(\boldsymbol{y})\big\rangle^{(2,2)}\Big]K_G(\boldsymbol{y})\\
+\mathrm{g}K_G(\boldsymbol{x})\,\boldsymbol{e}_3\Big[&\alpha_G\Big(\nabla_y^T\big\langle\Phi^{(0,0)}(\boldsymbol{y})\big\rangle C_{K\Phi}^{(2,2)}(\boldsymbol{y},\boldsymbol{x}) + \Big(\nabla_y^T\big\langle\Phi^{(0,2)}(\boldsymbol{y})\big\rangle + \frac{1}{2}\sigma_\beta^2\nabla_y^T\big\langle\Phi^{(0,0)}(\boldsymbol{y})\big\rangle\Big)C_{K\Phi}^{(2,0)}(\boldsymbol{y},\boldsymbol{x})\Big)\\
&+\alpha_G\big\langle K_s'(\boldsymbol{y})\Phi'(\boldsymbol{x})\nabla_y^T\Phi'(\boldsymbol{y})\big\rangle^{(2,2)} + \big\langle\alpha' K_s'(\boldsymbol{y})\Phi'(\boldsymbol{x})\nabla_y^T\Phi'(\boldsymbol{y})\big\rangle^{(2,2)}\\
&+\big\langle\Phi^{(0,0)}(\boldsymbol{x})\big\rangle\big\langle\alpha' K'(\boldsymbol{y})\nabla_y^T\Phi'(\boldsymbol{y})\big\rangle^{(2,2)} + \nabla_y^T\big\langle\Phi^{(0,0)}(\boldsymbol{y})\big\rangle\big\langle\alpha' K_s'(\boldsymbol{y})\Phi'(\boldsymbol{x})\big\rangle^{(2,2)}\Big]\\
+K_G(\boldsymbol{x})\Big[&\big\langle K'(\boldsymbol{y})\nabla_x^T\Phi'(\boldsymbol{x})\big\rangle^{(2,2)}\nabla_y^T\big\langle\Phi^{(0,0)}(\boldsymbol{y})\big\rangle + \big\langle K_s'(\boldsymbol{y})\nabla_x^T\Phi'(\boldsymbol{x})\big\rangle^{(2,0)}\nabla_y^T\big\langle\Phi^{(0,2)}(\boldsymbol{y})\big\rangle\\
&+\big\langle K_s'(\boldsymbol{y})\nabla\Phi'(\boldsymbol{x})\nabla_y^T\Phi'(\boldsymbol{y})\big\rangle^{(2,2)}\Big]\\
+\mathrm{g}K_G(\boldsymbol{x})\Big[&\alpha_G\Big(\big\langle K_s'(\boldsymbol{y})\nabla_x\Phi'(\boldsymbol{x})\big\rangle^{(2,2)}\big\langle\Phi^{(0,0)}(\boldsymbol{y})\big\rangle + \big\langle K_s'(\boldsymbol{y})\nabla_x\Phi'(\boldsymbol{x})\big\rangle^{(2,0)}\Big(\big\langle\Phi^{(0,2)}(\boldsymbol{y})\big\rangle + \frac{1}{2}\sigma_\beta^2\big\langle\Phi^{(0,0)}(\boldsymbol{y})\big\rangle\Big)\Big)\\
&+\alpha_G\big\langle K_s'(\boldsymbol{y})\nabla_x\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\big\rangle^{(2,2)} + \big\langle\alpha' K_s'(\boldsymbol{y})\nabla_x\Phi'(\boldsymbol{x})\big\rangle^{(2,2)}\big\langle\Phi^{(0,0)}(\boldsymbol{y})\big\rangle\Big]\boldsymbol{e}_3^T
\end{aligned}
\tag{3-47}
$$

3.3.3 Approximations for $C_{Yq}(x, y)$

Rewriting (2-30) in terms of mean quantities and fluctuations about these means, then collecting terms of same order in σ_Y and σ_β, we obtain expressions for the cross-covariance between the natural logarithm of saturated hydraulic conductivity and flux up to second order in σ_Y and σ_β,

$$\begin{aligned} C_{Yq}^{(2,0)}(x,y) &= \langle Y'(x) q'(y) \rangle^{(2,0)} \\ &= -K_G(y)\langle Y'(x)\nabla\Phi'(y)\rangle^{(2,0)} - C_Y(x,y)K_G(y)\nabla\langle\Phi^{(0,0)}(y)\rangle \\ &\quad - g\alpha_G K_G(y)\left[\langle Y'(x)\Phi'(y)\rangle^{(2,0)} + C_Y(x,y)\langle\Phi^{(0,0)}(y)\rangle\right] e_3 \end{aligned} \tag{3-48}$$

$$\begin{aligned} C_{Yq}^{(2,2)}(x,y) &= \langle Y'(x) q'(y) \rangle^{(2,2)} \\ &= -K_G(y)\left(\nabla_y C_{Y\Phi}^{(2,2)}(x,y) + C_Y(x,y)\nabla\langle\Phi^{(0,2)}(y)\rangle\right) - \langle Y'(x)K_s'(y)\nabla\Phi'(y)\rangle^{(2,2)} \\ &\quad - g\left[\alpha_G K_G(y)\left(C_{Y\Phi}^{(2,2)}(x,y) + \frac{1}{2}\sigma_\beta^2 C_{Y\Phi}^{(2,0)}(x,y)\right) + \alpha_G\langle Y'(x)K_s'(y)\Phi'(y)\rangle^{(2,2)} \right. \\ &\quad + \alpha_G K_G(y) C_Y(x,y)\left(\langle\Phi^{(0,2)}(y)\rangle + \frac{1}{2}\sigma_\beta^2\langle\Phi^{(0,0)}(y)\rangle\right) + \\ &\quad \left. + K_G(y)\langle\alpha' Y'(x)\Phi'(y)\rangle^{(2,2)} + \langle\alpha' Y'(x)K_s'(y)\Phi'(y)\rangle^{(2,2)}\right] e_3 \end{aligned} \tag{3-49}$$

All terms on the right hand sides of (3-48)-(3-49) are derived in Appendix C.

3.3.4 Approximations for $C_{\beta q}(x, y)$

Similarly, rewriting (2-31) in terms of mean quantities and corresponding fluctuations, then collecting terms of same order in σ_Y and σ_β, we obtain expressions for the cross-covariance between β and flux up to second order in σ_Y and σ_β,

$$C_{\beta q}^{(0,2)}(y) = \langle \beta' q'(y) \rangle^{(0,2)} = -K_G(y)\left[\nabla R_{\beta\Phi}^{(0,2)}(y) + g\alpha_G\left(R_{\beta\Phi}^{(0,2)}(y) + \sigma_\beta^2\langle\Phi^{(0,0)}(y)\rangle\right) e_3\right] \tag{3-50}$$

$$
\begin{aligned}
\boldsymbol{C}_{\beta q}^{(2,2)}(\boldsymbol{y}) &= \left\langle \beta' \boldsymbol{q}'(\boldsymbol{y}) \right\rangle^{(2,2)} \\
&= -K_G(\boldsymbol{y}) \left[\nabla R_{\beta\Phi}^{(2,2)}(\boldsymbol{y}) + \frac{1}{2}\sigma_Y^2(\boldsymbol{y}) \nabla R_{\beta\Phi}^{(0,2)}(\boldsymbol{y}) \right] - \left\langle \beta' K_s'(\boldsymbol{y}) \nabla \Phi'(\boldsymbol{y}) \right\rangle^{(2,2)} \\
&\quad - g\alpha_G K_G(\boldsymbol{y}) \left[\left(R_{\beta\Phi}^{(2,2)}(\boldsymbol{y}) + \frac{1}{2}\sigma_Y^2(\boldsymbol{y}) R_{\beta\Phi}^{(0,2)}(\boldsymbol{y}) \right) + \sigma_\beta^2 \left(\left\langle \Phi^{(2,0)}(\boldsymbol{y}) \right\rangle + \frac{1}{2}\sigma_Y^2(\boldsymbol{y}) \left\langle \Phi^{(0,0)}(\boldsymbol{y}) \right\rangle \right) \right] \boldsymbol{e}_3 \\
&\quad - g \left[K_G(\boldsymbol{y}) \left\langle \alpha' \beta' \Phi'(\boldsymbol{y}) \right\rangle^{(2,2)} + \alpha_G \left\langle \beta' K_s'(\boldsymbol{y}) \Phi'(\boldsymbol{y}) \right\rangle^{(2,2)} + \left\langle \alpha' \beta' K_s'(\boldsymbol{y}) \Phi'(\boldsymbol{y}) \right\rangle^{(2,2)} \right] \boldsymbol{e}_3
\end{aligned}
\tag{3-51}
$$

CHAPTER 4
FINITE ELEMENT SOLUTIONS OF RECURSIVE CONDITIONAL MOMENT EQUATIONS

4.1 INTRODUCTION

In this study, we consider steady state unsaturated flow in a two-dimensional vertical plane. The flow domain is discretized into a number of elements. Soil properties, such as saturated hydraulic conductivity, are defined over elements, i.e., they are considered to be constant inside an element but may vary from element to element. However, flow properties, such as pressure head and its transformed variable Φ, are evaluated at nodes, and their values at points other than nodes can be interpolated using weight functions, which are defined later.

We solve the recursive conditional moment equations by a Galerkin finite element scheme on a rectangular vertical grid, using bilinear weight functions. For simplicity, we consider only deterministic forcing terms. For illustration purposes, we show only the derivation of numerical solutions for recursive conditional mean equations and covariance functions in detail. Appendix D is devoted to the detailed derivation of all other quantities (related to the mean and covariance equations).

4.2 FINITE ELEMENT SOLUTIONS OF CONDITIONAL MEAN FLOW EQUATIONS

4.2.1 Mean Transformed Variables

Consider Galerkin orthogonalization of (3-9). Application of Green's first identity yields

$$\begin{aligned}&\int_{\Omega} K_G(\boldsymbol{x})\left(\nabla\left\langle\Phi^{(0,0)}(\boldsymbol{x})\right\rangle + g\alpha_G\left\langle\Phi^{(0,0)}(\boldsymbol{x})\right\rangle \boldsymbol{e}_2\right)\cdot\nabla\xi_n(\boldsymbol{x})d\Omega \\ &\quad = \int_{\Gamma_D} K_G(\boldsymbol{x})\nabla\left\langle\Phi^{(0,0)}(\boldsymbol{x})\right\rangle\xi_n(\boldsymbol{x})\cdot\boldsymbol{n}(\boldsymbol{x})d\Gamma + \int_{\Gamma_N}\left\langle Q(\boldsymbol{x})\right\rangle\xi_n(\boldsymbol{x})d\Gamma + \int_{\Omega}\left\langle f(\boldsymbol{x})\right\rangle\xi_n(\boldsymbol{x})d\Omega\end{aligned} \tag{4-1}$$

where, $\boldsymbol{e}_3$ in (3-9) has been changed to $\boldsymbol{e}_2=(0,1)^T$ for two-dimensional flow. Let

$$\left\langle\Phi^{(0,0)}(\boldsymbol{x})\right\rangle = \sum_{m=1}^{NN}\left\langle\Phi_m^{(0,0)}\right\rangle\xi_m(\boldsymbol{x}) \tag{4-2}$$

where ξ_m is the weight function defined in (D-2), NN is the total number of nodes used for discretization of the flow domain, and $\langle\Phi_m^{(0,0)}\rangle$ is $\langle\Phi^{(0,0)}(\boldsymbol{x})\rangle$ evaluated at global node m. It should be pointed out that in the following derivation, a node number (such as m here) may denote either a global node or a local node, which should be evident from the context. Substituting (4-2) into the first integral of (4-1), and defining

$$\begin{aligned}A_{nm} &= \sum_e A_{nm}^{(e)} = \int_{\Omega} K_G(\boldsymbol{x})\nabla\xi_n(\boldsymbol{x})\cdot\nabla\xi_m(\boldsymbol{x})d\Omega \\ \boldsymbol{B}_{nm} &= \sum_e \boldsymbol{B}_{nm}^{(e)} = \int_{\Omega} K_G(\boldsymbol{x})\xi_n(\boldsymbol{x})\nabla\xi_m(\boldsymbol{x})d\Omega\end{aligned} \tag{4-3}$$

leads to

$$\begin{aligned}\sum_{m=1}^{NN}\left(A_{nm} + g\alpha_G\boldsymbol{e}_2^T\boldsymbol{B}_{nm}\right)\left\langle\Phi_m^{(0,0)}\right\rangle &= \int_{\Gamma_D} K_G(\boldsymbol{x})\nabla\left\langle\Phi^{(0,0)}(\boldsymbol{x})\right\rangle\xi_n(\boldsymbol{x})\cdot\boldsymbol{n}(\boldsymbol{x})d\Gamma \\ &\quad + \int_{\Gamma_N}\left\langle Q(\boldsymbol{x})\right\rangle\xi_n(\boldsymbol{x})d\Gamma + \int_{\Omega}\left\langle f(\boldsymbol{x})\right\rangle\xi_n(\boldsymbol{x})d\Omega \qquad n = 1,2,\ldots NN\end{aligned} \tag{4-4}$$

where integrals containing prescribed mean flux $\langle Q\rangle$ and source/sink term $\langle f\rangle$ need to be evaluated, but the integral over Dirichlet boundary can be ignored. In fact, for any node $n\notin\Gamma_D$, since $\xi_n(y)=0$ on Γ_D, the first boundary integral in (4-4) vanishes. For any $n\in\Gamma_D$, we can drop the n-th equation, since the value of $\langle\Phi_n^{(0,0)}\rangle$ is prescribed on Γ_D, or we can simply assign coefficient matrices

$$\tilde{A}_{nm}=\begin{cases}A_{nm}+g\alpha_G\boldsymbol{e}_2^T\boldsymbol{B}_{mn} & \text{if } n\notin\Gamma_D\\ 1 & \text{if } n\in\Gamma_D \text{ and } n=m\\ 0 & \text{if } n\in\Gamma_D \text{ and } n\neq m\end{cases}\tag{4-5}$$

and

$$\tilde{b}_n=\begin{cases}\left\langle H_n^{(0,0)}\right\rangle & \text{if n} \in\Gamma_D\\ \displaystyle\sum_{e\in E_n}\frac{w_1^{(e)}w_2^{(e)}}{4}\langle f(e)\rangle+\sum_{e\in E_n'}\frac{d^{(e)}}{2}\left\langle Q^{(e)}\right\rangle & \text{if n}\notin\Gamma_D\end{cases}\tag{4-6}$$

so that (4-4) can be rewritten as

$$\sum_{m=1}^{NN}\tilde{A}_{nm}\Phi_m^{(0,0)}=\tilde{b}_n\tag{4-7}$$

This scheme is easier to implement, because we do not need to distinguish between types of boundary nodes (Neumann boundary nodes or Dilichlet boundary nodes) in assembling element matrices into global matrices. Here $\langle H_n^{(0,0)}\rangle$ is the mean value of the Kirchhoff-transformed variable specified at the Dirichlet boundary node n, as evaluated in (A-10) of Appendix A. Definitions for other terms are illustrated in Figure 4-1. Here we assumed that prescribed flux is uniformly distributed along the Neumann boundary of each boundary element. If flux is prescribed at boundary nodes, the coefficent matrix in (4-6) should be modified accordingly.

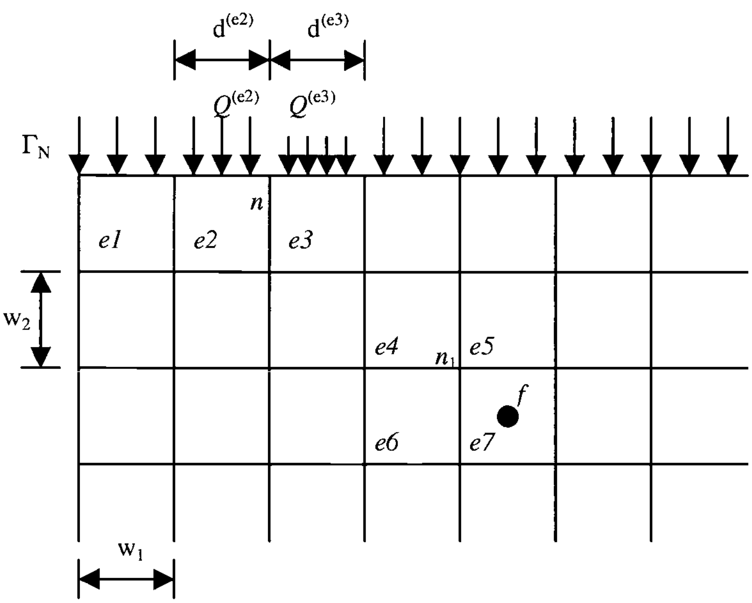


Figure 4-1. Diagram showing how the contribution of prescribed flux and the source/sink term is evaluated in formulating element matrices, i.e., (4-7). For global node n_1, E_n in (4-7) consists of element $e4$, $e5$, $e6$, and $e7$, and the source f in e7 contributes one quarter of strength to this node; the contribution from influx to the global node n consists of half of influx in element $e2$ and half from $e3$.

We note that all the recursive equations (3-9), (3-12), (3-18) and (3-23) have the same structure. This leads to corresponding finite element equations with the same format as (4-5) with exactly the same $\tilde{A}$ matrix but different $\tilde{b}$. The finite element equation for $\langle \Phi^{(0,2)}(\boldsymbol{x}) \rangle$ can be written as

$$\sum_{m=1}^{NN} \tilde{A}_{nm} \Phi_m^{(0,2)} = \tilde{b}_n \tag{4-8}$$

where

$$\tilde{b}_n = \begin{cases} \left\langle H_n^{(0,2)} \right\rangle & \text{if } n \in \Gamma_D \\ -g\sum_{m=1}^{NN}\left(\frac{\sigma_\beta^2}{2}\left\langle \Phi_m^{(0,0)} \right\rangle + R_{\alpha\Phi,m}^{(0,2)} \right) e_2^T \boldsymbol{B}_{mn} & \text{if } n \notin \Gamma_D \end{cases} \tag{4-9}$$

Here, $R_{\alpha\Phi,m}^{(0,2)}$ is the covariance function $R_{\alpha\Phi}^{(0,2)}$ evaluated at node m, and $\left\langle H_n^{(0,2)} \right\rangle$ is defined in (A-9). Derivation of $\langle \Phi^{(2,0)}(\boldsymbol{x}) \rangle$ is somewhat more complicated. Following the same procedure as we did for $\langle \Phi^{(0,0)}(\boldsymbol{x}) \rangle$, we obtain

$$\begin{aligned} &\int_\Omega K_G(\boldsymbol{x})\left(\nabla\left\langle \Phi^{(2,0)}(\boldsymbol{x}) \right\rangle + g\alpha_G\left\langle \Phi^{(2,0)}(\boldsymbol{x}) \right\rangle e_2 \right)\cdot\nabla\xi_n(\boldsymbol{x})d\Omega \\ &\quad = \int_{\Gamma_D}\Big[K_G(\boldsymbol{x})\left(\nabla\left\langle \Phi^{(2,0)}(\boldsymbol{x}) \right\rangle + 0.5\sigma_Y^2(\boldsymbol{x})\nabla\left\langle \Phi^{(2,0)}(\boldsymbol{x}) \right\rangle \right) - \boldsymbol{r}^{(2,0)}(\boldsymbol{x}) \\ &\qquad + g\left(\alpha_G K_G(\boldsymbol{x})\left(\left\langle \Phi^{(2,0)}(\boldsymbol{x}) \right\rangle + 0.5\sigma_Y^2(\boldsymbol{x})\nabla\left\langle \Phi^{(0,0)}(\boldsymbol{x}) \right\rangle \right) + \alpha_G R_{K\Phi}^{(2,0)}(\boldsymbol{x}) \right) e_3 \Big]\xi_n(\boldsymbol{x})\cdot\boldsymbol{n}(\boldsymbol{x})d\Gamma \\ &\qquad + \int_\Omega\left(\boldsymbol{r}^{(2,0)}(\boldsymbol{x}) - \frac{1}{2}g\alpha_G K_G(\boldsymbol{x})\sigma_Y^2(\boldsymbol{x})\left\langle \Phi^{(0,0)}(\boldsymbol{x}) \right\rangle e_2 - g\alpha_G R_{K\Phi}^{(2,0)}(\boldsymbol{x})e_2 \right)\cdot\nabla\xi_n(\boldsymbol{x})d\Omega \end{aligned} \tag{4-10}$$

For $\forall \boldsymbol{x} \in e$, multiplying (D-15) of Appendix D by $K_G^{(e)}(\boldsymbol{x})$, taking the derivative with respect to $\boldsymbol{y}$, and then setting $\boldsymbol{y} = \boldsymbol{x}$, gives

$$\begin{aligned} &\boldsymbol{r}^{(2,0)(e)}(\boldsymbol{x}) = \boldsymbol{R}^{(2,0)(e)}(\boldsymbol{x},\boldsymbol{x}) = \left\langle K_s'(\boldsymbol{x})\nabla\Phi'(\boldsymbol{x}) \right\rangle^{(2,0)(e)} = K_G(\boldsymbol{x})\left\langle Y'(\boldsymbol{x})\nabla\Phi'(\boldsymbol{x}) \right\rangle^{(2,0)(e)} \\ &= \sum_{e'} C_Y(e,e')K_G^{(e)}(\boldsymbol{x})\sum_{j=1}^{N}\sum_{k=1}^{N}\sum_{p=1}^{N} G_{jk}^{(0,0)(e',e)}\left\langle \Phi_p^{(0,0)(e')} \right\rangle * \left(A_{jp}^{(e')} + g\alpha_G \boldsymbol{e}_2^T \boldsymbol{B}_{pj}^{(e')} \right)\nabla\xi_k^{(e)}(\boldsymbol{x}) \end{aligned} \tag{4-11}$$

where $G_{jk}^{(0,0)(e',e)}$ is $G^{(0,0)}$ associated with node j in element e' and node k in element e (Figure 4-2), $\langle \Phi_p^{(0,0)(e')} \rangle$ is $\langle \Phi^{(0,0)}(\boldsymbol{x}) \rangle$ at local node p in element e', N is the number of nodes in an element, $\xi_k^{(e)}$ is weight function ξ associated with node k in element e, and $\xi_j^{(e')}$ is ξ associated with node j in element e'.

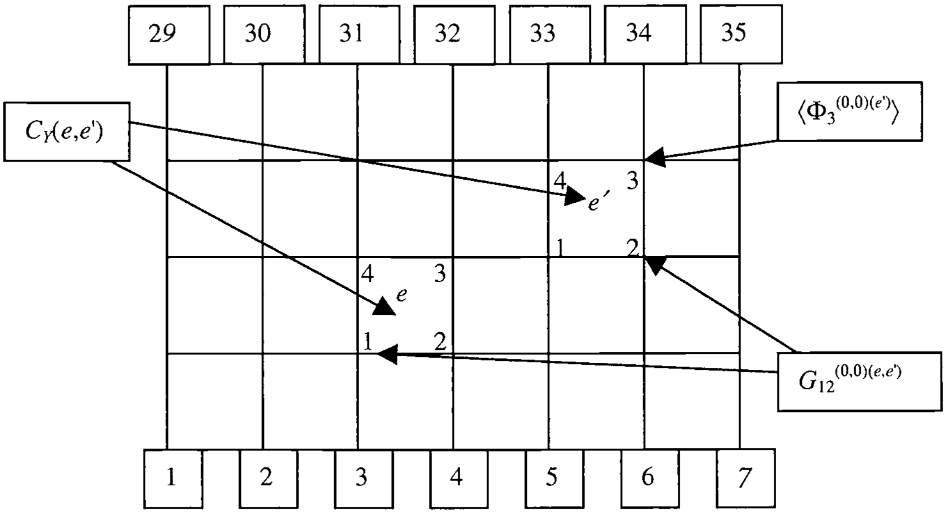


Figure 4-2. Diagram illustrating the numbering of nodes and elements. The boxed numbers are global nodal numbers, and the numbers inside elements are local nodal numbers. It also shows the meanings of some terms appearing in equations.

From (4-11), we obtain

$$\begin{aligned}&\int_\Omega \boldsymbol{r}^{(2,0)(e)}(\boldsymbol{x})\cdot\nabla\xi_n(\boldsymbol{x})d\Omega\\&=\sum_e\sum_{e'}C_Y(e,e')\sum_{j=1}^N\sum_{k=1}^N\sum_{p=1}^N G_{jk}^{(0,0)(e',e)}\left\langle\Phi_p^{(0,0)(e')}\right\rangle*\left(A_{jp}^{(e')}+g\alpha_G\boldsymbol{e}_2^T\boldsymbol{B}_{pj}^{(e')}\right)\int_\Omega K_G^{(e)}(\boldsymbol{x})\nabla\xi_k^{(e)}(\boldsymbol{x})\cdot\nabla\xi_n^{(e)}(\boldsymbol{x})d\Omega\\&=\sum_e\sum_{e'}C_Y(e,e')\sum_{j=1}^N\sum_{k=1}^N\sum_{p=1}^N G_{jk}^{(0,0)(e',e)}\left\langle\Phi_p^{(0,0)(e')}\right\rangle*\left(A_{jp}^{(e')}+g\alpha_G\boldsymbol{e}_2^T\boldsymbol{B}_{pj}^{(e')}\right)A_{nk}^{(e)}\end{aligned}\tag{4-12}$$

Similarly,

$$\begin{aligned}&\int_\Omega R_{K\Phi}^{(2,0)(e)}(\boldsymbol{x})\boldsymbol{e}_2\cdot\nabla\xi_n(\boldsymbol{x})d\Omega\\&=-\sum_e\sum_{e'}C_Y(e,e')\sum_{j=1}^N\sum_{k=1}^N\sum_{p=1}^N G_{jk}^{(0,0)(e',e)}\left\langle\Phi_p^{(0,0)(e')}\right\rangle*\left(A_{jp}^{(e')}+g\alpha_G\boldsymbol{e}_2^T\boldsymbol{B}_{pj}^{(e')}\right)\boldsymbol{e}_2^T\boldsymbol{B}_{kn}^{(e)}\end{aligned}\tag{4-13}$$

Derivations of the remaining terms in (4-10) re straightforward. We finally obtain

$$\sum_{m=1}^{NN} \tilde{A}_{nm} \Phi_m^{(2,0)} = \tilde{b}_n \tag{4-14}$$

$$\begin{aligned} \tilde{b}_n = &-\frac{1}{2}\sum_e \sigma_Y^{2(e)} \sum_{m=1}^{4} \left(A_{nm}^{(e)} + g\alpha_G e_2^T \boldsymbol{B}_{mn}^{(e)} \right) \left\langle \Phi_m^{(0,0)(e)} \right\rangle \\ &+ \sum_e \sum_{e'} C_Y(e,e') \sum_{m,l,p=1}^{4} \left\langle G_{ml}^{(0,0)(e,e')} \right\rangle \left(A_{pm}^{(e)} + g\alpha_G e_2^T \boldsymbol{B}_{pm}^{(e)} \right) \left(A_{\ln}^{(e')} + g\alpha_G e_2^T \boldsymbol{B}_{\ln}^{(e')} \right) \left\langle \Phi_p^{(0,0)(e)} \right\rangle \end{aligned} \tag{4-15}$$

for $n \notin \Gamma_D$, and $\tilde{b}_n$=0 otherwise. Lastly, from (3-23), the component $\tilde{b}_n$ in the finite element equation for $\langle \Phi^{(2,2)}(\boldsymbol{x}) \rangle$ is zero for $n \in \Gamma_D$, otherwise

$$\begin{aligned} \tilde{b}_n = &-\frac{1}{2}\sum_e \sigma_Y^{2(e)} \sum_{m=1}^{N} \left(A_{nm}^{(e)} + \alpha_G e_2^T \boldsymbol{B}_{mn}^{(e)} \right) \left\langle \Phi_m^{(0,2)(e)} \right\rangle + \sum_e \left(r_1^{(2,2)(e)} C_{1n} + r_2^{(2,2)(e)} C_{2n} \right) \\ &-\frac{1}{2} g\alpha_G \sigma_\beta^2 e_2^T \sum_e \sum_{m=1}^{N} \boldsymbol{B}_{mn}^{(e)} \left\langle \Phi_m^{(2,0)(e)} \right\rangle - \frac{1}{4} g\alpha_G \sigma_\beta^2 e_2^T \sum_e \sigma_Y^{2(e)} \sum_{m=1}^{N} \boldsymbol{B}_{mn}^{(e)} \left\langle \Phi_m^{(0,0)(e)} \right\rangle \\ &- g\alpha_G \sum_e \left(R_{K\Phi}^{(2,2)(e)} + \frac{1}{2} \sigma_\beta^2 R_{K\Phi}^{(2,0)(e)} \right) C_{2n} \\ &- g\alpha_G \sum_e \sum_{m=1}^{N} \left(R_{\alpha\Phi,m}^{(2,2)(e)} + \frac{1}{2} \sigma_Y^{2(e)} R_{\alpha\Phi,m}^{(0,2)(e)} \right) e_2^T \boldsymbol{B}_{mn}^{(e)} \\ &- g\alpha_G \sum_e R_{\alpha K\Phi}^{(2,2)(e)} C_{2n} \qquad \text{if } n \notin \Gamma_D \end{aligned} \tag{4-16}$$

where $r_1^{(2,2)(e)}$ and $r_2^{(2,2)(e)}$ are components of $\boldsymbol{r}^{(2,2)}$ at element e, $R_{\alpha K\Phi}^{(2,2)(e)}$is $R_{\alpha K\Phi}^{(2,2)}$ at element e, $\sigma_Y^{2(e)}$ is the conditional variance of Y at element e, and

$$\begin{aligned} C_{1n}^{(e)} &= \int_{\Omega_e} \frac{\partial \xi_n^{(e)}(\boldsymbol{x})}{\partial x_1} d\Omega \\ C_{2n}^{(e)} &= \int_{\Omega_e} \frac{\partial \xi_n^{(e)}(\boldsymbol{x})}{\partial x_2} d\Omega \end{aligned} \tag{4-17}$$

All these terms are evaluated in Appendix D.

4.2.2 Conditional Mean Fluxes

Mean flow can be computed to second-order after solving equations for mean Φ and other covariance functions (presented in the next section). As an example, the equation for $\langle \boldsymbol{q}^{(0,0)} \rangle$ is derived from (3-29) as

$$\left\langle \boldsymbol{q}^{(0,0)}(\boldsymbol{x}) \right\rangle = -K_G(\boldsymbol{x})\left(\nabla\left\langle \Phi^{(0,0)}(\boldsymbol{x}) \right\rangle + g\alpha_G \left\langle \Phi^{(0,0)}(\boldsymbol{x}) \right\rangle \boldsymbol{e}_2\right) \qquad \boldsymbol{x} \in \Omega \tag{4-18}$$

Basically, $\langle \boldsymbol{q}^{(0,0)} \rangle$ can be obtained in two ways from (4-18). One approach consists of computing $\langle \boldsymbol{q}^{(0,0)} \rangle$ directly at any point $\boldsymbol{x}$ inside an element e by using the weight functions ξ,

$$\left\langle \boldsymbol{q}^{(0,0)(e)}(\boldsymbol{x}) \right\rangle = -K_G^{(e)}(\boldsymbol{x})\sum_{m=1}^{N}\left\langle \Phi_m^{(0,0)(e)} \right\rangle \left(\nabla\xi_m^{(e)}(\boldsymbol{x}) + g\alpha_G \xi_m^{(e)}(\boldsymbol{x})\boldsymbol{e}_2\right) \qquad \boldsymbol{x} \in \Omega \tag{4-19}$$

where m is the node number in element e. The zero-order flux at the center of a rectangular element is

$$\left\langle \boldsymbol{q}^{(0,0)(e)} \right\rangle = K_G^{(e)} \begin{pmatrix} \dfrac{1}{2w_1^{(e)}}\left(\left\langle \Phi_1^{(0,0)(e)} \right\rangle + \left\langle \Phi_4^{(0,0)(e)} \right\rangle - \left\langle \Phi_2^{(0,0)(e)} \right\rangle - \left\langle \Phi_3^{(0,0)(e)} \right\rangle\right) \\ \dfrac{1}{2w_2^{(e)}}\left(\left\langle \Phi_1^{(0,0)(e)} \right\rangle + \left\langle \Phi_2^{(0,0)(e)} \right\rangle - \left\langle \Phi_3^{(0,0)(e)} \right\rangle - \left\langle \Phi_4^{(0,0)(e)} \right\rangle\right) \end{pmatrix} + \frac{1}{4} g\alpha_G K_G^{(e)} \sum_{i=1}^{4} \left\langle \Phi_i^{(0,0)(e)} \right\rangle \tag{4-20}$$

where $w_1^{(e)}$ and $w_2^{(e)}$ are the dimensions of element e in the x_1 and x_2 directions (Figure 4-1), and the subscripts 1-4 of $\left\langle \Phi^{(0,0)(e)} \right\rangle$ denote the values of $\left\langle \Phi^{(0,0)} \right\rangle$ at local nodes in element e. The scheme is very simple and easy to implement. One problem is that the calculated flux is defined inside the element. It is not convenient if one needs to compare closeness of the solution with prescribed flux on the boundary, when the flux is prescribed at boundary nodes.

Another approach is based on writing a finite element algorithm for (4-18) and solving for the mean flux defined at the same nodes as mean Φ. At first glance, it seems that solving equations for $\langle \boldsymbol{q}^{(n,m)} \rangle$ by the finite element method, instead of direct calculation, involves an average scheme that may lower the accuracy of the solution. However, since expressions for $\langle \boldsymbol{q}^{(n,m)} \rangle$ usually contain quantities defined at both nodes and elements, some kind of averaging is inevitable.

Multiplying (4-18) by the weigh function $\xi_n(\boldsymbol{x})$, integrating over the flow domain Ω, and setting

$$\begin{aligned} \left\langle \boldsymbol{q}^{(0,0)}(\boldsymbol{x}) \right\rangle &= \sum_{m=1}^{NN} \left\langle \boldsymbol{q}_m^{(0,0)} \right\rangle \xi_n(x) \\ \left\langle \Phi^{(0,0)}(\boldsymbol{x}) \right\rangle &= \sum_{m=1}^{NN} \left\langle \Phi_m^{(0,0)} \right\rangle \xi_n(x) \end{aligned} \tag{4-21}$$

where $\left\langle \Phi_m^{(0,0)} \right\rangle$ and $\left\langle \boldsymbol{q}_m^{(0,0)} \right\rangle$ are $\left\langle \Phi^{(0,0)}(x) \right\rangle$ and $\left\langle \boldsymbol{q}^{(0,0)}(\boldsymbol{x}) \right\rangle$ evaluated at global node m, respectively, gives

$$\sum_{m=1}^{NN} \left\langle \boldsymbol{q}_m^{(0,0)} \right\rangle \int_\Omega \xi_m(\boldsymbol{x}) \xi_n(\boldsymbol{x}) d\Omega = -\sum_{m=1}^{NN} \left\langle \Phi_m^{(0,0)} \right\rangle \int_\Omega K_G(\boldsymbol{x}) [\nabla \xi_m(\boldsymbol{x}) + g\alpha_G \xi_m(\boldsymbol{x}) \boldsymbol{e}_2]\, \xi_n(\boldsymbol{x}) d\Omega \tag{4-22}$$

or

$$\sum_{m=1}^{NN} D_{nm} \left\langle \boldsymbol{q}_m^{(0,0)} \right\rangle = -\sum_{m=1}^{NN} (\boldsymbol{B}_{nm} + g\alpha_G S_{nm} \boldsymbol{e}_2) \left\langle \Phi_m^{(0,0)} \right\rangle \qquad n=\overline{1, NN} \tag{4-23}$$

where

$$\begin{aligned} D_{nm} &= \sum_e D_{nm}^{(e)} = \int_\Omega \xi_n(\boldsymbol{x}) \xi_m(\boldsymbol{x}) d\Omega \\ S_{nm} &= \sum_e S_{nm}^{(e)} = \int_\Omega K_G(\boldsymbol{x}) \xi_n(\boldsymbol{x}) \xi_m(\boldsymbol{x}) d\Omega \end{aligned} \tag{4-24}$$

which are evaluated in Appendix D.

In a similar manner, the finite element equations for higher-order approximations of mean flux can be formulated as

$$\sum_{m=1}^{NN} D_{nm}\left\langle q_m^{(2,0)}\right\rangle = -\sum_e \sum_{m=1}^{N}\left[\left(B_{nm}^{(e)} + g\alpha_G S_{nm}^{(e)} e_2\right)\left(\left\langle \Phi_m^{(2,0)(e)}\right\rangle + \frac{1}{2}\sigma_Y^{2(e)}\left\langle \Phi_m^{(0,0)(e)}\right\rangle\right)\right] + \sum_e\left(r^{(2,0)(e)} - g\alpha_G R_{K\Phi}^{(2,0)(e)} e_2\right)T_n^{(e)} \qquad n=\overline{1, NN} \tag{4-25}$$

$$\sum_{m=1}^{NN} D_{nm}\left\langle q_m^{(0,2)}\right\rangle = -\sum_e \sum_{m=1}^{N}\left[\left(B_{nm}^{(e)} + g\alpha_G S_{nm}^{(e)} e_2\right)\left\langle \Phi_m^{(0,2)(e)}\right\rangle + \frac{1}{2} g\alpha_G \sigma_\beta^2 S_{nm}^{(e)}\left\langle \Phi_m^{(0,0)(e)}\right\rangle e_2\right] - g\sum_e \sum_{m=1}^{N} R_{\alpha\Phi}^{(0,2)(e)} S_{nm}^{(e)} e_2 \qquad n=\overline{1, NN} \tag{4-26}$$

$$\begin{aligned}\sum_{m=1}^{NN} D_{nm}\left\langle q_m^{(2,2)}\right\rangle = &-\sum_e \sum_{m=1}^{N} B_{nm}^{(e)}\left(\left\langle \Phi_m^{(2,2)(e)}\right\rangle + \frac{\sigma_Y^{2(e)}}{2}\left\langle \Phi_m^{(0,2)(e)}\right\rangle\right)\\ &- g\alpha_G \sum_e \sum_{m=1}^{N}\left(\left\langle \Phi_m^{(2,2)(e)}\right\rangle + \frac{\sigma_\beta^2}{2}\left\langle \Phi_m^{(2,0)(e)}\right\rangle + \frac{\sigma_Y^{2(e)}}{2}\left\langle \Phi_m^{(0,2)(e)}\right\rangle + \frac{\sigma_\beta^2\sigma_Y^{2(e)}}{4}\left\langle \Phi_m^{(0,2)(e)}\right\rangle\right) S_{nm}^{(e)} e_2\\ &- g\sum_e \sum_{m=1}^{N}\left(R_{\alpha\Phi,m}^{(2,2)(e)} + \frac{\sigma_Y^{2(e)}}{2} R_{\alpha\Phi,m}^{(0,2)(e)}\right) S_{nm}^{(e)} e_3\\ &+ \sum_e r^{(2,2)(e)} T_n^{(e)} - g\alpha_G \sum_e \sum_{m=1}^{N}\left(R_{K\Phi,m}^{(2,2)(e)} + \frac{\sigma_\beta^2}{2} R_{K\Phi,m}^{(2,0)(e)}\right) T_n^{(e)} e_2\\ &- g\sum_e \sum_{m=1}^{N} R_{\alpha K\Phi}^{(2,2)(e)} T_n^{(e)} e_2 \qquad n=\overline{1, NN}\end{aligned} \tag{4-27}$$

where $R_{K\Phi,m}^{(2,2)(e)}$ and $R_{K\Phi,m}^{(2,0)(e)}$ are second order cross-covariances $R_{K\Phi}^{(2,2)}$ and $R_{K\Phi}^{(2,0)}$ between K_s in element e and Φ at node m of element e, $R_{\alpha\Phi,m}^{(2,2)(e)}$ and $R_{\alpha\Phi,m}^{(0,2)(e)}$ are second order cross-covariances $R_{\alpha\Phi}^{(2,2)}$ and $R_{\alpha\Phi}^{(0,2)}$ between α and Φ at node m of element e, $R_{\alpha K\Phi,m}^{(2,2)(e)}$ is $R_{\alpha K\Phi}^{(2,2)}$ associated with K_s at element e and Φ at node m of element e, and

$$T_n = \sum_e T_n^{(e)} = \int_\Omega \xi_n(x)d\Omega \tag{4-28}$$

4.3 FINITE ELEMENT SOLUTION OF CONDITIONAL SECOND MOMENT EQUATIONS

4.3.1 Covariance Function of Φ

For deterministic driving forces, $C_\Phi^{(2,0)}$ is zero. Similar to first moment equations, applying Galerkin orthogonalization to (3-39), the equation for $C_\Phi^{(2,0)}$, using Green's first identity, and again assuming deterministic boundary conditions, gives

$$
\begin{aligned}
&\int_\Omega K_G(\boldsymbol{x})\left(\nabla_x C_\Phi^{(2,0)}(\boldsymbol{x},\boldsymbol{y}) + g\alpha_G C_\Phi^{(2,0)}(\boldsymbol{x},\boldsymbol{y})\boldsymbol{e}_2\right)\cdot\nabla\xi_n(\boldsymbol{x})d\Omega \\
&\quad = -\int_\Omega \left(\nabla_x C_{K\Phi}^{(2,0)}(\boldsymbol{x},\boldsymbol{y}) + g\alpha_G C_{K\Phi}^{(2,0)}(\boldsymbol{x},\boldsymbol{y})\boldsymbol{e}_2\right)\left\langle\Phi^{(0,0)}(\boldsymbol{x})\right\rangle\cdot\nabla\xi_n(\boldsymbol{x})d\Omega \\
&\qquad + \int_{\Gamma_D}\Big[K_G(\boldsymbol{x})\,\nabla_x C_\Phi^{(2,0)}(\boldsymbol{x},\boldsymbol{y}) + C_{K\Phi}^{(2,0)}(\boldsymbol{x},\boldsymbol{y})\,\nabla\left\langle\Phi^{(0,0)}(\boldsymbol{x})\right\rangle \\
&\qquad\quad + \mathrm{g}\,\alpha_{\mathrm{G}}\left(K_G(\boldsymbol{x})\,C_\Phi^{(2,0)}(\boldsymbol{x},\boldsymbol{y}) + C_{K\Phi}^{(2,0)}(\boldsymbol{x},\boldsymbol{y})\left\langle\Phi^{(0,0)}(\boldsymbol{x})\right\rangle\right)\boldsymbol{e}_3\Big]\xi_n\cdot\boldsymbol{n}(\boldsymbol{x})d\Gamma
\end{aligned}
\tag{4-29}
$$

Let

$$C_\Phi^{(2,0)}(\boldsymbol{x},\boldsymbol{y}) = \sum_{m=1}^{NN} C_{\Phi,mp}^{(2,0)}\xi_m(\boldsymbol{x}) \tag{4-30}$$

be the second-order (in σ_Y) approximation of the covariance of Φ between point $\boldsymbol{x}$ and point $\boldsymbol{y}$, which is taken to coincide with node p of our finite element mesh, then (4-29) becomes

$$
\begin{aligned}
&\sum_{m=1}^{NN}\left(A_{nm} + g\alpha_G\boldsymbol{e}_2^T\boldsymbol{B}_{mn}\right)C_{\Phi,mp}^{(2,0)} \\
&\quad = -\sum_e\sum_{m=1}^{N} A_{p,nm}^{(2,0)(e)}\left\langle\Phi_m^{(0,0)}\right\rangle - g\alpha_G\sum_e\sum_{m=1}^{N} C_{K\Phi,p}^{(2,0)(e)}B_{2,mn}^{(e)}\left\langle\Phi_m^{(0,0)}\right\rangle + I(\Gamma_D) \qquad n = 1,2,\ldots NN
\end{aligned}
\tag{4-31}
$$

where $I(\Gamma_D)$ is the integral over Dirichlet boundary as shown in (4-29), $C_{K\Phi,p}^{(2,0)(e)}$ is the cross-covariance $C_{K\Phi}^{(2,0)}(\boldsymbol{x},\boldsymbol{y})$ evaluated at $\boldsymbol{x}\in e$ and $\boldsymbol{y}$ at global node p, and

$$
\begin{aligned}
A_{p,mn}^{(2,0)(e)} &= \int_{\Omega_e} C_{K\Phi}^{(2,0)}(\boldsymbol{x},\boldsymbol{y}=p)\nabla\xi_m(\boldsymbol{x})\cdot\nabla\xi_n(\boldsymbol{x})d\Omega \\
B_{1,mn}^{(e)} &= \int_{\Omega_e} \xi_m(\boldsymbol{x})\frac{\partial\xi_n(\boldsymbol{x})}{\partial x_1}d\Omega \\
B_{2,mn}^{(e)} &= \int_{\Omega_e} \xi_m(\boldsymbol{x})\frac{\partial\xi_n(\boldsymbol{x})}{\partial x_2}d\Omega
\end{aligned} \tag{4-32}
$$

Using (4-6), (4-31) can be rewritten as

$$
\sum_{m=1}^{NN} \tilde{A}_{nm} C_{\Phi,mp}^{(2,0)} = \tilde{b}_n \tag{4-33}
$$

where

$$
\tilde{b}_n = \begin{cases} C_{H\Phi,np}^{(2,0)} & \text{if } \mathrm{n} \in \Gamma_\mathrm{D} \\ -\sum_e \sum_{m=1}^{N} A_{p,nm}^{(e)} \langle \Phi_m^{(0,0)} \rangle - g\alpha_G \sum_e \sum_{m=1}^{N} C_{K\Phi,p}^{(2,0)(e)} B_{2,mn}^{(e)} \langle \Phi_m^{(0,0)} \rangle & \text{if } \mathrm{n} \notin \Gamma_\mathrm{D} \end{cases} \tag{4-34}
$$

and $C_{H\Phi,np}^{(2,0)}$ is the cross-covariance between H at Dirichlet boundary node n and Φ at any node p. For any given node p, the solution of (4-33) is the covariance of Φ between all nodes with respect to p. Therefore, solving (4-33) for each node p in the flow domain yields the covariance of Φ between all nodes. It should be pointed out that the covariance function between Φ at a node with that at a reference point on the Dilichlet boundary may not be zero if the driving forces are not deterministic.

The equations for $C_\Phi{}^{(0,2)}$, and $C_\Phi{}^{(2,2)}$ have the same format as (4-33), with different $\tilde{b}_n$.

For $C_\Phi{}^{(0,2)}$ and any fixed $\boldsymbol{y}$ at node p, $C_{\alpha\Phi}^{(0,2)}(\boldsymbol{y}) = C_{\alpha\Phi,p}^{(0,2)}$, we get

$$
\tilde{b}_n = \begin{cases} C_{H\Phi,np}^{(0,2)} & \text{if } \mathrm{n} \in \Gamma_\mathrm{D} \\ -gR_{\alpha\Phi,p}^{(0,2)} \sum_e \sum_{m=1}^{4} B_{mn}^{(e)} \langle \Phi_m^{(0,0)} \rangle & \text{if } \mathrm{n} \notin \Gamma_\mathrm{D} \end{cases} \tag{4-35}
$$

Similarly, the vector $\tilde{b}_n$ needed for the computation of $C_\Phi{}^{(2,2)}$ is obtained (when considering any fixed $\boldsymbol{y}$ at node p and $\boldsymbol{x}\in e$) upon interpolating some terms in (3-40) such as

$$\begin{aligned}
&C_\Phi^{(0,2)}(\boldsymbol{x},\boldsymbol{y}) = \sum_{m=1}^{N} C_{\Phi,mp}^{(0,2)(e)}\xi_m^{(e)} \\
&\left\langle K_s'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Phi'(\boldsymbol{x})\right\rangle_{\boldsymbol{x}\in e,\boldsymbol{y}=p}^{(i,j)} = \left\langle K_s'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Phi'(\boldsymbol{x})\right\rangle_p^{(i,j)(e)} \\
&\left\langle \alpha'\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle_{\boldsymbol{x}\in e,\boldsymbol{y}=p}^{(i,j)} = \sum_{m=1}^{N}\left\langle \alpha'\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle_{mp}^{(i,j)(e)}\xi_m^{(e)}
\end{aligned} \tag{4-36}$$

where i, j denote the order of terms, as

$$\tilde{\boldsymbol{b}}_n = \begin{cases}
C_{H\Phi,np}^{(2,2)} & \text{if } \mathrm{n}\in\Gamma_{\mathrm{D}} \\[2ex]
-\dfrac{1}{2}\sum_e \sigma_Y^2(e)\sum_{m=1}^{N} C_{\Phi,mp}^{(0,2)(e)}A_{mn}^{(e)} - \sum_e\left\langle K_s'(\boldsymbol{x})\Phi'(\boldsymbol{y})\nabla\Phi'(\boldsymbol{x})\right\rangle_p^{(2,2)(e)} C_{2n} \\
-\sum_e\sum_{m=1}^{N} A_{p,nm}^{(2,0)(e)}\left\langle\Phi_m^{(0,2)}\right\rangle - \dfrac{1}{2}g\alpha_G\sum_e\sum_{m=1}^{N}\left(\sigma_Y^2(e)C_{\Phi,mp}^{(0,2)(e)} + \sigma_\beta^2 C_{\Phi,mp}^{(2,0)(e)}\right)B_{mn}^{(e)} \\
-g\alpha_G\sum_e\left(\left\langle K_s'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Phi'(\boldsymbol{x})\right\rangle_p^{(2,2)(e)} + \dfrac{1}{2}\sigma_\beta^2\left\langle K_s'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Phi'(\boldsymbol{x})\right\rangle_p^{(2,0)(e)}\right)C_{2n} \\
-g\sum_e\sum_{m=1}^{N}\left(\left\langle\alpha'\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle_{mp}^{(2,2)(e)} + \dfrac{1}{2}\sigma_Y^2(e)\left\langle\alpha'\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle_{mp}^{(0,2)(e)}\right)B_{mn}^{(e)} \\
-g\sum_e\left\langle\alpha' K_s'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Phi'(\boldsymbol{x})\right\rangle_p^{(2,2)(e)} C_{2n} \\
-g\sum_e\sum_{m=1}^{N}\left(R_{\alpha\Phi,p}^{(2,2)(e)}\left\langle\Phi_m^{(0,0)}\right\rangle + R_{\alpha\Phi,p}^{(0,2)(e)}\left\langle\Phi_m^{(2,0)}\right\rangle + \dfrac{1}{2}\sigma_Y^2(e)R_{\alpha\Phi,p}^{(0,2)(e)}\left\langle\Phi_m^{(0,0)}\right\rangle\right)B_{mn}^{(e)} \\
-g\alpha_G\sum_e\sum_{m=1}^{N}\left(C_{K\Phi,p}^{(2,2)(e)}\left\langle\Phi_m^{(0,0)}\right\rangle + C_{K\Phi,p}^{(2,0)(e)}\left\langle\Phi_m^{(0,2)}\right\rangle + \dfrac{1}{2}\sigma_\beta^2 C_{K\Phi,p}^{(2,0)(e)}\left\langle\Phi_m^{(0,0)}\right\rangle\right)C_{2n} \\
-g\sum_e\sum_{m=1}^{N} C_{\alpha K\Phi,p}^{(2,2)(e)}C_{2n}\left\langle\Phi_m^{(0,0)}\right\rangle & \text{if } \mathrm{n}\notin\Gamma_{\mathrm{D}}
\end{cases} \tag{4-37}$$

where

$$A_{p,mn}^{(2,2)(e)} = \int_{\Omega_e} C_{K\Phi}^{(2,2)}(\boldsymbol{x},\boldsymbol{y}=p)\nabla\xi_m(\boldsymbol{x})\cdot\nabla\xi_n(\boldsymbol{x})d\Omega \tag{4-38}$$

4.3.2 Covariance Tensor of Flux

For simplicity, we compute the covariance tensor of flux directly from (3-42)-(3-45). Let

$$\begin{aligned} C_{\Phi}^{(i,j)(e,e')}(\boldsymbol{x},\boldsymbol{y}) &= \sum_{m,n=1}^{N} C_{\Phi,mn}^{(i,j)(e,e')}\xi_m^{(e)}(\boldsymbol{x})\xi_n^{(e')}(\boldsymbol{y}) \\ C_{Y\Phi}^{(i,j)(e,e')}(\boldsymbol{x},\boldsymbol{y}) &= \sum_{n=1}^{N} C_{Y\Phi,n}^{(i,j)(e)}\xi_n^{(e')}(\boldsymbol{y}) \end{aligned} \tag{4-39}$$

be the (i, j)-order components (in σ_Y and σ_β, respectively) of the covariance of Φ and cross-covariance of Φ at point $\boldsymbol{y}$ in element e' and Y at point $\boldsymbol{x}$ in element e. Substituting (4-39) into (3-42), for example, yields

$$\begin{aligned} C_q^{(0,0)}(\boldsymbol{x},\boldsymbol{y}) = K_G^{(e)}(\boldsymbol{x}) \sum_{m,n=1}^{N} C_{\Phi,mn}^{(0,0)(e,e')}\Big[&\nabla_x\xi_m^{(e)}(\boldsymbol{x})\nabla_y^T\xi_n^{(e')}(\boldsymbol{y}) + g\alpha_G\nabla_x\xi_m^{(e)}(\boldsymbol{x})\xi_n^{(e')}(\boldsymbol{y})\boldsymbol{e}_2^T \\ &+g\alpha_G\,\boldsymbol{e}_2\xi_m^{(e)}(\boldsymbol{x})\nabla_y^T\xi_n^{(e')}(\boldsymbol{y}) + g\alpha_G^2\xi_m^{(e)}(\boldsymbol{x})\xi_n^{(e')}(\boldsymbol{y})\boldsymbol{E}_2\Big]K_G^{(e')}(\boldsymbol{y}) \end{aligned} \tag{4-40}$$

which is zero if driving forces are deterministic. Similarly, from (3-43)-(3-45), the rest terms of the covariance tensor of flux up to second order are

$$\begin{aligned} &C_q^{(0,2)}(\boldsymbol{x},\boldsymbol{y}) \\ &= \sum_{m,n=1}^{N} K_G^{(e)}(\boldsymbol{x})C_{\Phi,mn}^{(0,2)(e,e')}\Big[\nabla_x\xi_m^{(e)}(\boldsymbol{x})\nabla_y^T\xi_n^{(e')}(\boldsymbol{y}) + g\alpha_G\nabla_x\xi_m^{(e)}(\boldsymbol{x})\xi_n^{(e')}(\boldsymbol{y})\boldsymbol{e}_2^T + g\alpha_G\boldsymbol{e}_2\xi_m^{(e)}(\boldsymbol{x})\nabla_y^T\xi_n^{(e')}(\boldsymbol{y}) \\ &\qquad + g\alpha_G^2\xi_m^{(e)}(\boldsymbol{x})\xi_n^{(e')}(\boldsymbol{y})\boldsymbol{E}_2\Big]K_G^{(e')}(\boldsymbol{y}) \\ &\quad + g\alpha_G\sum_{m,n=1}^{N} R_{\alpha\Phi,m}^{(0,2)(e')}K_G^{(e)}(\boldsymbol{x})\Big[\nabla_x\xi_m^{(e)}(\boldsymbol{x})\xi_n^{(e')}(\boldsymbol{y})\boldsymbol{e}_2^T + \xi_m^{(e)}(\boldsymbol{x})\xi_n^{(e')}(\boldsymbol{y})\boldsymbol{E}_2\Big]K_G^{(e')}(\boldsymbol{y}) \\ &\quad + g\alpha_G\sum_{m,n=1}^{N} R_{\alpha\Phi,n}^{(0,2)(e)}K_G^{(e)}(\boldsymbol{x})\Big[\boldsymbol{e}_2\xi_m^{(e)}(\boldsymbol{x})\nabla_y^T\xi_n^{(e')}(\boldsymbol{y}) + \xi_m^{(e)}(\boldsymbol{x})\xi_n^{(e')}(\boldsymbol{y})\boldsymbol{E}_2\Big]K_G^{(e')}(\boldsymbol{y}) \\ &\quad + g\alpha_G\sigma_\beta^2\sum_{m,n=1}^{N}\left\langle\Phi_m^{(0,0)(e)}\right\rangle\left\langle\Phi_n^{(0,0)(e')}\right\rangle K_G^{(e)}(\boldsymbol{x})\xi_m^{(e)}(\boldsymbol{x})\boldsymbol{E}_2\xi_n^{(e')}(\boldsymbol{y})K_G^{(e')}(\boldsymbol{y}) \end{aligned} \tag{4-41}$$

$$C_q^{(2,0)}(\boldsymbol{x},\boldsymbol{y})=\sum_{m,n=1}^{N}\Big[C_{\Phi,mn}^{(2,0)(e,e')}+C_{Y\Phi,m}^{(2,0)(e')}\left\langle\Phi_n^{(0,0)(e')}\right\rangle+C_{Y\Phi,n}^{(2,0)(e)}\left\langle\Phi_m^{(0,0)(e)}\right\rangle+\left\langle\Phi_m^{(0,0)(e)}\right\rangle\left\langle\Phi_n^{(0,0)(e')}\right\rangle\Big]$$
$$*K_G^{(e)}(\boldsymbol{x})\Big[\nabla_x\xi_m^{(e)}(\boldsymbol{x})\nabla_y^T\xi_n^{(e')}(\boldsymbol{y})+g\alpha_G\nabla_x\xi_m^{(e)}(\boldsymbol{x})\xi_n^{(e')}(\boldsymbol{y})\boldsymbol{e}_2^T \tag{4-42}$$
$$+g\alpha_G\boldsymbol{e}_2\xi_m^{(e)}(\boldsymbol{x})\nabla_y^T\xi_n^{(e')}(\boldsymbol{y})+g\alpha_G^2\xi_m^{(e)}(\boldsymbol{x})\xi_n^{(e')}(\boldsymbol{y})\boldsymbol{E}_2\Big]K_G^{(e')}(\boldsymbol{y})$$

$$C_q^{(2,2)}(\boldsymbol{x},\boldsymbol{y})=\boldsymbol{U}_1(\boldsymbol{x},\boldsymbol{y})+\boldsymbol{U}_2(\boldsymbol{x},\boldsymbol{y})+\boldsymbol{V}_1(\boldsymbol{x},\boldsymbol{y})+\boldsymbol{V}_1^T(\boldsymbol{x},\boldsymbol{y})+\boldsymbol{V}_2(\boldsymbol{x},\boldsymbol{y})+\boldsymbol{V}_2^T(\boldsymbol{x},\boldsymbol{y}) \tag{4-43}$$

where

$$U_1(\boldsymbol{x},\boldsymbol{y})=\sum_{m,n=1}^{N}K_G^{(e)}(\boldsymbol{x})\Bigg[\left(C_{\Phi,mn}^{(2,2)}+\frac{1}{2}\left(\sigma_Y^{2(e)}+\sigma_Y^{2(e')}\right)C_{\Phi,mn}^{(0,2)}\right)\nabla_x\xi_m(\boldsymbol{x})\nabla_y^T\xi_n(\boldsymbol{y})$$
$$+\left\langle\Phi_m^{(0,0)}\right\rangle\nabla_x\xi_m(\boldsymbol{x})\left\langle Y'(\boldsymbol{x})Y'(\boldsymbol{y})\nabla_y^T\Phi'(\boldsymbol{y})\right\rangle_n^{(2,2)(e)}\xi_n(\boldsymbol{y})$$
$$+\left\langle\Phi_n^{(0,0)}\right\rangle\nabla\xi_n(\boldsymbol{y})\left\langle Y'(\boldsymbol{x})Y'(\boldsymbol{y})\nabla_x^T\Phi'(\boldsymbol{x})\right\rangle_m^{(2,2)(e')}\xi_m(\boldsymbol{x}) \tag{4-44}$$
$$+\left\langle Y'(\boldsymbol{x})Y'(\boldsymbol{y})\nabla_x\Phi'(\boldsymbol{x})\nabla_y^T\Phi'(\boldsymbol{y})\right\rangle_{mn}^{(2,2)}\xi_m(\boldsymbol{x})\xi_n(\boldsymbol{y})$$
$$+C_Y(e,e')\left(\left\langle\Phi_m^{(0,2)}\right\rangle\left\langle\Phi_n^{(0,0)}\right\rangle+\left\langle\Phi_n^{(0,2)}\right\rangle\left\langle\Phi_m^{(0,0)}\right\rangle\right)\nabla_x\xi_m(\boldsymbol{x})\nabla_y^T\xi_n(\boldsymbol{y})$$
$$+g\alpha_G^2\xi_m^{(e)}(\boldsymbol{x})\xi_m^{(e')}(\boldsymbol{y})\boldsymbol{E}_2\Big]K_G^{(e')}(\boldsymbol{y})$$

$$U_2(\boldsymbol{x},\boldsymbol{y})$$
$$=g\sum_{m,n=1}^{N}K_G^{(e)}(\boldsymbol{x})\Bigg[\alpha_G^2\left(C_{\Phi,mn}^{(2,2)}+\frac{1}{2}\left(\sigma_Y^{2(e)}+\sigma_Y^{2(e')}\right)C_{\Phi,mn}^{(0,2)}+\sigma_\beta^2C_{\Phi,mn}^{(2,0)}\right)$$
$$+\alpha_G\left(R_{\alpha\Phi,m}^{(2,2)}\left\langle\Phi_n^{(0,0)}\right\rangle+R_{\alpha\Phi,m}^{(0,2)(e)}\left(\left\langle\Phi_n^{(2,0)}\right\rangle+\frac{1}{2}\left(\sigma_Y^{2(e)}+\sigma_Y^{2(e')}\right)\left\langle\Phi_n^{(0,0)}\right\rangle\right)\right)$$
$$+\alpha_G\left(R_{\alpha\Phi,n}^{(2,2)}\left\langle\Phi_m^{(0,0)}\right\rangle+R_{\alpha\Phi,n}^{(0,2)}\left(\left\langle\Phi_m^{(2,0)}\right\rangle+\frac{1}{2}\left(\sigma_Y^{2(e)}+\sigma_Y^{2(e')}\right)\left\langle\Phi_m^{(0,0)}\right\rangle\right)\right)$$
$$+\alpha_G^2\sigma_\beta^2\left(\left\langle\Phi_m^{(2,0)}\right\rangle\left\langle\Phi_n^{(0,0)}\right\rangle+\left\langle\Phi_m^{(0,0)}\right\rangle\left\langle\Phi_n^{(2,0)}\right\rangle+\frac{1}{2}\left(\sigma_Y^{2(e)}+\sigma_Y^{2(e')}\right)\left\langle\Phi_m^{(0,0)}\right\rangle\left\langle\Phi_n^{(0,0)}\right\rangle\right)$$
$$+\left\langle\alpha'^2\Phi'(\boldsymbol{y})\right\rangle_n^{(2,2)}\left\langle\Phi_m^{(0,0)}\right\rangle+\left\langle\alpha'^2\Phi'(\boldsymbol{x})\right\rangle_m^{(2,2)}\left\langle\Phi_n^{(0,0)}\right\rangle \tag{4-45}$$
$$+2\alpha_G\left\langle\alpha'\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle_{mn}^{(2,2)}+\left\langle\alpha'^2\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle_{mn}^{(2,2)}$$
$$+\alpha_G^2C_Y(e,e')\left[\left\langle\Phi_m^{(0,2)}\right\rangle\left\langle\Phi_n^{(0,0)}\right\rangle+\left\langle\Phi_m^{(0,0)}\right\rangle\left\langle\Phi_n^{(0,2)}\right\rangle+2\sigma_\beta^2\left\langle\Phi_m^{(0,0)}\right\rangle\left\langle\Phi_n^{(0,0)}\right\rangle\right]$$
$$+\alpha_G^2\left\langle Y'(\boldsymbol{x})Y'(\boldsymbol{y})\Phi'(\boldsymbol{x})\right\rangle_m^{(2,2)(e')}\left\langle\Phi_n^{(0,0)}\right\rangle+\alpha_G^2\left\langle Y'(\boldsymbol{x})Y'(\boldsymbol{y})\Phi'(\boldsymbol{x})\right\rangle_n^{(2,2)(e)}\left\langle\Phi_m^{(0,0)}\right\rangle$$
$$+2\alpha_G\left\langle\alpha'Y'(\boldsymbol{x})Y'(\boldsymbol{y})\Phi'(\boldsymbol{y})\right\rangle_n^{(2,2)(e)}\left\langle\Phi_m^{(0,0)}\right\rangle+2\alpha_G\left\langle\alpha'Y'(\boldsymbol{x})Y'(\boldsymbol{y})\Phi'(\boldsymbol{x})\right\rangle_m^{(2,2)(e')}\left\langle\Phi_n^{(0,0)}\right\rangle$$
$$+\alpha_G^2\left\langle Y'(\boldsymbol{x})Y'(\boldsymbol{y})\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle_{mn}^{(2,2)}\Bigg]\xi_m^{(e)}(\boldsymbol{x})\xi_n^{(e')}(\boldsymbol{y})\boldsymbol{E}_2$$

$$
\begin{aligned}
&V_1(\boldsymbol{x},\boldsymbol{y}) \\
&= \mathrm{g}\sum_{n,m=1}^{N} K_G^{(e)}\boldsymbol{E}_2\Big[\alpha_G^2\Big(C_{K\Phi,m}^{(2,2)(e')}\left\langle\Phi_n^{(0,0)}\right\rangle + C_{K\Phi,m}^{(2,0)(e')}\Big(\left\langle\Phi_n^{(0,2)}\right\rangle + \sigma_\beta^2\left\langle\Phi_n^{(0,0)}\right\rangle\Big)\Big) \\
&\qquad + \alpha_G^2\left\langle K_s'(\boldsymbol{y})\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle_{mn}^{(2,2)} + \alpha_G\left\langle\Phi_m^{(0,0)}\right\rangle\left\langle\alpha' K_s'(\boldsymbol{y})\Phi'(\boldsymbol{y})\right\rangle_n^{(2,2)} \\
&\qquad + 2\alpha_G\left\langle\Phi_n^{(0,0)}\right\rangle\left\langle\alpha' K'(\boldsymbol{y})\Phi'(\boldsymbol{x})\right\rangle_{mn}^{(2,2)} + 2\alpha_G\left\langle\alpha' K_s'(\boldsymbol{y})\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle_{mn}^{(2,2)} \\
&\qquad + \left\langle\Phi_m^{(0,0)}\right\rangle\left\langle\alpha'^2 K_s'(\boldsymbol{y})\Phi'(\boldsymbol{y})\right\rangle_n^{(2,2)} + \left\langle\Phi_n^{(0,0)}\right\rangle\left\langle\alpha'^2 K_s'(\boldsymbol{y})\Phi'(\boldsymbol{x})\right\rangle_{mn}^{(2,2)}\Big]\xi_m(\boldsymbol{x})\xi_n(\boldsymbol{y}) \\
&\quad + \mathrm{g}\sum_{m,n=1}^{N} K_G^{(e)}\boldsymbol{e}_2\Big[\alpha_G\Big(C_{\Phi,mn}^{(2,2)} + \frac{1}{2}\Big(\sigma_Y^{2(e)} + \sigma_Y^{2(e')}\Big)C_{\Phi,mn}^{(0,2)} + \frac{1}{2}\sigma_\beta^2 C_{\Phi,mn}^{(2,0)}\Big) \\
&\qquad + R_{\alpha\Phi,n}^{(2,2)}\left\langle\Phi_m^{(0,0)}\right\rangle + R_{\alpha\Phi,n}^{(0,2)}\Big(\left\langle\Phi_m^{(2,0)}\right\rangle + \frac{1}{2}\Big(\sigma_Y^{2(e)} + \sigma_Y^{2(e')}\Big)\left\langle\Phi_m^{(0,0)}\right\rangle\Big) \\
&\qquad + \alpha_G C_Y^{(e,e')}\Big(\left\langle\Phi_m^{(0,2)}\right\rangle\left\langle\Phi_n^{(0,0)}\right\rangle + \left\langle\Phi_m^{(0,0)}\right\rangle\left\langle\Phi_n^{(0,2)}\right\rangle + \frac{1}{2}\sigma_\beta^2\left\langle\Phi_m^{(0,0)}\right\rangle\left\langle\Phi_n^{(0,0)}\right\rangle\Big) \\
&\qquad + \left\langle\alpha'\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle_{mn}^{(2,2)} + \left\langle\alpha' Y'(\boldsymbol{x})Y'(\boldsymbol{y})\Phi'(\boldsymbol{x})\right\rangle_m^{(2,2)}\left\langle\Phi_n^{(0,0)}\right\rangle \\
&\qquad + \alpha_G\left\langle Y'(\boldsymbol{x})Y'(\boldsymbol{y})\Phi'(\boldsymbol{x})\right\rangle_m^{(2,2)}\left\langle\Phi_n^{(0,0)}\right\rangle + \left\langle\alpha' Y'(\boldsymbol{x})Y'(\boldsymbol{y})\Phi'(\boldsymbol{y})\right\rangle^{(2,2)}\left\langle\Phi_m^{(0,0)}\right\rangle \\
&\qquad + \alpha_G\left\langle Y'(\boldsymbol{x})Y'(\boldsymbol{y})\Phi'(\boldsymbol{y})\right\rangle_n^{(2,2)}\left\langle\Phi_m^{(0,0)}\right\rangle + \alpha_G\left\langle Y'(\boldsymbol{x})Y'(\boldsymbol{y})\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle_{mn}^{(2,2)} \\
&\qquad + \left\langle\alpha' Y'(\boldsymbol{x})\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle_{mn}^{(2,2)}\Big]K_G^{(e')}\xi_m(\boldsymbol{x})\nabla_y^T\xi_n(\boldsymbol{y})
\end{aligned}
\tag{4-46}
$$

$$
\begin{aligned}
&V_2(\boldsymbol{x},\boldsymbol{y}) \\
&= \mathrm{g}\sum_{m,n=1}^{N} K_G^{(e)}\boldsymbol{e}_2\Big[\alpha_G\Big(C_{K\Phi,m}^{(2,2)(e')}\left\langle\Phi_n^{(0,0)}\right\rangle + C_{K\Phi,m}^{(2,0)(e')}\Big(\left\langle\Phi_n^{(0,2)}\right\rangle + \frac{1}{2}\sigma_\beta^2\left\langle\Phi_n^{(0,0)}\right\rangle\Big)\Big) \\
&\qquad + \alpha_G\left\langle K_s'(\boldsymbol{y})\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle_{mn}^{(2,2)} + \left\langle\alpha' K_s'(\boldsymbol{y})\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle_{mn}^{(2,2)} \\
&\qquad + \left\langle\Phi_m^{(0,0)}\right\rangle\left\langle\alpha' K'(\boldsymbol{y})\Phi'(\boldsymbol{y})\right\rangle_n^{(2,2)} + \left\langle\Phi_n^{(0,0)}\right\rangle\left\langle\alpha' K_s'(\boldsymbol{y})\Phi'(\boldsymbol{x})\right\rangle_m^{(2,2)(e')}\Big]\xi_m(\boldsymbol{x})\nabla_y^T\xi_n(\boldsymbol{y}) \\
&\quad + \sum_{m,n=1}^{N} K_G^{(e)}\Big[C_{K\Phi,m}^{(2,2)(e')}\left\langle\Phi_n^{(0,0)}\right\rangle + C_{K\Phi,m}^{(2,0)(e')}\left\langle\Phi_n^{(0,2)}\right\rangle^{(2,0)} + \left\langle K_s'(\boldsymbol{y})\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle_{mn}^{(2,2)}\Big]\nabla_x\xi_m(\boldsymbol{x})\nabla_y^T\xi_n(\boldsymbol{y}) \\
&\quad + \mathrm{g}\sum_{m,n=1}^{N} K_G(\boldsymbol{x})\Big[\alpha_G\Big(C_{K\Phi,m}^{(2,2)(e')}\left\langle\Phi_n^{(0,0)}\right\rangle + C_{K\Phi,m}^{(2,0)(e')}\Big(\left\langle\Phi_n^{(0,2)}\right\rangle + \frac{1}{2}\sigma_\beta^2\left\langle\Phi_n^{(0,0)}\right\rangle\Big)\Big) \\
&\qquad + \alpha_G\left\langle K_s'(\boldsymbol{y})\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle_{mn}^{(2,2)} + \left\langle\alpha' K_s'(\boldsymbol{y})\nabla_x\Phi'(\boldsymbol{x})\right\rangle_m^{(2,2)}\left\langle\Phi_n^{(0,0)}\right\rangle\Big]\nabla_x\xi_m(\boldsymbol{x})\xi_n(\boldsymbol{y})\boldsymbol{e}_3^T
\end{aligned}
\tag{4-47}
$$

where the superscripts e and e' have been dropped except where this may cause confusion, and n and m are node numbers in element e and e', respectively. For gravity-free flow, g = 0 and (4-42) simplifies to (45) of *Guadagnini and Neuman* [1999a] for saturated flow.

4.3.3 Cross-covariance Function of Y and *q*

Finite element equations for the cross-covariance between Y at point $\boldsymbol{x}$ in element e and $\boldsymbol{q}$ at point $\boldsymbol{y}$ in element e' can be calculated directly from (3-48) and (3-49). By interpolating some terms in the equations, for example,

$$\begin{aligned}
\langle Y'(\boldsymbol{x})\nabla\Phi'(\boldsymbol{y})\rangle^{(i,j)}_{x\in e,y\in e'} &= \sum_{m=1}^{N}\langle Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle^{(i,j)(e)}_{n}\nabla_y\xi^{(e')}_{n} \\
\langle Y'(\boldsymbol{x})Y'(\boldsymbol{y})\nabla\Phi'(\boldsymbol{y})\rangle^{(i,j)}_{x\in e,y\in e'} &= \sum_{m=1}^{N}\langle Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle^{(i,j)(e)}_{n}\nabla_y\xi^{(e')}_{n}
\end{aligned} \tag{4-48}$$

where (i, j) designate orders of approximation in σ_Y and σ_β, respectively, we have

$$C^{(2,0)}_{Yq}(\boldsymbol{x},\boldsymbol{y}) = -\sum_{n=1}^{N}K^{(e')}_{G}(\boldsymbol{y})\left[C^{(2,0)(e)}_{Y\Phi,n} + C_Y(e,e')\langle\Phi^{(0,0)}_{n}\rangle\right]\left(\nabla_y\xi_n(\boldsymbol{y}) + g\alpha_G\xi_n(\boldsymbol{y})\boldsymbol{e}_2\right) \tag{4-49}$$

$$\begin{aligned}
C^{(2,2)}_{Yq}(\boldsymbol{x},\boldsymbol{y}) = &-\sum_{n=1}^{N}K^{(e')}_{G}(\boldsymbol{y})\left[C^{(2,2)(e)}_{Y\Phi,n} + C_Y(e,e')\langle\Phi^{(0,2)}_{n}\rangle\right]\left(\nabla_y\xi_n(\boldsymbol{y}) + g\alpha_G\xi_n(\boldsymbol{y})\boldsymbol{e}_2\right) \\
&-\sum_{n=1}^{N}K^{(e')}_{G}(\boldsymbol{y})\langle Y'(\boldsymbol{x})Y'(\boldsymbol{y})\nabla\Phi'(\boldsymbol{y})\rangle^{(2,2)(e)}_{n}\xi_n(\boldsymbol{y}) \\
&-\frac{1}{2}g\alpha_G\sigma^2_\beta\sum_{n=1}^{N}K^{(e')}_{G}(\boldsymbol{y})\left[C^{(2,0)(e)}_{Y\Phi,n} + C_Y(e,e')\langle\Phi^{(0,0)}_{n}\rangle\right]\xi_n(\boldsymbol{y})\boldsymbol{e}_2 \\
&-g\sum_{n=1}^{N}K^{(e')}_{G}(\boldsymbol{y})\left[\langle\alpha' Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle^{(2,2)(e)}_{n} + \langle\alpha' Y'(\boldsymbol{x})Y'(\boldsymbol{y})\Phi'(\boldsymbol{y})\rangle^{(2,2)(e)}_{n}\right]\xi_n(\boldsymbol{y})\boldsymbol{e}_2
\end{aligned} \tag{4-50}$$

where, for example, $C^{(2,0)(e)}_{Y\Phi,n}$ denotes the cross-covariance function $C^{(2,0)}_{Y\Phi}$ associated with Y in element e and Φ at node n in element e'.

4.3.4 Cross-covariance Function of β and *q*

The finite element equations for the covariance function of β and q can be readily derived from (3-49) and (3-49). The equations are, to second order,

$$C_{\beta q}^{(0,2)}(y) = -\sum_{m,n=1}^{N} K_G^{(e)}(y) R_{\beta\Phi,n}^{(0,2)} \left(\nabla_y \xi_n(y) + g\alpha_G \xi_n(y) e_2\right) - g\alpha_G \sigma_\beta^2 \sum_{m,n=1}^{N} K_G^{(e)}(y) \left\langle \Phi_n^{(0,0)} \right\rangle \xi_n(y) e_2 \tag{4-51}$$

$$\begin{aligned} C_{\beta q}^{(2,2)}(y) = & -K_G^{(e)}(y) \sum_{n=1}^{N} \left(R_{\beta\Phi,n}^{(2,2)} + \frac{1}{2}\sigma_Y^2(e) R_{\beta\Phi,n}^{(0,2)} \right) \left(\nabla \xi_n(y) + g\alpha_G \xi_n(y) e_2\right) \\ & - \sum_{n=1}^{N} \left\langle \beta' K_s'(y) \Phi'(y) \right\rangle_n^{(2,2)} \nabla \xi_n(y) \\ & - g\alpha_G \sigma_\beta^2 K_G^{(e)}(y) \sum_{n=1}^{N} \left(\left\langle \Phi_n^{(2,0)} \right\rangle + \frac{1}{2}\sigma_Y^2(e) \left\langle \Phi_n^{(0,0)} \right\rangle \right) \xi_n(y) e_2 \\ & - g\alpha_G \sum_{n=1}^{N} \left[K_G^{(e)}(y) \left\langle \beta'^2 \Phi'(y) \right\rangle_n^{(2,2)} + \left\langle \beta' K_s'(y) \Phi'(y) \right\rangle_n^{(2,2)} + \left\langle \beta'^2 K_s'(y) \Phi'(y) \right\rangle_n^{(2,2)} \right] \xi_n(y) e_2 \end{aligned} \tag{4-52}$$

CHAPTER 5
DERIVATIONS OF MEAN PRESSURE HEAD AND ITS (CO)VARIANCES

5.1 MEAN PRESSURE HEAD

Once we know the mean field of the transformed variable $\Phi(\boldsymbol{x})$ and its associated variances and covariance, we can calculate the mean field and covariance of the original variable, i.e., pressure head. Rewrite equation (2-8) as

$$\alpha\psi(\boldsymbol{x}) = \ln(\alpha\ \Phi(\boldsymbol{x})) \tag{5-1}$$

Replacing each random variable or function in (5-1) by its conditional mean plus a perturbation, and recalling expansions for $\langle\alpha\rangle$ and $\langle\Phi(\boldsymbol{x})\rangle$, i.e., (3-2) and (3-3), we have

$$\langle\alpha\rangle\langle\psi(\boldsymbol{x})\rangle + \langle\alpha\rangle\psi'(\boldsymbol{x}) + \alpha'\langle\psi(\boldsymbol{x})\rangle + \alpha'\psi'(\boldsymbol{x}) = \ln\left(\alpha_G\left\langle\Phi^{(0,0)}(\boldsymbol{x})\right\rangle\right) + \beta' + B(\boldsymbol{x}) + O(b^3(\boldsymbol{x})) \tag{5-2}$$

where

$$B(\boldsymbol{x}) = b(\boldsymbol{x}) - \frac{1}{2}b^2(\boldsymbol{x}) \tag{5-3}$$

and

$$b(\boldsymbol{x}) = \frac{\Phi'(\boldsymbol{x})}{\left\langle\Phi^{(0,0)}(\boldsymbol{x})\right\rangle} + \sum_{n+m\neq 0}^{\infty}\frac{\left\langle\Phi^{(n,m)}(\boldsymbol{x})\right\rangle}{\left\langle\Phi^{(0,0)}(\boldsymbol{x})\right\rangle} \tag{5-4}$$

Taking conditional mean of (5-2) yields:

$$\langle\alpha\rangle\langle\psi(\boldsymbol{x})\rangle + \langle\alpha'\psi'(\boldsymbol{x})\rangle = \ln\left(\alpha_G\left\langle\Phi^{(0,0)}(\boldsymbol{x})\right\rangle\right) + \langle B(\boldsymbol{x})\rangle + O\left(\left\langle b^3(\boldsymbol{x})\right\rangle\right) \tag{5-5}$$

To eliminate $\langle\alpha'\psi'(\boldsymbol{x})\rangle$ from the above equation, one multiplies (5-2) by α' and takes conditional mean,

$$\langle\alpha\rangle\langle\alpha'\psi'(\boldsymbol{x})\rangle + \left\langle\alpha'^2\right\rangle\langle\psi(\boldsymbol{x})\rangle + \left\langle\alpha'^2\psi'(\boldsymbol{x})\right\rangle = \langle\alpha'\beta'\rangle + \langle\alpha' B(\boldsymbol{x})\rangle + HO \tag{5-6}$$

where HO represents higher-order terms. Multiplying (5-2) by α'^2 and taking conditional mean gives

$$\langle\alpha'^2\rangle\langle\alpha\rangle\langle\psi(\boldsymbol{x})\rangle+\langle\alpha\rangle\langle\alpha'^2\psi'(\boldsymbol{x})\rangle=\langle\alpha'^2\rangle\ln\left(\alpha_G\langle\Phi^{(0,0)}(\boldsymbol{x})\rangle\right)+\langle\alpha'^2B(\boldsymbol{x})\rangle+HO \tag{5-7}$$

From (5-5), (5-6), and (5-7), we obtain an equation for mean pressure head

$$\begin{aligned}\langle\alpha\rangle^3\langle\psi(\boldsymbol{x})\rangle &=\left(\langle\alpha\rangle^2+\langle\alpha'^2\rangle\right)\ln\left(\alpha_G\langle\Phi^{(0,0)}(\boldsymbol{x})\rangle\right)+\langle\alpha\rangle^2\langle B(\boldsymbol{x})\rangle+\langle\alpha'^2B(\boldsymbol{x})\rangle\\ &\quad-\langle\alpha\rangle\left[\langle\alpha'\beta'\rangle+\langle\alpha'B(\boldsymbol{x})\rangle\right]+HO\end{aligned} \tag{5-8}$$

Expanding (5-8) in powers of σ_Y and σ_β, and equating terms of same order in both sides, we obtain solutions for the conditional mean pressure head to second order in σ_Y and σ_β

$$\begin{aligned}
\langle\psi^{(0,0)}(\boldsymbol{x})\rangle &= \frac{1}{\alpha_G}\left[\ln\left(\alpha_G\langle\Phi^{(0,0)}(\boldsymbol{x})\rangle\right)-\frac{1}{2}\frac{C_\Phi^{(0,0)}(\boldsymbol{x},\boldsymbol{x})}{\langle\Phi^{(0,0)}(\boldsymbol{x})\rangle^2}\right]\\
\langle\psi^{(2,0)}(\boldsymbol{x})\rangle &= \frac{1}{\alpha_G}\left[\frac{\langle\Phi^{(2,0)}(\boldsymbol{x})\rangle}{\langle\Phi^{(0,0)}(\boldsymbol{x})\rangle}-\frac{1}{2}\frac{C_\Phi^{(2,0)}(\boldsymbol{x},\boldsymbol{x})}{\langle\Phi^{(0,0)}(\boldsymbol{x})\rangle^2}\right]\\
\langle\psi^{(0,2)}(\boldsymbol{x})\rangle &= -\frac{\sigma_\beta^2}{\alpha_G}+\frac{\sigma_\beta^2}{2\alpha_G}\ln\left(\alpha_G\langle\Phi^{(0,0)}(\boldsymbol{x})\rangle\right)+\frac{1}{\alpha_G}\left[\frac{\langle\Phi^{(0,2)}(\boldsymbol{x})\rangle}{\langle\Phi^{(0,0)}(\boldsymbol{x})\rangle}-\frac{C_\Phi^{(0,2)}(\boldsymbol{x},\boldsymbol{x})}{2\langle\Phi^{(0,0)}(\boldsymbol{x})\rangle^2}+\frac{\sigma_\beta^2}{4}\frac{C_\Phi^{(0,0)}(\boldsymbol{x},\boldsymbol{x})}{\langle\Phi^{(0,0)}(\boldsymbol{x})\rangle^2}\right.\\
&\qquad\left.-\frac{R_{\alpha\Phi}^{(0,2)}(\boldsymbol{x})}{\alpha_G\langle\Phi^{(0,0)}(\boldsymbol{x})\rangle}+\frac{\langle\alpha'\Phi'^2(\boldsymbol{x})\rangle^{(0,2)}}{2\alpha_G\langle\Phi^{(0,0)}(\boldsymbol{x})\rangle^2}+\frac{\langle\alpha'^2\Phi'(\boldsymbol{x})\rangle^{(0,2)}}{\alpha_G^2\langle\Phi^{(0,0)}(\boldsymbol{x})\rangle}-\frac{\langle\alpha'^2\Phi'^2(\boldsymbol{x})\rangle^{(0,2)}}{2\alpha_G^2\langle\Phi^{(0,0)}(\boldsymbol{x})\rangle^2}\right]\\
\langle\psi^{(2,2)}(\boldsymbol{x})\rangle &= \frac{1}{\alpha_G}\left[\frac{\langle\Phi^{(2,2)}(\boldsymbol{x})\rangle}{\langle\Phi^{(0,0)}(\boldsymbol{x})\rangle}+\frac{\sigma_\beta^2}{2}\frac{\langle\Phi^{(2,0)}(\boldsymbol{x})\rangle}{\langle\Phi^{(0,0)}(\boldsymbol{x})\rangle}-\frac{\langle\Phi^{(2,0)}(\boldsymbol{x})\rangle\langle\Phi^{(0,2)}(\boldsymbol{x})\rangle}{\langle\Phi^{(0,0)}(\boldsymbol{x})\rangle^2}\right]\\
&\quad-\frac{1}{2\alpha_G\langle\Phi^{(0,0)}(\boldsymbol{x})\rangle^2}\left[C_\Phi^{(2,2)}(\boldsymbol{x},\boldsymbol{x})-\frac{\sigma_\beta^2}{2}C_\Phi^{(2,0)}(\boldsymbol{x},\boldsymbol{x})\right]\\
&\quad-\frac{1}{\alpha_G^2\langle\Phi^{(0,0)}(\boldsymbol{x})\rangle}\left[R_{\alpha\Phi}^{(2,2)}(\boldsymbol{x})-\frac{\langle\Phi^{(2,0)}(\boldsymbol{x})\rangle}{\langle\Phi^{(0,0)}(\boldsymbol{x})\rangle}R_{\alpha\Phi}^{(0,2)}(\boldsymbol{x})-\frac{\langle\alpha'^2\Phi'(\boldsymbol{x})\rangle^{(2,2)}}{\alpha_G}+\frac{\langle\alpha'^2\Phi'(\boldsymbol{x})\rangle^{(0,2)}}{\alpha_G}\frac{\langle\Phi^{(2,0)}(\boldsymbol{x})\rangle}{\langle\Phi^{(0,0)}(\boldsymbol{x})\rangle}\right.\\
&\qquad\left.+\frac{\langle\alpha'^2\Phi'^2(\boldsymbol{x})\rangle^{(2,2)}}{2\alpha_G\langle\Phi^{(0,0)}(\boldsymbol{x})\rangle}-\frac{\langle\alpha'\Phi'^2(\boldsymbol{x})\rangle^{(0,2)}}{2\langle\Phi^{(0,0)}(\boldsymbol{x})\rangle}\right]
\end{aligned} \tag{5-9}$$

For the case of deterministic driving forces, the first two equations in (5-9) simplify to (45)-(46) of *Tartakovsky et al.* [1999], in which α is also taken as deterministic constant.

5.2 PRESSURE HEAD COVARIANCE FUNCTIONS

Multiplying (5-1) by itself in terms of $\boldsymbol{y}$, we have

$$\alpha^2\psi(\boldsymbol{x})\psi(\boldsymbol{y}) = \ln[\alpha\Phi(\boldsymbol{x})]\ \ln[\alpha\Phi(\boldsymbol{y})] \tag{5-10}$$

Replacing all terms in their mean and perturbation, and taking conditional mean, the left hand side becomes

$$\begin{aligned}\langle L\rangle &= \langle\alpha\rangle^2\langle\psi(\boldsymbol{x})\rangle\langle\psi(\boldsymbol{y})\rangle + \langle\alpha\rangle^2 C_\psi(\boldsymbol{x},\boldsymbol{y}) + 2\langle\alpha\rangle\langle\psi(\boldsymbol{x})\rangle\langle\alpha'\psi'(\boldsymbol{y})\rangle \\ &\quad + 2\langle\alpha\rangle\langle\psi(\boldsymbol{y})\rangle\langle\alpha'\psi'(\boldsymbol{x})\rangle + 2\langle\alpha\rangle\langle\alpha'\psi'(\boldsymbol{x})\psi'(\boldsymbol{y})\rangle + \langle\alpha'^2\rangle\langle\psi(\boldsymbol{x})\rangle\langle\psi(\boldsymbol{y})\rangle \\ &\quad + \langle\psi(\boldsymbol{x})\rangle\langle\alpha'^2\psi'(\boldsymbol{y})\rangle + \langle\psi(\boldsymbol{y})\rangle\langle\alpha'^2\psi'(\boldsymbol{x})\rangle + \langle\alpha'^2\psi'(\boldsymbol{x})\psi'(\boldsymbol{y})\rangle\end{aligned} \tag{5-11}$$

To eliminate higher-order terms, we note that

$$\begin{aligned}\langle\alpha' L\rangle &= \langle\alpha\rangle^2\langle\psi(\boldsymbol{x})\rangle\langle\alpha'\psi'(\boldsymbol{y})\rangle + \langle\alpha\rangle^2\langle\psi(\boldsymbol{y})\rangle\langle\alpha'\psi'(\boldsymbol{x})\rangle + \langle\alpha\rangle^2\langle\alpha'\psi'(\boldsymbol{x})\psi'(\boldsymbol{y})\rangle \\ &\quad + 2\langle\alpha\rangle\langle\psi(\boldsymbol{x})\rangle\langle\psi(\boldsymbol{y})\rangle\langle\alpha'^2\rangle + 2\langle\alpha\rangle\langle\psi(\boldsymbol{x})\rangle\langle\alpha'^2\psi'(\boldsymbol{y})\rangle \\ &\quad + 2\langle\alpha\rangle\langle\psi(\boldsymbol{y})\rangle\langle\alpha'^2\psi'(\boldsymbol{x})\rangle + 2\langle\alpha\rangle\langle\alpha'^2\psi'(x)\psi'(\boldsymbol{y})\rangle + HO\end{aligned} \tag{5-12}$$

and

$$\begin{aligned}\langle\alpha'^2 L\rangle &= \langle\alpha\rangle^2\langle\psi(\boldsymbol{x})\rangle\langle\psi(\boldsymbol{y})\rangle\langle\alpha'^2\rangle + \langle\alpha\rangle^2\langle\psi(\boldsymbol{x})\rangle\langle\alpha'^2\psi'(\boldsymbol{y})\rangle \\ &\quad + \langle\alpha\rangle^2\langle\psi(\boldsymbol{y})\rangle\langle\alpha'^2\psi'(\boldsymbol{x})\rangle + \langle\alpha\rangle^2\langle\alpha'^2\psi'(\boldsymbol{x})\psi'(\boldsymbol{y})\rangle + HO\end{aligned} \tag{5-13}$$

Multiplying (5-11), (5-12) and (5-13) by $\langle\alpha\rangle^2$, -2$\langle\alpha\rangle$ and 3, respectively, and summing them yields

$$\langle\alpha\rangle^2\langle L\rangle - 2\langle\alpha\rangle\langle\alpha' L\rangle + 3\langle\alpha'^2 L\rangle = \langle\alpha\rangle^4\langle\psi(\boldsymbol{x})\rangle\langle\psi(\boldsymbol{y})\rangle + \langle\alpha\rangle^4 C_\psi(\boldsymbol{x},\boldsymbol{y}) + HO \tag{5-14}$$

The second term on the right hand side of (5-14) is the covariance of pressure head. Equation (5-14) could also be derived from (5-10) upon multiplying the left hand side by $\langle\alpha\rangle^2$-2$\langle\alpha\rangle\alpha'$+3$\alpha'^2$ and taking the conditional mean,

$$\begin{aligned}&\langle\alpha\rangle^4\langle\psi(\boldsymbol{x})\rangle\langle\psi(\boldsymbol{y})\rangle + \langle\alpha\rangle^4 C_\psi(\boldsymbol{x},\boldsymbol{y}) \\ &= \Big\langle\big(\langle\alpha\rangle^2 - 2\langle\alpha\rangle\alpha' + 3\alpha'^2\big)\Big[\ln\big(\alpha_G\langle\Phi^{(0,0)}(\boldsymbol{x})\rangle\big) + \beta + B(\boldsymbol{x})\Big]\Big[\ln\big(\alpha_G\langle\Phi^{(0,0)}(\boldsymbol{y})\rangle\big) + \beta + B(\boldsymbol{y})\Big]\Big\rangle + HO\end{aligned} \tag{5-15}$$

Expanding (5-15) in powers of σ_Y and σ_β and comparing terms of same order on both sides of (5-15) yield, recursive approximations to the second order in σ_Y and σ_β

$$
\begin{aligned}
C_\psi^{(0,0)}(\boldsymbol{x},\boldsymbol{y}) &= \frac{1}{\alpha_G^2}\Big[C_\phi^{(0,0)}(\boldsymbol{x},\boldsymbol{y}) - \frac{1}{2}\left\langle \phi'^2(\boldsymbol{x})\phi'(\boldsymbol{y})\right\rangle^{(0,0)} - \frac{1}{2}\left\langle \phi'(\boldsymbol{x})\phi'^2(\boldsymbol{y})\right\rangle^{(0,0)} + \frac{1}{4}\left\langle \phi'^2(\boldsymbol{x})\phi'^2(\boldsymbol{y})\right\rangle^{(0,0)} \\
&\qquad - \frac{1}{4}C_\phi^{(0,0)}(\boldsymbol{x},\boldsymbol{x})C_\phi^{(0,0)}(\boldsymbol{y},\boldsymbol{y})\Big] \\
C_\psi^{(2,0)}(\boldsymbol{x},\boldsymbol{y}) &= \frac{1}{\alpha_G^2}\left[F_1(\boldsymbol{x},\boldsymbol{y}) + F_1(\boldsymbol{y},\boldsymbol{x})\right] \\
C_\psi^{(0,2)}(\boldsymbol{x},\boldsymbol{y}) &= \frac{1}{\alpha_G^2}\left[F_2(\boldsymbol{x},\boldsymbol{y}) + F_2(\boldsymbol{y},\boldsymbol{x})\right] \\
C_\psi^{(2,2)}(\boldsymbol{x},\boldsymbol{y}) &= -2\sigma_\beta^2 C_\psi^{(2,0)}(\boldsymbol{x},\boldsymbol{y}) + \frac{1}{\alpha_G^2}\left[F_3(\boldsymbol{x},\boldsymbol{y}) + F_3(\boldsymbol{y},\boldsymbol{x})\right]
\end{aligned}
\tag{5-16}
$$

where

$$
\phi(\boldsymbol{x}) = \Phi(\boldsymbol{x})/\Phi^{(0,0)}(\boldsymbol{x}) \qquad \phi'(\boldsymbol{x}) = \Phi'(\boldsymbol{x})/\Phi^{(0,0)}(\boldsymbol{x}) \tag{5-17}
$$

$$
F_1(\boldsymbol{x},\boldsymbol{y}) = \frac{1}{2}\left[C_\phi^{(2,0)}(\boldsymbol{x},\boldsymbol{y}) + \left\langle \phi'^2(\boldsymbol{x})\phi'(\boldsymbol{y})\right\rangle^{(2,0)} - C_\phi^{(0,0)}(\boldsymbol{x},\boldsymbol{x})\left(\left\langle \phi^{(2,0)}(\boldsymbol{y})\right\rangle - \frac{1}{2}C_\phi^{(2,0)}(\boldsymbol{y},\boldsymbol{y}) \right)\right] \tag{5-18}
$$

$$
\begin{aligned}
F_2(\boldsymbol{x},\boldsymbol{y}) &= \frac{\sigma_\beta^2}{2}\left[\ln\left(\alpha_G\left\langle \Phi^{(0,0)}(\boldsymbol{x})\right\rangle\right) - 1\right]\left[\ln\left(\alpha_G\left\langle \Phi^{(0,0)}(\boldsymbol{y})\right\rangle\right) - 1\right] + \frac{5\sigma_\beta^2}{8}C_\phi^{(0,0)}(\boldsymbol{x},\boldsymbol{x})C_\phi^{(0,0)}(\boldsymbol{y},\boldsymbol{y}) \\
&\quad + \frac{1}{4}\left(C_\phi^{(0,2)}(\boldsymbol{x},\boldsymbol{y}) - \left\langle \phi'^2(\boldsymbol{x})\phi'(\boldsymbol{y})\right\rangle^{(0,2)} - \left\langle \phi'(\boldsymbol{x})\phi'^2(\boldsymbol{y})\right\rangle^{(0,2)} + \left\langle \phi'^2(\boldsymbol{x})\phi'^2(\boldsymbol{y})\right\rangle^{(0,2)}\right) \\
&\quad + \frac{\sigma_\beta^2}{2}\left(C_\phi^{(0,0)}(\boldsymbol{x},\boldsymbol{y}) - \left\langle \phi'^2(\boldsymbol{x})\phi'(\boldsymbol{y})\right\rangle^{(0,0)} - \left\langle \phi'(\boldsymbol{x})\phi'^2(\boldsymbol{y})\right\rangle^{(0,0)} + \left\langle \phi'^2(\boldsymbol{x})\phi'^2(\boldsymbol{y})\right\rangle^{(0,0)}\right) \\
&\quad - \left\langle \beta'\phi'(\boldsymbol{x})\phi'(\boldsymbol{y})\right\rangle^{(0,2)} + \frac{1}{2}\left\langle \beta'\phi'(\boldsymbol{x})\phi'^2(\boldsymbol{y})\right\rangle^{(0,2)} + \frac{1}{2}\left\langle \beta'\phi'^2(\boldsymbol{x})\phi'(\boldsymbol{y})\right\rangle^{(0,2)} - \frac{1}{4}\left\langle \beta'\phi'^2(\boldsymbol{x})\phi'^2(\boldsymbol{y})\right\rangle^{(0,2)} \\
&\quad + \left(\frac{1}{2}C_\phi^{(0,0)}(\boldsymbol{y},\boldsymbol{y}) - \ln\left(\alpha_G\left\langle \Phi^{(0,0)}(\boldsymbol{x})\right\rangle\right) + 1\right)\left(\left\langle \beta'\phi'(\boldsymbol{x})\right\rangle^{(0,2)} - \frac{1}{2}\left\langle \beta'\phi'^2(\boldsymbol{x})\right\rangle^{(0,2)}\right) \\
&\quad + \left[\frac{1}{4}C_\phi^{(0,0)}(\boldsymbol{y},\boldsymbol{y}) + 2\left(\ln\left(\alpha_G\left\langle \Phi^{(0,0)}(\boldsymbol{x})\right\rangle\right) - 1\right)\right]\left\langle \beta'^2\phi'(\boldsymbol{x})\right\rangle^{(0,2)} \\
&\quad - \frac{1}{2}\left[\frac{1}{2}C_\phi^{(0,0)}(\boldsymbol{y},\boldsymbol{y}) + 2\left(\ln\left(\alpha_G\left\langle \Phi^{(0,0)}(\boldsymbol{x})\right\rangle\right) - 1\right)\right]\left\langle \beta'^2\phi'^2(\boldsymbol{x})\right\rangle^{(0,2)} \\
&\quad + \frac{1}{2}\left[\left\langle \phi^{(0,2)}(\boldsymbol{y})\right\rangle - \frac{1}{2}C_\phi^{(0,2)}(\boldsymbol{y},\boldsymbol{y}) - \sigma_\beta^2\left(\ln\left(\alpha_G\left\langle \Phi^{(0,0)}(\boldsymbol{x})\right\rangle\right) - 1\right)\right]C_\phi^{(0,0)}(\boldsymbol{x},\boldsymbol{x})
\end{aligned}
\tag{5-19}
$$

$$
\begin{aligned}
F_3(\boldsymbol{x},\boldsymbol{y}) = {} & \frac{1}{2}\left\langle \phi^{(2,2)}(\boldsymbol{x})\right\rangle \left(\left\langle \phi'(\boldsymbol{x})\phi'^2(\boldsymbol{y})\right\rangle^{(0,0)} - C_\phi^{(0,0)}(\boldsymbol{y},\boldsymbol{y}) - 2C_\phi^{(0,0)}(\boldsymbol{x},\boldsymbol{y})\right) \\
& + \frac{1}{\alpha_G^2}\left\langle \phi^{(2,0)}(\boldsymbol{x})\right\rangle \Big[3\alpha_G^2\sigma_\beta^2 \left(1 - \ln\left(\alpha_G \left\langle \Phi^{(0,0)}(\boldsymbol{y})\right\rangle\right)\right) - \alpha_G \left\langle \alpha'\phi'(\boldsymbol{y})\right\rangle^{(0,2)} \\
& \qquad - \alpha_G \left(1 - \ln\left(\alpha_G \left\langle \Phi^{(0,0)}(\boldsymbol{y})\right\rangle\right)\right)\left\langle \alpha'\phi'(\boldsymbol{x})\right\rangle^{(0,2)} + 2\left\langle \alpha'^2\phi'(\boldsymbol{y})\right\rangle^{(0,2)} \\
& \qquad + 2\left(1 - \ln\left(\alpha_G \left\langle \Phi^{(0,0)}(\boldsymbol{y})\right\rangle\right)\right)\left\langle \alpha'^2\phi'(\boldsymbol{x})\right\rangle^{(0,2)} - \frac{3}{2}\alpha_G \left\langle \alpha'\phi'^2(\boldsymbol{y})\right\rangle^{(0,2)} \\
& \qquad - \left\langle \alpha'^2\phi'^2(\boldsymbol{y})\right\rangle^{(0,2)} - \alpha_G^2 \left\langle \phi'(\boldsymbol{x})\phi'(\boldsymbol{y})\right\rangle^{(0,2)} + \frac{1}{2}\alpha_G^2 \left\langle \phi'(\boldsymbol{x})\phi'^2(\boldsymbol{y})\right\rangle^{(0,2)} \\
& \qquad - 2\alpha_G \left\langle \alpha'\phi'(\boldsymbol{x})\phi'(\boldsymbol{y})\right\rangle^{(0,2)} - \alpha_G \left\langle \alpha'\phi'(\boldsymbol{x})\phi'^2(\boldsymbol{y})\right\rangle^{(0,2)} \\
& \qquad - 3\left\langle \alpha'^2\phi'(\boldsymbol{x})\phi'(\boldsymbol{y})\right\rangle^{(0,2)} + \frac{3}{2}\alpha_G \left\langle \alpha'^2\phi'(\boldsymbol{x})\phi'^2(\boldsymbol{y})\right\rangle^{(0,2)} \Big] \\
& + \left\langle \phi^{(0,2)}(\boldsymbol{x})\right\rangle \left[-\left\langle \phi'(\boldsymbol{x})\phi'(\boldsymbol{y})\right\rangle^{(2,0)} + \frac{1}{2}\left\langle \phi'(\boldsymbol{x})\phi'^2(\boldsymbol{y})\right\rangle^{(2,0)} \right] \\
& + \left\langle \phi^{(0,2)}(\boldsymbol{x})\right\rangle \left\langle \phi^{(2,0)}(\boldsymbol{x})\right\rangle \left[\left\langle \phi'(\boldsymbol{x})\phi'(\boldsymbol{y})\right\rangle^{(0,0)} - \frac{1}{2}C_\phi^{(0,0)}(\boldsymbol{y},\boldsymbol{y}) \right] \\
& + \frac{C_\phi^{(2,0)}(\boldsymbol{x},\boldsymbol{x})}{2\alpha_G^2} \Big[-\alpha_G \left\langle \alpha'\phi'(\boldsymbol{y})\right\rangle^{(0,2)} + \frac{1}{2}\alpha_G \left\langle \alpha'\phi'^2(\boldsymbol{y})\right\rangle^{(0,2)} + \left\langle \alpha'^2\phi'(\boldsymbol{y})\right\rangle^{(0,2)} - \frac{1}{2}\alpha_G^2\sigma_\beta^2 C_\phi^{(0,0)}(\boldsymbol{y},\boldsymbol{y}) \\
& \qquad - \frac{1}{2}\alpha_G^2 C_\phi^{(0,2)}(\boldsymbol{y},\boldsymbol{y}) + \alpha_G^2\sigma_\beta^2 \left(1 - \ln\left(\alpha_G \left\langle \Phi^{(0,0)}(\boldsymbol{y})\right\rangle\right)\right) \Big] \\
& + \frac{1}{\alpha_G}\left(1 - \ln\left(\alpha_G \left\langle \Phi^{(0,0)}(\boldsymbol{y})\right\rangle\right)\right)\left[\left\langle \alpha'\phi'(\boldsymbol{x})\right\rangle^{(2,2)} - \frac{1}{2}\left\langle \alpha'\phi'^2(\boldsymbol{x})\right\rangle^{(2,2)} \right] + \frac{2}{\alpha_G^2}\left\langle \alpha'^2\phi'(\boldsymbol{x})\right\rangle^{(2,2)} \ln\left(\alpha_G \left\langle \Phi^{(0,0)}(\boldsymbol{y})\right\rangle\right) \\
& - \frac{1}{2}\left(C_\phi^{(2,2)}(\boldsymbol{x},\boldsymbol{y}) - 4\sigma_\beta^2 C_\phi^{(2,0)}(\boldsymbol{x},\boldsymbol{y})\right) - \frac{1}{2}\left(\left\langle \phi'(\boldsymbol{x})\phi'^2(\boldsymbol{y})\right\rangle^{(2,2)} + \sigma_\beta^2 \left\langle \phi'(\boldsymbol{x})\phi'^2(\boldsymbol{y})\right\rangle^{(2,0)} \right) \\
& + \left\langle \beta'\phi'(\boldsymbol{x})\right\rangle^{(2,2)} + \frac{2}{\alpha_G}\left\langle \beta'\phi'(\boldsymbol{x})\phi'(\boldsymbol{y})\right\rangle^{(2,2)} - \frac{1}{\alpha_G}\left\langle \beta'\phi'(\boldsymbol{x})\phi'^2(\boldsymbol{y})\right\rangle^{(2,2)} \\
& + \frac{1}{8}\left\langle \phi'^2(\boldsymbol{x})\phi'^2(\boldsymbol{y})\right\rangle^{(2,2)} + \frac{1}{2}\sigma_\beta^2 \left\langle \phi'^2(\boldsymbol{x})\phi'^2(\boldsymbol{y})\right\rangle^{(2,0)} + \frac{1}{8\alpha_G}\left\langle \alpha'\phi'^2(\boldsymbol{x})\phi'^2(\boldsymbol{y})\right\rangle^{(2,2)}
\end{aligned}
\tag{5-20}
$$

For deterministic α and driving forces, from (5-16), the variance of mean pressure head simplifies to

$$
C_\psi^{(2,0)}(\boldsymbol{x},\boldsymbol{x}) = C_\phi^{(2,0)}(\boldsymbol{x},\boldsymbol{x}) = \frac{C_\Phi^{(2,0)}(\boldsymbol{x},\boldsymbol{x})}{\alpha_G^2 \left\langle \Phi^{(0,0)}(\boldsymbol{x})\right\rangle^2} \tag{5-21}
$$

which is identical to (47) of *Tartakovsky et al.* [1999].

5.3 CROSS-COVARIANCE FUNCTION $C_{Y\psi}(X, Y)$

Multiplying (5-2) by $Y'(\boldsymbol{x})$, taking conditional mean, and noting that $\langle\alpha' Y'(\boldsymbol{x})\rangle=0$,

$$\langle\alpha\rangle C_{Y\Phi}(\boldsymbol{x},\boldsymbol{y})+\langle\alpha' Y'(\boldsymbol{x})\psi'(\boldsymbol{y})\rangle=\langle Y'(\boldsymbol{x})B(\boldsymbol{y})\rangle+HO \tag{5-22}$$

To eliminate the second term in the above equation, multiply (5-2) by $\alpha' Y'(\boldsymbol{x})$ and taking conditional mean, to give

$$\langle\alpha\rangle\langle\alpha' Y'(\boldsymbol{x})\psi'(\boldsymbol{y})\rangle+\langle\alpha'^2 Y'(\boldsymbol{x})\psi'(\boldsymbol{y})\rangle=\langle\alpha' Y'(\boldsymbol{x})B(\boldsymbol{y})\rangle+HO \tag{5-23}$$

Again, the second term in (5-23) can be formulated upon multiplying (5-2) by $\alpha'^2 Y'(\boldsymbol{x})$ and taking conditional mean,

$$\langle\alpha\rangle\langle\alpha'^2 Y'(\boldsymbol{x})\psi'(\boldsymbol{y})\rangle=\langle\alpha'^2 Y'(\boldsymbol{x})B(\boldsymbol{y})\rangle+HO \tag{5-24}$$

From (5-22)-(5-24) we get an equation for the cross-covariance function $C_{Y\psi}(\boldsymbol{x},\boldsymbol{y})$,

$$\langle\alpha\rangle^3 C_{Y\psi}(\boldsymbol{x},\boldsymbol{y})=\langle\alpha\rangle^2\langle Y'(\boldsymbol{x})B(\boldsymbol{y})\rangle-\langle\alpha\rangle\langle\alpha' Y'(\boldsymbol{x})B(\boldsymbol{y})\rangle+\langle\alpha'^2 Y'(\boldsymbol{x})B(\boldsymbol{y})\rangle+HO \tag{5-25}$$

Expanding (5-25) in powers of σ_Y and σ_β and equating the terms of same order on both sides yields approximations for the cross-covariance function $C_{Y\psi}(\boldsymbol{x}, \boldsymbol{y})$ to the second order,

$$\begin{aligned}
&C_{Y\psi}^{(0,0)}(\boldsymbol{x},\boldsymbol{y})=C_{Y\psi}^{(0,1)}(\boldsymbol{x},\boldsymbol{y})=C_{Y\psi}^{(0,2)}(\boldsymbol{x},\boldsymbol{y})=0\\
&C_{Y\psi}^{(1,0)}(\boldsymbol{x},\boldsymbol{y})=C_{Y\psi}^{(1,1)}(\boldsymbol{x},\boldsymbol{y})=C_{Y\psi}^{(1,2)}(\boldsymbol{x},\boldsymbol{y})=0\\
&C_{Y\psi}^{(2,0)}(\boldsymbol{x},\boldsymbol{y})=\frac{C_{Y\Phi}^{(2,0)}(\boldsymbol{x},\boldsymbol{y})}{\alpha_G\langle\Phi^{(0,0)}(\boldsymbol{y})\rangle}\\
&C_{Y\psi}^{(2,1)}(\boldsymbol{x},\boldsymbol{y})=0\\
&C_{Y\psi}^{(2,2)}(\boldsymbol{x},\boldsymbol{y})=\frac{C_{Y\Phi}^{(2,2)}(\boldsymbol{x},\boldsymbol{y})}{\alpha_G\langle\Phi^{(0,0)}(\boldsymbol{y})\rangle}-\frac{C_{Y\Phi}^{(2,0)}(\boldsymbol{x},\boldsymbol{y})}{\alpha_G\langle\Phi^{(0,0)}(\boldsymbol{y})\rangle^2}\left[\langle\Phi^{(0,2)}(\boldsymbol{y})\rangle+\frac{\sigma_\beta^2}{2}\langle\Phi^{(0,0)}(\boldsymbol{y})\rangle\right]
\end{aligned} \tag{5-26}$$

5.4 CROSS-COVARIANCE FUNCTION $C_{\beta\psi}(X, Y)$

Multiplying (5-2) by $(\langle\alpha\rangle-\alpha')\beta'$ and taking conditional mean yields

$$\begin{aligned}\langle\alpha\rangle^2 C_{\beta\psi}(x) = {} & \langle\alpha\rangle\left(\langle\beta'\beta'^2\rangle+\langle\beta' B(\boldsymbol{x})\rangle\right)-\langle\alpha'\beta' B(\boldsymbol{x})\rangle \\ & -\langle\alpha'\beta'\rangle\ln\left(\alpha_G\langle\Phi^{(0,0)}(\boldsymbol{x})\rangle\right)+HO\end{aligned} \tag{5-27}$$

where $B(\boldsymbol{x})$ is defined in (5-3). Expanding (5-27) in powers of σ_Y and σ_β, and equating terms of same order in both sides yields the following recursive approximations to the second order in σ_Y and σ_β

$$\begin{aligned}C^{(0,2)}_{\beta\psi}(\boldsymbol{x}) &= \frac{1}{\alpha_G}\left[\sigma_\beta^2-\sigma_\beta^2\ln\left(\alpha_G\langle\Phi^{(0,0)}(\boldsymbol{x})\rangle\right)+\frac{C^{(0,2)}_{\beta\Phi}(\boldsymbol{x})}{\langle\Phi^{(0,0)}(\boldsymbol{x})\rangle}\right] \\ C^{(2,2)}_{\beta\psi}(\boldsymbol{x}) &= \frac{1}{\alpha_G\langle\Phi^{(0,0)}(\boldsymbol{x})\rangle^2}\left[C^{(2,2)}_{\beta\Phi}(\boldsymbol{x})\langle\Phi^{(0,0)}(\boldsymbol{x})\rangle-C^{(0,2)}_{\beta\Phi}(\boldsymbol{x})\langle\Phi^{(2,0)}(\boldsymbol{x})\rangle\right] \\ & \quad -\frac{\langle\alpha'\beta'\Phi'(\boldsymbol{x})\rangle^{(2,2)}}{\alpha_G^2\langle\Phi^{(0,0)}(\boldsymbol{x})\rangle}-\frac{1}{2}\frac{\langle\beta'\Phi'^2(\boldsymbol{x})\rangle^{(2,2)}}{\alpha_G\langle\Phi^{(0,0)}(\boldsymbol{x})\rangle^2}+\frac{1}{2}\frac{\langle\alpha'\beta'\Phi'^2(\boldsymbol{x})\rangle^{(2,2)}}{\alpha_G^2\langle\Phi^{(0,0)}(\boldsymbol{x})\rangle^2}\end{aligned} \tag{5-28}$$

CHAPTER 6
NUMERICAL EXAMPLES OF TWO-DIMENSIONAL VERTICAL STEADY STATE UNSATURATED FLOW

6.1 DESCRIPTION OF PROBLEM

This section describes problem samples that illustrate the nonlocal finite element methodology. In our main example, denoted as Case 1, we consider a rectangular grid of 20 x 40 square elements in the vertical plane (Fig. 6.1) having a width $L_1 = 4\lambda$, a height $L_2 = 8\lambda$, and elements with sides 0.2λ, where λ is the auto-correlation scale of $Y = \ln K_s$. The boundary conditions consist of no-flow on the left and right sides ($x_1=0$ and $x_1 = 4.0\lambda$), a constant deterministic flux Q = 0.5 (all terms are given in arbitrary consistent units) at the top boundary ($x_2 = 8.0\lambda$), and zero pressure head at the bottom ($x_2 = 0$). A point source of magnitude QS = 1 is placed inside the domain to render the flow locally divergent.

The saturated hydraulic conductivity field is made statistically non-homogeneous through conditioning at three points, two above and one below the source. In most cases of practical interest, conditioning points are sparse enough to ensure that conditional mean quantities vary more slowly in space than do their random counterparts. Hence one can resolve the former (by an algorithm such as we propose) on a coarser grid than is required to resolve the latter (by Monte Carlo simulation). Here we nevertheless use a fine grid to allow comparing our direct finite element solution of the recursive moment equations with a finite element Monte Carlo solution of the original stochastic flow equations.

To solve the original stochastic flow equations by Monte Carlo simulation using standard finite elements, we assume that Y is multivariate Gaussian. Prior to conditioning, Y is statistically homogeneous and isotropic with exponential auto-covariance

$$C_Y(\xi) = \sigma_Y^2 e^{-\xi/\lambda} \tag{6-1}$$

where ξ is separation distance and σ_Y^2 is the variance of Y. We started by generating one unconditional random Y field on the grid using a Gaussian sequential simulator, GCOSIM [*Gómez-Hernández* 1991], with unconditional $\langle Y \rangle = 1$, $\sigma_Y^2 = 2$ and $\lambda=1$. We took its values at the conditioning points to represent exact "measurements" and generated NMC = 3000 realizations of a corresponding non-homogeneous conditional Y field by the same method. Our choice of number of Monte Carlo simulations (NMC) is based on numerical simulations that will be discussed in Section 6.4. For purposes of flow analysis by conditional Monte Carlo (MC) simulation, we assigned to each element a constant Y value corresponding to the point value generated at its center by GCOSIM. To ensure that the generated fields possess the desired properties, we examined the conditional ensemble mean and variance of these fields. Since generation of conditional fields starts from unconditional fields, we need to examine the quality of unconditional fields first. Figure 6.2 shows images of a single unconditional realization, unconditional sample mean $\langle Y(\boldsymbol{x}) \rangle$ and variance $\sigma_Y^2(\boldsymbol{x})$ obtained from 3000 Monte Carlo simulations with unconditional $\langle Y \rangle=1.0$, $\sigma_Y^2=2.0$, and $\lambda=1.0$. Even though hydraulic conductivity values in any single realization may fluctuate significantly (Fig. 6.2A), unconditional sample mean and variance of these realizations are close to specified unconditional $\langle Y \rangle$ and σ_Y^2, as shown in contour maps (Fig. 6.2B-C) and two cross-sections (Figs. 6.3-6.4), where the sample mean ranges from 0.93 to 1.07 and the sample variance from 1.85 to 2.12. Comparison between unconditional auto-covariance C_Y obtained from Monte Carlo simulations and calculated C_Y using (6.1) shows that they are very close (Fig. 6.5). These results ensure the quality of the generated unconditional log hydraulic conductivity fields.

For conditional log hydraulic conductivity fields, Figure 6.6 shows images of a single conditional realization of Y, conditional sample mean $\langle Y(\boldsymbol{x}) \rangle$ and variance $\sigma_Y^2(\boldsymbol{x})$ obtained from 3000 Monte Carlo conditional simulations with unconditional $\langle Y \rangle=1.0$, $\sigma_Y^2=2.0$, and $\lambda=1.0$. Cross-sectional views of conditional sample mean $\langle Y(\boldsymbol{x}) \rangle$ and variance $\sigma_Y^2(\boldsymbol{x})$ are presented in Figures 6.7 and 6.8. Comparison between conditional auto-covariance C_Y obtained from Monte Carlo simulations and calculated unconditional C_Y using equation (6.1) is illustrated in Figure 6.9.

We solved (2-1)-(2-4) for each realization of log hydraulic conductivity, together with a constant $\ln\alpha = -1$ by the standard finite element method. As an example, Figure 6.10 depicts solutions of pressure head, transverse flux and longitudinal flux corresponding to the single conditional realization of Y shown in Figure 6.6A. We then calculated sample mean pressure head and flux at each node, as well as sample variance and covariance of head and flux across the grid, based on solutions from all realizations. This completed our conditional Monte Carlo simulation of flow in Case 1.

Our nonlocal solution does not require generating any random field realizations, and is free of any distributional assumptions. Nevertheless, to render it consistent with the Monte Carlo solution, we based it on the same conditional mean and auto-covariance of Y generated earlier by GCOSIM. In other words, the geometric mean $K_G(\boldsymbol{x})=\exp(\langle Y(\boldsymbol{x})\rangle)$ and the conditional auto-covariance, $C_Y(\boldsymbol{x}, \boldsymbol{y})$, of Y used in our nonlocal conditional moment equations were those obtained from generated realizations (Figures 6.6B-C). In practical applications, one would normally infer these conditional moments geostatistically from measurements by methods such as kriging. It should be noted that the conditional Y fields are non-stationary with conditional mean $\langle Y(\boldsymbol{x})\rangle$ and auto-covariance $C_Y(\boldsymbol{x}, \boldsymbol{y})$ that depend on the coordinates $\boldsymbol{x}$ and $\boldsymbol{y}$. From Figures 6.6B-C we note that the sample mean field is much smoother than a single realization of Y (Figure 6.6A), whose values range from -3 to 6 on natural log scale, which is equivalent to 3 orders of magnitude on arithmetic scale of K_s. The pattern of the mean field is controlled largely by the conditioning points. The conditional variance of Y is zero at the conditioning points, increases rapidly with distance from these points, and is as high as the unconditional variance in some areas near the boundary.

6.2 CONDITIONAL MOMENTS OF HYDRAULIC HEAD

6.2.1 Mean Conditional Pressure Head

Figure 6.11(A) depicts two-dimensional contours of conditional mean head obtained by Monte Carlo simulation, zero-order local solutions, and second-order nonlocal solutions with parameters defined in Figure 6.1. Throughout the rest of this chapter, we use solid, dash-dotted and dashed lines to denote results from Monte Carlo simulations, zero-order and second-order solutions, respectively, unless stated otherwise. Figure 6.11(B) is a vertical profile passing through one of the conditional points, and Figure 6.11(C) is a vertical profile passing through the source. Whereas the second-order mean pressure head virtually coincides with Monte Carlo (MC) results (maximum deviation of 0.82% and average deviation of 0.26%, from MC results), the zero-order solution deviates from them slightly (maximum deviation of 10.48% and average deviation of 3.2% from MC results), especially near the upper flux boundary.

6.2.2 Conditional Variance and Covariance of Pressure Head

Figure 6.12A depicts two-dimensional contours of conditional head variance as computed by MC and nonlocal finite elements. Figures 6.12B-C show how this variance varies along profiles indicated in Figure 6.12A. Although our nonlocal results represents only the lowest possible order of approximating second moments, the variance of pressure head computed from our second-order solutions is close to the Monte Carlo results, even for such a large unconditional variance as σ_Y^2=2.0. Generally, along the longitudinal (vertical) direction, the head variance is zero on the Dirichlet boundary at the bottom and increases upwards. The variance exhibits a peak at the source (Fig 6.12C).

The covariance between pressure head ψ at all nodes and ψ at various reference points P is illustrated in Figure 6.13, where the first diagram in each row is a contour map while the other two are vertical profiles identified in the first diagram. Though the nonlocal and Monte Carlo simulation yield similar patterns, there is a notable numerical difference between them when σ_Y^2=2.0. The difference diminishes when σ_Y^2=1.0 (Fig. 6.14). It should be noted that the variance of pressure head at a point P might be less than the covariance of pressure heads between point P and other points. Indeed, the peaks of covariance are offset from the reference point P in Figures. 6.13A, D, and J. *Guadagnini and Neuman* [1999a] noted the same and ascribed it to the non-uniformity of the conditioning variance. We also find that the auto-covariance of pressure head in our examples is always positive, though it is not clear if this must always be the case.

6.2.3 Cross-covariance between Y and ψ

The cross-covariance between pressure head values at nodes and Y in various elements P (Y is a constant in any element) is illustrated in Figure 6.15. It seems that the cross-covariance is almost always negative except for a small area below element P. That is, any increase in Y within element P causes pressure head to decrease nearly everywhere except in an area under element P. Intuitively, since the overall flow in the domain is fixed (due to the flux boundary at the top and fixed inflow from point sources), according to Darcy's law, an increase in hydraulic conductivity within an element must decrease the hydraulic gradient. Therefore, pressure head tends to decrease in the upstream side of point P and increase in the downstream side of P.

6.3 CONDITIONAL MOMENTS OF FLUX

6.3.1 Conditional Mean Flux

Figure 6.16 compares mean flux in the longitudinal (vertical, x_2) direction as obtained by Monte Carlo simulation, zero-order and second-order solutions. The figure shows a contour map and cross-sections identified on this contour map. Though both the zero- and second-order solutions yield good results (average deviation of 1.23% and 3.03% from MC results, respectively), the second-order solution is closer to the Monte Carlo results.

The pattern of the contours in Figure 6.16 is largely controlled by the conditioning points of hydraulic conductivity and the point source, which render the flow field non-uniform. Three peaks correspond to three conditioning points. For convenience of discussion, we denote the conditioning point below the source as c1, the other two points from left to right as c2 and c3. The highest peak in the flux field corresponds to the largest mean hydraulic conductivity (Fig. 6.6) and lowest peak to the lowest mean hydraulic conductivity.

Figure 6.17 compares the mean flux in the transverse (horizontal, x_1) direction obtained from Monte Carlo simulation, zero- and second-order solutions. Again, both solutions are good, but the second-order solution is somewhat better than the zero-order solution (average discrepancy 0.015 for the second-order solution and 0032 for zero-order the solution).

Due to the highest hydraulic conductivity value at conditioning point c1, upstream of this point, the flow tends to converge to it, producing positive horizontal components to its upper-left and negative components to its upper-right. Similarly, downstream of point c1, the flow diverges from this point, which yields negative horizontal components to its lower-left and positive components to its lower right. The pattern of transverse component at c1 is almost symmetric except to its upper-right, where the transverse flux is affect by the point source. The pattern around the point source is also close to symmetric, with negative components to its left and positive components to its right.

6.3.2 Conditional Variance and Covariance Tensor of Flux

Figures 6.18-6.20 compare components of the conditional variance tensor of flux, as obtained by Monte Carlo simulation and second-order moment solutions. Figure 6.18A shows contours of the conditional variance (covariance at a zero lag) of longitudinal flux, $C_{q2q2}^{(2,0)}(\boldsymbol{x},\boldsymbol{x})$, and Figures 6.18B-C show vertical profiles along two lines passing through a conditioning point and the point source, respectively. The conditional variance of transverse flux $C_{q1q1}^{(2,0)}(\boldsymbol{x},\boldsymbol{x})$ is shown in Figure 6.19, and the cross-covariance $C_{q1q2}^{(2,0)}(\boldsymbol{x},\boldsymbol{x})$, which is equivalent to $C_{q2q1}^{(2,0)}(\boldsymbol{x},\boldsymbol{x})$, in Figure 6.20. There is an excellent agreement between the second-order and Monte Carlo results.

Figures 6.18-20 show that the point source does not have significant impact on $C_{q1q1}^{(2,0)}(\boldsymbol{x},\boldsymbol{x})$ and $C_{q1q2}^{(2,0)}(\boldsymbol{x},\boldsymbol{x})$, but it has significant effect on the conditional variance of longitudinal flux, $C_{q2q2}^{(2,0)}(\boldsymbol{x},\boldsymbol{x})$. The variance, $C_{q2q2}^{(2,0)}(\boldsymbol{x},\boldsymbol{x})$, starting from zero on the upper Neumann boundary, increases markedly near the point source. Unlike *Guadagnini and Neuman* (1999) who had found that conditioning tends to reduce the variance of longitudinal flux, here the effect of conditioning on this variance is mixed. For example, in Figure 6.18(C), there is a valley at conditioning point c3, but a peak at conditioning point c1.

The conditional variance of transverse flux (Fig. 6.19) is zero along the lateral, vertical no-flow boundaries, where transverse flux is prescribed to be zero. It is also zero on the bottom (the constant pressure head boundary) along which a same deterministic constant pressure head is prescribed at all nodes and so transverse flux is zero. The variance is reduced near conditioning point c3 (Fig 6.19C), but has a peak at conditioning point c1. The peak at c1 is not surprising if we recall from Figure 6.17A that near this point, the transverse flow changes dramatically. In fact, in any vicinity of this point, the flux may have a positive or negative horizontal component, which decreases the predictability of transverse flux at this point and thus the variance is large.

The term $C_{q1q2}(\boldsymbol{x},\boldsymbol{x})$ represents cross-covariance between transverse flux and longitudinal flux at a zero lag. Figure 6.20 shows that near conditioning point c1, it has a more-or-less symmetric pattern with respect to a vertical line passing through the middle of the domain, especially in the lower half of the domain. One possible reason for lack of symmetry in the upper half is that conditioning points c2, c3, and the point source are too close to each other to allow the formation of a clear pattern.

The conditional auto-covariance tensor of flux between all nodes and point P at the center of the grid are depicted in Figures 6.21-6.24. Each of these figures includes a contour map and two vertical profiles, one passing through a conditioning point and the other through the point source. Unlike the auto-covariance of flux with a zero lag ($\boldsymbol{x} = \boldsymbol{y}$), which is symmetric, $C_{q1q2}(\boldsymbol{x},\boldsymbol{y})$ is generally not equal to $C_{q2q1}(\boldsymbol{x},\boldsymbol{y})$ when $\boldsymbol{x} \neq \boldsymbol{y}$. The second-order moment solution of the conditional covariance tensor of flux is close to Monte Carlo results.

The auto-covariance of the longitudinal flux with reference to point P at the center of the grid, $C^{(2,0)}_{q2q2}(P,\boldsymbol{y})$, exhibits a peak at P and decays more-or-less monotonically with distance from P (Fig. 6.21). The rate of decay is slower in the longitudinal than in the transverse direction, where the covariance soon becomes negative. This implies that the correlation scale of longitudinal flux is longer in the longitudinal direction than in the transverse direction. Since we prescribe a constant flux along the upper Neumann boundary and a constant rate of injection at the point source, an increase in longitudinal flux at one point must cause a decrease at some other location along the same horizontal cross-section, which explains the negative covariance in the figure. The covariance of transverse flux with reference to point P, $C^{(2,0)}_{q1q1}(P,\boldsymbol{y})$, in Figure 6.22, also shows a sharp peak at P, together with a small negative peak downstream of it. The positive peak is elongated in the transverse direction, which means that the correlation scale of transverse flux is longer in the transverse direction than in the longitudinal direction. Both $C^{(2,0)}_{q2q2}(P,\boldsymbol{y})$ and $C^{(2,0)}_{q1q1}(P,\boldsymbol{y})$ are more-or-less symmetric with respect to horizontal and vertical lines passing through the reference point.

The contour map of $C^{(2,0)}_{q1q2}(P,\boldsymbol{y})$, which represents the cross-covariance between transverse flux at reference point P and longitudinal flux at other points, shows a more-or-less anti-symmetric pattern with respect to the vertical line passing through the reference point P (Fig. 6.23). Similar results have been found by *Rubin* [1990] for an unbounded saturated flow domain and by *Osnes* [1997] for a bounded saturated flow domain. Contours of $C^{(2,0)}_{q2q1}(P,y)$ in Figure 6.24, the cross-covariance between longitudinal flux at reference point P and transverse flux at other points, shows a somewhat similar pattern.

It should be noted that both the point source and conditioning points do not have significant effects on the pattern of the above covariance of the flux, except in the case of zero separation lag, i.e., the variance of flux.

6.3.3 Cross-covariance of Y and *q*

Figure 6.25 depicts the cross-covariance between Y and longitudinal flux with a zero separation distance, i.e., $C_{Yq2}(x,x)$, obtained from Monte Carlo simulation and our second-order solution, and Figure 6.26 shows the cross-covariance between Y and the transverse flux, $C_{Yq1}(x,x)$. Each of these figures includes a contour and two vertical profiles passing through a conditioning point and the point source, respectively. It is seen from these figures that the second-order solution is close to Monte Carlo results, even though the variability of the medium is high (σ_Y^2=2.0). The figures for $C_{Yq2}(x,x)$ illustrate some very interesting features (Fig. 6.25). First, this quantity is always negative. In fact, intuitively, any increase in Y at a point x tends to increase the flow rate at this point. Since the mean flow is downward (opposite to the vertical coordinate x_2 which is upward), an increase in flow rate implies that the flow rate becomes more negative. Thus the cross-covariance $C_{Yq2}(x,x)$ is negative. In addition, the value of the cross-covariance, starting from zero along the deterministic Neumann boundary (the upper boundary), increases gradually toward the lower boundary, except for areas near the point source or conditioning points. At the point source, the cross-covariance exhibits a sharp peak (Fig. 6.25C). At conditioning points, the cross-covariance is zero because there is no variability of Y at these points. The cross-covariance $C_{Yq1}(\boldsymbol{x},\boldsymbol{x})$ has a slightly different pattern (Fig. 6.26). Near the point source, instead of a sharp peak as seen for $C_{Yq2}(\boldsymbol{x},\boldsymbol{x})$, it exhibits one positive peak and one negative peak, i.e., an anti-symmetric pattern with respect to a vertical line passing through the source. The same is true at conditioning points (Fig. 6.26).

We also examined how the cross-covariance $C_{Yq2}(P,\boldsymbol{x})$ changes with various locations of point P (Figures 6.27B-F), where only the second-order solution is depicted, since it is very close to Monte Carlo results (not shown). In all these cases, $C_{Yq2}(P,\boldsymbol{x})$ shows a negative peak at the reference point P, which means that an increase in Y at point P will increase the magnitude of the longitudinal flux. The negative sign is due to our choice of vertical coordinate, which is opposite to the downward mean flow direction. Away from point P, $C_{Yq2}(P,\boldsymbol{x})$ decays rapidly with distance from P, especially in the transverse direction, where this drop is accompanied by a change of sign, as explained earlier.

Similar depictions of the cross-covariance between Y and transverse flux are shown in Figures 6.28B-F, most of which exhibit some degree of anti-symmetric behavior (positive on one side and negative on the other side). Take Figure 6.28F as an example, where reference point P is located in the center of the domain. Around point P, there are two positive peaks to its upper-left and lower-right and two negative peaks to its upper-right and lower-left. This can be explained as follows. For any increase in Y at point P, the flow on upstream side of the point tends to converge toward it, producing positive transverse components to its upper-left and negative transverse component to its upper-right. This yields a positive peak in the upper-left and a negative peak in the upper-right. The two peaks downstream of point P can be explained in a similar fashion.

6.4 FACTORS AFFECTING SOLUTIONS

In section 6.3 we illustrated that, compared to zero-order solutions, our second-order solutions are closer to Monte Carlo results, even when unconditional variance is as high as 2. Here, we discuss some factors that may affect our solutions. The factors considered include conditioning, type of boundaries imposed, and number of Monte Carlo simulations.

6.4.1 Effect of Conditioning Points

Consider a case, Case 2, the unconditional equivalent of Case 1. The unconditional ensemble mean log hydraulic field and auto-covariance have been shown in Figure 5-2. The results are presented in Figures 6.29-6.39. Although the second-order solution of mean pressure head is very close to the Monte Carlo results in both the conditional (Fig. 6.11) and unconditional (Fig. 6.29) cases, the zero-order solution is less closer. A comparison of Figure 6.12 (the conditional case) and Figure 6.30 (the unconditional case) shows that conditioning reduces the variance of pressure head and improves the quality of the second-order solution (i.e., the latter is closer to Monte Carlo results). Without conditioning, the variance of mean pressure head obtained from the second-order solution differs noticeably from Monte Carlo results. The unconditional mean flux fields obtained from zero-order, second-order and Monte Carlo solutions are illustrated in Figures 6.31-6.32. The unconditional solution of mean flux (Figs. 6.31-6.32) exhibits a very different pattern than does the conditional solution (Figs. 6.16-6.17). Though the second-order solutions for fluxes are superior to the zero-order solutions in both the conditional and unconditional cases, the zero-order solutions are nevertheless close to Monte Carlo results in both cases.

Figures 6.33-6.39 depict the (co)variance tensor of flux. In contrast to the variance of mean pressure head, our second-order solutions for (co)variance of mean flux are very close to Monte Carlo results, even without conditioning. Comparison between Figure 6.33 and Figure 6.18 (the variance of longitudinal flex) shows that the effect of conditioning on the variance of longitudinal flux is mixed. Comparing to the unconditional case, the variance is reduced around conditioning points c2 and c3, but around conditional point c1, the variance is much larger in the conditional case than in the unconditional case. Similar is true for the variance of transverse flux. This may be due to the effect of the point source.

To isolate the effect of conditioning, two numerical experiments have been conducted. In one experiment (Case 3), we considered a soil with $\langle Y \rangle = 0.0$, $\sigma_Y^2 = 1.0$, $\lambda = 1.0$, $\langle \beta \rangle = -1.0$, $\sigma_\beta^2 = 0.0$, and without any point source and conditioning points. The mean and variance of unconditional realizations of log hydraulic conductivity are shown in Figure 6.40. Case 4 is the same as Case 3, but there are four conditioning points as shown in Figure 6.41. Numerical results from these two experiments are illustrated in Figures 6.42-6.57.

Figure 6.42 compares mean pressure head computed from cases with and without conditioning points, where diagrams (A) and (C) show contours for unconditional and conditional cases, and diagrams (B) and (D) show vertical profiles identified in (A) and (C), respectively. Since there is no significant difference between mean pressure head computed from MC and second-order solutions when $\sigma_Y^2 = 1.0$, only the second-order solutions are plotted in Figure 6.42. Figure 6.42D includes two vertical profiles, one passing through two conditioning points, and the other through the middle of the domain. Conditioning has clearly changed the mean flow field considerably. A part of the flow field even becomes saturated, due to small values of hydraulic conductivity in the lower-right area (Fig. 6.40). The impact of conditioning on the variance of pressure head is illustrated in Figure 6.43, where the variance increases monotonically from bottom to top in the unconditional case (Fig. 6.43A-B), but it diminishes near conditioning points in the conditional case (Fig. 6.43C-D).

The effect of conditioning on conditional cross-covariances between log hydraulic conductivity at various locations and pressure head, $C_{Y\psi}$, are also examined (Figs. 6.44-6.45). It is seen that conditioning generally reduces the magnitude of the cross-covariance $C_{Y\psi}$. The cross-covariance is a measure of how well one can predict one variable, given information about the other. More specifically, $C_{Y\psi}$ is a measure of how an increase in Y at one point affects pressure head at other points. In the conditional case, the effect of knowing of hydraulic conductivity at any particular point on pressure head prediction is less than in the unconditional case, because hydraulic conductivity date are given at conditioning points. Therefore, the cross-covariance is lower in the conditional case than in the unconditional case. Figures 6.44-45 also show that log hydraulic conductivity and pressure head may be positively or negatively correlated in the conditional case, while in the unconditional case, they are always negatively correlated.

The mean longitudinal and transverse fluxes derived from unconditional and conditional cases (Case 3 and Case 4) are shown in Figures 6.46-47. Each of these figures includes contours for unconditional and conditional cases as well as scatter plots showing comparisons between Monte Carlo, zero- and second-order solutions. Although our second-order solutions are superior to zero-order solutions in all cases, the zero-order solutions are very close to Monte Carlo results in the conditional case (Figs. 6.46E-F, 6.47E-F), but much less so in the unconditional cases (Figs. 6.46B-C, 6.47B-C). This implies that zero-order mean flux may be accurate enough when conditioning points are available. In addition, as discussed in Section 6.3, conditioning has a visible impact on the flow pattern. The mean flux (especially the mean transverse flux) is controlled largely by conditioning points (Fig. 6.47D). Without conditioning, the flow rate is more-or-less uniform and close to that prescribed at the Neumann boundary, as shown in Figures 6.46A-C and 6.47A-C. In the conditional case, however, there may be divergent or convergent flow around conditioning points.

Figures 6.48-6.49 suggest that conditioning reduces uncertaintites of flux predictions. Figure 6.48 compares the variance of longitudinal flux for both unconditional and conditional cases (Cases 3 and 4), where (A) and (C) are contours for unconditional and conditional cases, respectively, and (B) and (D) are vertical profiles indicated in their corresponding contour maps (A) and (C), respectively. The profile A-A' in Figure 6.48D passes through two of the conditioning points, and the other through the middle of the flow domain. The figure indicates that conditioning does not change the overall pattern but reduces the variance of longitudinal flux locally around conditioning points. In fact, at all conditioning points, the contour map shows valleys (Fig. 6.48C-D). The same holds for transverse flow (Fig. 6.49).

Covariance of flux has been discussed by many researchers, but most of these studies are only applicable to saturated flow in unbounded statistically isotropic domains. *Rubin* [1990] derived analytical expressions of unconditional velocity covariances in a two-dimensional statistically isotropic domain of infinite extent under uniform mean flow and concluded that the variance of longitudinal flux is three times as large as the variance of transverse flux. Additional analytical expressions for two- or three-dimensional statistically isotropic domains were given by *Rubin and Dagan* [1992], *Zhang and Neuman* [1992], *Hsu* et al. [1996], and *Hsu* [1999]. *Osnes* [1997] presented expressions for velocity covariance in a bounded domain. In unsaturated flow, *Russo* [1993, 1995] derived expressions for velocity covariance in an unbounded domain under a mean uniform hydraulic gradient.

Simple calculation for the unconditional case shows that our results are smaller than values calculated from Rubin's expressions. For example, in the central part of the domain (where the effect of boundaries is minimum), the second-order approximation $C_{q2q2}(\boldsymbol{x}, \boldsymbol{x}) \cong 0.06$, $C_{q1q1}(\boldsymbol{x}, \boldsymbol{x}) \cong 0.015$, thus the ratio of longitudinal velocity variance to transverse velocity variance, which is equivalent to the ratio of the corresponding flux variances, is approximately equal to 4, not 3 as predicted by Rubin's expressions. The discrepancy is mainly due to the boundary effect. For instance, since $C_{q1q1}(\boldsymbol{x}, \boldsymbol{x})$ is zero at lateral boundaries and the lower boundary, its values in whole domain are small in the cases of relatively small domain. In fact, for large domain, our data fit Rubin's expressions quite well (next section).

The auto-covariance of flux has been examined for both unconditional and conditional cases (Case 3 and 4), and results are displayed in Figures 6.50-53. Figure 6.50 depicts the auto-covaraince of the longitudinal flux between a fixed point at the center of the domain and all other points. The magnitude of the auto-covarince is seen to be reduced by conditioning. In addition, unlike the unconditional case where the peak is at the reference point, in the conditional case the peak is shifted slightly away from the reference point. This is also true for the covariance of the transverse flux (Fig. 6.51).

Several authors have noticed that the flux covariance exhibits anisotropy (i.e., the correlation scale of the flux variance varies with the angle from the mean flow direction) in two-dimensional [*Rubin*, 1990; *Shapiro and Cvetkovic*, 1990; *Osnes*, 1997] and three-dimensional [*Shapiro and Cvetkovic*, 1990] saturated flow. It seems that our results do not support *Russo*'s [1993] conclusion that, under unsatuared conditions, the auto-correlation scale of the velocity covariance (equivalent to flux covariance) is not sensitive to the angle from the mean flow direction. In fact, the auto-covariances of longitudinal and transverse flux exhibit anisotropy under both unconditional and conditional cases, as shown in Figures 6.50-51. Anisotropy of the flux auto-convariance is strongly influenced by boundaries, suggesting that *Russo*'s [1993] conclusion may be valid only for unbounded domains.

The cross-covariance $C_{q1q2}(\boldsymbol{x}, \mathrm{P})$ between longitudinal and transverse flux at a reference point P, located at the center of the domain, are illustrated in Figure 6.52 for unconditional (A-C) and conditional cases (D-F). The figure includes two contours for unconditional and conditional cases, and cross-sections along two diagonal lines of each contour map (dashed curves represent second-order solutions). Compared to the unconditional case, the cross-covariance $C_{q1q2}(\boldsymbol{x}, \mathrm{P})$ for the conditional case is smaller in magnitude, especially near conditioning points. Compared to the unconditional case where the contour map shows a more-or-less anti-symmetric pattern with respect to a vertical line and a horizontal line passing through reference point P, in the conditional case, symmetry is less obvious. Even when it shows some kind of symmetry, the symmetry is not with respect to point P but some other point shifted away from point P (Figs. 6.52D, 6.53D).

We also examined the cross-covariance between flux and log hydraulic conductivity at various points in the domain for both unconditional and conditional cases, as shown in Figures 6.54-6.57, where the first diagram in each figure is the cross-covariance of flux and Y with zero lag distance. These figures indicate that conditioning does not have a significant impact on the cross-covariances C_{Yq1} and C_{Yq2}, except at zero lag. It appears that this observation contradicts our previous finding which states that conditioning has impact on cross-covariance between pressure head and Y. One possible explanation is that, even though increasing Y at one point (say P1) may cause an increase or a decrease in pressure head at other point (say P2), it does not necessarily cause a change in hydraulic gradient at P2 and therefore the flux may not be affected.

6.4.2 Effect of Boundary Types

To illustrate the possible effect of boundary type on solutions, we ran two cases with unconditional realizations (2,000 realizations with unconditional mean $\langle Y \rangle$=1.0, σ_Y^2=0.5, λ=1.0.) of log hydraulic conductivity fields that yield the mean and auto-covariance, as shown in Figure 6.58. In Case 5, we imposed impermeable boundaries on both lateral (vertical) sides, and prescribed deterministic pressure head on both the lower boundary and at the upper boundary. In Case 6, we replaced the prescribed pressure head at the upper boundary in Case 5 by a prescribed deterministic flux. The major difference between Case 6 and the previous unconditional case (Case 3) is that the domain size is doubled in Case 6. To isolate effect of boundary types, there are neither conditioning points nor point sources in Cases 5 and 6. Strictly speaking, one may need to run Case 5 to find the mean flux at the top boundary and impose this flux as the prescribed flux for Case 6, or run Case 6 to obtain mean pressure head at the top boundary and impose it as prescribed pressure head for Case 5. However, this is not necessary, since we are concerned only with the general pattern of mean flow and associated (co)variances for different boundary types. The results from these two runs are shown in Figures 6.59-70. Each of these figures shows contour maps and vertical profiles along the middle of the domain. There is a noticeable discrepancy between pressure head from the zero-order and MC solutions in Case 6 (Fig. 6.59C-D), in Case 5, however, the zero-order pressure head is very close to MC results (Fig. 6.59A-B). This may stem from the fact that the variability of pressure head is much smaller when pressure heads are prescribed on both the upper and lower boundaries (Fig. 6.60A-B). In either case, the second-order solution is almost identical to MC results. Unlike Case 6 where the variance of pressure head increases with elevation (Fig. 6.60C-D), the variance of pressure head in Case 5 increases from the bottom, reaches a maximum and then decreases to zero at the upper boundary (Fig. 6.60A-B). Even though the zero-order mean pressure head in Case 5 is very close to that of MC, the zero-order mean flux is different from that of MC, as shown in Figures 6.61B-C, where Figure 6.61B is a vertical profile passing through the middle of the domain and Figure 6.61C is a scatter plot of zero-order solution against MC results. This may be due to the fact that zero-order mean flux is calculated from zero-order mean pressure head, while the mean flux of MC simulations is computed from the flux of all realizations, not directly from the averaged pressure head of MC results. Another reason is that a small difference in pressure head may cause a relatively large gradient (due to small grid size) and thus the difference is magnified in terms of flux. In either case, flux computed from second-order solutions is closer to that obtained from MC than computed from zero-order solutions (Fig. 6.61-64).

The variance of flux is depicted in Figures 6.65-66. As we mentioned previously, due to significant boundary effect, the variance of flux does not fit Rubin's expressions for our cases with a small domain. For the current numerical examples, our simple calculation shows that Rubin's expressions are more-or-less applicable for large domain. In Case 6, for example, the second-order approximation of $C_{q2q2}(\boldsymbol{x}, \boldsymbol{x})\cong 0.075$, and $C_{q1q1}(\boldsymbol{x}, \boldsymbol{x})\cong 0.025$, thus the ratio of the longitudinal velocity variance to the transverse velocity variance (equivalent to the ratio of corresponding flux variances) is approximately equal to 3, as predicted by his expressions. Figures 6.65-66 also indicate that the effect of boundaries on the velocity covariance extends across about one correlation scale, which means that expressions for unbounded domain may be applicable for an area that is several correlation scales away from the boundary.

Figure 6.67 compares the auto-covariance between longitudinal flux at reference point P in the center of the domain for Case 5 and Case 6. Since magnitudes of mean longitudinal fluxes in these two cases are different from each other, we may need to normalize them by the square of their mean longitudinal fluxes, respectively. For example, the normalized peak value in Case 6 (Fig. 6.67D) is $0.054/0.5^2=0.216$, and the normalized peak value in Case 5 (Figure 6.67B) is $0.009/0.14^2=0.46$. Other cross-covariance terms of flux components are illustrated in Figures 6.68-70. One conclusion we can draw from these figures is that the cross-covariance of flux computed from second-order solutions is closer to MC results in Case 6 than in Case 5.

6.4.3 Effect of Number of Monte Carlo Simulations (NMC)

As we mentioned in Chapter 1, there are no rigorous criteria to determine if Monte Carlo simulations converge or not. Even if they converge to a solution, it may not converge to the true solution of the problem. Intuitively, one way to check the convergence of Monte Carlo simulations is to plot quantities of interest (such as pressure head, flux and their variances) at any given point over the number of Monte Carlo simulations. Figure 6.71 shows mean pressure head, longitudinal flux, variance of mean pressure head, and variance of longitudinal flux for Case 1 over the number of Monte Carlo simulations at two points (x_1=2.0, x_2=2.0; and x_1=2.0, x_2=6.0). The figure shows that solutions for mean pressure head and mean longitudinal flux stabilize at NMC = 2000, but relatively large fluctuations are observed for the variance of mean pressure head and the variance of the longitudinal flux at NMC = 2000. These quantities seems to stabilize when NMC = 3000. We also examined the effect of heterogeneity (variance of log hydraulic conductivity) on the convergence of Monte Carlo simulations. Figure 6.72 depicts mean pressure head, longitudinal flux, variance of mean pressure head, and variance of longitudinal flux over the number of Monte Carlo simulations at (x_1 = 1.1, x_2 = 1.1) and (x_1 = 1.1, x_2 = 3.1), for Case 4, i.e., the conditional case with σ_Y^2 = 1.0, λ = 1.0, $\langle\beta\rangle$ = -1, σ_β^2 = 0.0. For comparison, the similar cases with variance σ_Y^2 = 0.1 and σ_Y^2 = 2.0 are plotted in Figures 6.73 and 6.74, respectively. Comparison between Figures 6.72-74 indicates that high heterogeneity usually requires more realizations to render the solution stable. However, there are several problems with this technique. First, Monte Carlo simulations converging at some points do not guarantee convergence at all points in the domain. In addition, different quantities may have different rates of convergence. Furthermore, when variances are our concern, the number of Monte Carlo simulations required for convergence will be much larger. It takes many more realizations to make variances converge even when the mean is stable.

The second-order solutions presented so far are based on ensemble mean and covariance of log hydraulic conductivity derived from generated realizations, and our comparisons between Monte Carlo simulations and the second-order solutions are consistent in this sense. As we said earlier, one of merits in our approach is to avoid generating random realizations. However, one question remaining is whether our second-order solutions obtained from these ensemble quantities, with increase of the number of realizations, converge to the solutions with soil properties inferred from measurements, instead of from generated realizations. For this purpose, we designed three cases and generated 5,000 unconditional realizations of log hydraulic conductivity fields with $\langle Y \rangle = 1.0$, $\sigma_Y^2 = 0.5$. Parameter β is taken as $\langle \beta \rangle = -1.0$, $\sigma_\beta^2 = 0.0$. In the first case, we use mean Y and C_Y calculated from the first 2,000 realizations as input to our nonlocal recursive equations. In the second case, all 5,000 realizations are used to obtain mean Y and C_Y. Lastly, we use analytical values for Y and C_Y, i.e., $\langle Y \rangle$=1.0 and C_Y computed using (6-1). For all these cases, deterministic constant pressure head is imposed at the bottom, impermeable boundaries on both sides, and deterministic constant flux at the top. The second-order solutions from these cases are compared in Figures 6.75-78, which show that these solutions are very close.

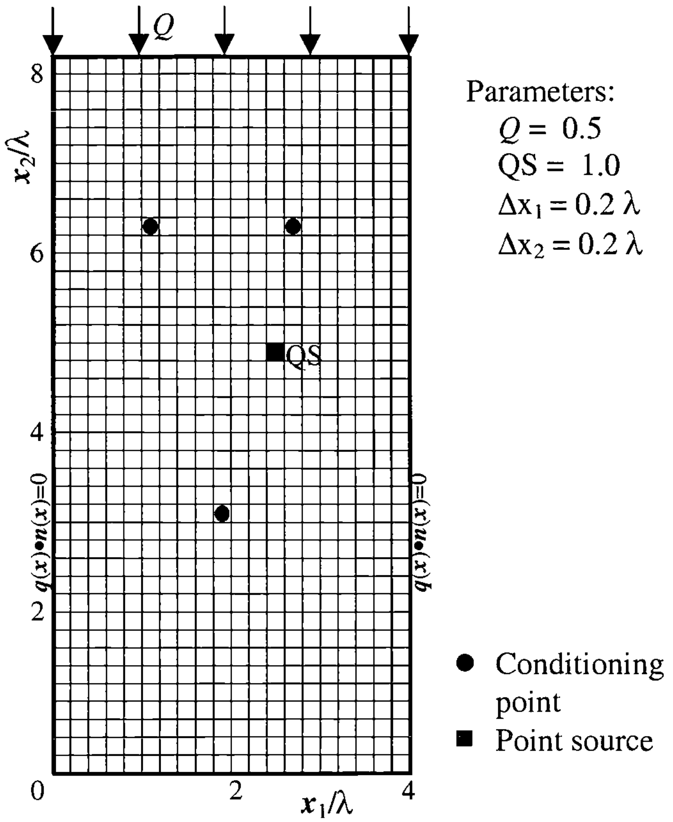


Figure 6.1. Problem definition, associated grid, and soil properties for Case 1.

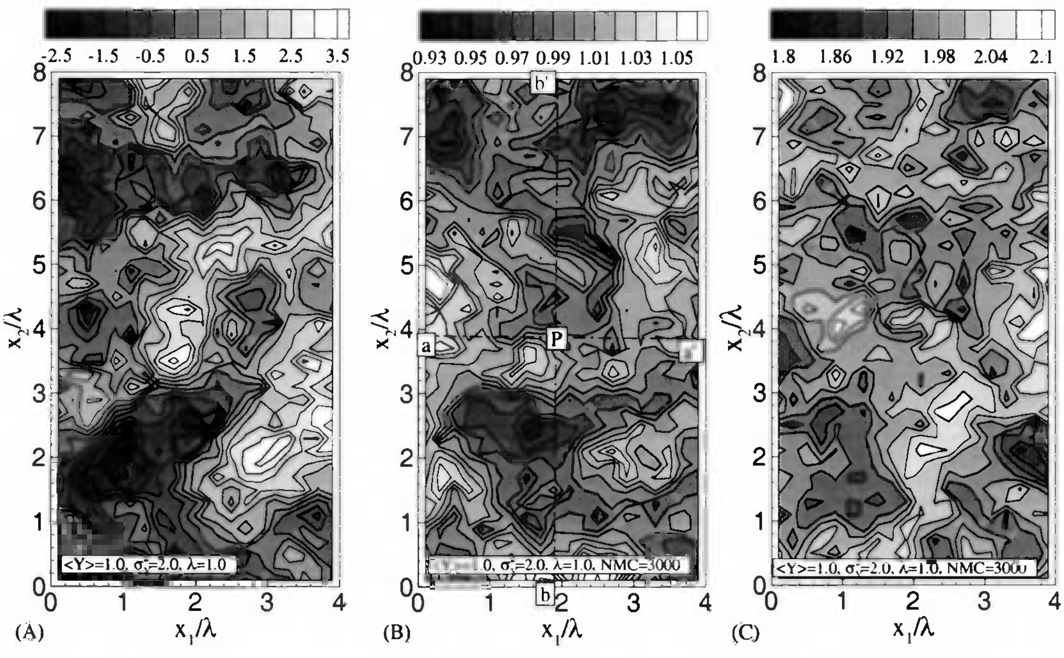


Figure 6.2. Images of (A) a single unconditional realization of Y, (B) unconditional ensemble mean $\langle Y(\boldsymbol{x})\rangle$, and (C) unconditional variance $\sigma_Y^2(\boldsymbol{x})$. (B) and (C) are obtained from 3000 Monte Carlo unconditional simulations with unconditional mean $\langle Y\rangle$=1.0, variance σ_Y^2=2.0, and λ=1.0.

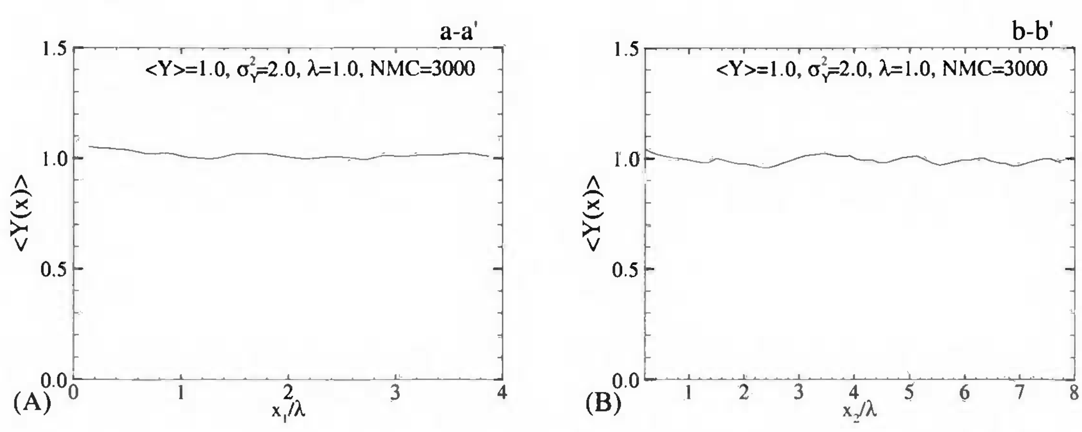


Figure 6.3. Cross-sections of unconditional mean $\langle Y(\boldsymbol{x})\rangle$ along horizontal profile a-a' and vertical profile b-b' identified in Figure 6.2.

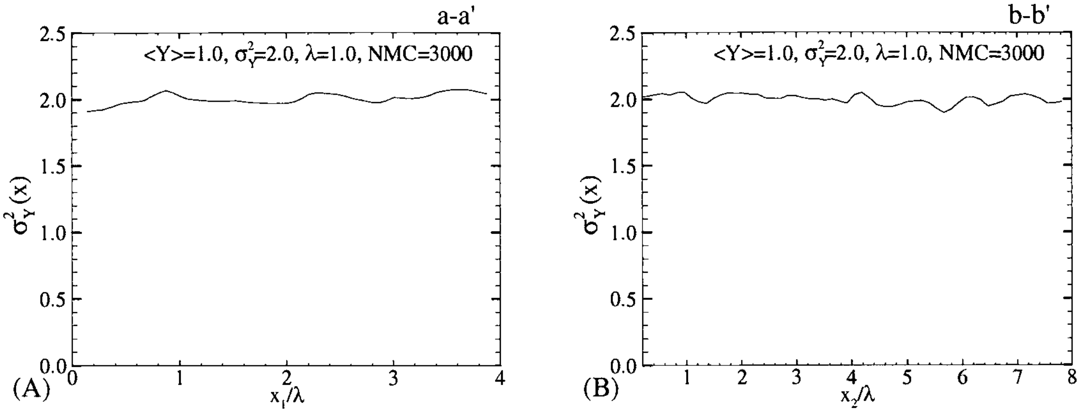


Figure 6.4. Cross-sections of unconditional variance $\sigma_Y^2(x)$ along horizontal profile a-a' and vertical profile b-b' identified in Figure 6.2.

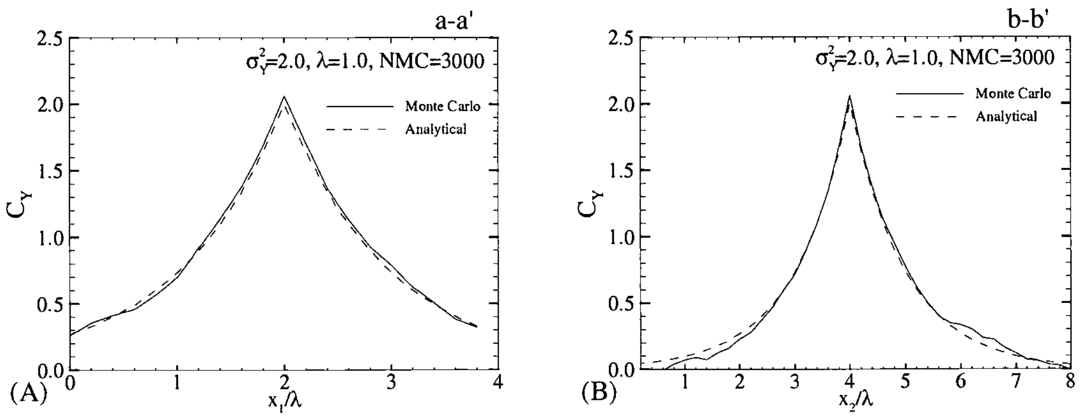


Figure 6.5. Auto-covariance between Y at reference point P and Y at points along horizontal and vertical sections identified in Figure 6.2.

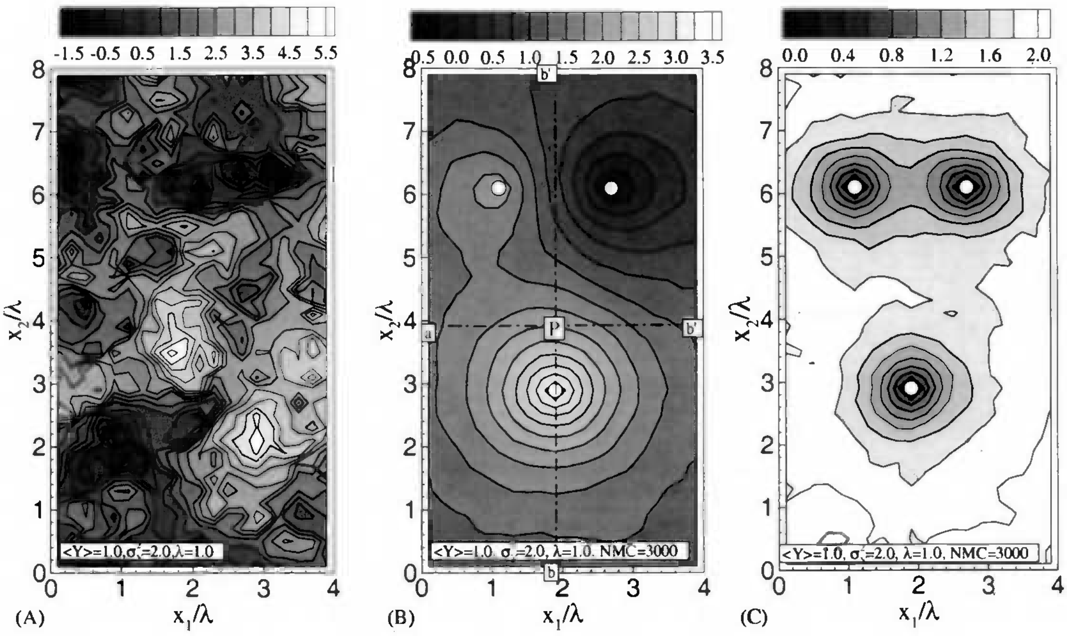


Figure 6.6. Images of (A) a single conditional realization of Y, (B) conditional ensemble mean $\langle Y(\boldsymbol{x})\rangle$, and (C) conditional variance $\sigma_Y^2(\boldsymbol{x})$. (B) and (C) are obtained from 3000 conditional Monte Carlo simulations with unconditional mean $\langle Y\rangle$=1.0, variance σ_Y^2=2.0, and λ=1.0.

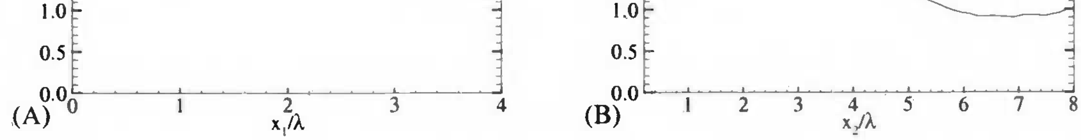


Figure 6.7. Cross-sections of conditional mean $\langle Y(\boldsymbol{x})\rangle$ along horizontal profile a-a' and vertical profile b-b' identified in Figure 6.6.

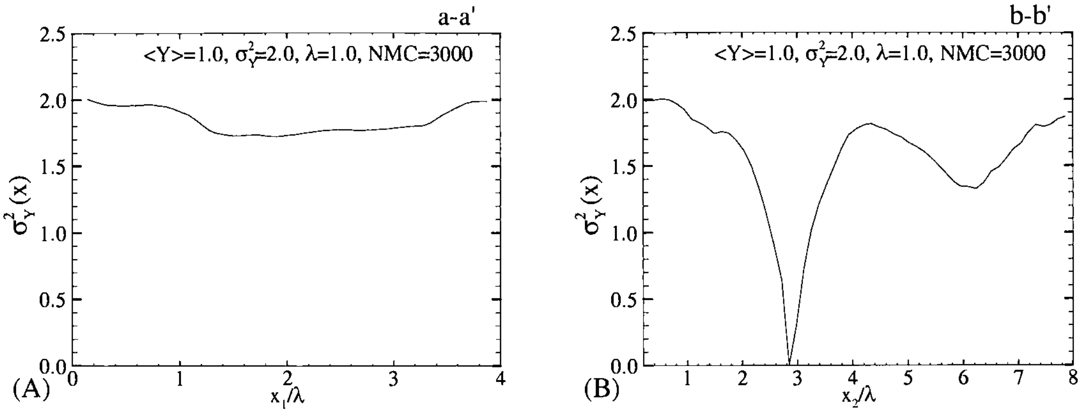


Figure 6.8. Cross-sections of conditional variance $\sigma_Y^2(x)$ along horizontal profile a-a' and vertical profile b-b' identified in Figure 6.6.

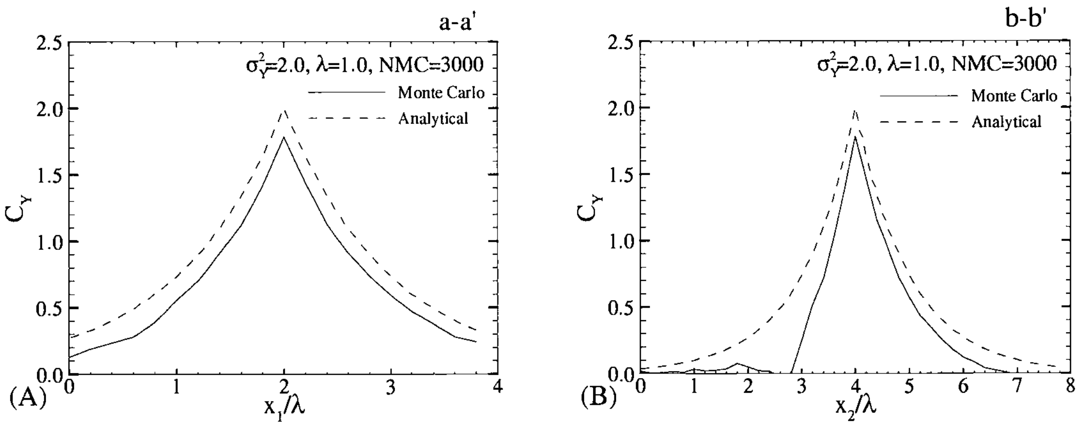


Figure 6.9. Conditional auto-covariance between Y at reference point P and that at points along horizontal and vertical sections identified in Figure 6.6.

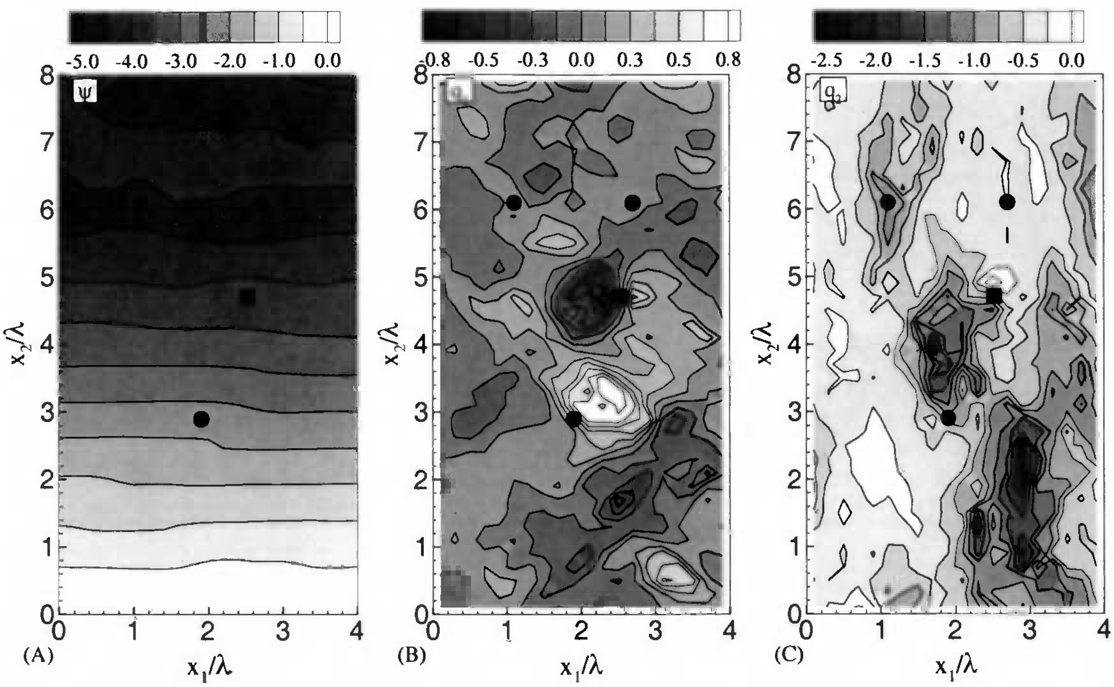


Figure 6.10. Images of (A) pressure head; (B) transverse flux; and (C) longitudinal flux, corresponding to the single conditional realization of Y presented in Figure 6.6.

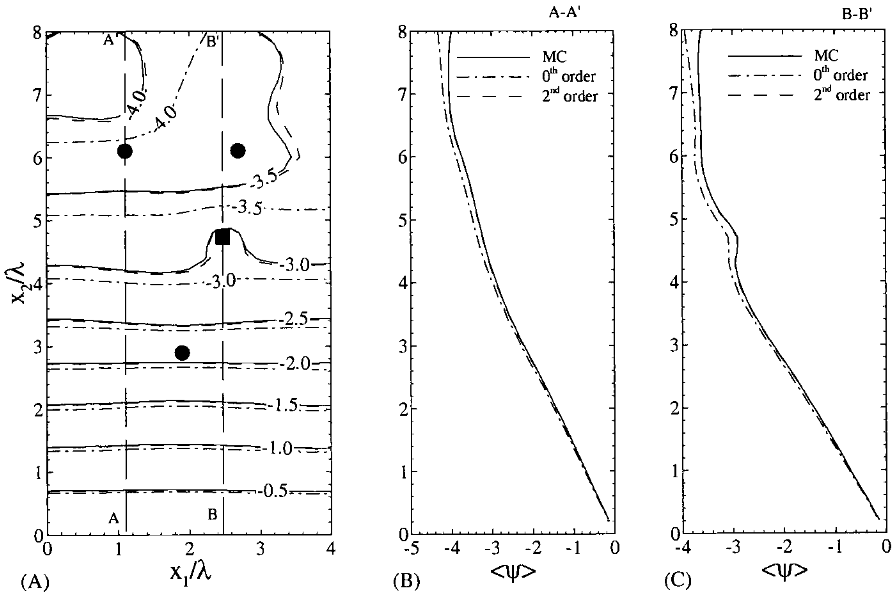


Figure 6.11. Mean pressure head obtained from Monte Carlo simulations (MC), zero-order and second-order solutions for Case 1. (A) A contour map; (B) vertical profile passing through a conditional point; and (C) vertical profile passing through the source.

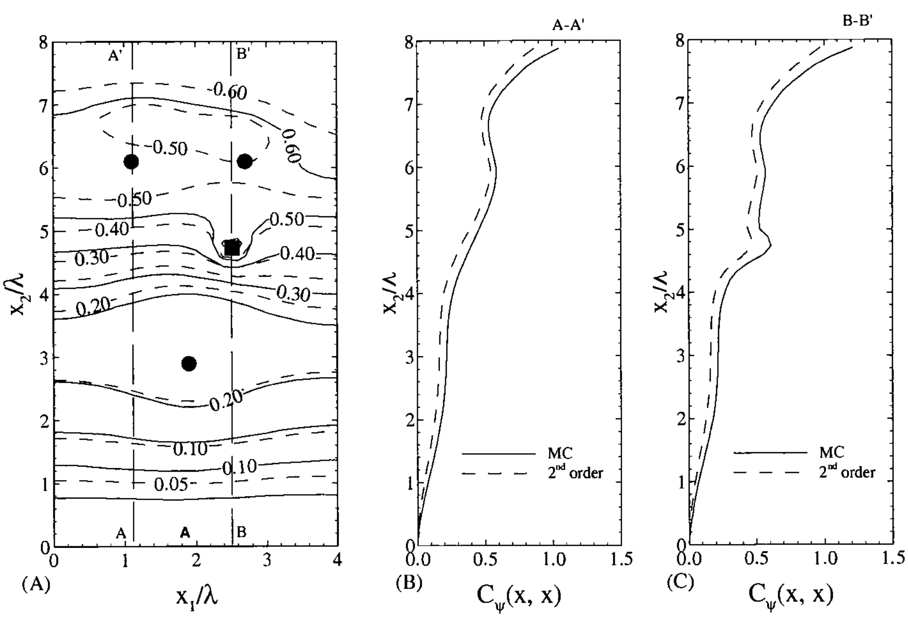


Figure 6.12. Variance of pressure head computed from MC, zero- and second-order solutions for Case 1. (A) A contour map; (B) vertical profile passing a conditional point, and (C) vertical profile passing the source.

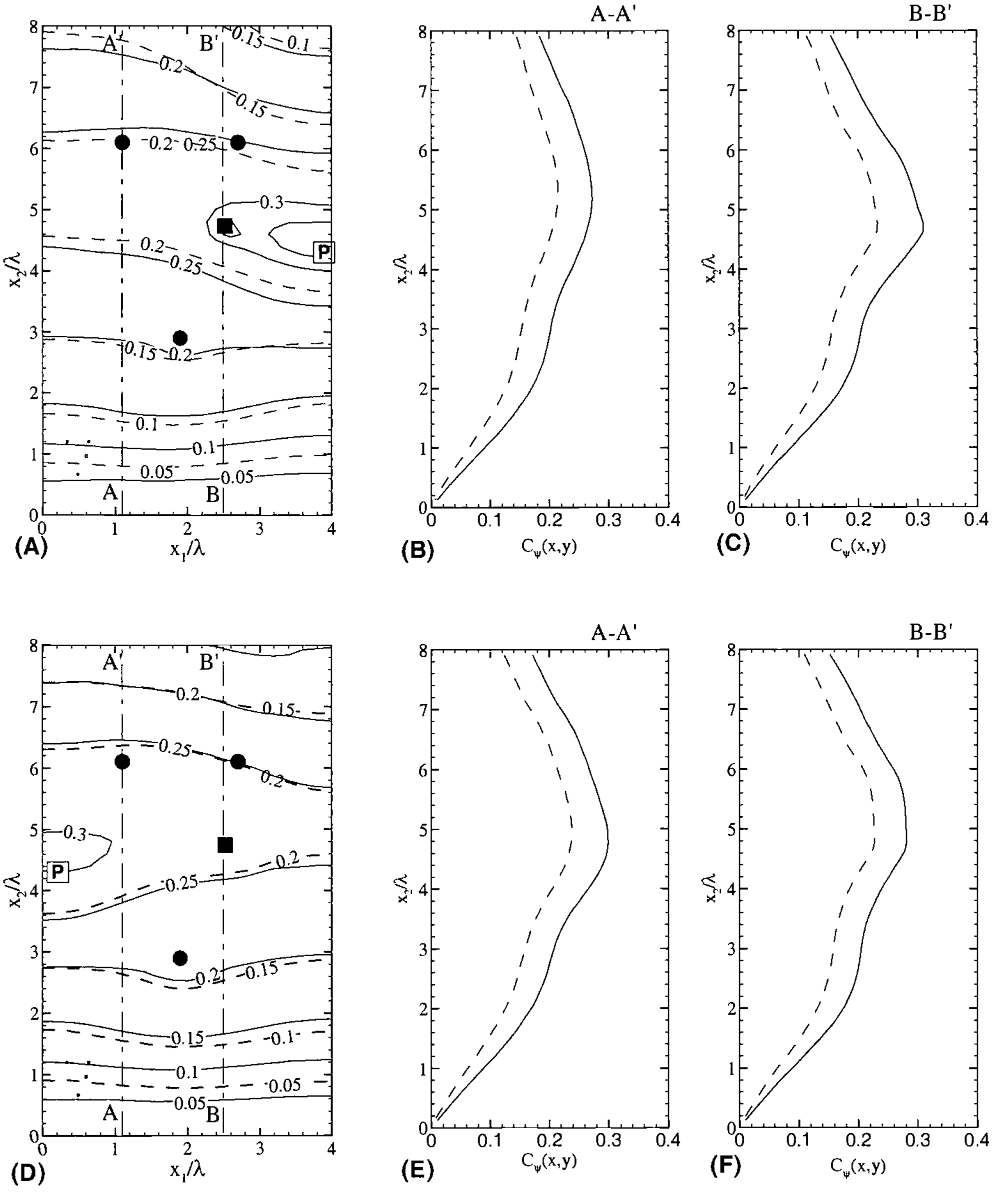


Figure 6.13. Conditional covariance function $C_\psi(\boldsymbol{x}, \boldsymbol{y})$ between ψ at all nodes and ψ at various reference points P for Case 1. The first diagram in each row is a contour map and the others are vertical profiles identified in the first diagram.

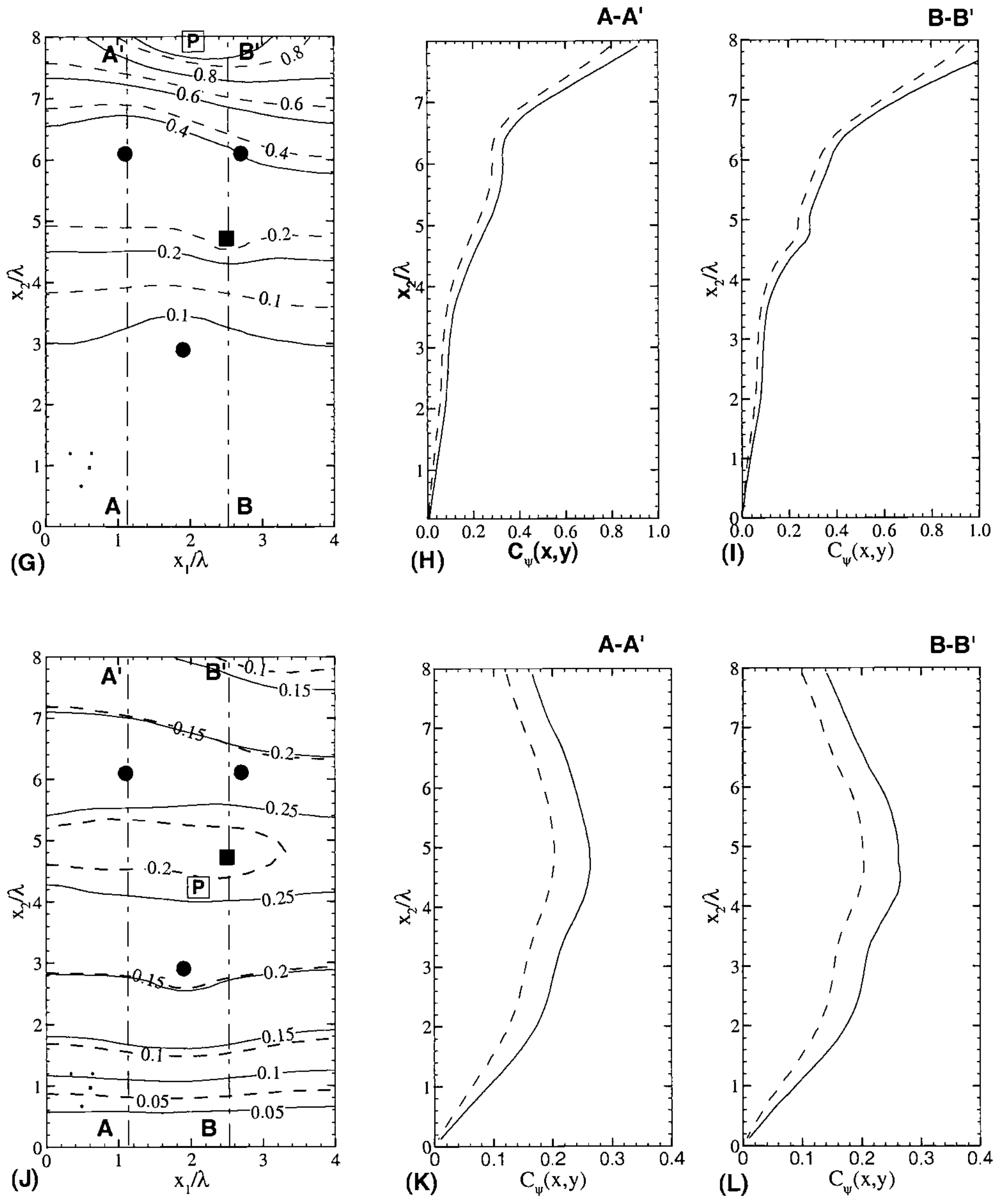


Figure 6.13 Continued

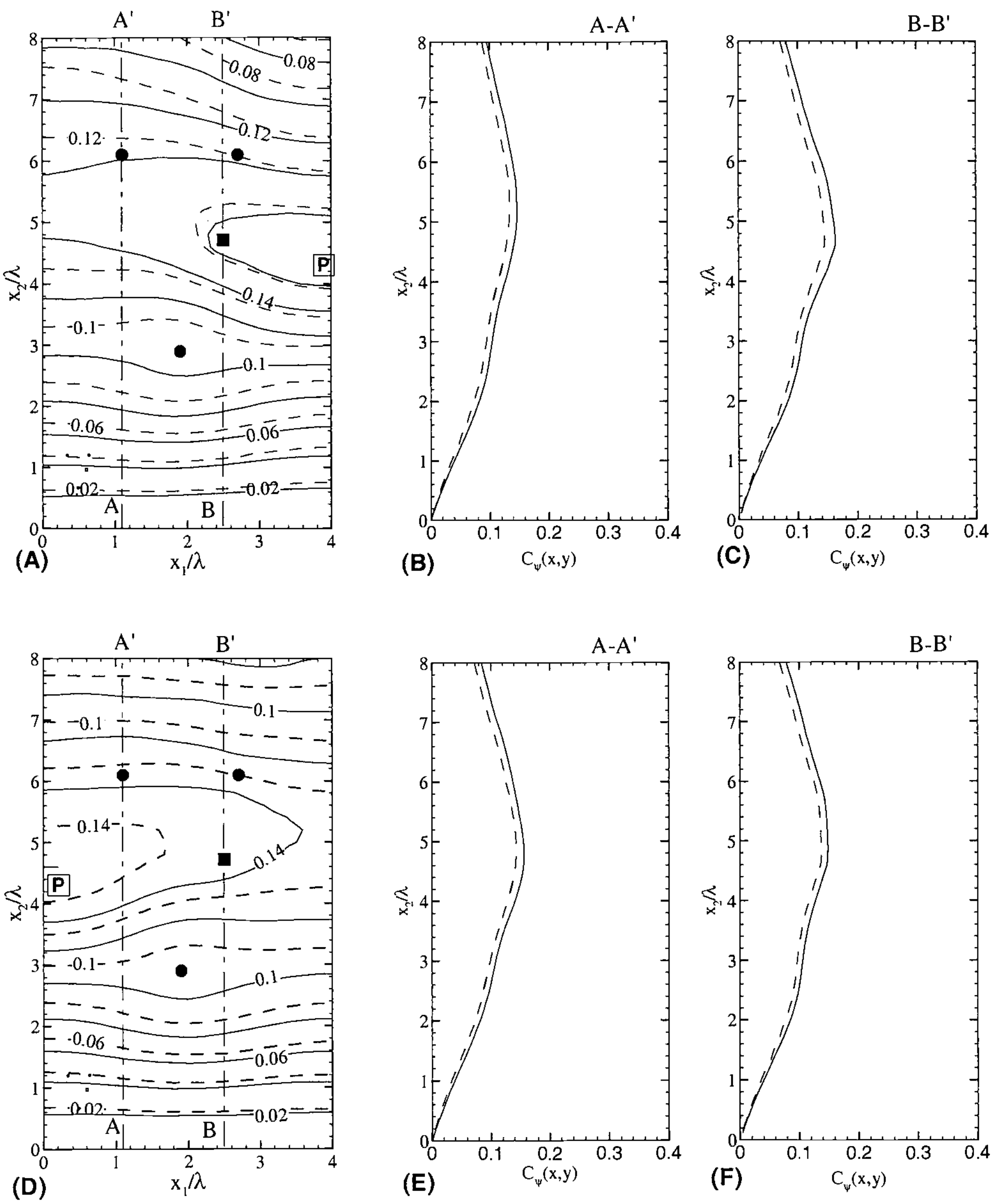


Figure 6.14. Conditional covariance function $C_\psi(x, y)$ between ψ at all nodes and ψ at various reference points P. All parameters and symbols are the same as those in Figure 6.13 except for $\sigma_Y^2=1.0$.

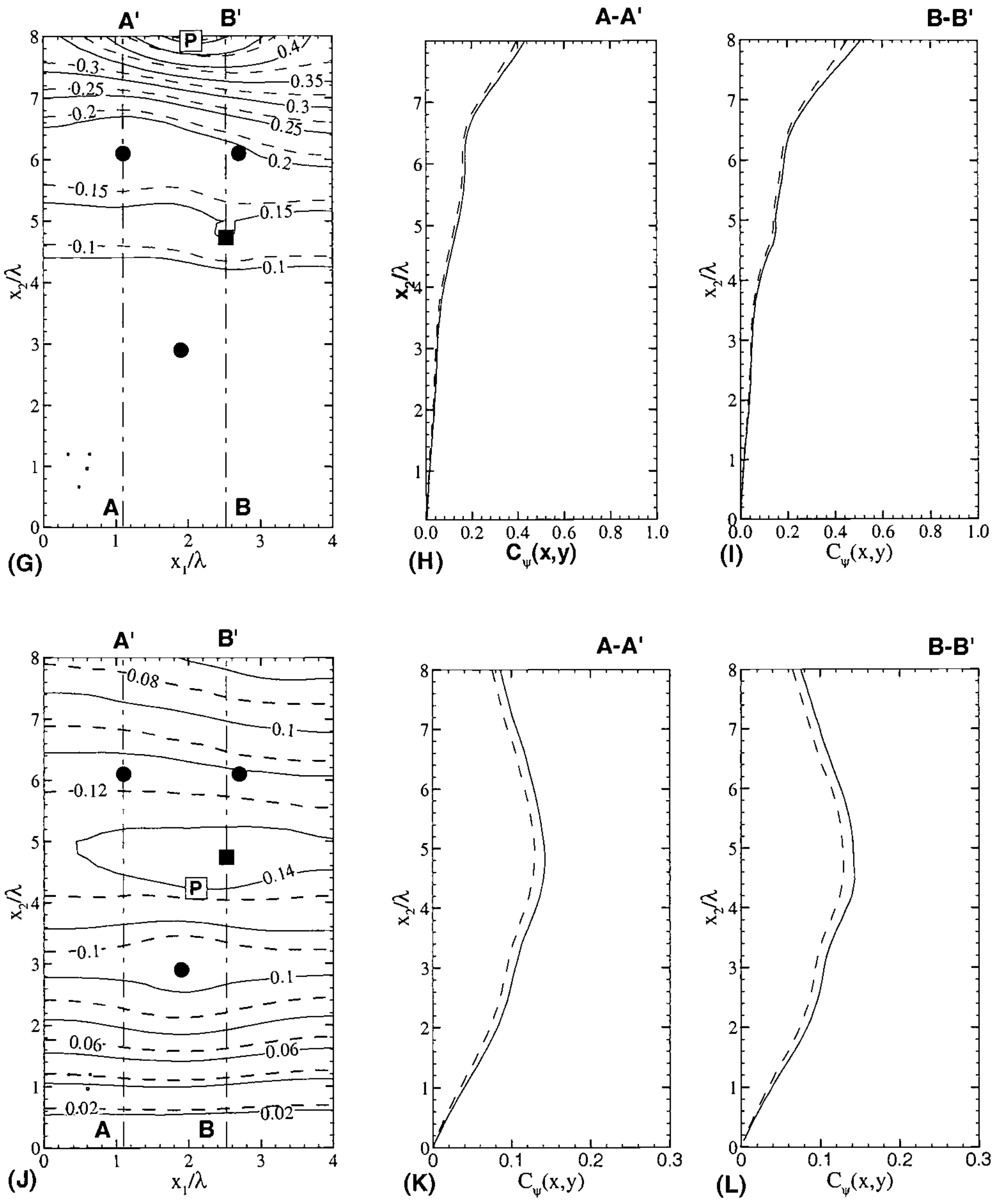


Figure 6.14. Continued.

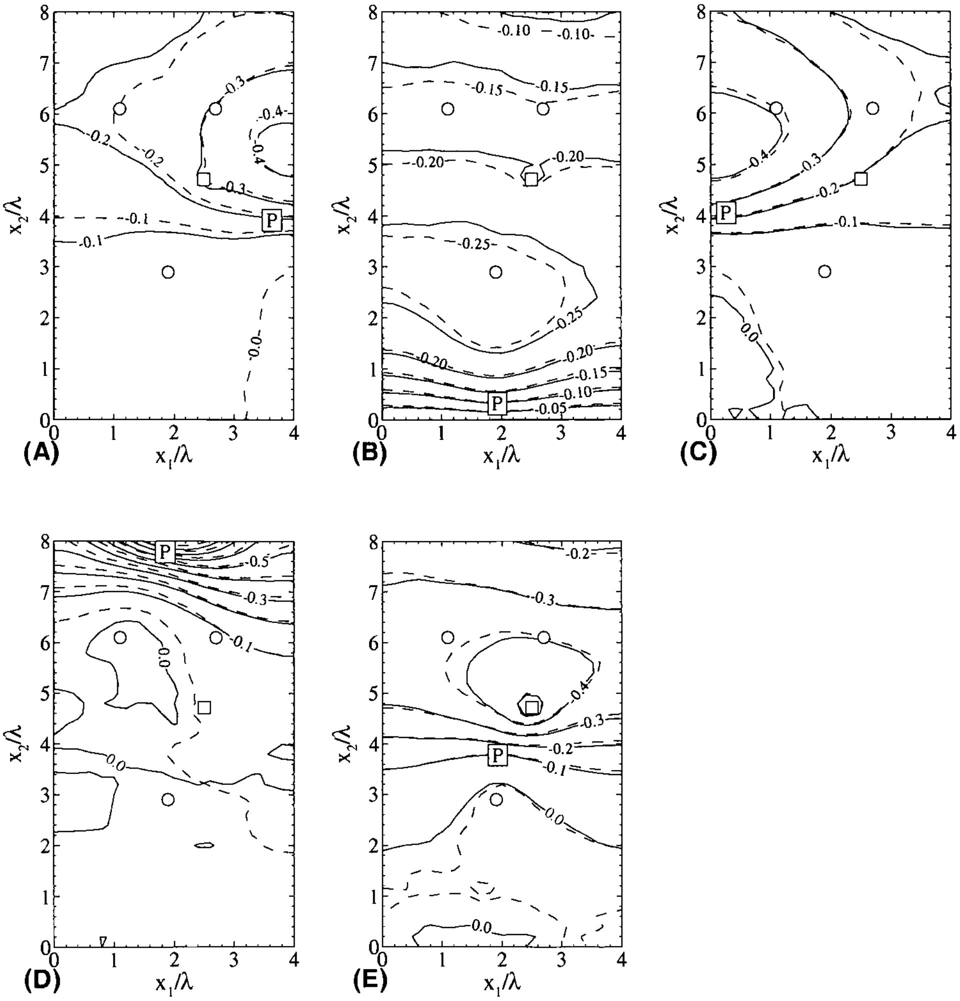


Figure 6.15. Cross-covariance between Y in various elements P and pressure head at all nodes, computed from MC (solid lines) and second-order nonlocal solutions (dashed lines) for Case 1.

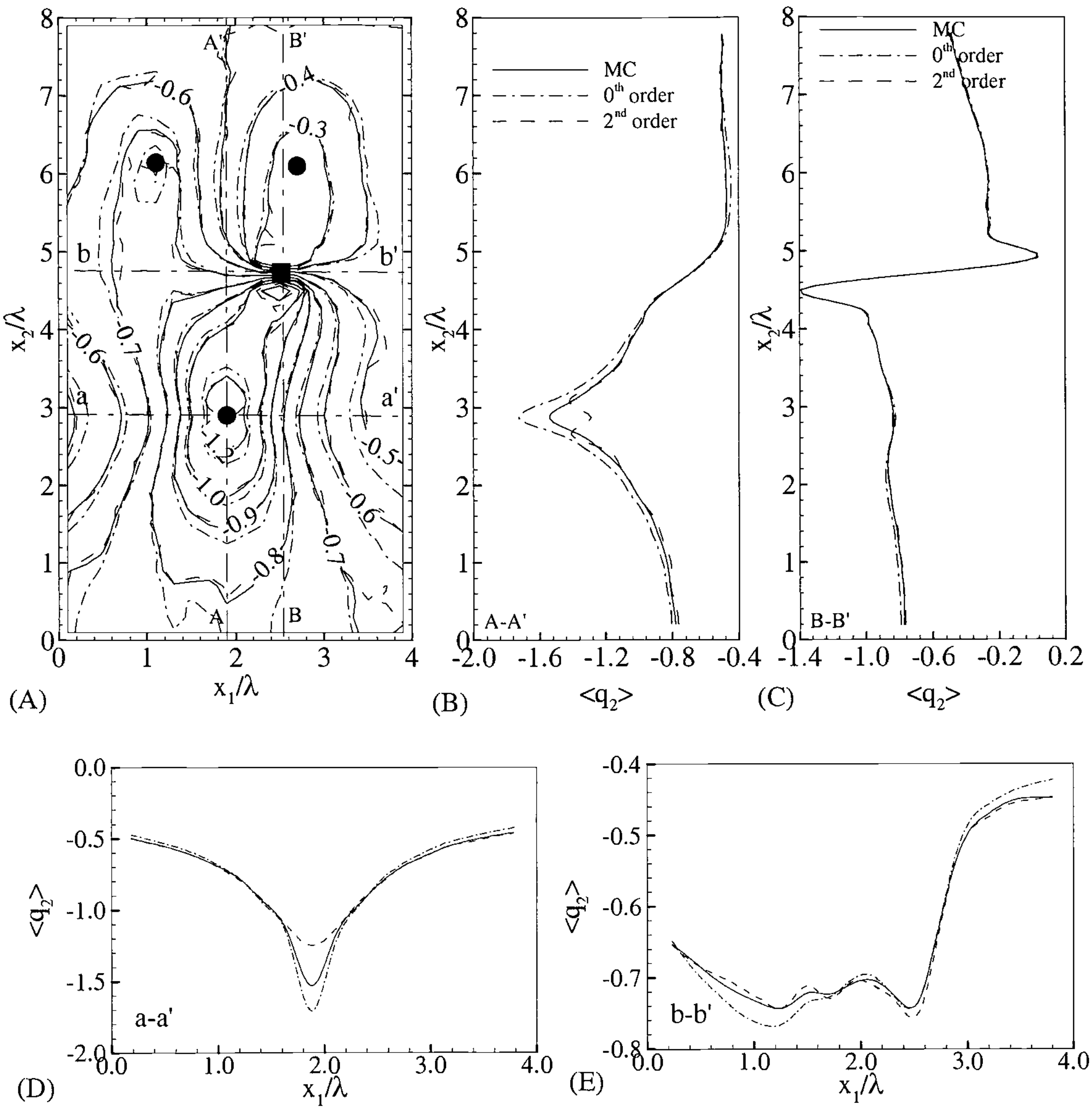


Figure 6.16. Mean flux in the longitudinal direction (x_2) using three solution methods in Case 1. Contour map (A) and various cross sections identified in (A).

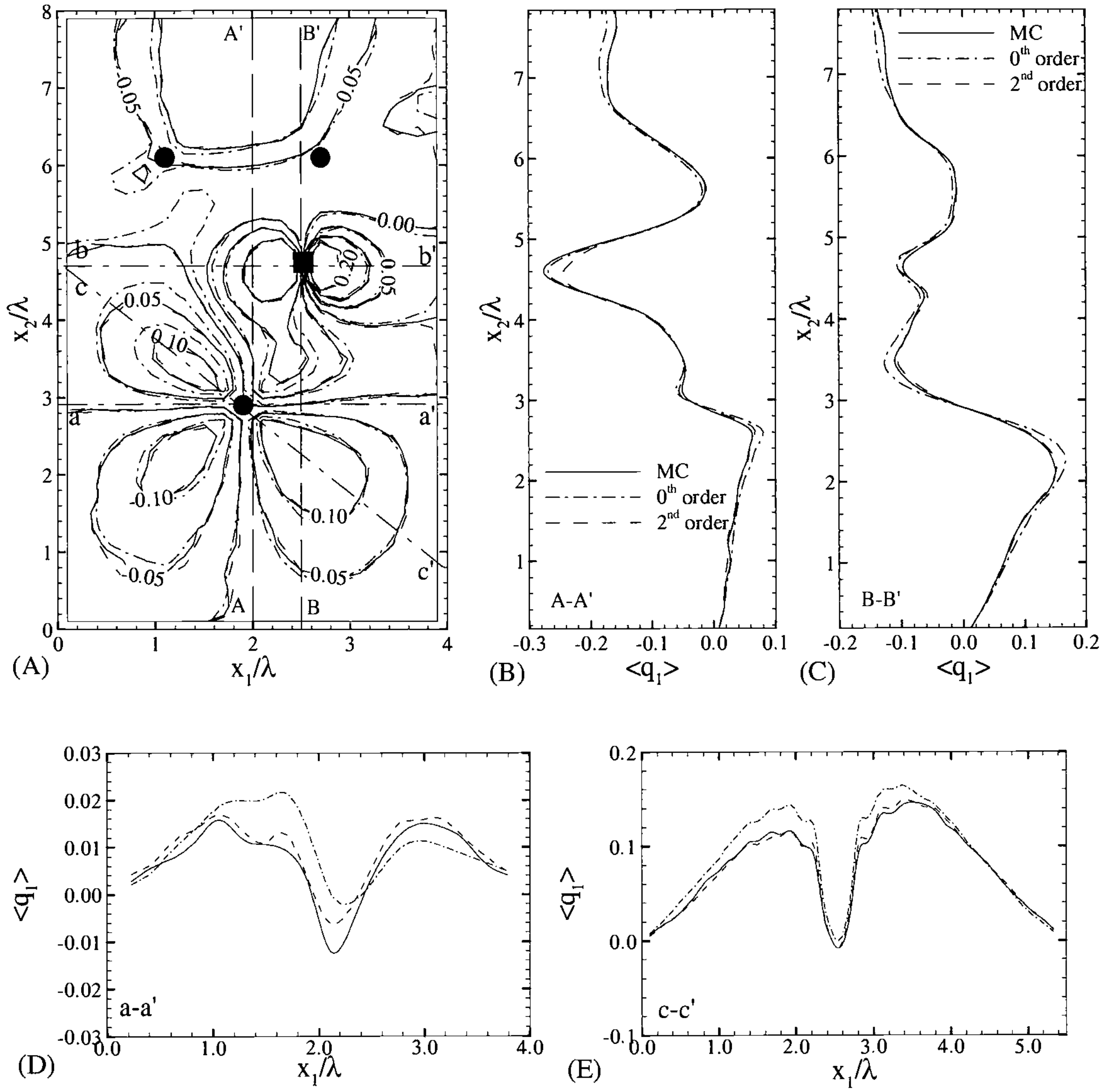


Figure 6.17. Mean flux in the transverse direction (x_1) using three solution methods in Case 1. Contour map (A) and four cross-sections identified in (A).

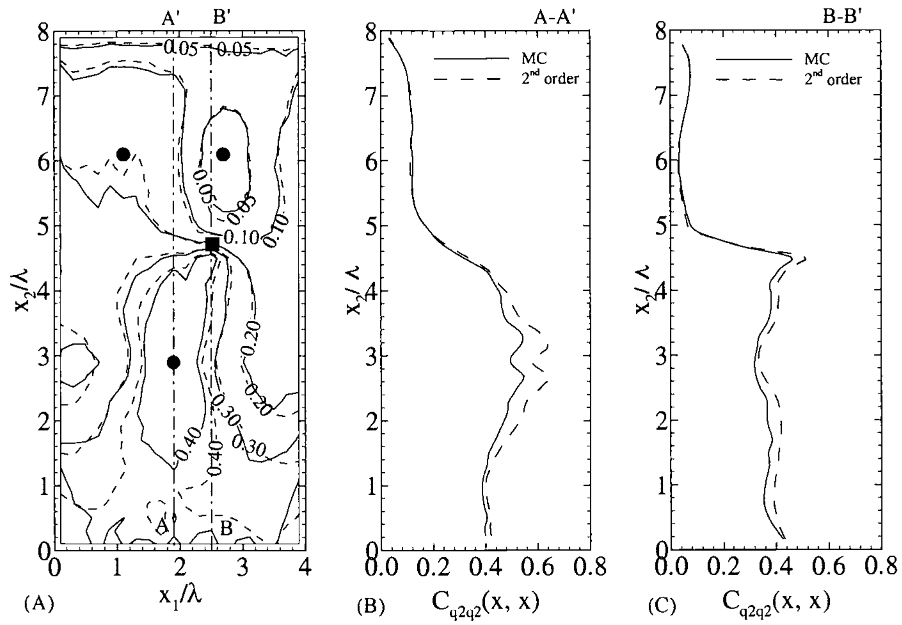


Figure 6.18. Conditional variance of longitudinal flux computed from Monte Carlo simulation and second-order solutions in Case 1. (A) A contour map, (B) a vertical profile passing through a conditional point, and (C) vertical profile passing through the source.

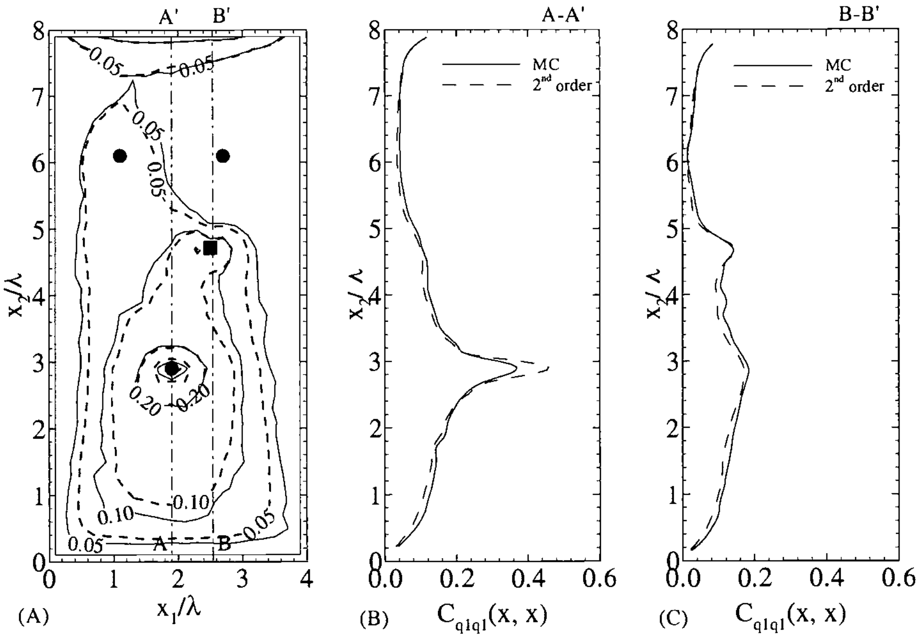


Figure 6.19. Conditional variance of transverse flux for the same case as in Figure 6.18.

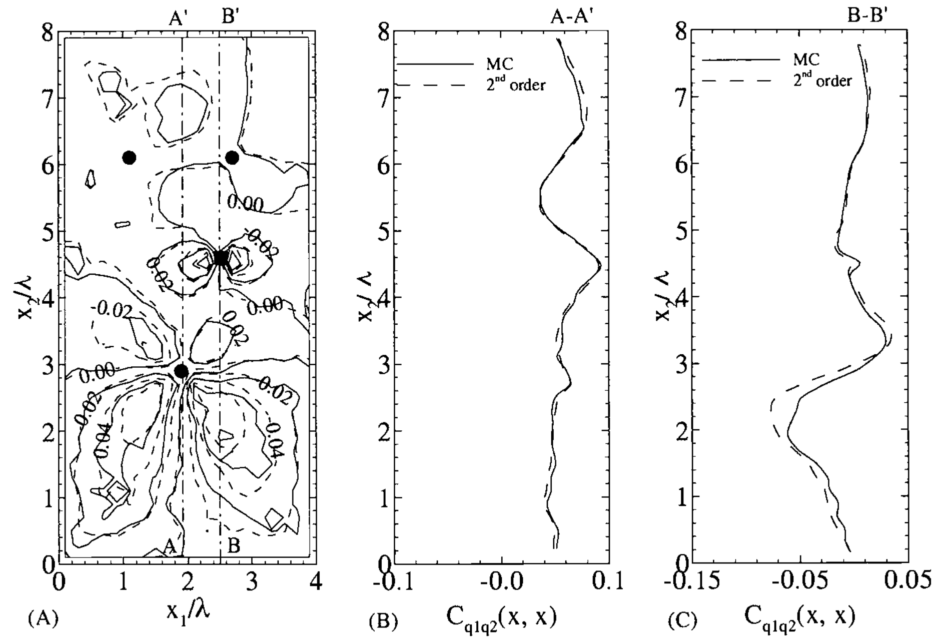


Figure 6.20. Conditional covariance between transverse flux and longitudinal flux at a zero lag for Case 1. (A) A contour map, and (B)-(C) profiles along A-A' and B-B'.

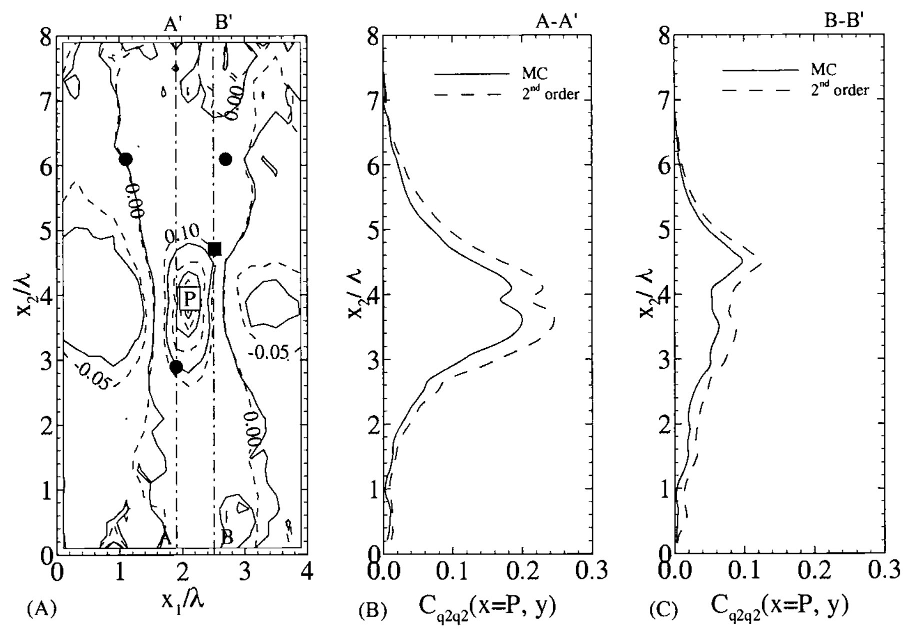


Figure 6.21. Auto-covariance of longitudinal flux with respect to a reference point P at the center of the domain, computed from MC and second-order solutions for Case 1. (A) A contour map; and (B)-(C) profiles along A-A' and B-B', respectively.

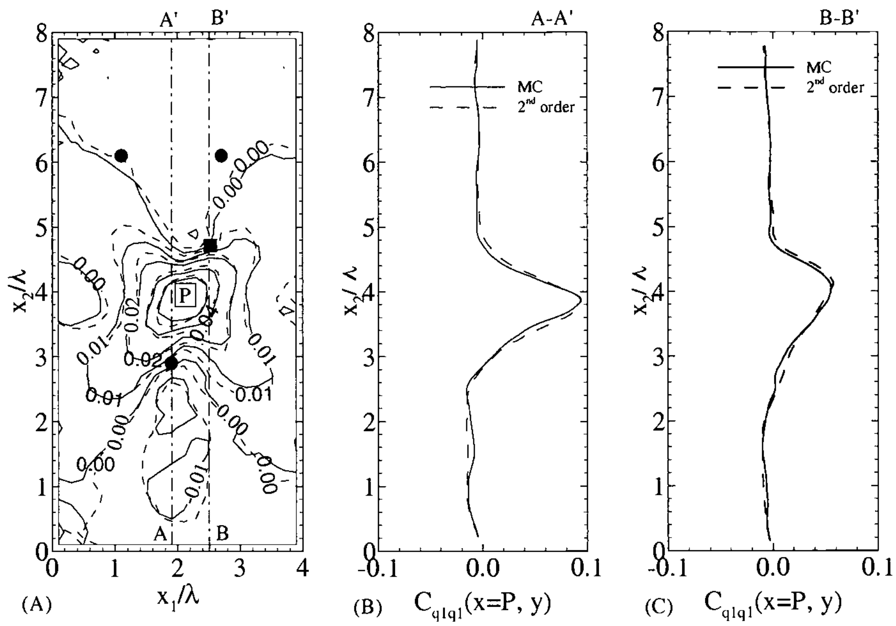


Figure 6.22. Auto-covariance of transverse flux with a reference point P at the center of the domain, for Case 1. (A) A contour map, and (B)-(C) profiles along A-A' and B-B'.

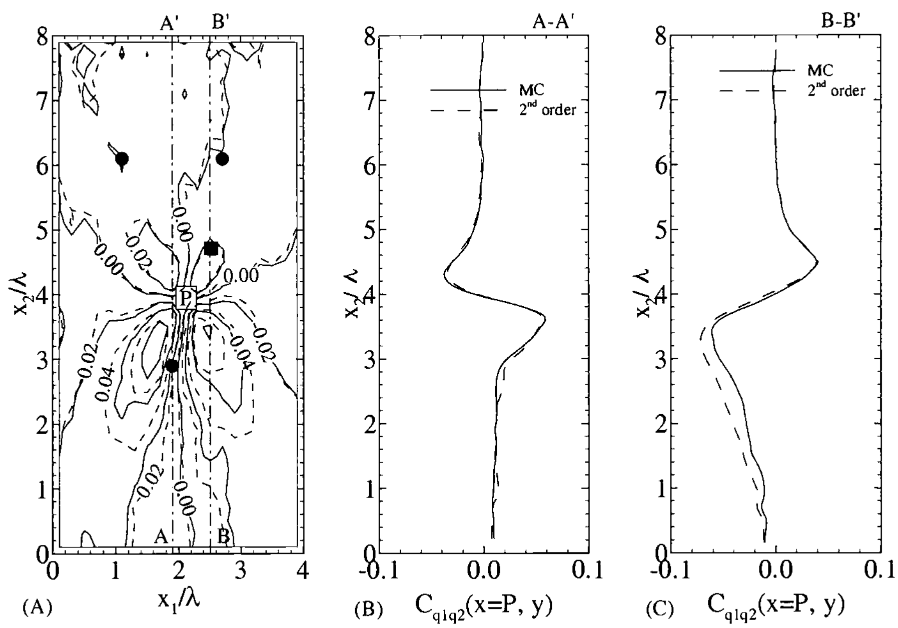
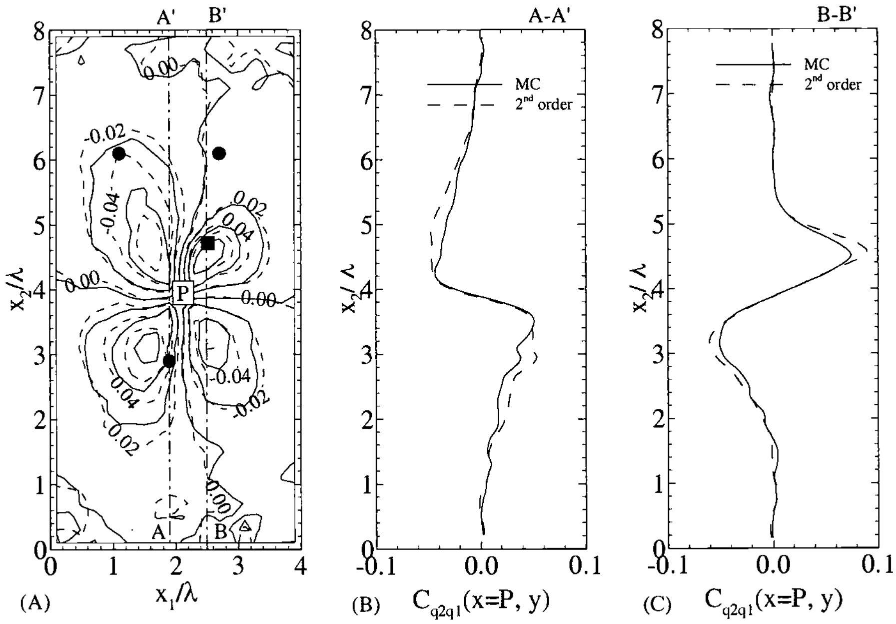
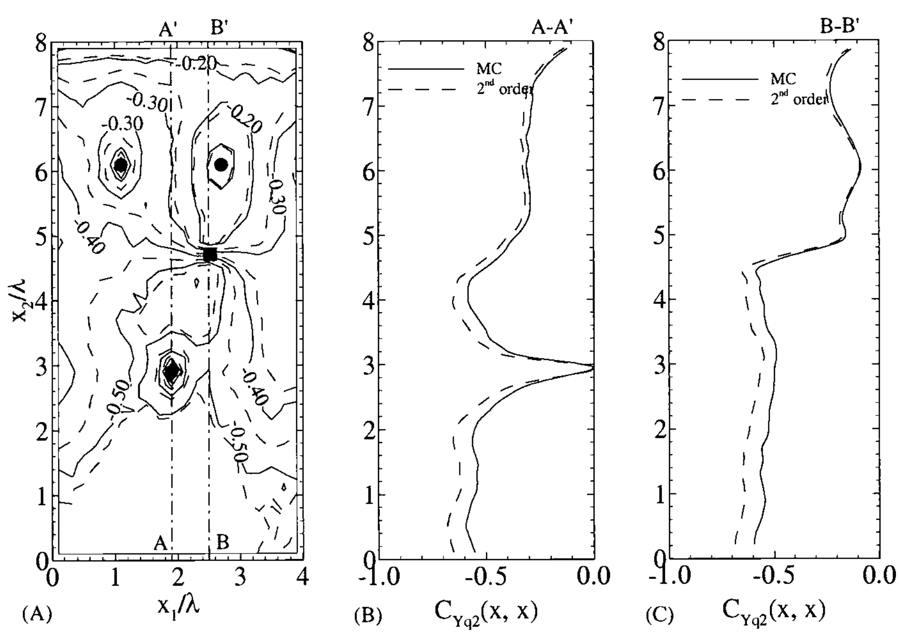


Figure 6.23. Cross-covariance between longitudinal flux at all nodes and transverse flux at a reference point P at the center of the domain, for Case 1. (A) A contour map, and (B)-(C) profiles along A-A' and B-B'.



(A) (B) (C)

Figure 6.24. Cross-covariance between transverse flux at all nodes and longitudinal flux at the center of the domain, for Case 1. (A) A contour map, and (B)-(C) profiles along A-A' and B-B'.



(A) (B) (C)

Figure 6.25. Cross-covariance between longitudinal flux and Y at a zero lag, for Case 1. (A) A contour map; and (B)-(C) profiles along A-A' and B-B', respectively.

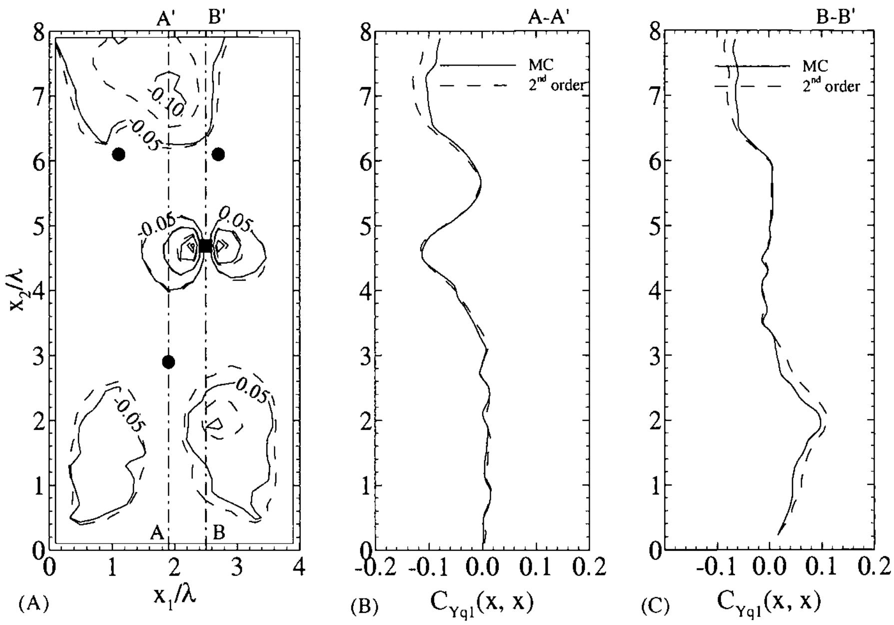


Figure 6.26. Cross-covariance between transverse flux and Y at a zero lag, for Case 1. (A) A contour map; and (B)-(C) profiles along A-A' and B-B', respectively.

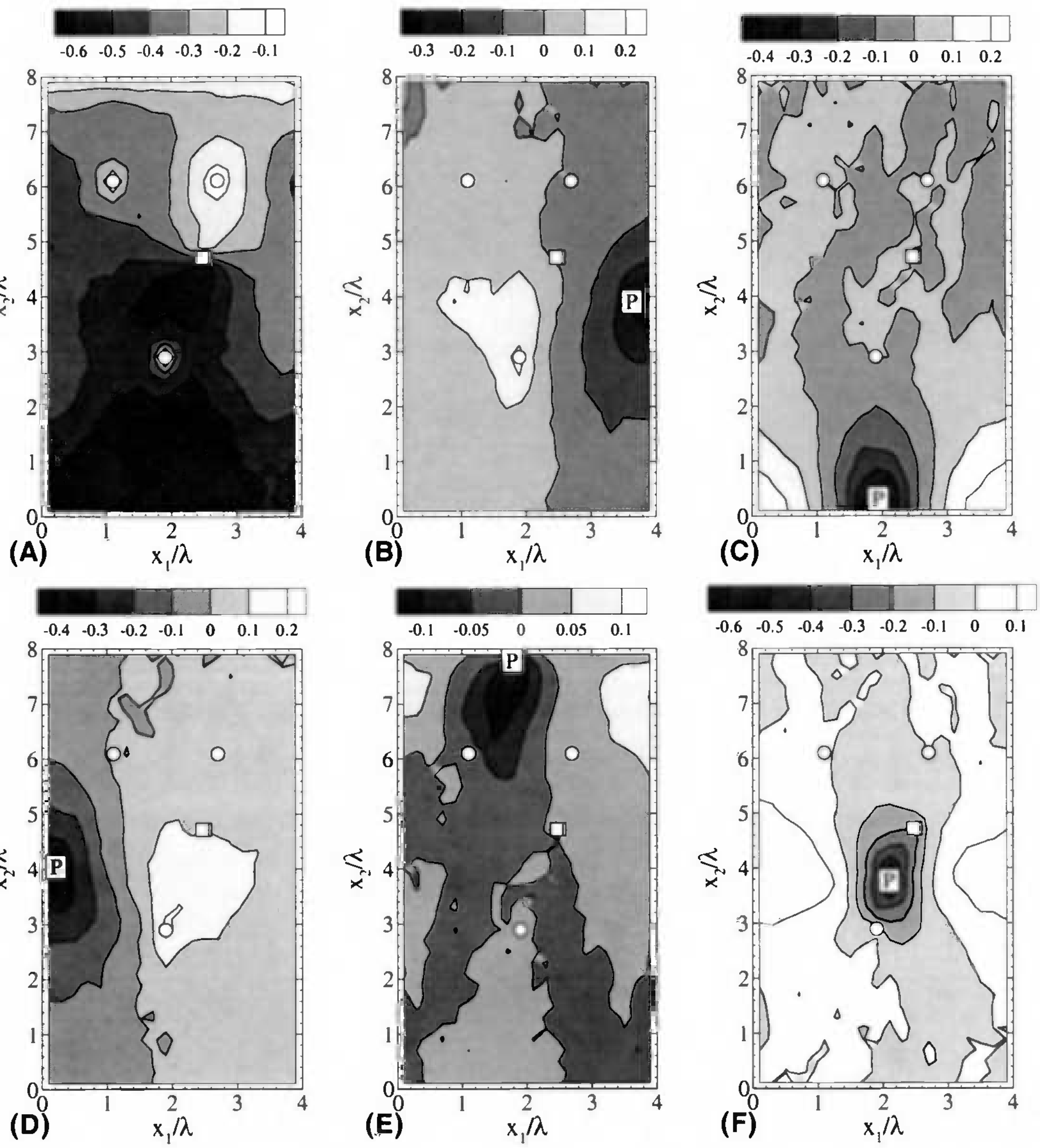


Figure 6.27. Cross-covariance between longitudinal flux at all nodes and Y in various elements P in the domain, for Case 1.

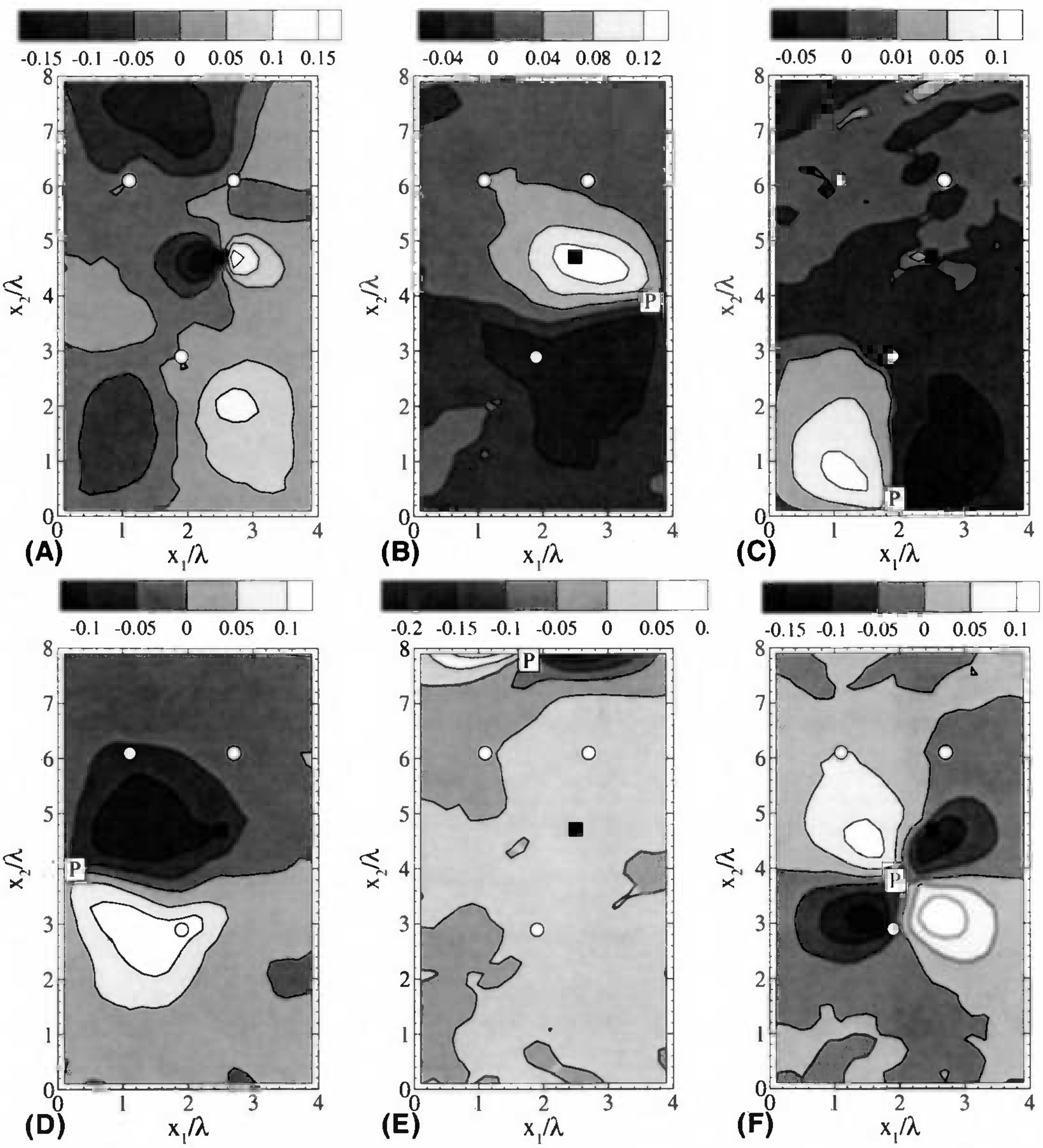


Figure 6.28. Cross-covariance between transverse flux at all nodes and *Y* in various elements P in the domain, for Case 1.

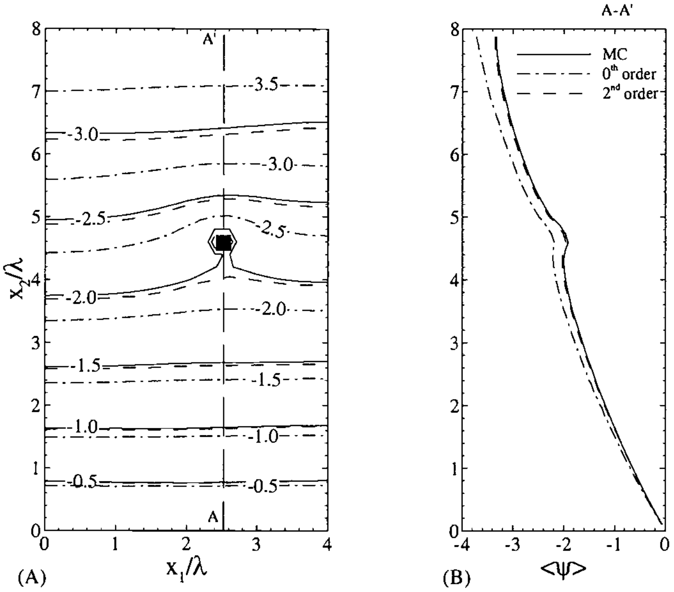


Figure 6.29. Mean pressure head obtained from Monte Carlo simulations (MC), zero-order and second-order solutions in Case 2. (A) A contour map; and (B) a vertical profile passing through the source.

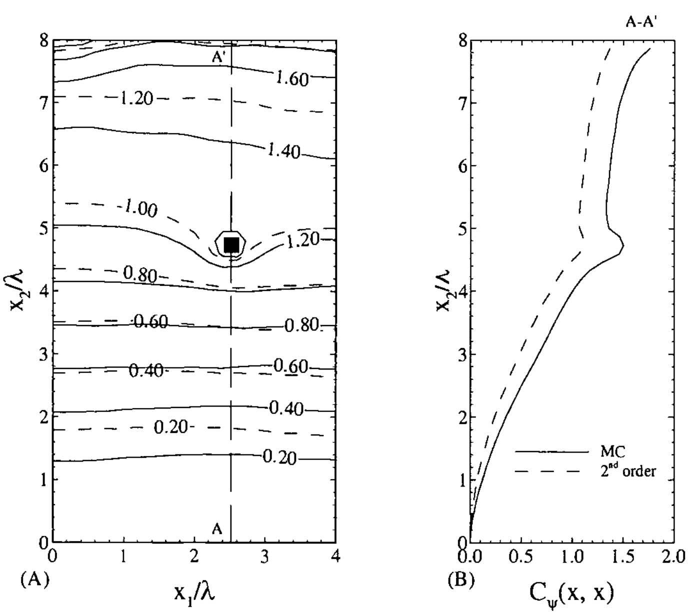


Figure 6.30. Pressure head variance obtained from Monte Carlo simulations (MC) and second-order solutions in Case 2. (A) A contour map; and (B) a vertical profile passing through the source.

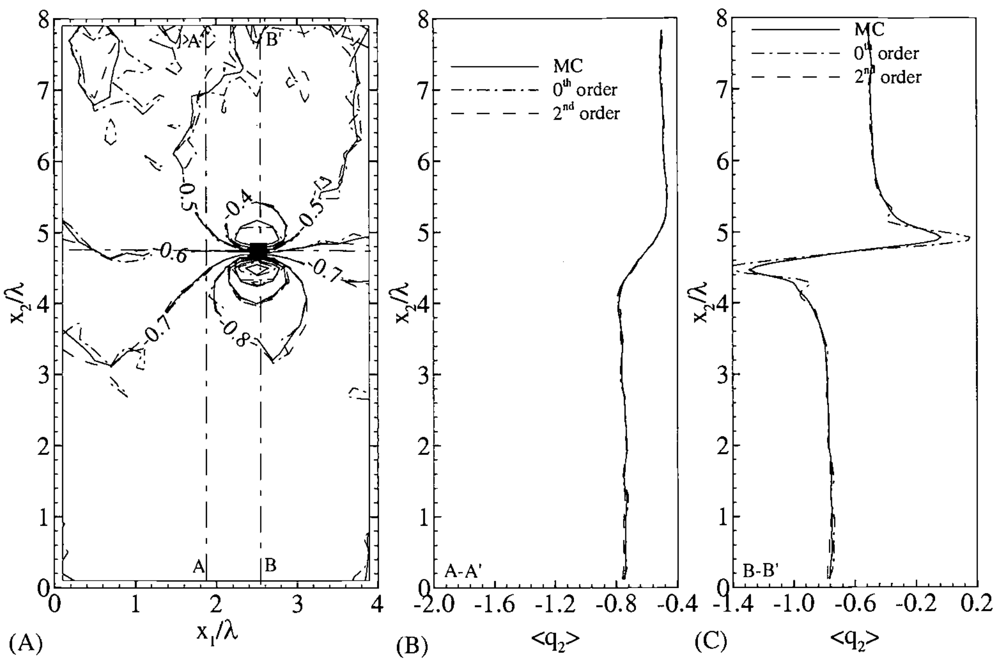


Figure 6.31. Mean flux in the longitudinal direction (x_2) using three solution methods in Case 2. A contour map (A) and various cross sections identified in (A).

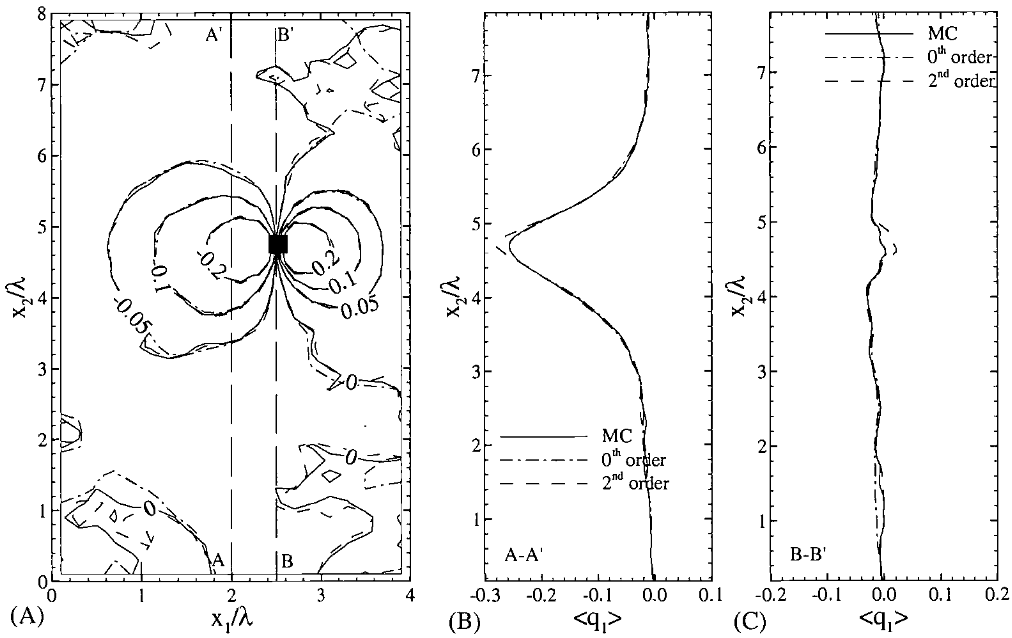


Figure 6.32. Mean flux in the transverse direction (x_1) using three methods in Case 2. A contour map (A) and various cross sections identified in (A).

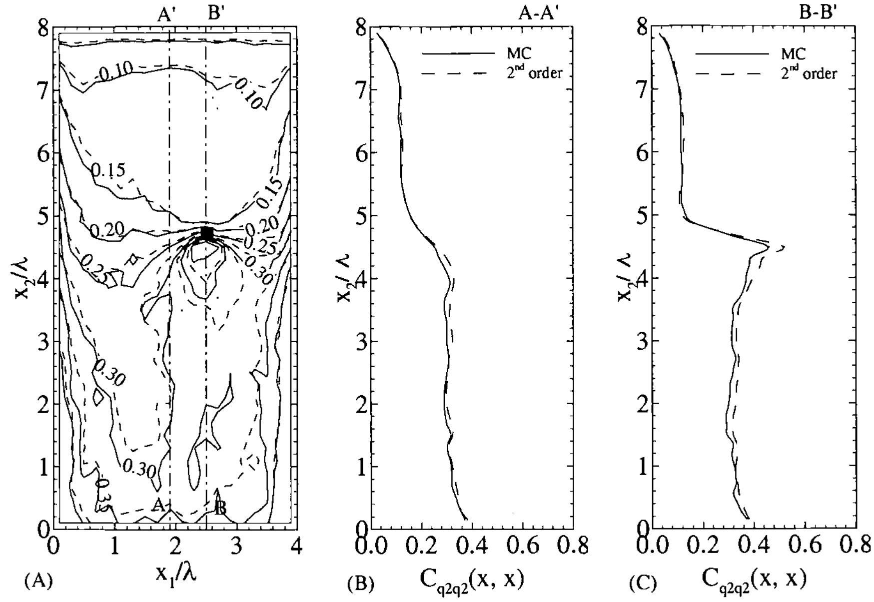


Figure 6.33. Unconditional variance of longitudinal flux computed from Monte Carlo simulation and second-order solutions in Case 2. A contour map (A) and two profiles.

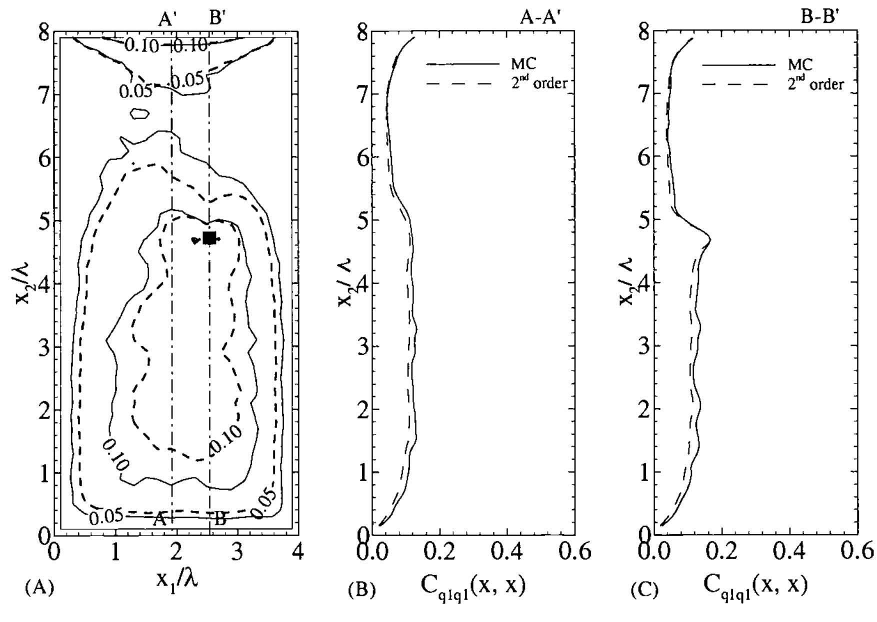


Figure 6.34. Unconditional variance of transverse flux in Case 2.

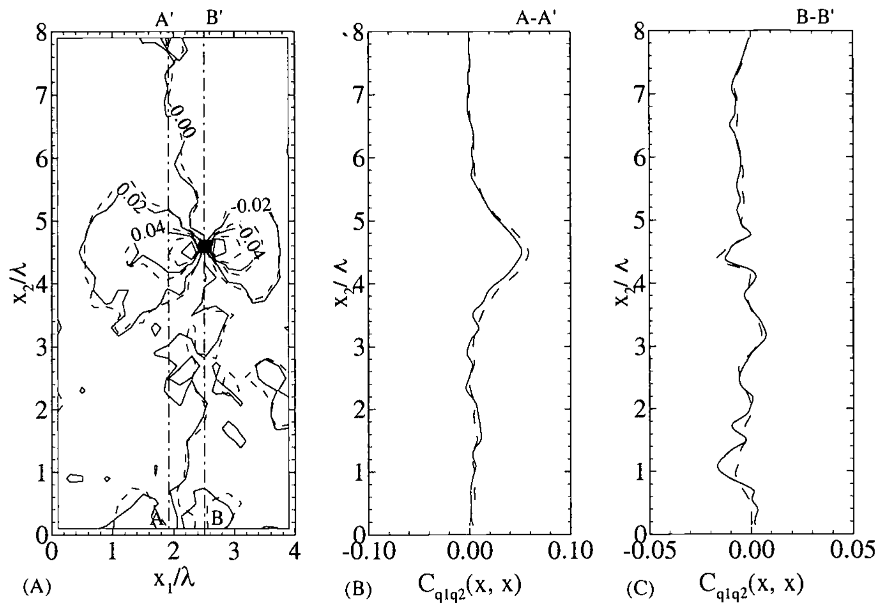


Figure 6.35. Unconditional covariance between transverse flux and longitudinal flux at a zero lag in Case 2.

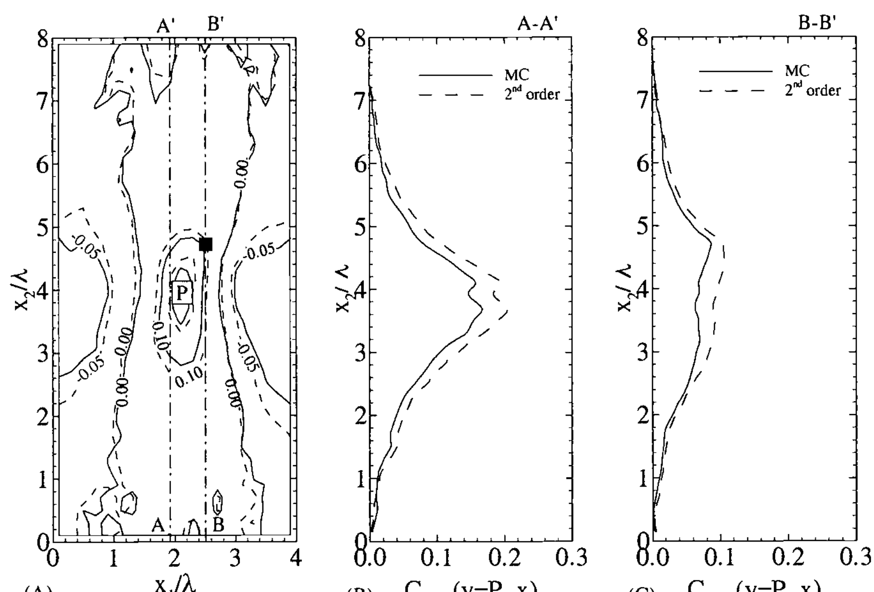


Figure 6.36. Auto-covariance of longitudinal flux with a reference point P at the center of the domain, computed from MC and second-order solutions in Case 2. (A) A contour map; and (B)-(C) profiles along A-A' and B-B', respectively.

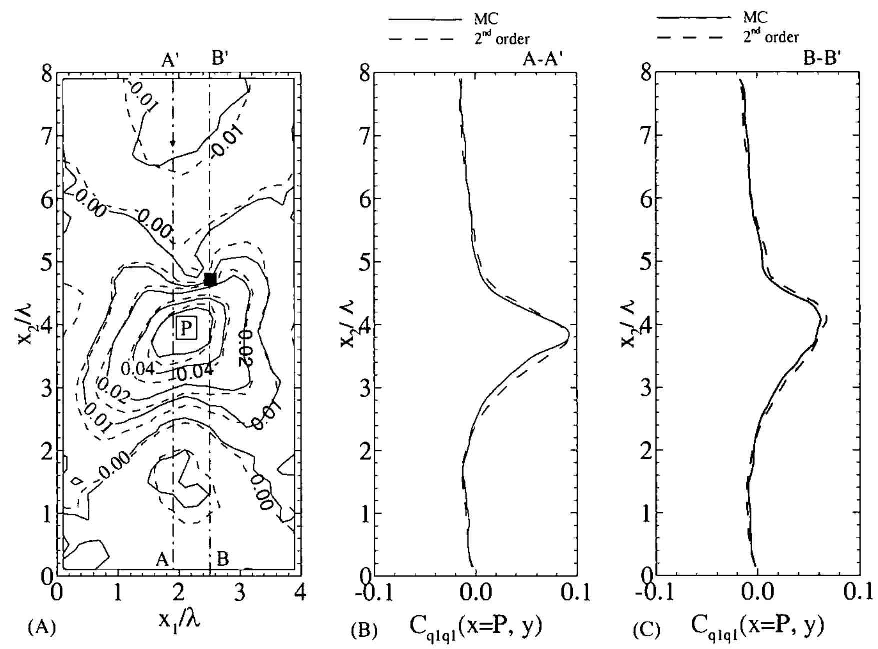


Figure 6.37. Auto-covariance of transverse flux with a reference point P at the center of the domain, for Case 2. (A) A contour map; and (B)-(C) profiles along A-A' and B-B', respectively.

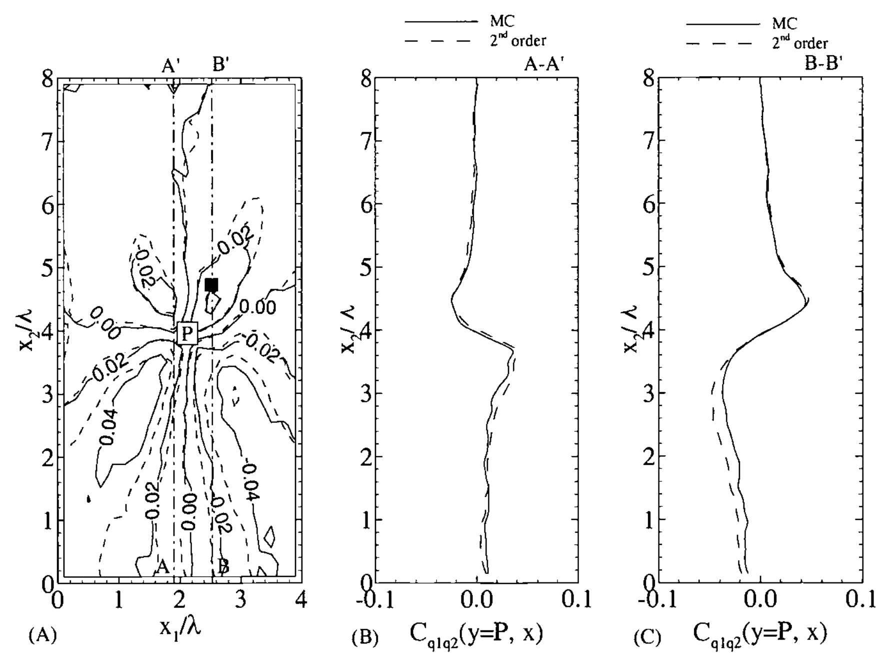


Figure 6.38. Cross-covariance between longitudinal flux at all nodes and transverse flux at a reference point P at the center of the domain, for Case 2. (A) A contour map; and (B)-(C) profiles along A-A' and B-B', respectively.

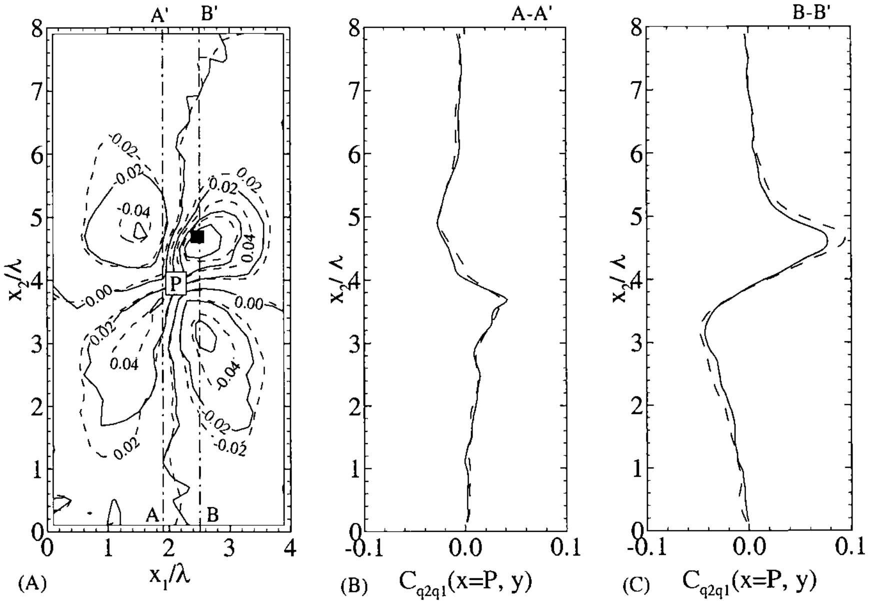


Figure 6.39. Cross-covariance between transverse flux at all nodes and longitudinal flux at the center of the domain in Case 2. (A) A contour map; and (B)-(C) profiles along A-A' and B-B', respectively.

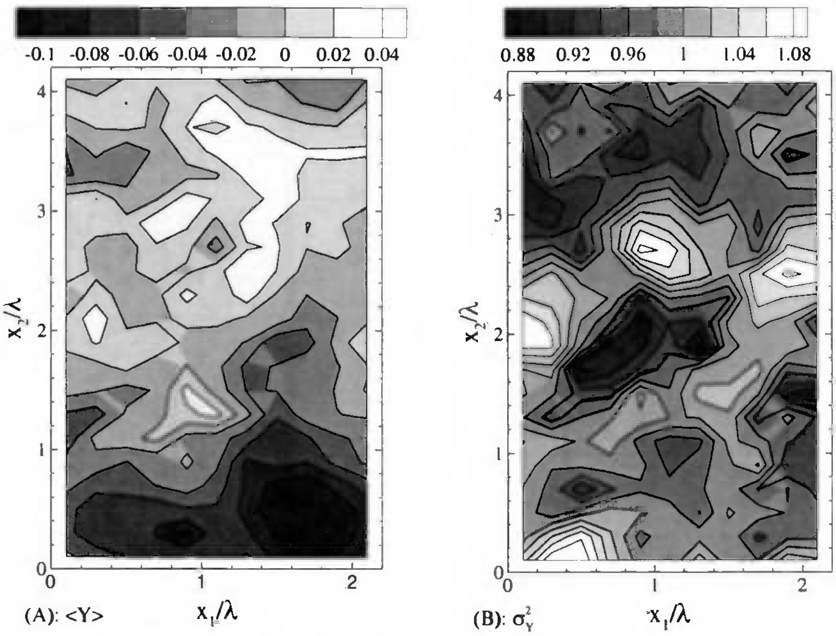


Figure 6.40. Image of (A) an unconditional mean log hydraulic conductivity field, and (B) covariance calculated from 2,000 unconditional realizations with $\langle Y\rangle$=0.0, $\sigma_Y{}^2$=1.0, λ=1.0, and an 11x21 grid with Δx_1=Δx_2=0.2λ. (Case 3)

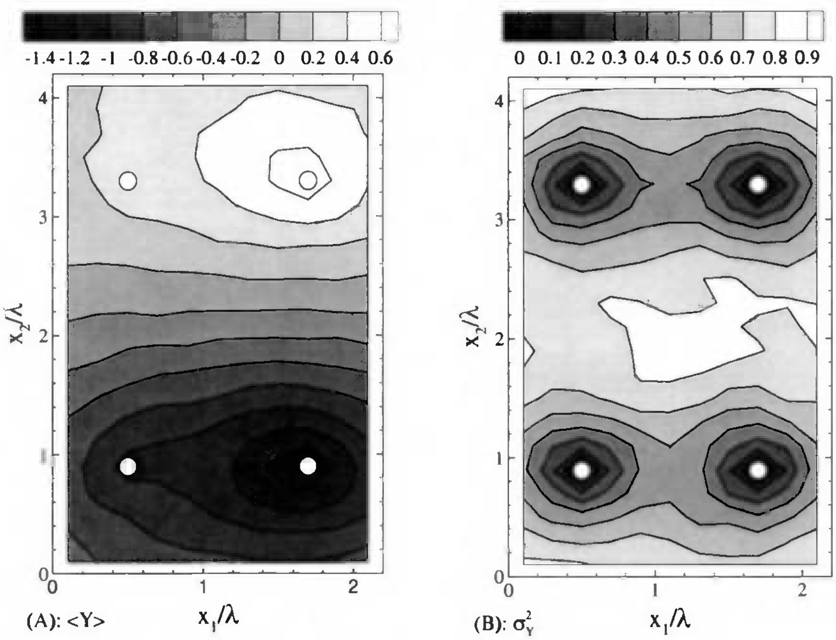


Figure 6.41. Images of (A) a conditional mean log hydraulic conductivity and (B) covariance calculated from 2,000 conditional realizations with $\langle Y\rangle$=0.0, $\sigma_Y{}^2$=1.0, λ=1.0, and an 11x21 grid with Δx_1=Δx_2=0.2λ. (Case 4)

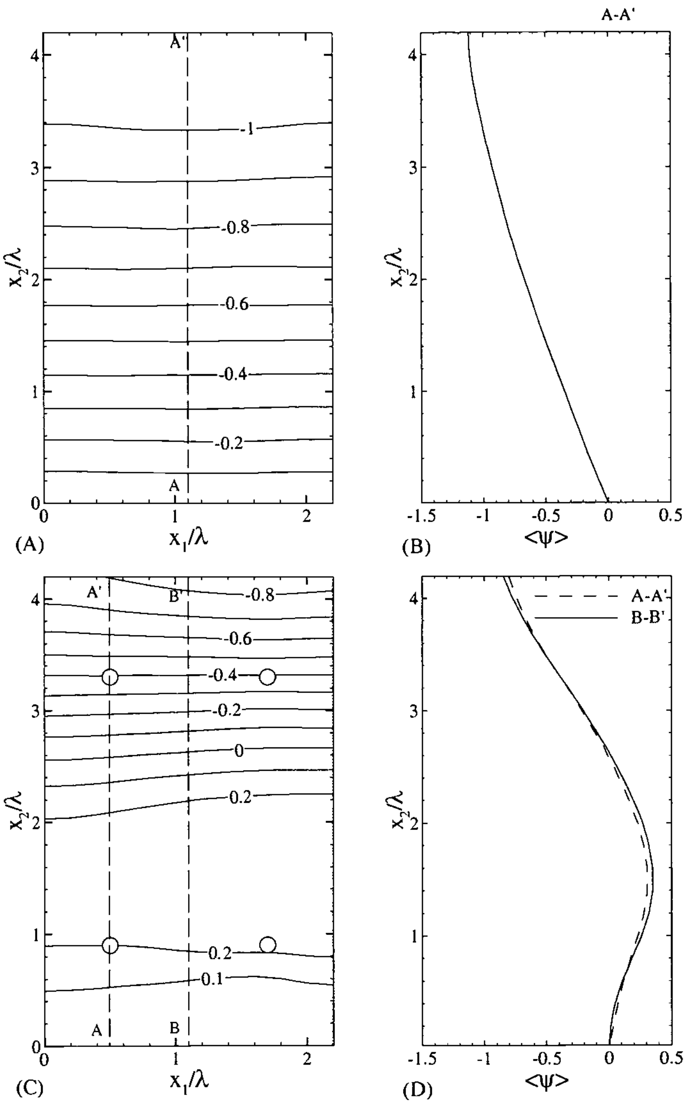


Figure 6.42. Mean pressure heads computed for cases with and without conditioning points. (A) and (C) are contours for unconditional case (Case 3) and conditional case (case 4), and (B) and (D) are profiles corresponding to (A) and (C), respectively.

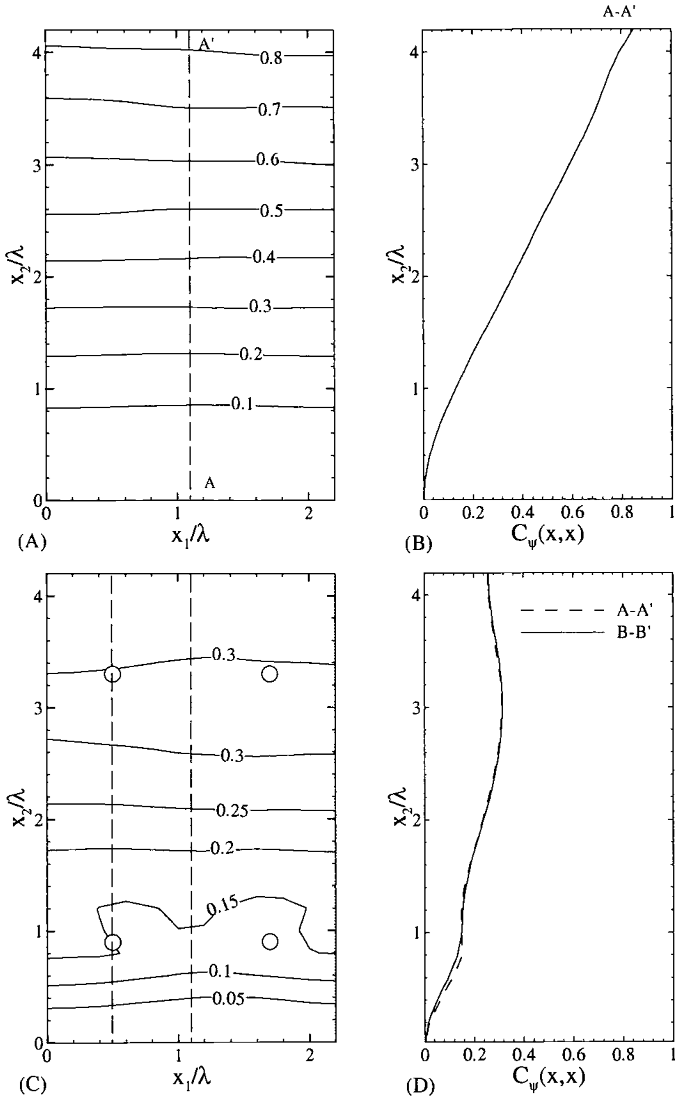


Figure 6.43. Variance of pressure head computed for cases with and without conditioning points. (A) and (C) are contours for unconditional case (Case 3) and conditional case (case 4), and (B) and (D) are profiles corresponding to (A) and (C), respectively.

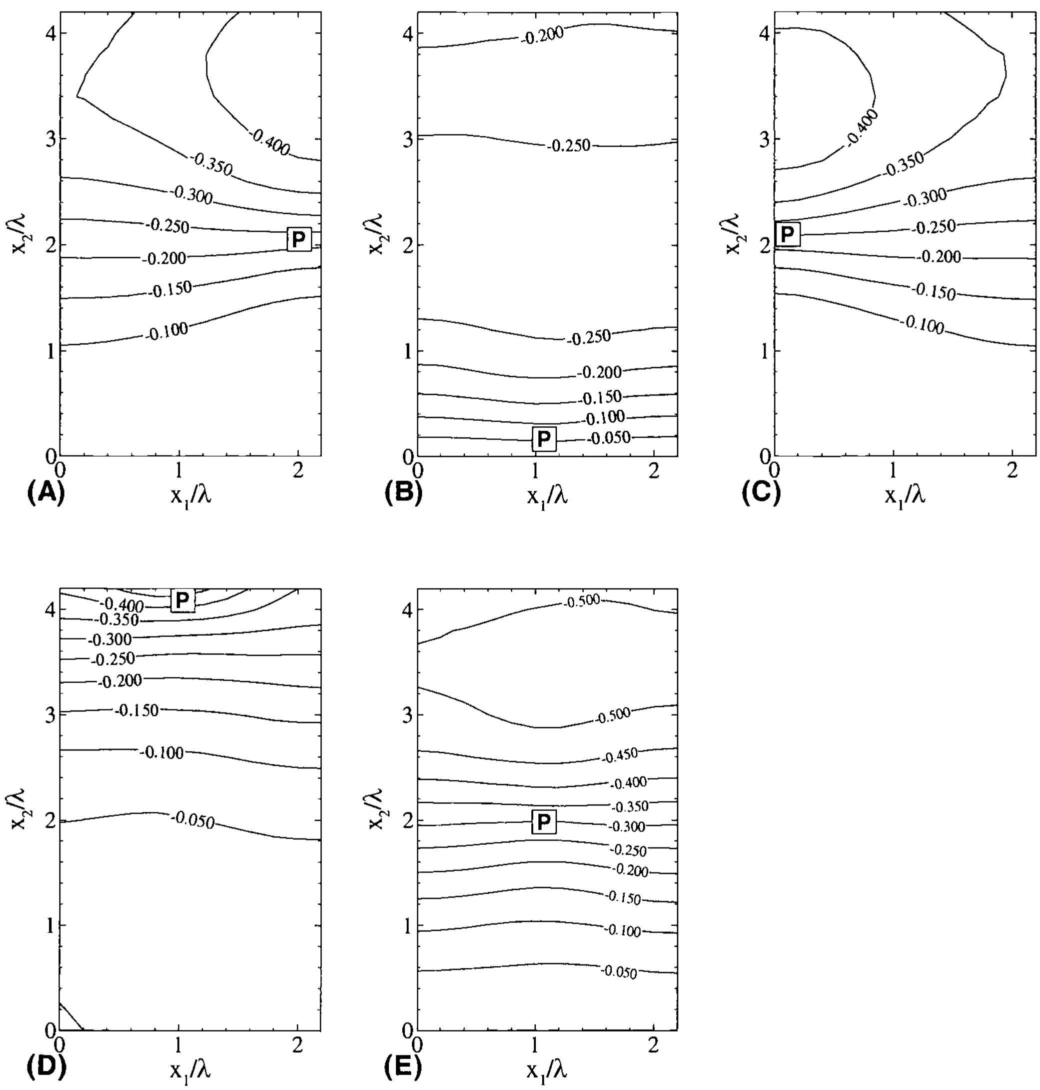


Figure 6.44. Cross-covariance between pressure head and log hydraulic conductivity at various locations P, $C_{Y\psi}(\mathrm{P}, \boldsymbol{x})$, for Case 3.

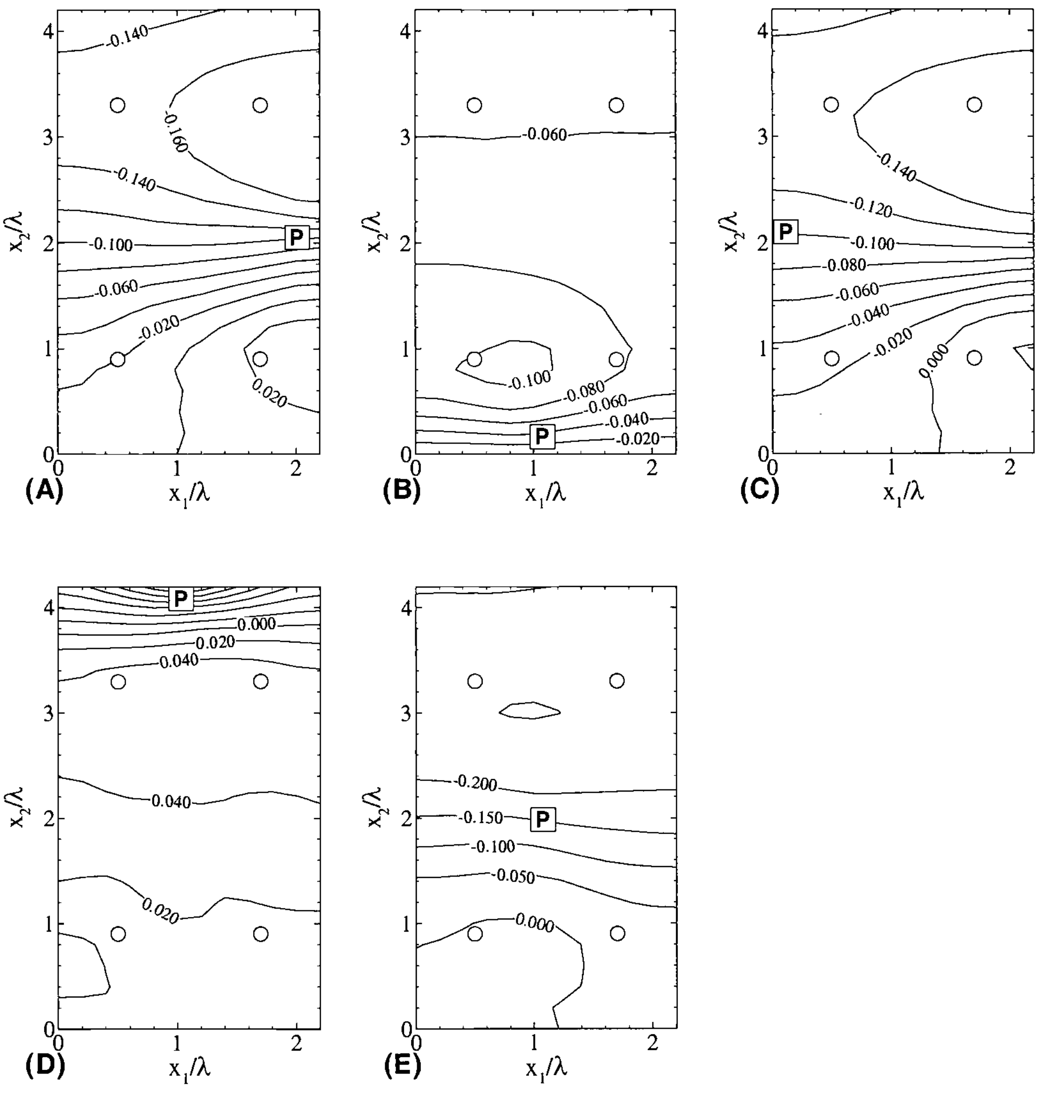


Figure 6.45. Cross-covariance between pressure head and log hydraulic conductivity at various locations, $C_{Y\psi}(\mathrm{P}, \boldsymbol{x})$, for Case 4.

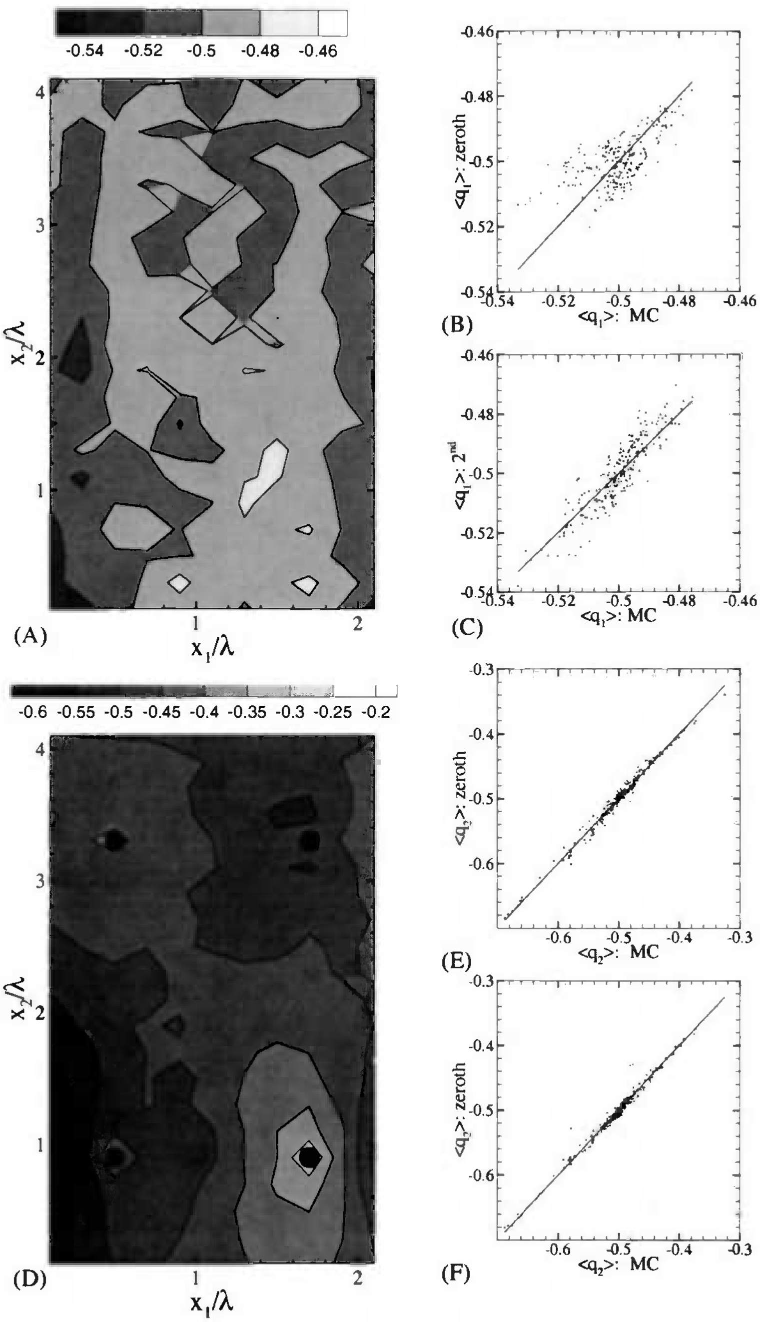


Figure 6.46. Longitudinal flux for unconditional (A-C) and conditional cases (D-F). The contours are plotted from second-order solutions.

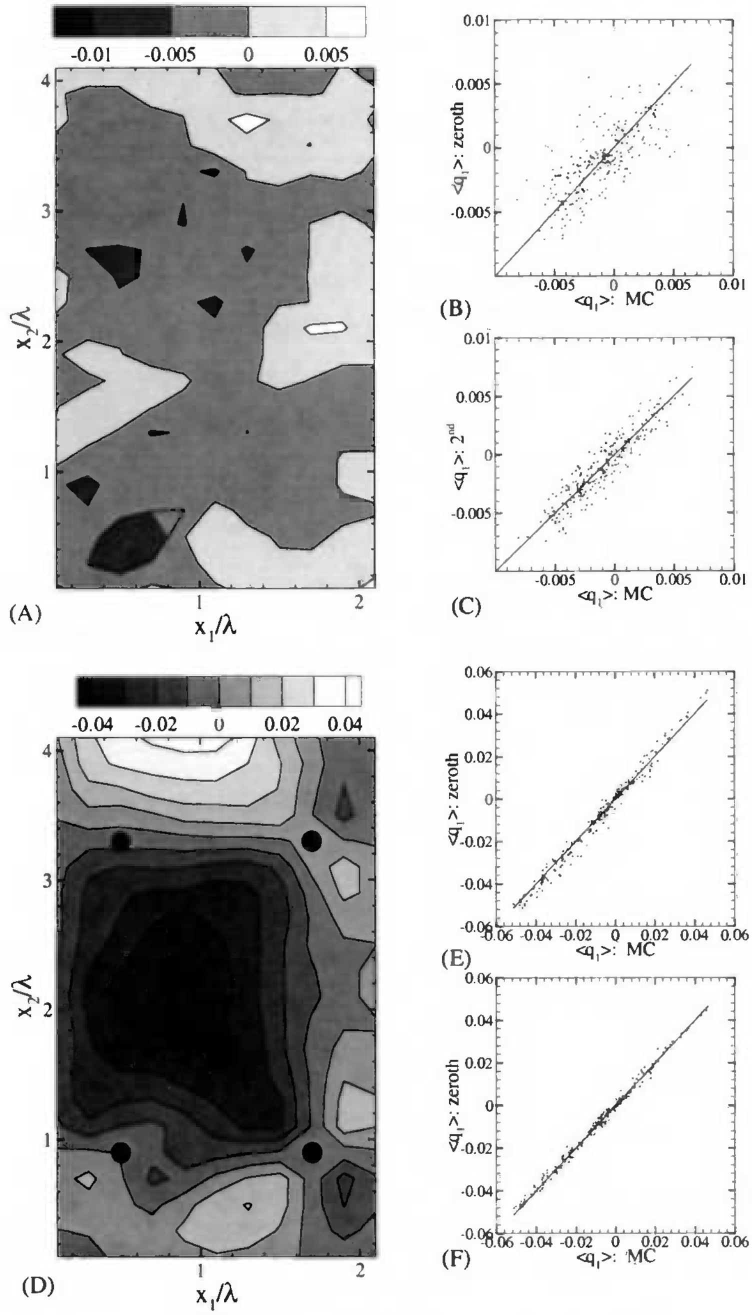


Figure 6.47. Transverse flux for unconditional (A-C) and conditional cases (D-F). The contours are plotted from second-order solutions.

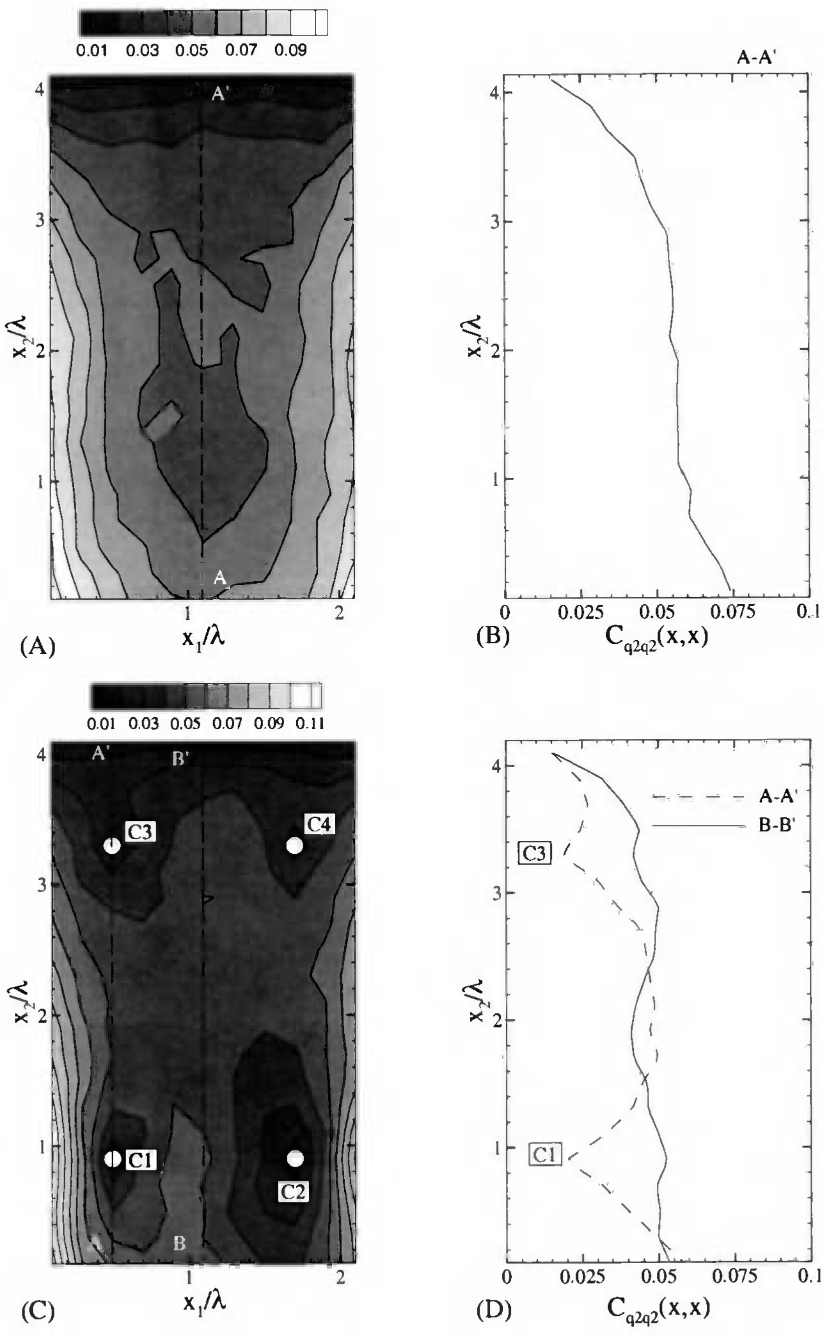


Figure 6.48. Variance of longitudinal flux (second-order solutions) for unconditional (A-B) and conditional cases (C-D).

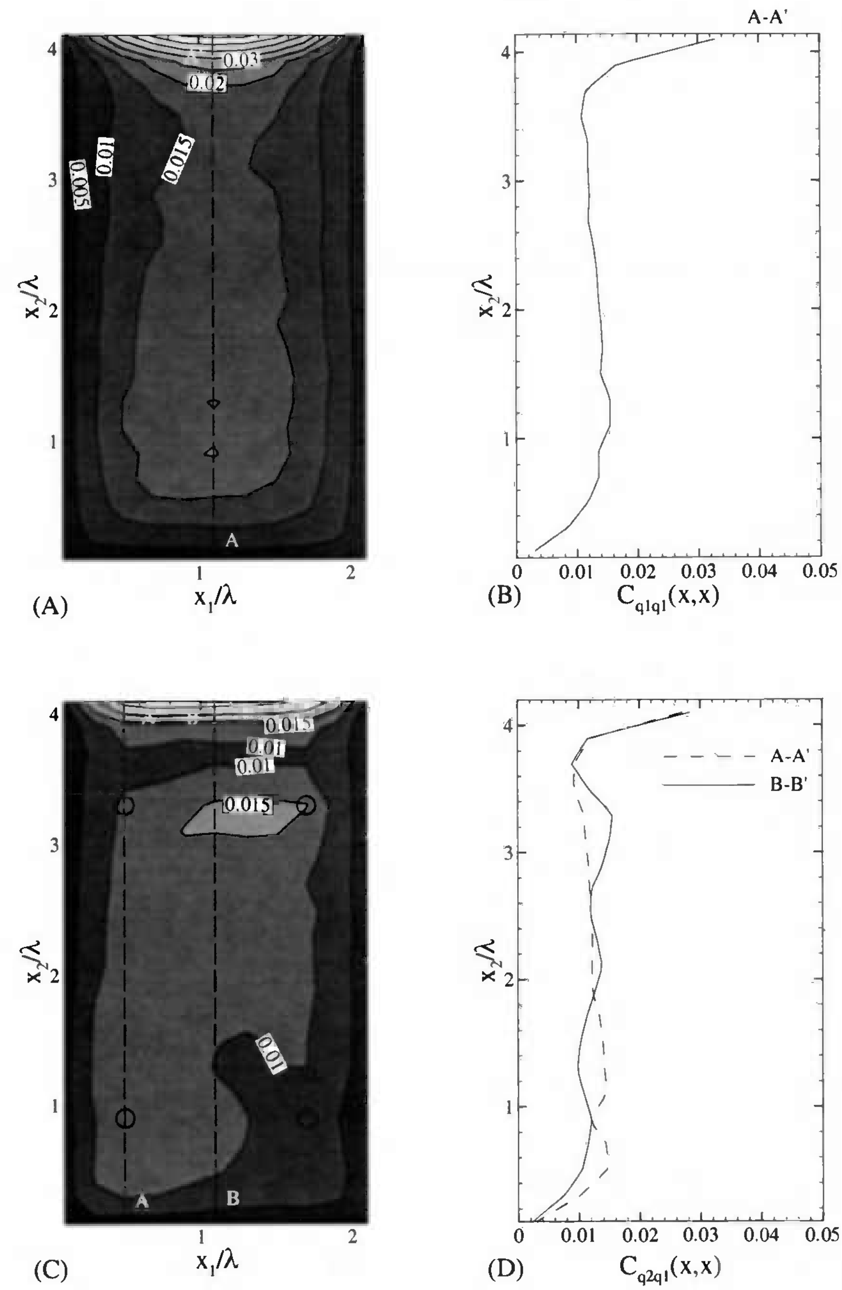


Figure 6.49. Variance of transverse flux (second-order solutions) for unconditional (A-B) and conditional cases (C-D).

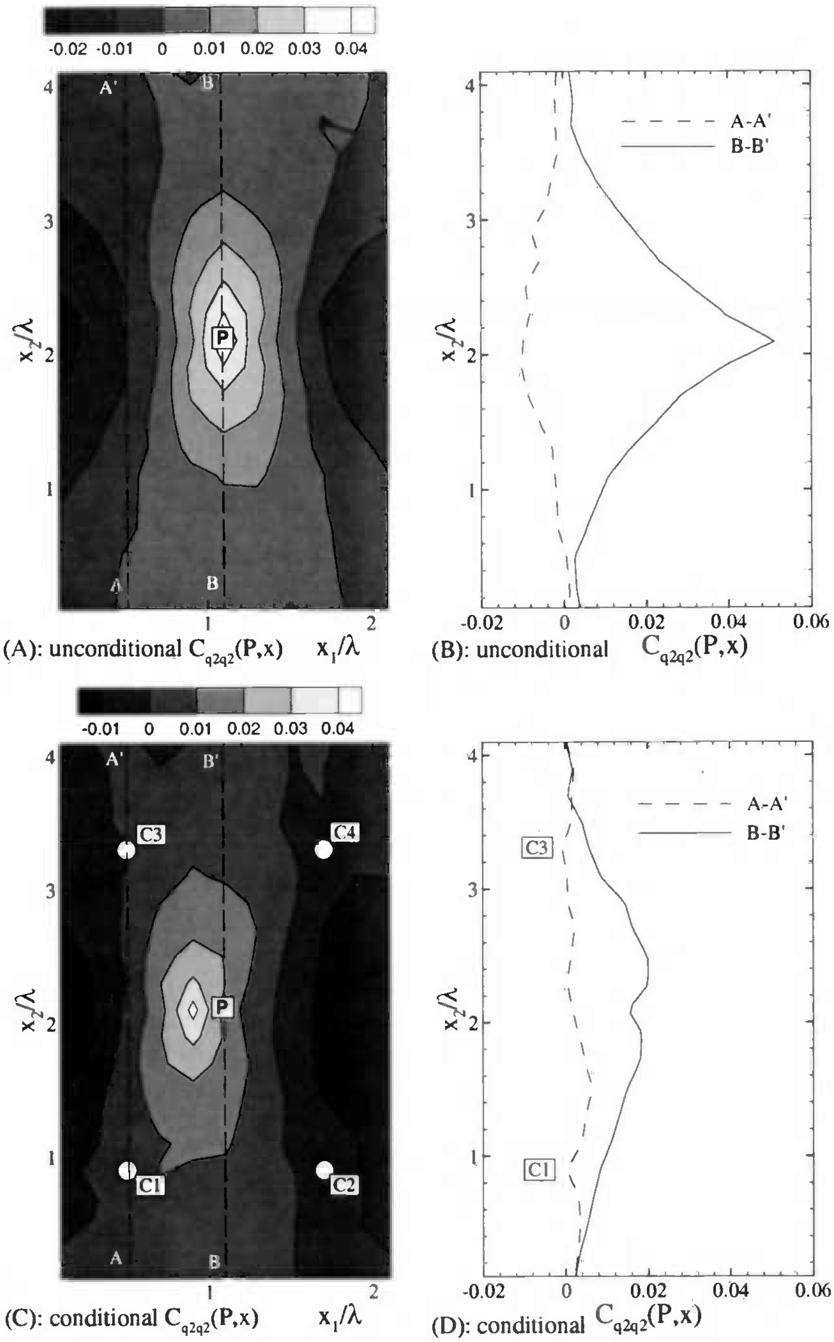


Figure 6.50. Auto-covariance of the longitudinal flux with respect to reference point P located at the center of the domain for unconditional (A-B) and conditional cases (C-D).

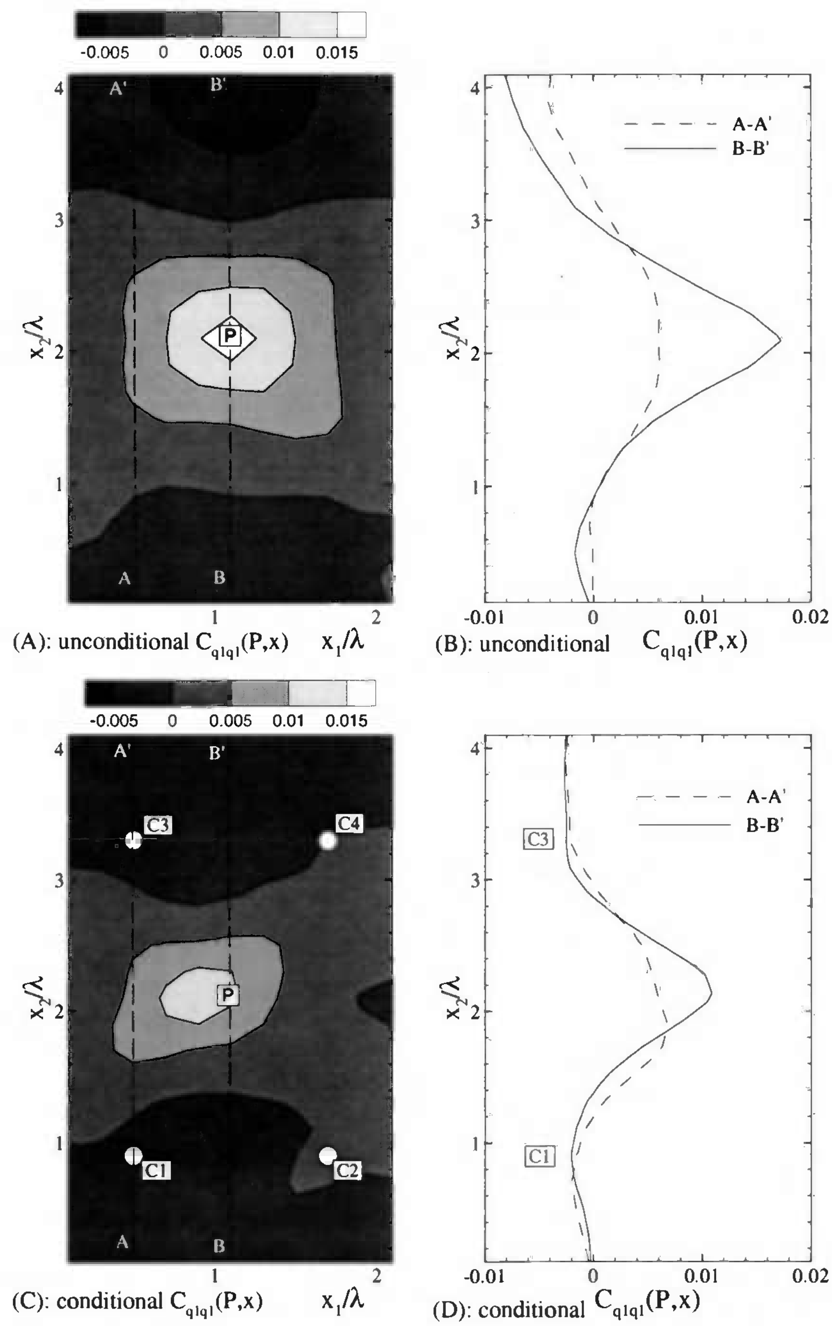


Figure 6.51. Auto-covariance of the transverse flux with respect to reference point P located at the center of the domain for unconditional (A-B) and conditional cases (C-D).

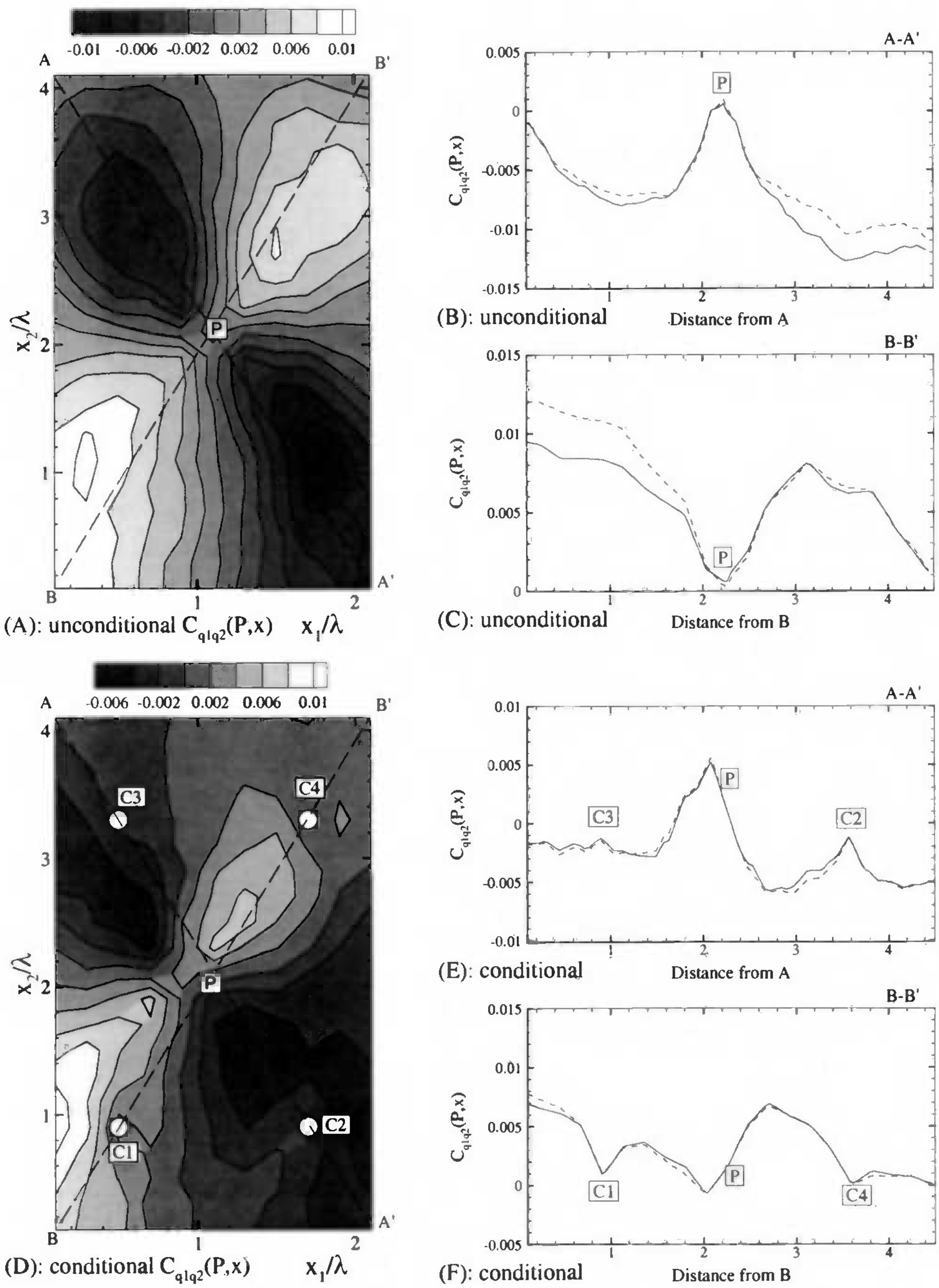


Figure 6.52. Cross-covariance between the longitudinal flux and the transverse flux at a reference point P located at the center of the domain for unconditional (A-C) and conditional cases (D-F). Dash lines in cross-sectional diagrams are results from Monte Carlo simulations and all solid lines represent results from second-order solutions.

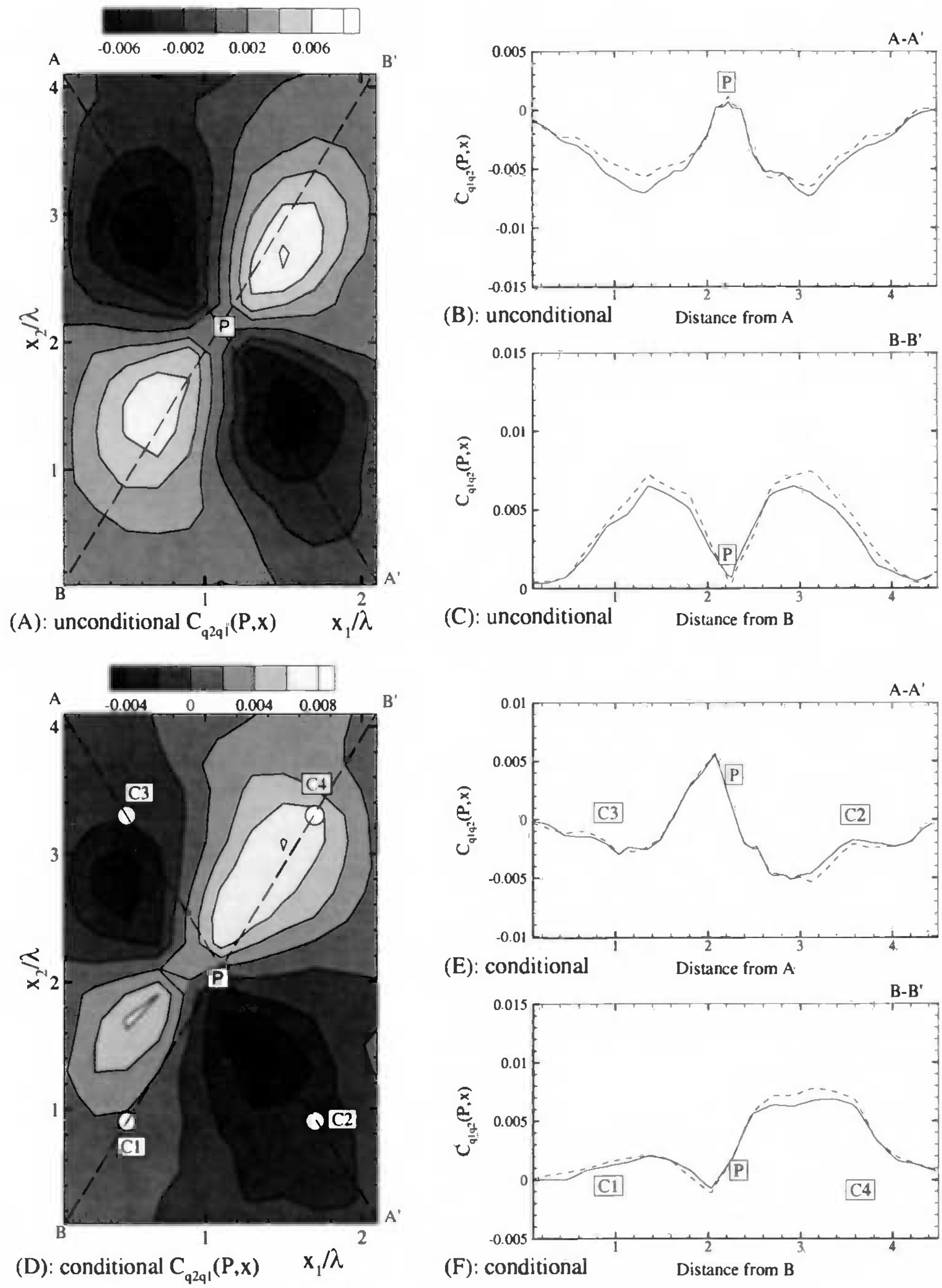


Figure 6.53. Cross-covariance between transverse flux and longitudinal flux at a reference point *P* located at the center of the domain for unconditional (A-C) and conditional cases (D-F). Dash lines in cross-sectional diagrams are results from Monte Carlo simulations and all solid lines are results from our second-order solutions.

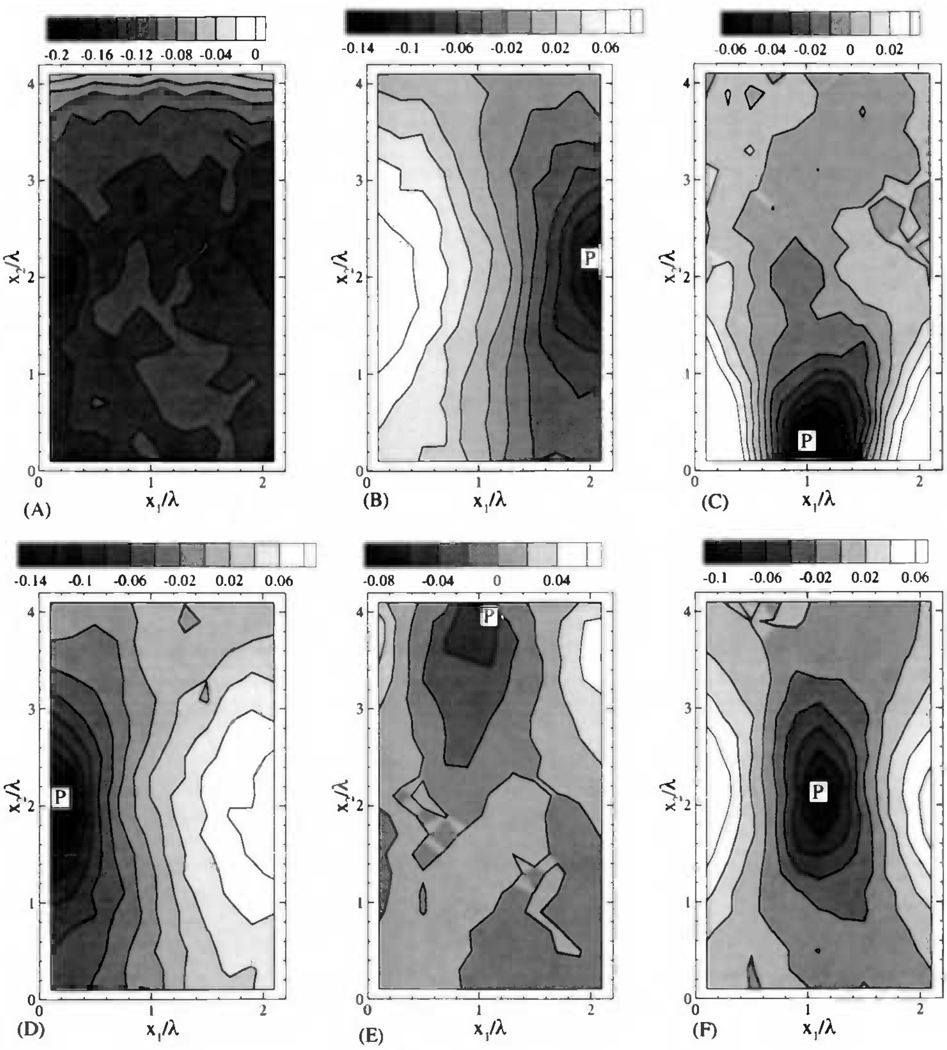


Figure 6.54. Cross-covariance between the longitudinal flux and log hydraulic conductivity Y at various locations for the unconditional case (Case 3).

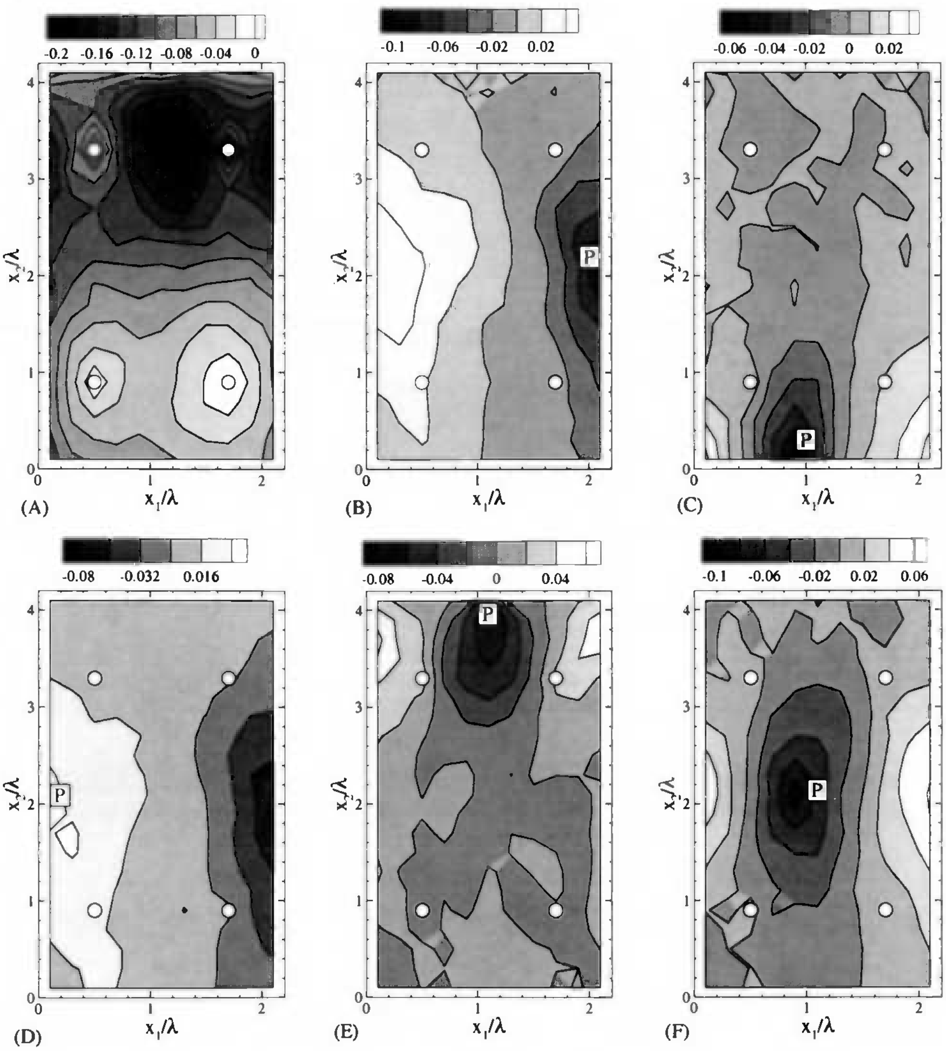


Figure 6.55. Cross-covariance between the longitudinal flux and log hydraulic conductivity Y at various locations P for the conditional case (Case 4).

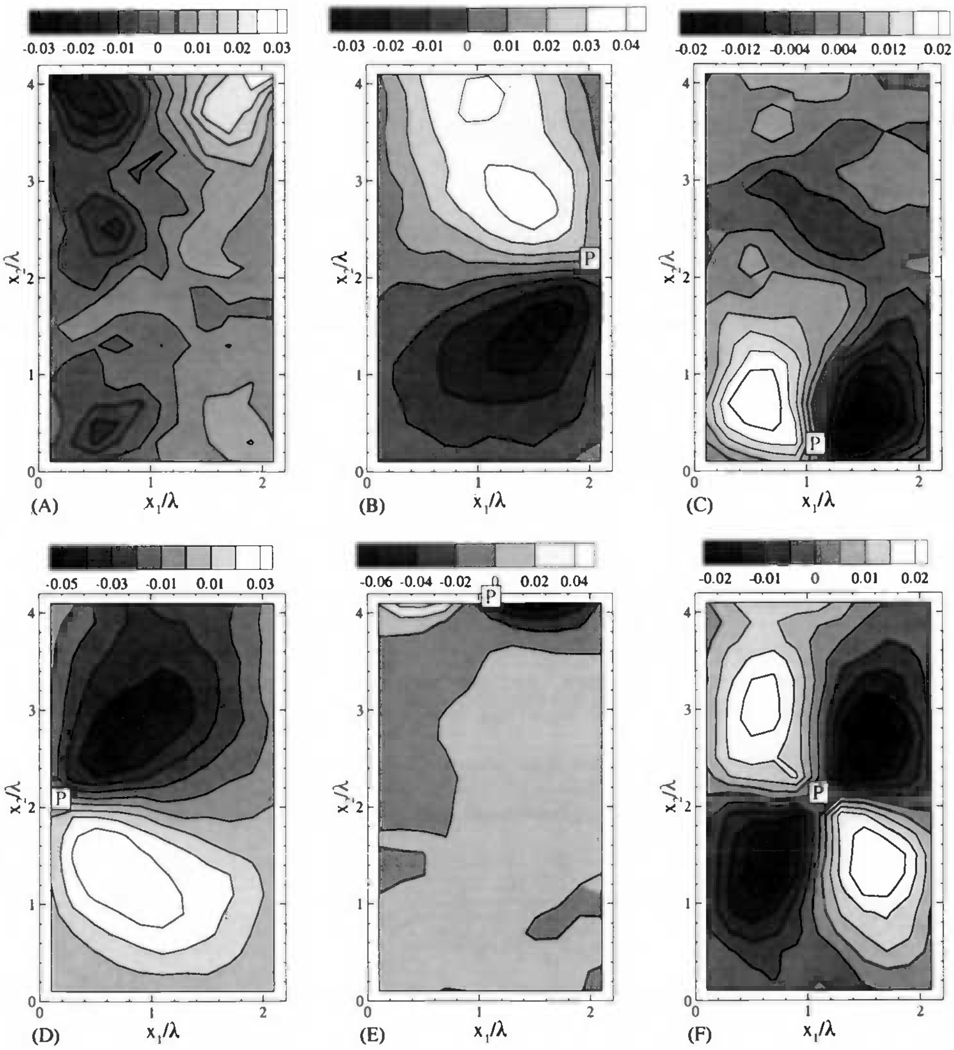


Figure 6.56. Cross-covariance between the transverse flux and log hydraulic conductivity Y at various locations P in Case 3.

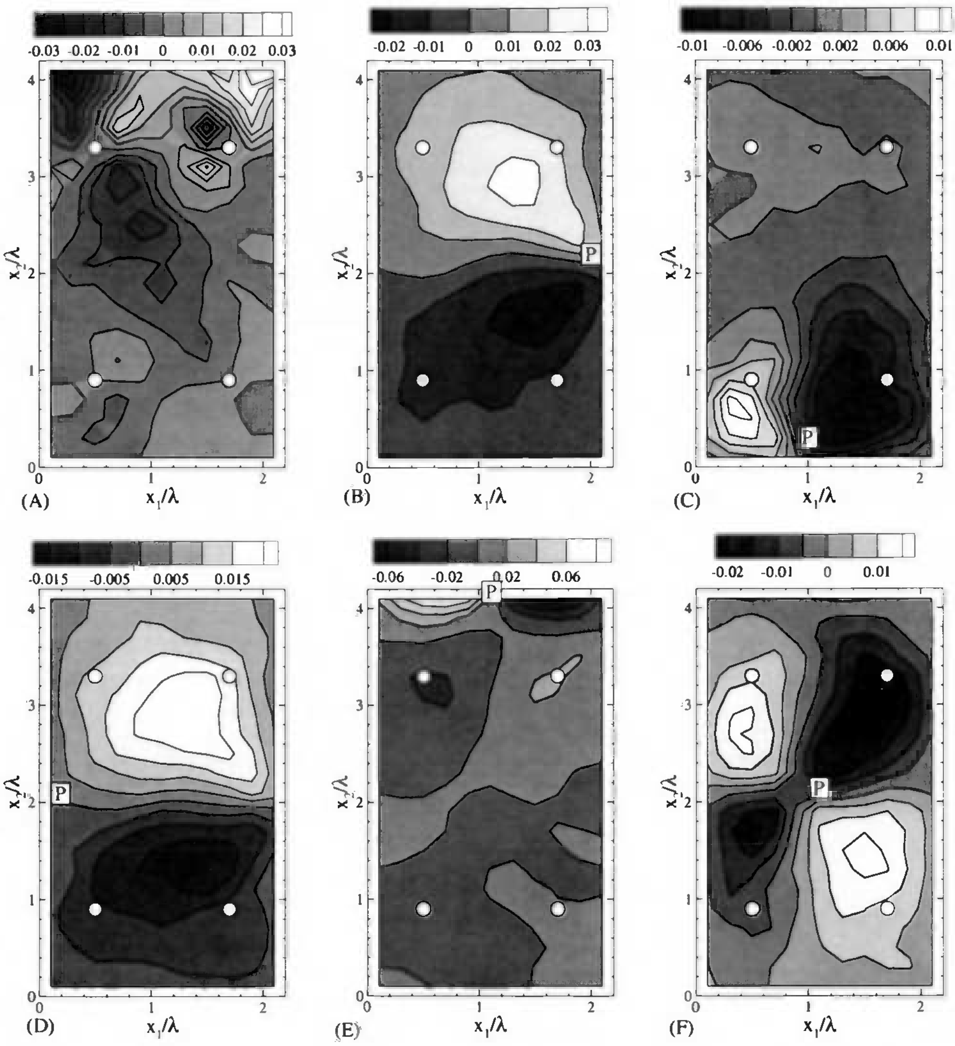


Figure 6.57. Cross-covariance between transverse flux and log hydraulic conductivity Y at various locations P in Case 4.

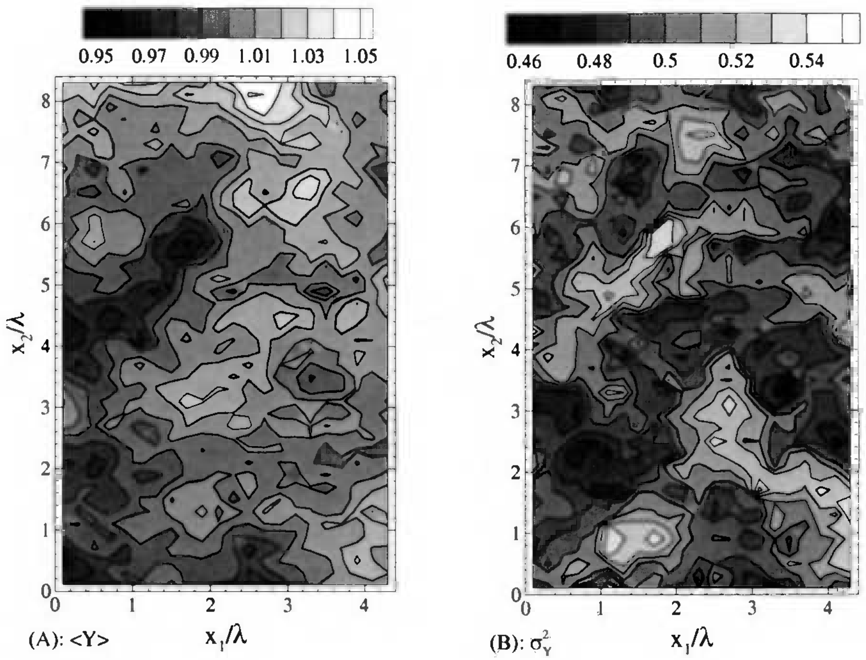


Figure 6.58. Image of (A) an unconditional mean log hydraulic conductivity field, and (B) covariance calculated from 2,000 unconditional realizations with $\langle Y \rangle=1.0$, $\sigma_Y{}^2=0.5$, $\lambda=1.0$, and a 22x42 grid with $\Delta x_1=\Delta x_2=0.2\lambda$.

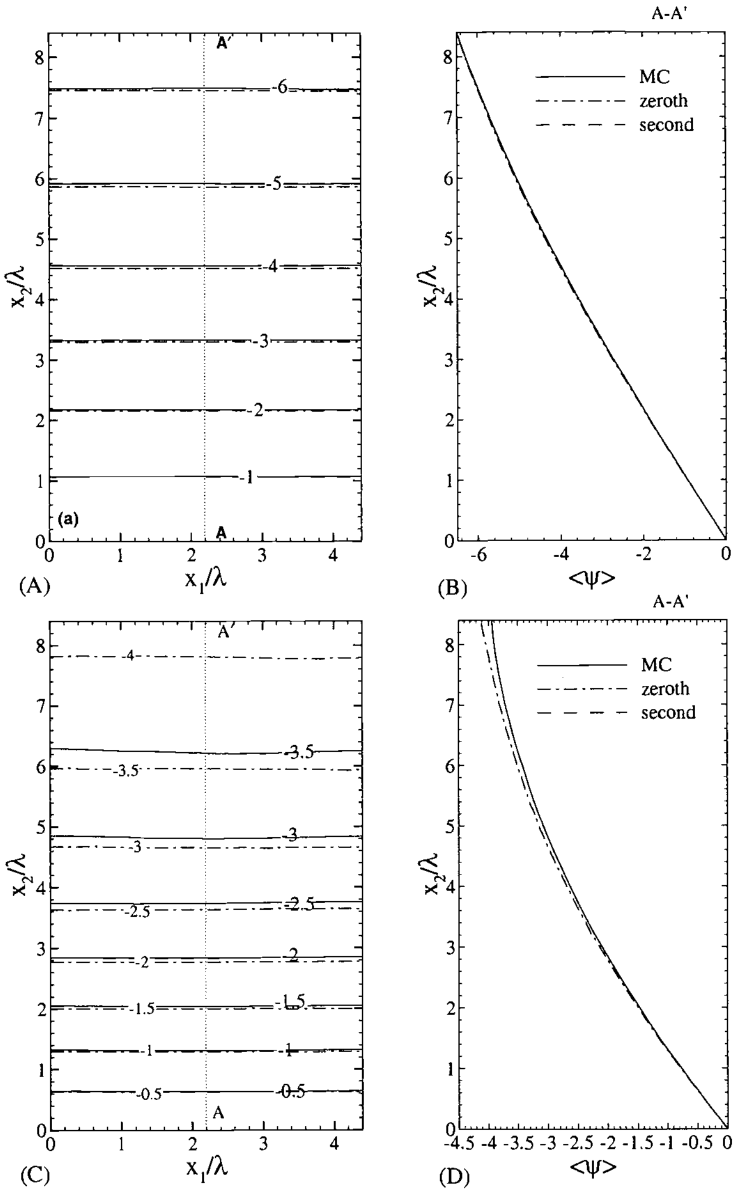


Figure 6.59. Mean pressure head computed from Monte Carlo simulation (MC), zero-order and second-order solutions for Case 5 (A-B) and Case 6 (C-D).

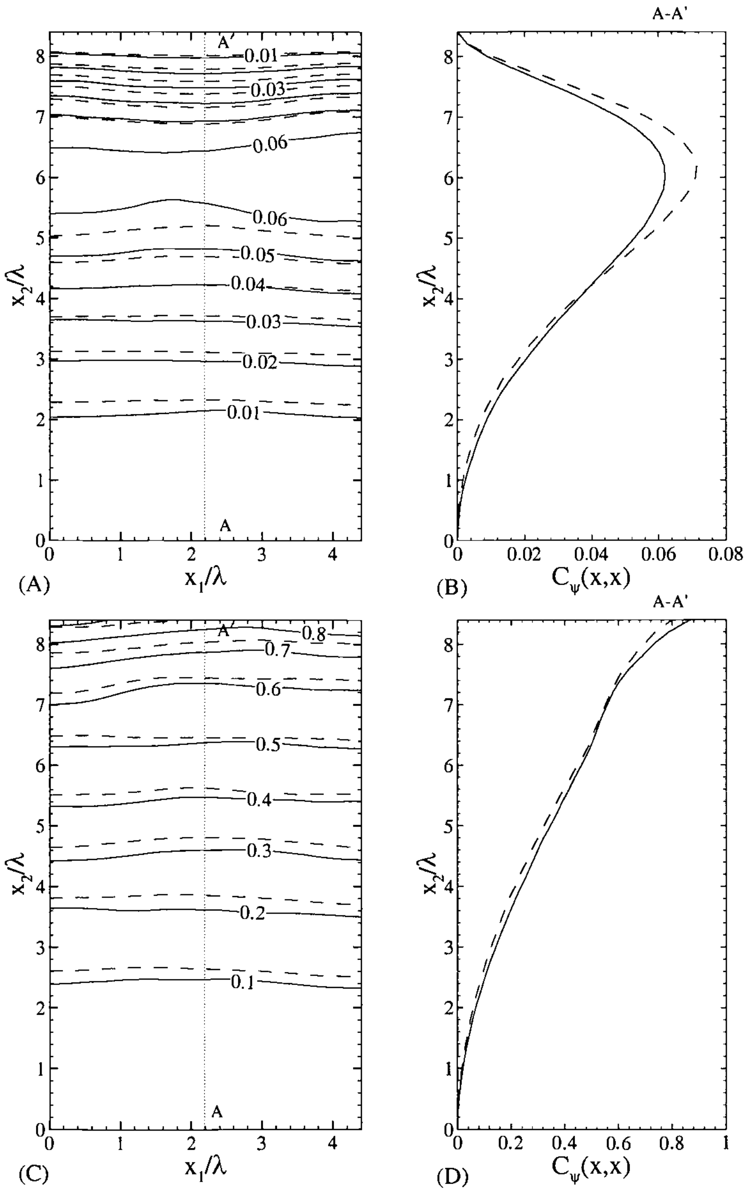


Figure 6.60. Variance of pressure head computed from Monte Carlo simulation (MC) and second-order solutions for Case 5 (A-B) and Case 6 (C-D).

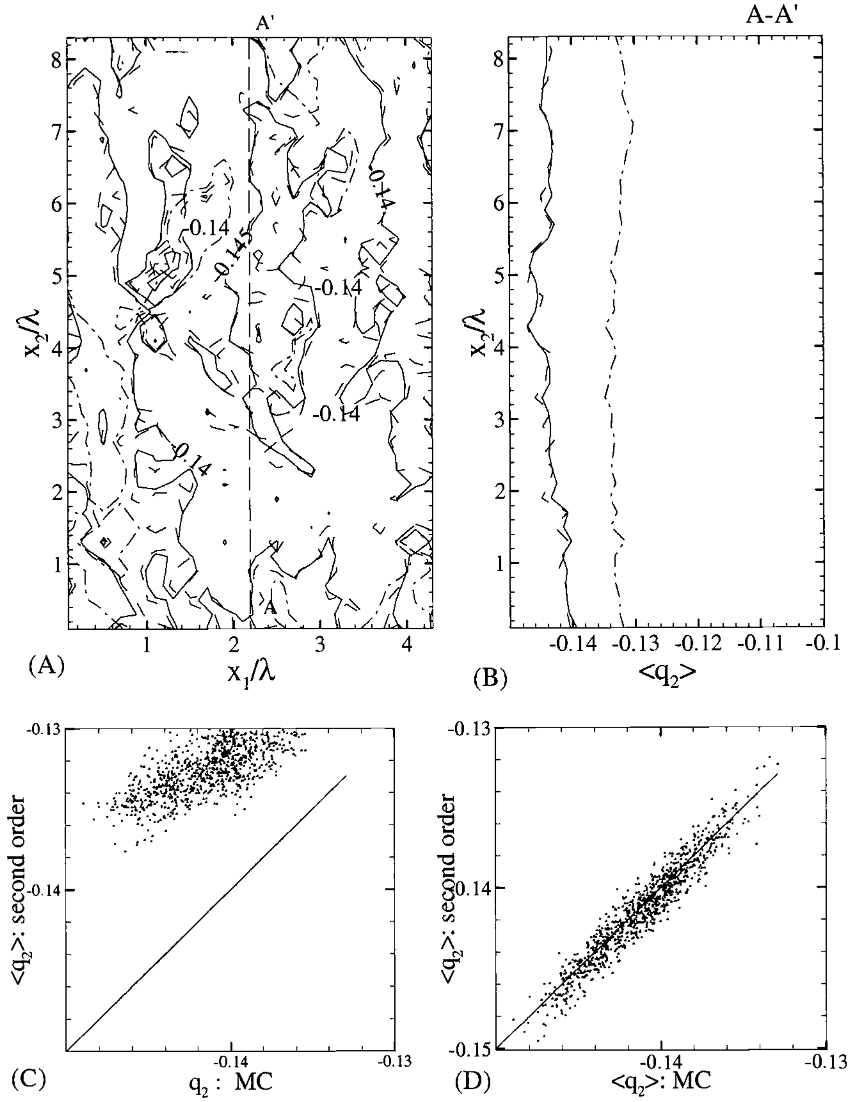


Figure 6.61. Mean longitudinal flux $\langle q_2 \rangle$ computed from Monte Carlo simulation (MC), zero-order and second-order solutions for Case 5 (prescribed pressure head at the upper boundary). (A) A contour map; (B) a profile along A-A'; (C)-(D) scatter plots of zero and second-order solutions against MC resluts.

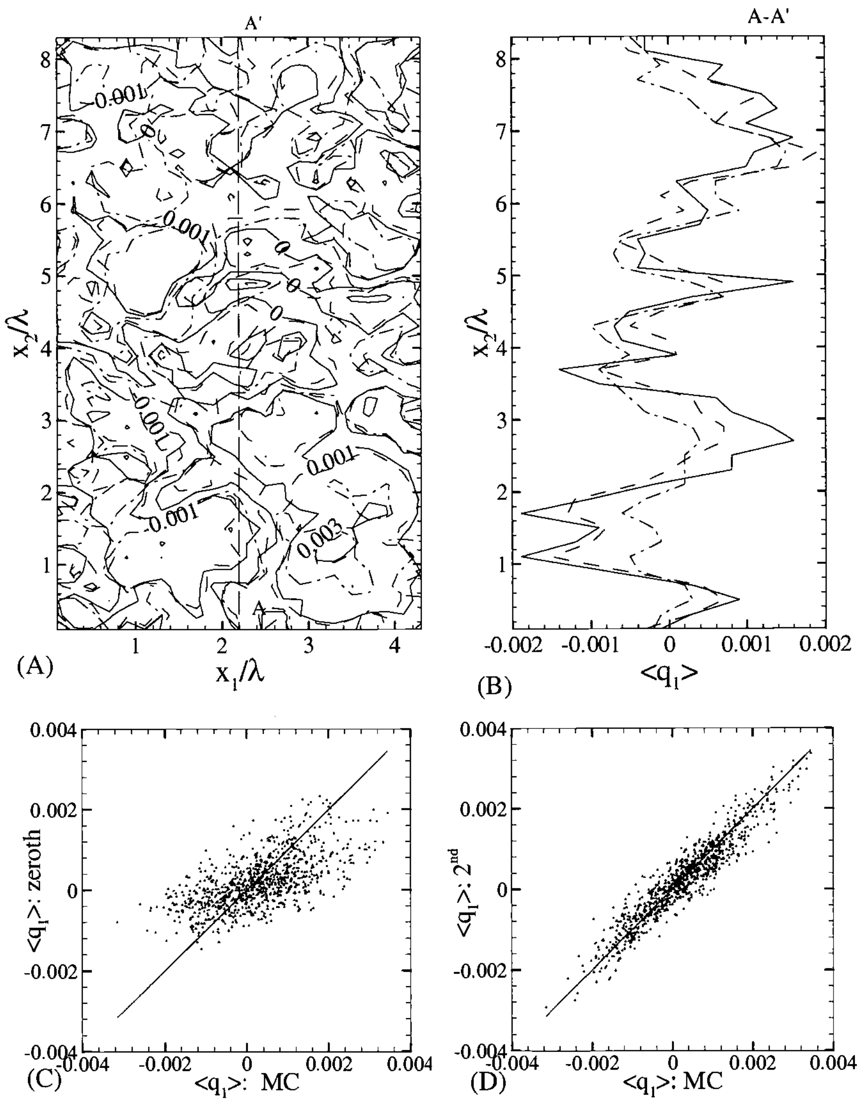


Figure 6.62. Mean transverse flux $\langle q_1 \rangle$ computed from Monte Carlo simulation (MC), zero-order and second-order solutions for Case 5 (prescribed pressure head at the upper boundary). (A) A contour map; (B) a profile along A-A'; (C)-(D) scatter plots of zero and second-order solutions against MC resluts.

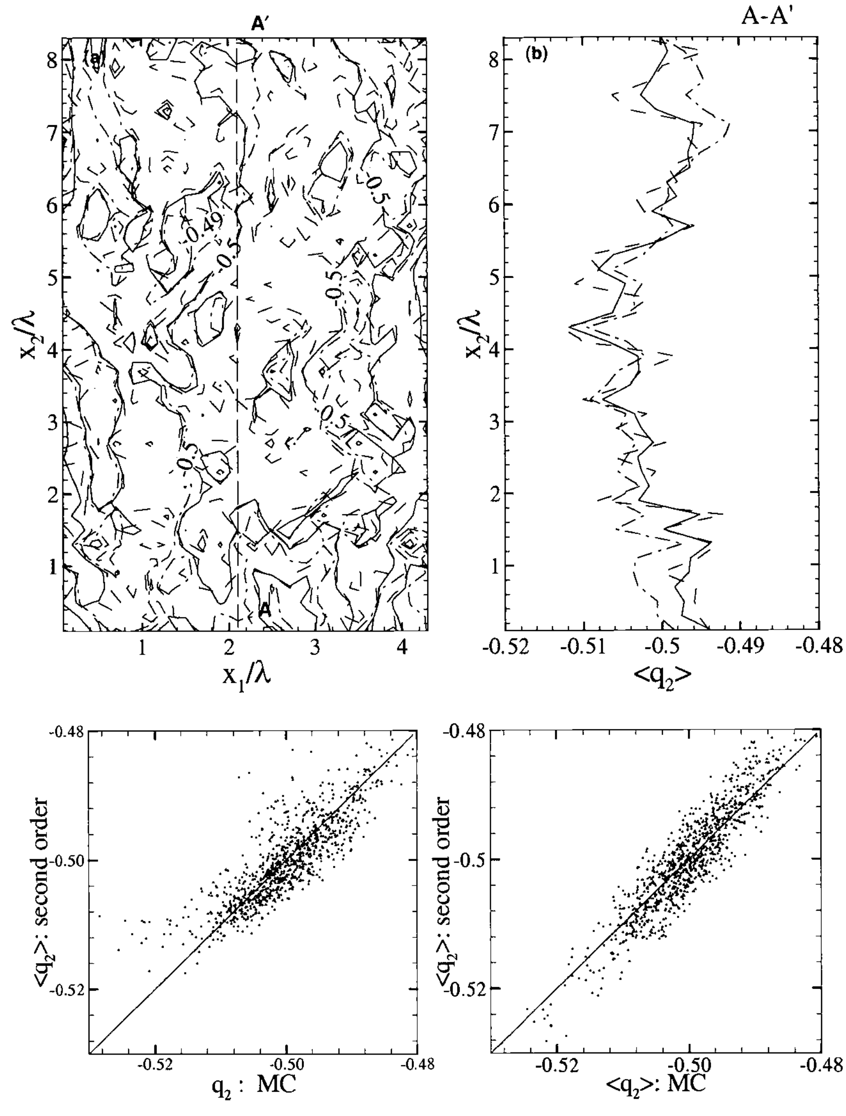


Figure 6.63. Mean longitudinal flux $\langle q_2 \rangle$ computed from Monte Carlo simulation (MC), zero-order and second-order solutions for Case 6 (prescribed flux at the upper boundary). (A) A contour map; (B) a profile along A-A'; (C)-(D) scatter plots of zero- and second-order solutions against MC resluts.

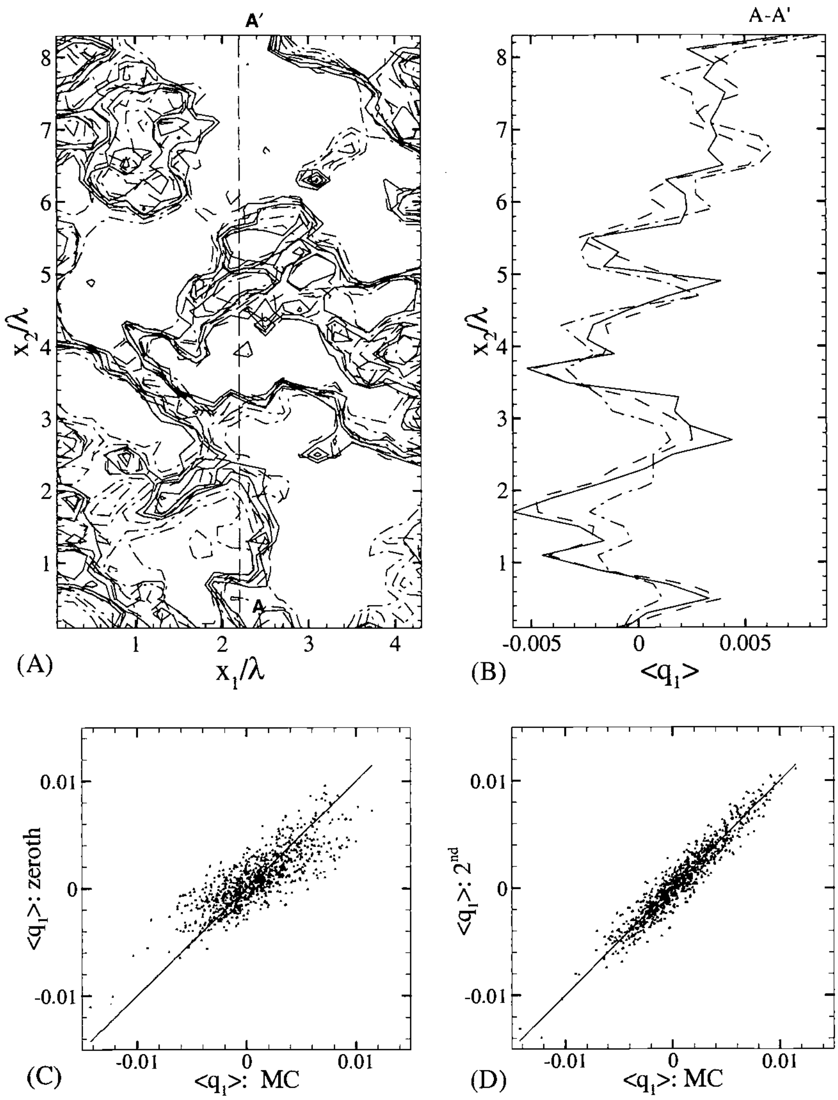


Figure 6.64. Mean transverse flux $\langle q_1 \rangle$ computed from Monte Carlo simulation (MC), zero-order and second-order solutions for Case 6 (prescribed flux at the upper boundary). (A) A contour map; (B) a profile along A-A'; (C)-(D) scatter plots of zero- and second-order solutions against MC resluts.

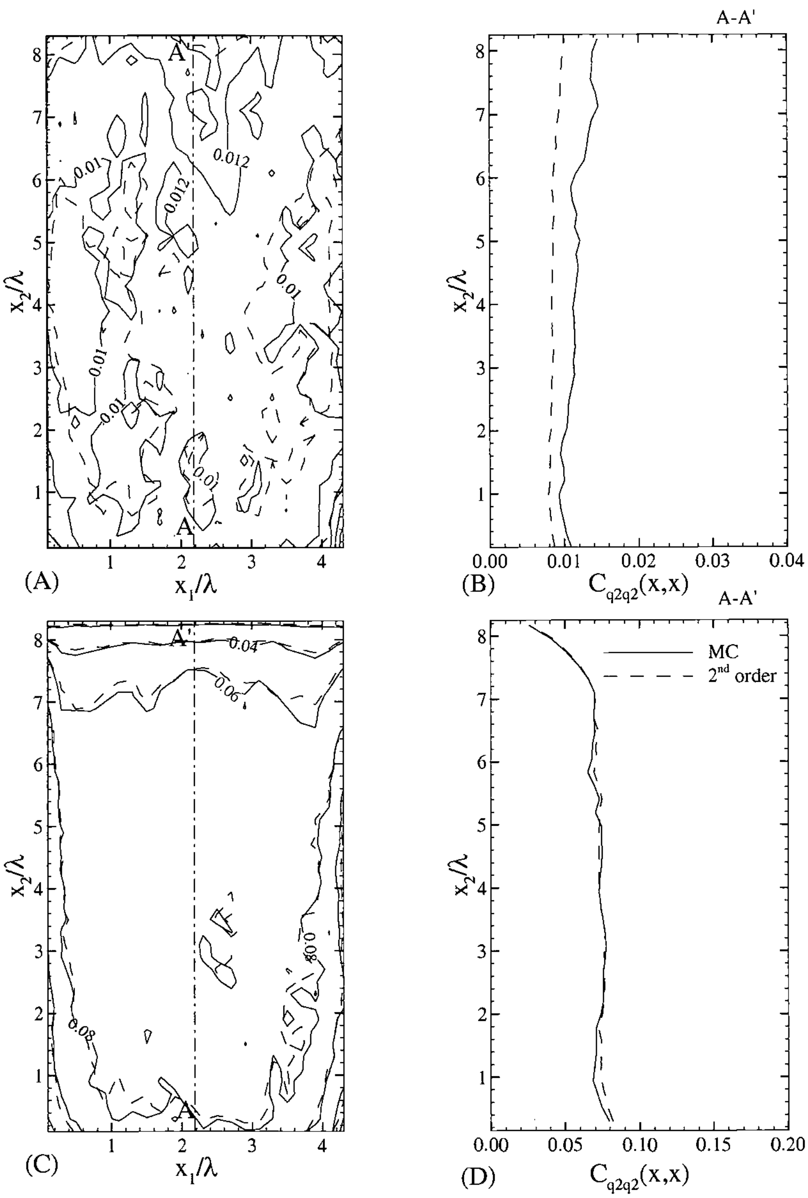


Figure 6.65. Variance of longitudinal flux computed from Monte Carlo simulation (solid), second-order solutions (dash) for Case 5 (A-B) and Case 6 (C-D).

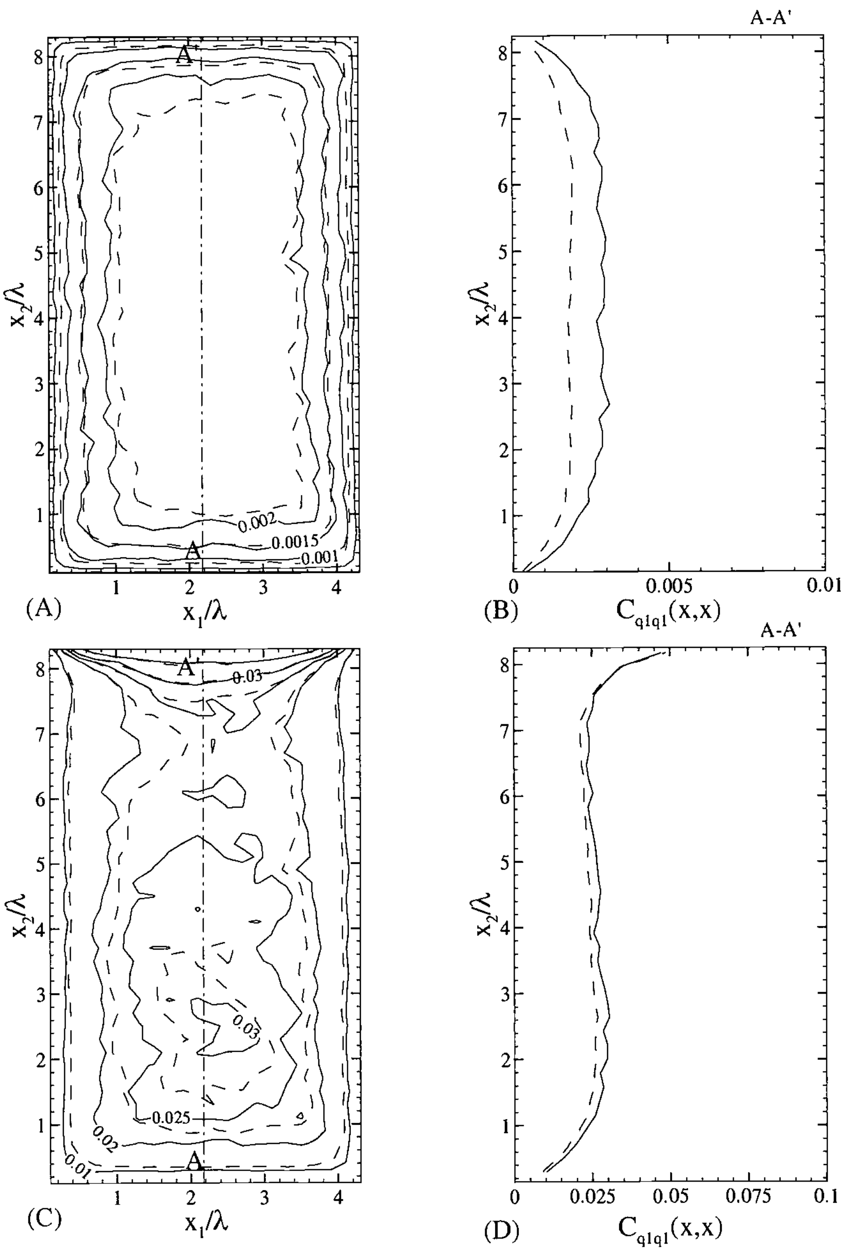


Figure 6.66. Variance of transverse flux computed from Monte Carlo simulation (solid) and second-order solutions (dash) for Case 5 (A-B) and Case 6 (C-D).

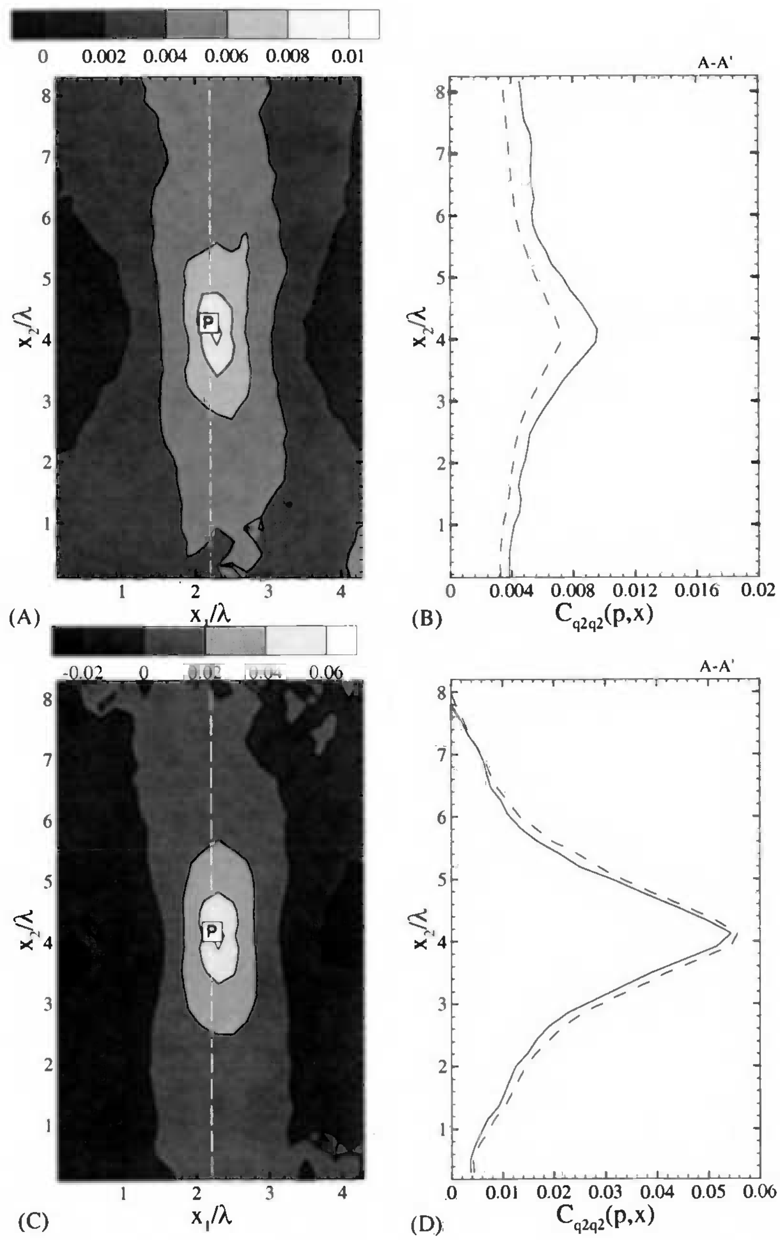


Figure 6.67. Auto-covariance of the longitudinal flux reference to point P, computed from Monte Carlo simulation (solid) and second-order solutions (dash) for Case 5 (A-B) and Case 6 (C-D).

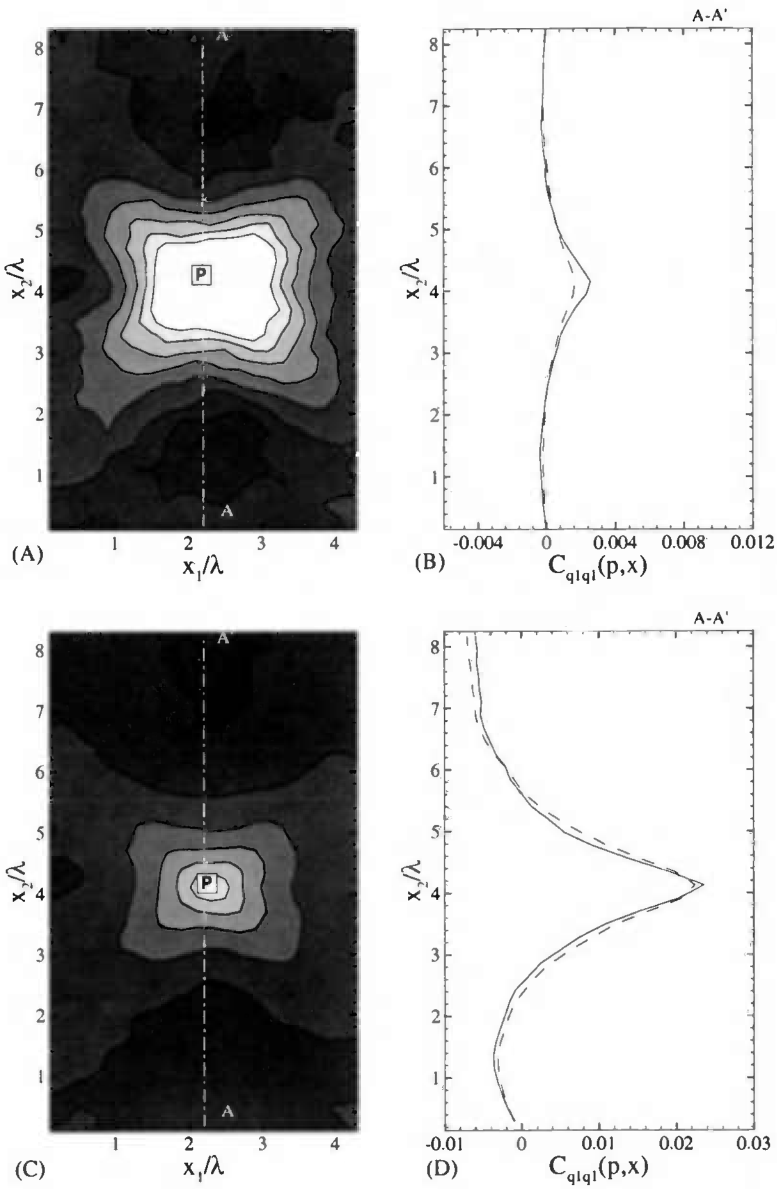


Figure 6.68. Auto-covariance of the transverse flux reference to point P, computed from Monte Carlo simulation (solid) and second-order solutions (dash) for Case 5 (A-B) and Case 6 (C-D).

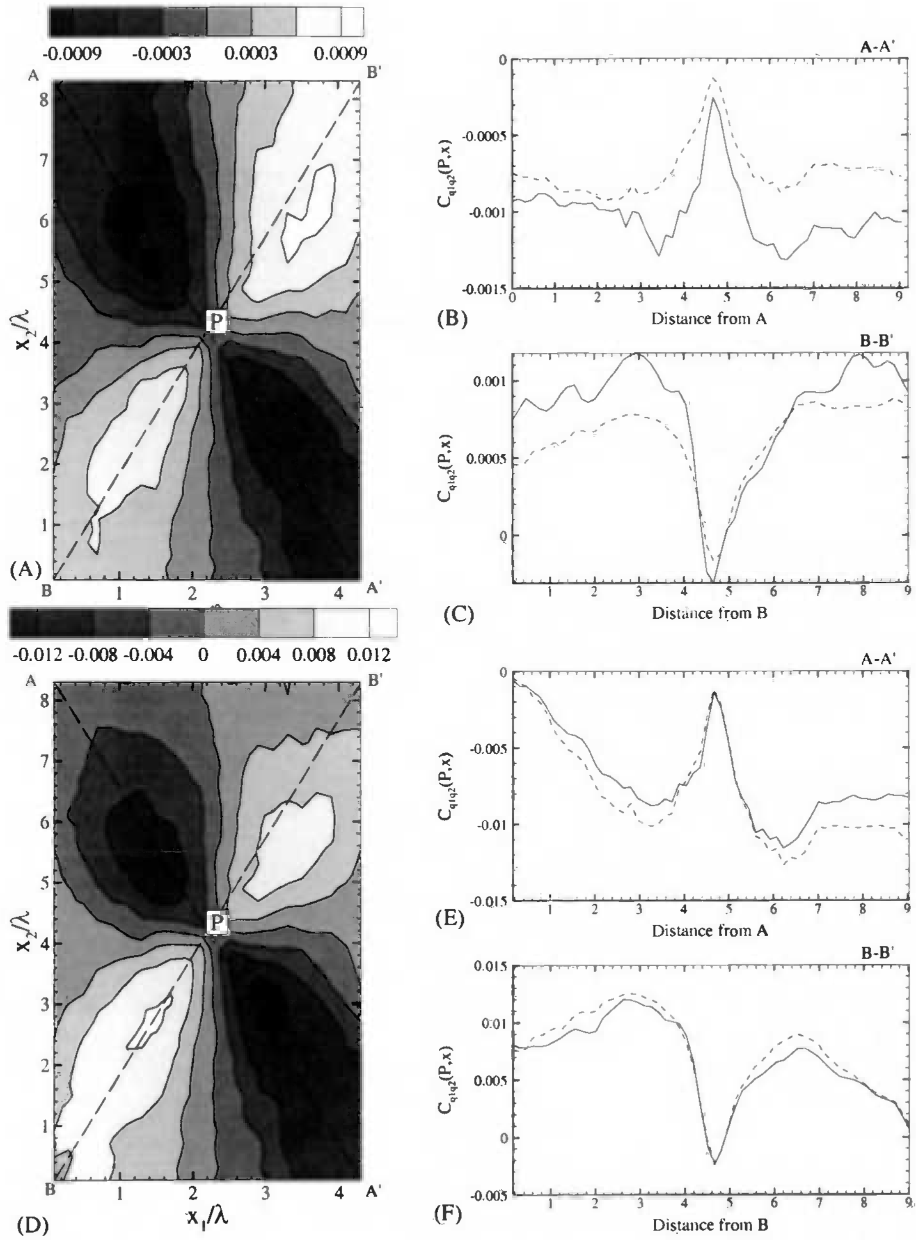


Figure 6.69. Cross-covariance between the longitudinal flux at all nodes and the transverse flux at pont P, computed from Monte Carlo simulation (solid), second-order solutions (dash) for Case 5 (A-C) and Case 6 (D-F).

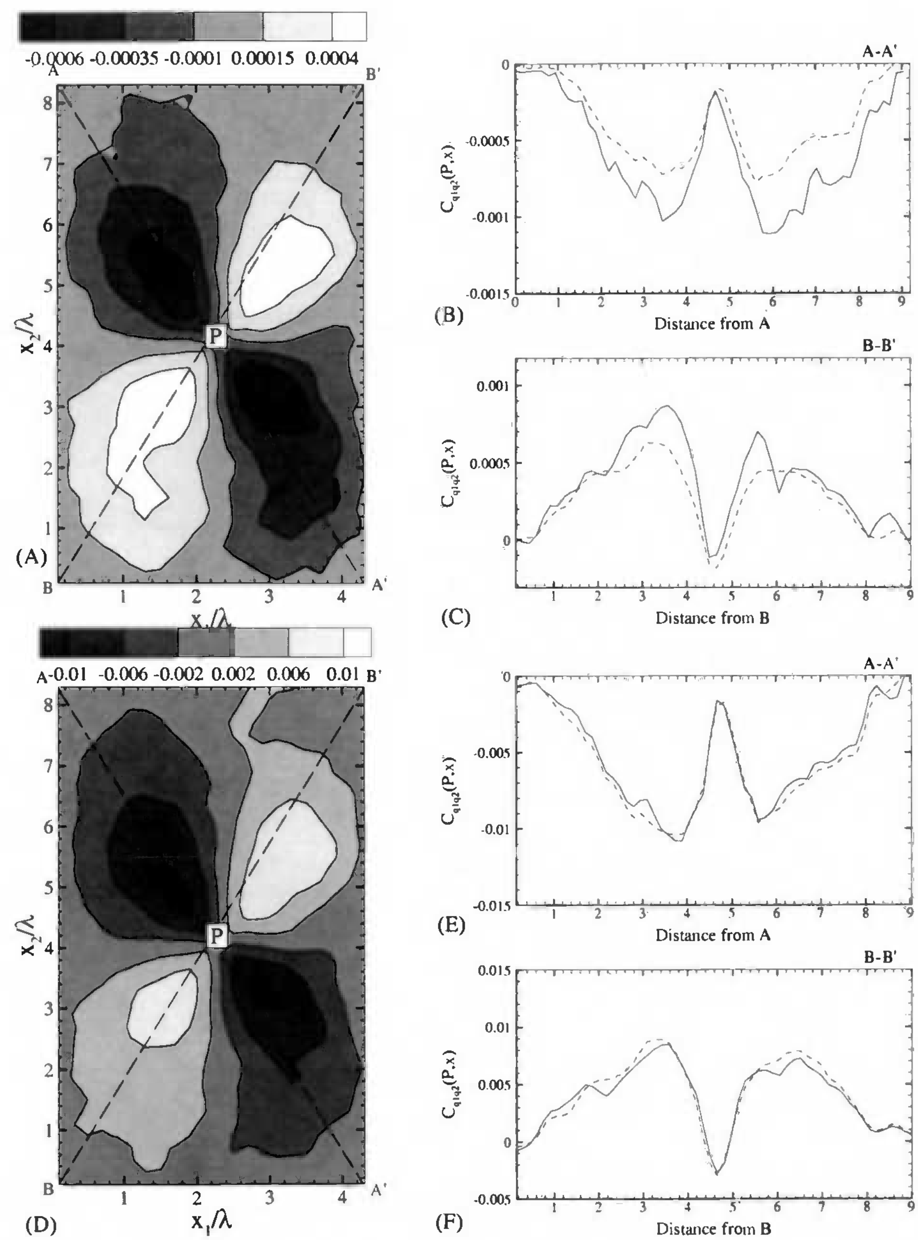


Figure 6.70. Cross-covariance between the transverse flux at all nodes and the longitudinal flux at pont P, computed from Monte Carlo simulation (solid), second-order solutions (dash) for Case 5 (A-C) and Case 6 (D-F).

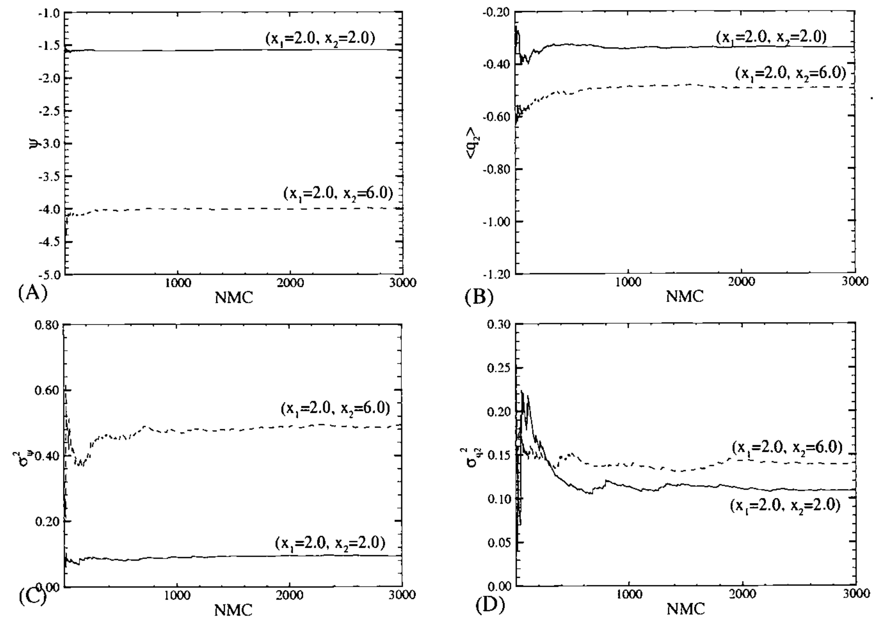


Figure 6.71. Convergence of MC simulations of (A) pressure head, (B) longitudinal flux, (C) variance of pressure head, and (D) variance of longitudinal flux for Case 1.

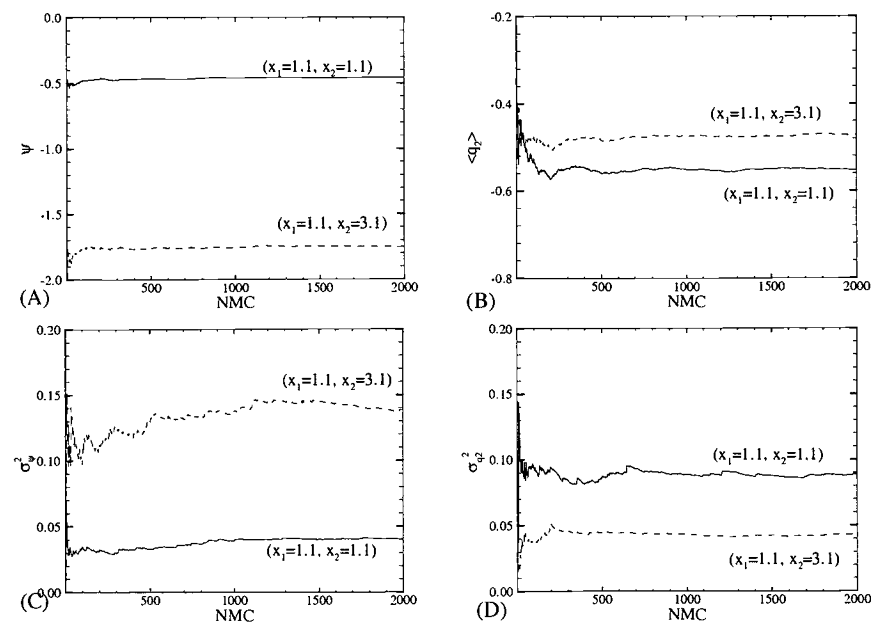


Figure 6.72. Convergence of MC simulations of (A) pressure head, (B) longitudinal flux, (C) variance of pressure head, and (D) variance of longitudinal flux for Case 4.

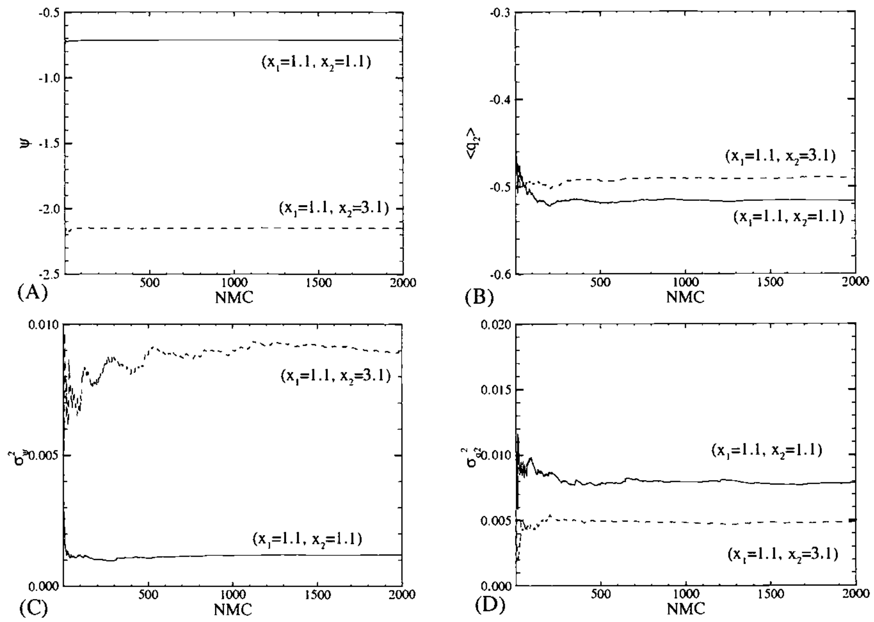


Figure 6.73. Convergence of MC simulations of (A) pressure head, (B) longitudinal flux, (C) variance of pressure head, and (D) variance of longitudinal flux for the case which is the same as Case 4 except for σ_Y^2=0.1.

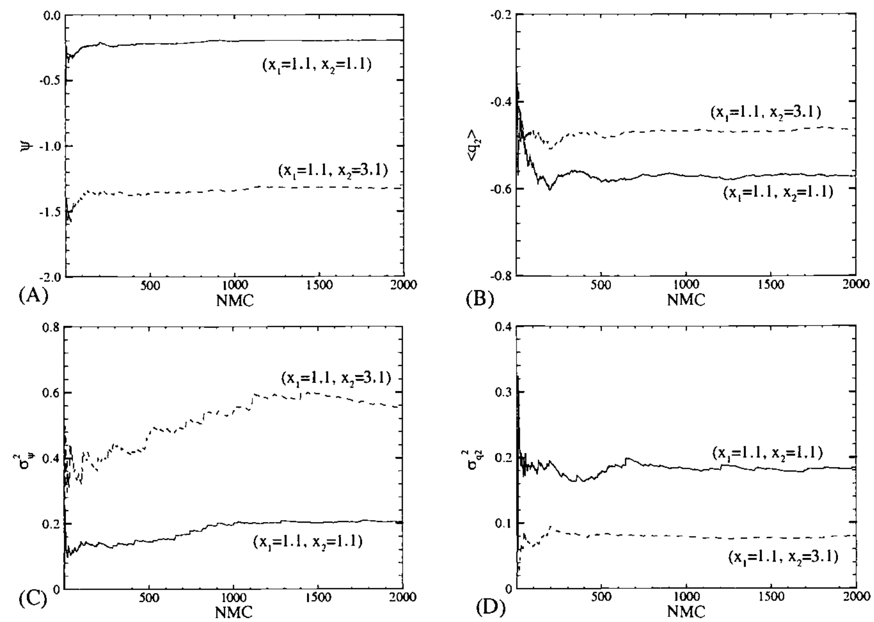


Figure 6.74. Convergence of MC simulations of (A) pressure head, (B) longitudinal flux, (C) variance of pressure head, and (D) variance of longitudinal flux for the case which is the same as Case 4 except for σ_Y^2=2.0..

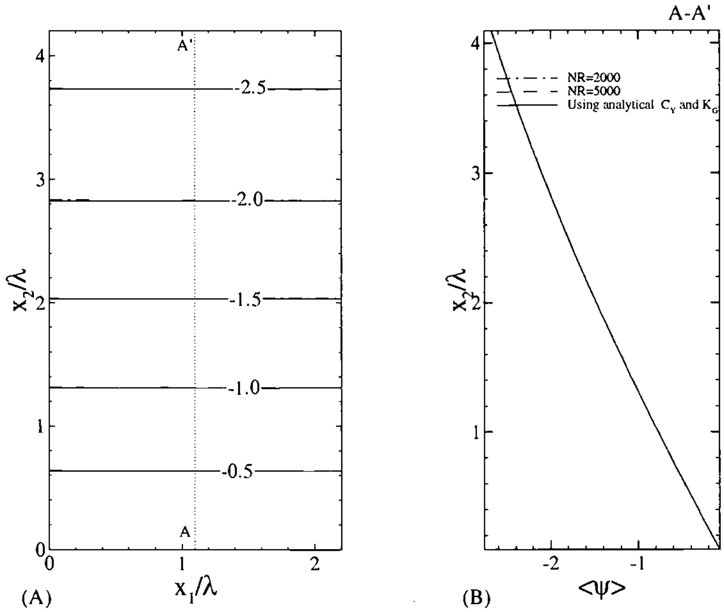


Figure 6.75. Second-order mean pressure head calcluated using 2,000 realizations (dash-dotted lines), 5,000 realizations (dashed lines), and analytical mean Y and C_Y (solid lines).

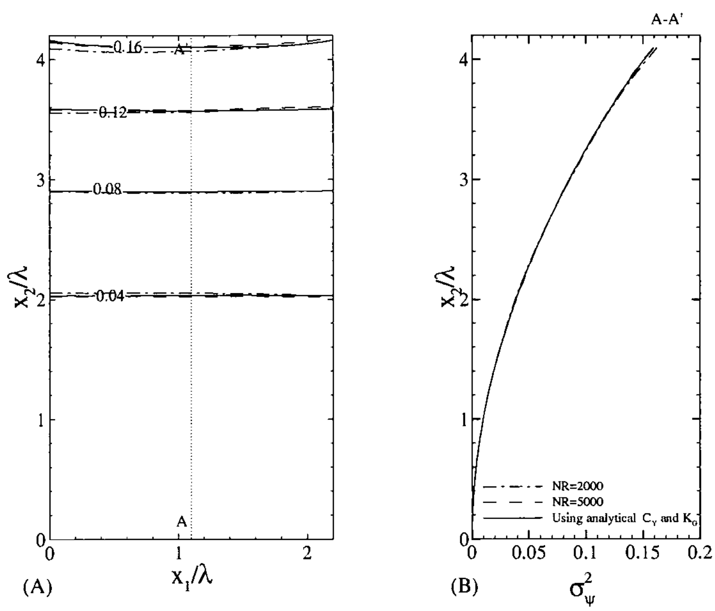


Figure 6.76. Variance of pressure head calcluated using 2,000 realizations (dash-dotted lines), 5,000 realizations (dashed lines), and analytical mean *Y* and C_Y (solid lines).

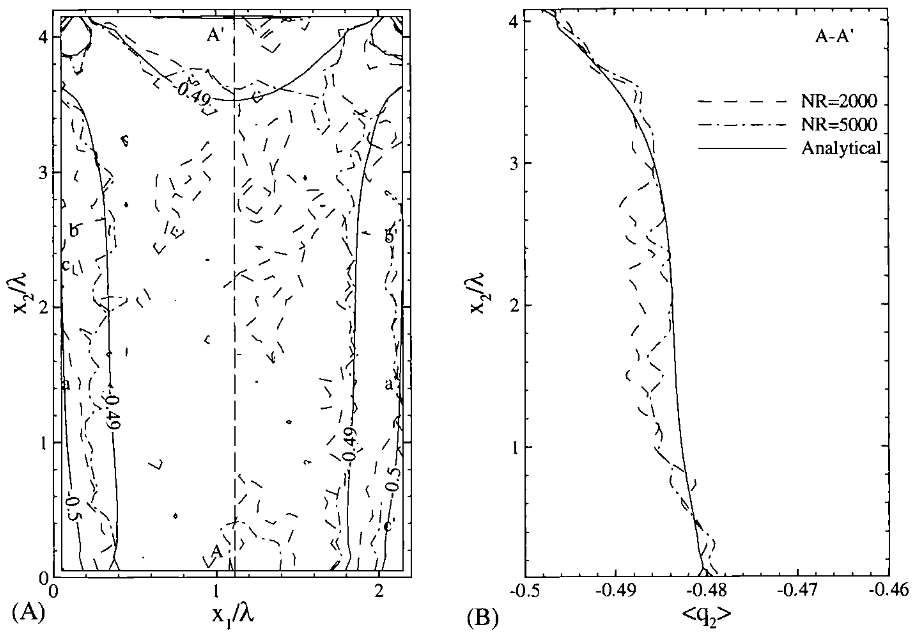


Figure 6.77. Longitudinal flux calcluated using 2,000 realizations (dash-dotted lines), 5,000 realizations (dashed lines), and analytical mena Y and C_Y (solid lines). (A) A contour map, and (B) a profile along A-A'.

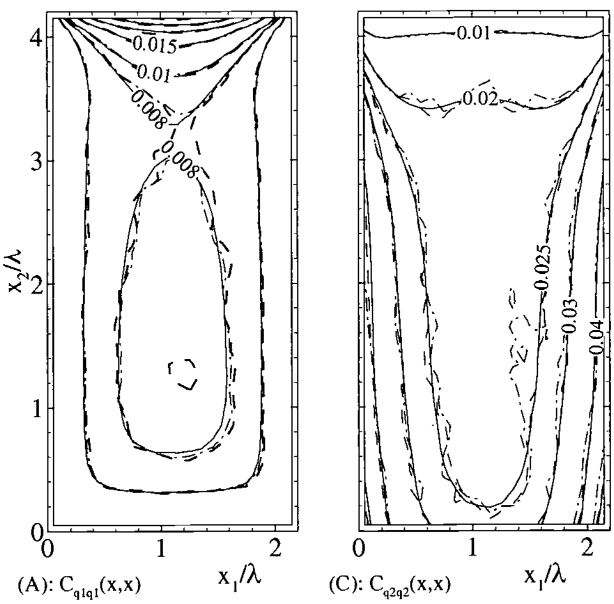


Figure 6.78. Variance of the transvere flux and longitudinal flux calcluated using 2,000 realizations (dash-dotted lines), 5,000 realizations (dashed lines), and analytical mena Y and C_Y (solid lines).

CHAPTER 7

CONCLUSIONS

On the line of *Tartakovsky et al* [1999], we developed a deterministic alternative to conditional Monte Carlo simulation to predict steady-state unsaturated flow in randomly heterogeneous soils with uncertainties in driving forces, without resorting to Monte Carlo simulation, upscaling or linearization of the constitutive relationship between unsaturated hydraulic conductivity and pressure head. By assuming that the Gardner model is valid and treating the corresponding exponent α as a random constant, the steady state unsaturated flow equations can be linearized by means of the Kirchhoff transformation. This allows us develop exact integro-differential equations for the conditional first and second moments of transformed pressure head and flux. The predictions of system states and fluxes are made by means of first ensemble moments, conditioned at measured values of soil properties. The uncertainties associated with these predictions, also conditioned at the measured values of the soil properties, are assessed by conditional second moments.

Although the derived conditional moment equations are exact, they are not workable unless some kinds of closure approximations are employed. The approximation we used in this research is perturbation analysis. Expending all related terms in exact conditional moment equations as powers of σ_Y and σ_β leads to recursive equations. These recursive equations are then solved numerically using finite element methods. The validity of the perturbation method is normally limited for flow in soils with mild heterogeneity. However, the method can be applied to strong heterogeneous soils, as long as the hydraulic properties are conditioned at some measurement points.

Our approach has several advantages over Monte Carlo simulations. First, the computational demand will be reduced. All conditional parameters in our conditional moment equations are smoother than their random counterpart in the original flow equations, and therefore these moment equations can be solved using a relative coarse grid. In Monte Carlo simulation, the number of times to solve flow equations required to make solution convergent increases as the heterogeneity of the soil increases, while in our approach, the number of times is fixed, since moment equations are deterministic. More importantly, even if Monte Carlo simulation converges, there is no guarantee that they converge to the true solution. Numerical examples show that our second-order nonlocal solutions are superior to zero-order local solutions and are much closer to Monte Carlo simulations, which makes our approach to be an excellent alternative.

Instead of assuming statistically homogeneous hydraulic conductivity field as most of existing models did, our moment equations are conditioned at some measurement points, which renders the hydraulic field statistically non-homogeneous. The effects of conditioning can be summarized as follows. First, numerical examples show that even a few conditioning points may allow us to model unsaturated flow in strongly heterogeneous soils (for example, $\sigma_Y^2 = 2$ in Case 1). Second, though conditioning does not change the mean pressure head field drastically, it reduces the uncertainty associated with mean pressure head prediction and improves the quality of our second-order nonlocal solutions (closer to Monte Carlo results). In addition, conditioning points affect the overall flow pattern significantly, but it does not necessarily reduce the variance of flux for all cases, especially when some other factors, such as point sources, are present. Furthermore, although our second-order solutions for flux are superior to zero-order solutions in all cases, the zero-order solutions are very close to Monte Carlo results in the conditional case. This means that the flux filed obtained from zero-order solutions may be accurate enough for well-conditioned soils.

Unlike some other models that are applicable only to statistically uniform flow (or statistically uniform mean hydraulic gradient), our model allows us to deal with non-uniform flows, which for example may be caused by point sources in the domain. Our numerical examples show that point sources have significant effect on mean flow and it associated variance. The point source increases the variance of pressure head and the variance of flux.

APPENDIX A
DIRICHLET BOUNDARY CONDITIONS RELATED TO THE TRANSFORMED VARIABLE

A.1 INTRODUCTION

In Chapter 2 we showed that the original nonlinear Richards equation could be transformed into a linear equation by means of the Kirchhoff transformation. However, the transformation transforms the prescribed pressure head $\Psi(\boldsymbol{x})$ on the Dirichlet boundary to

$$\Phi(\boldsymbol{x}) = H(\boldsymbol{x}), \quad H(\boldsymbol{x}) = \frac{1}{\alpha} e^{\alpha\Psi(\boldsymbol{x})} \qquad \boldsymbol{x} \in \Gamma_D \qquad \text{(A-1)}$$

which introduces some difficulties in dealing with this boundary condition, especially when the parameter α is not a deterministic constant. In solving for the mean Kirchhoff-transformed variable Φ, we need to know its value at the Dirichlet boundary. In addition, both implicit and explicit perturbation equations for Φ, i.e., (2-17) and (2-19), include a term related to H', the perturbation of H, either as a Dirichlet boundary condition or as a boundary integral over the Dirichlet boundary. Even in the case that the original pressure head is deterministic on the Dirichlet boundary, i.e., $\Psi' = 0$, the transformed variable Φ is not necessarily deterministic on the boundary. As a result, in each (cross-)covariance function associated with Φ, there exists a term related to H' that needs to be evaluated before solving for (cross-)covariance functions. In this appendix, we derived mean H to second order in section A.2; obtained an perturbation expression for H' in section A.3, which is the basis for formulating cross-moments; and in sections A.4 and A.5, we formulated all terms that are related to H'.

A.2 EXPRESSION FOR THE PRESCRIBED MEAN Φ, $\langle H(x)\rangle$, ON THE DIRICHLET BOUNDARY

Rewriting equation (2-10) as

$$\alpha H(\boldsymbol{x}) = \exp\left(\alpha\Psi(\boldsymbol{x})\right) \qquad \boldsymbol{x}\in\Gamma_D \tag{A-2}$$

expanding its left side

$$\langle\alpha\rangle\langle H(\boldsymbol{x})\rangle + \langle\alpha\rangle H'(\boldsymbol{x}) + \alpha'\langle H(\boldsymbol{x})\rangle + \alpha' H'(\boldsymbol{x}) = \exp\left(\alpha\Psi(\boldsymbol{x})\right) \qquad \boldsymbol{x}\in\Gamma_D \tag{A-3}$$

and multiplying (A-3) by $\langle\alpha\rangle^2$-$\langle\alpha\rangle\alpha'$+$\alpha'^2$ yields

$$\langle\alpha\rangle^3\langle H(\boldsymbol{x})\rangle + \langle\alpha\rangle^3 H'(\boldsymbol{x}) + \alpha'^3 H(\boldsymbol{x}) = \left(\langle\alpha\rangle^2 - \langle\alpha\rangle\alpha' + \alpha'^2\right)\exp\left(\alpha\Phi(\boldsymbol{x})\right) \qquad \boldsymbol{x}\in\Gamma_D \tag{A-4}$$

Splitting $\Psi(\boldsymbol{x})$ into its mean $\langle\Psi(\boldsymbol{x})\rangle$ and perturbation $\Psi'(\boldsymbol{x})$, expanding α as

$$\alpha = e^{\beta} = e^{\langle\beta\rangle+\beta'} = \alpha_G \sum_{m=0}^{\infty}\frac{\beta'^m}{m!} \tag{A-5}$$

where α_G is the geometric mean α, and substituting (A-5) into $\exp(\alpha\Psi(\boldsymbol{x}))$

$$
\begin{aligned}
&\exp[\alpha\Psi(x)] \\
&= \exp\left[\alpha_G\left(1+\beta'+\frac{1}{2}\beta'^2\right)\left(\langle\Psi(x)\rangle+\Psi'(x)\right)\right]+HO \\
&= e^{\alpha_G\langle\Psi(x)\rangle}\Bigg[1+\alpha_G\Psi'(x)+\alpha_G\langle\Psi(x)\rangle\beta'+\frac{1}{2}\alpha_G^2\Psi'^2(x)+\frac{1}{2}\alpha_G\langle\Psi(x)\rangle\left(1+\alpha_G\langle\Psi(x)\rangle\right)\beta'^2 \\
&\qquad +\alpha_G\left(1+\alpha_G\langle\Psi(x)\rangle\right)\beta'\Psi'(x)+\frac{1}{2}\alpha_G\left(1+3\alpha_G\langle\Psi(x)\rangle+\alpha_G^2\langle\Psi(x)\rangle^2\right)\beta'^2\Psi'(x) \\
&\qquad +\alpha_G^2\left(1+\frac{1}{2}\alpha_G\langle\Psi(x)\rangle\right)\beta'\Psi'^2(x)+\frac{1}{4}\alpha_G^2\left(4+5\alpha_G\langle\Psi(x)\rangle+\alpha_G^2\langle\Psi(x)\rangle^2\right)\beta'^2\Psi'^2(x)\Bigg]+HO
\end{aligned}
\tag{A-6}
$$

Here HO is the sum of higher-order terms, because we are only interested in terms that are up to second order in σ_β and σ_Ψ (this equation is independent of σ_Y). Since we assume that the prescribed pressure head Ψ on the Dirichlet boundary is independent of medium properties, its mean $\langle\Psi(x)\rangle$ does not need to be expanded in powers of σ_Y and σ_β. Substituting (A-6) into (A-4), taking conditional ensemble mean, and rearranging, yields an expression for $\langle H(x)\rangle$

$$
\begin{aligned}
&\langle\alpha\rangle^3\langle H(x)\rangle+HO \\
&= e^{\alpha_G\langle\Psi(x)\rangle}\Bigg[\left(\langle\alpha\rangle^2+\langle\alpha'^2\rangle\right)\left(1+\frac{1}{2}\alpha_G^2\sigma_\Psi^2(x)\right) \\
&\qquad +\frac{1}{2}\alpha_G\langle\alpha\rangle\langle\Psi(x)\rangle\left[\langle\alpha\rangle\left(1+\alpha_G\langle\Psi(x)\rangle\right)-2\alpha_G\right]\langle\beta'^2\rangle \\
&\qquad +\alpha_G^2\sigma_\Psi^2(x)\left(\frac{\langle\alpha\rangle}{4}\left(4+5\alpha_G\langle\Psi(x)\rangle+\alpha_G^2\langle\Psi(x)\rangle^2\right)-\frac{\alpha_G}{2}\left(2+\alpha_G\langle\Psi(x)\rangle\right)\right)\langle\alpha\rangle\langle\beta'^2\rangle\Bigg]
\end{aligned}
\tag{A-7}
$$

where $\sigma_\Psi^2 = \langle\Psi'^2\rangle$ is the variance of prescribed preesure head on the Dirichlet boundary. Taking emsenble mean of (A-5) and expanding $\langle H(x)\rangle$ in (A-7) in powers of σ_Y and σ_β,

$$
\langle H(x)\rangle=\sum_{n=0}^{\infty}\sum_{m=0}^{\infty}\langle H^{(n,m)}(x)\rangle \tag{A-8}
$$

where n and m designates terms including n^{th} power of σ_Y and m^{th} power of σ_β, and equating terms with the same order on the two sides gives

$$\left\langle H^{(0,0)}(\boldsymbol{x})\right\rangle = \frac{e^{\alpha_G\langle\Psi(\boldsymbol{x})\rangle}}{\alpha_G}\left(1+\frac{1}{2}\alpha_G^2\sigma_\Psi^2(\boldsymbol{x})\right)$$
$$\left\langle H^{(0,2)}(\boldsymbol{x})\right\rangle = \frac{\sigma_\beta^2}{2}\frac{e^{\alpha_G\langle\Psi(\boldsymbol{x})\rangle}}{\alpha_G}\left[1+\alpha_G\left\langle\Psi(\boldsymbol{x})\right\rangle\ \left(\alpha_G\left\langle\Psi(\boldsymbol{x})\right\rangle-1\right)+0.5\alpha_G^2\left(1+3\alpha_G\left\langle\Psi(\boldsymbol{x})\right\rangle+\alpha_G^2\left\langle\Psi(\boldsymbol{x})\right\rangle^2\right)\sigma_\Psi^2(\boldsymbol{x})\right]$$

(A-9)

Here we take $\langle\Psi(\boldsymbol{x})\rangle$ and $\sigma_\Psi^2(\boldsymbol{x})$ to be system inputs that do not depend on medium properties. Other lower-order terms, such as $\left\langle H^{(0,1)}(\boldsymbol{x})\right\rangle$ and $\left\langle H^{(2,0)}(\boldsymbol{x})\right\rangle$, are zero and have been omitted in (A-9). For deterministic pressure head boundary condition, i.e., $\sigma_\Psi^2(\boldsymbol{x}) \equiv 0$, (A-9) is simplified to

$$\left\langle H^{(0,0)}(\boldsymbol{x})\right\rangle = \frac{1}{\alpha_G}e^{\alpha_G\langle\Psi(\boldsymbol{x})\rangle}$$
$$\left\langle H^{(0,2)}(\boldsymbol{x})\right\rangle = \frac{\sigma_\beta^2}{2}\frac{e^{\alpha_G\langle\Psi(\boldsymbol{x})\rangle}}{\alpha_G}\left[1+\alpha_G\left\langle\Psi(\boldsymbol{x})\right\rangle\left(\alpha_G\left\langle\Psi(\boldsymbol{x})\right\rangle-1\right)\right] \qquad \text{(A-10)}$$

A.3 EXPRESSION FOR THE PERTURBATION TERM $H'(x)$

Substituting (A-6) into (A-4) yields an expression for H'

$$
\begin{aligned}
\langle\alpha\rangle^3 H'(\boldsymbol{x}) = e^{\alpha_G\langle\Psi(\boldsymbol{x})\rangle}\Big[&\langle\alpha\rangle^2 + \alpha_G\langle\alpha\rangle^2\Psi'(\boldsymbol{x}) + \alpha_G\langle\alpha\rangle^2\langle\Psi(\boldsymbol{x})\rangle\beta' - \langle\alpha\rangle\alpha' + \frac{1}{2}\alpha_G^2\langle\alpha\rangle^2\Psi'^2(\boldsymbol{x}) \\
&+\frac{1}{2}\alpha_G\langle\alpha\rangle^2\langle\Psi(\boldsymbol{x})\rangle\left(1+\alpha_G\langle\Psi(\boldsymbol{x})\rangle\right)\beta'^2 - \alpha_G\langle\alpha\rangle\langle\Psi(\boldsymbol{x})\rangle\alpha'\beta' + \alpha'^2 \\
&+\alpha_G\langle\alpha\rangle^2\left(1+\alpha_G\langle\Psi(\boldsymbol{x})\rangle\right)\beta'\Psi'(\boldsymbol{x}) - \alpha_G\langle\alpha\rangle\alpha'\Psi'(\boldsymbol{x}) \\
&+\frac{1}{2}\alpha_G\langle\alpha\rangle^2\left(1+3\alpha_G\langle\Psi(\boldsymbol{x})\rangle + \alpha_G^2\langle\Psi(\boldsymbol{x})\rangle^2\right)\beta'^2\Psi'(\boldsymbol{x}) \\
&-\alpha_G\langle\alpha\rangle\left(1+\alpha_G\langle\Psi(\boldsymbol{x})\rangle\right)\alpha'\beta'\Psi'(\boldsymbol{x}) + \alpha_G\alpha'^2\Psi'(\boldsymbol{x}) \\
&+\alpha_G^2\langle\alpha\rangle^2\left(1+\frac{1}{2}\alpha_G\langle\Psi(\boldsymbol{x})\rangle\right)\beta'\Psi'^2(\boldsymbol{x}) - \frac{1}{2}\alpha_G^2\langle\alpha\rangle\alpha'\Psi'^2(\boldsymbol{x}) \\
&+\frac{1}{4}\alpha_G^2\langle\alpha\rangle^2\left(4+5\alpha_G\langle\Psi(\boldsymbol{x})\rangle + \alpha_G^2\langle\Psi(\boldsymbol{x})\rangle^2\right)\beta'^2\Psi'^2(\boldsymbol{x}) \\
&-\alpha_G^2\langle\alpha\rangle\left(1+\frac{1}{2}\alpha_G\langle\Psi(\boldsymbol{x})\rangle\right)\alpha'\beta'\Psi'^2(\boldsymbol{x}) + \frac{1}{2}\alpha_G^2\langle\alpha\rangle\alpha'^2\Psi'^2(\boldsymbol{x})\Big] \\
-\langle\alpha\rangle^3\langle H(\boldsymbol{x})\rangle + HO&
\end{aligned}
\tag{A-11}
$$

This is the basis for formulating cross-moments associated with H'.

A.4 H'-RELATED TERMS AS BOUNDARY CONDITIONS

Recall the Dirichlet boundary condition of the implicit equation for Φ'

$$\Phi'(\boldsymbol{x}) = H'(\boldsymbol{x}) \qquad \boldsymbol{x}\in\Gamma_D \tag{A-12}$$

If we formulate a cross-moment associated with Φ' using the implicit equation for Φ', i.e., (2-17), we will have a term related to H' as its Dirichlet boundary condition. All this types of H'-related terms will be evaluated in this section.

A.4.1 Cross-covariance $\langle H'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle$

To evaluate the covariance function $C_\Phi(\boldsymbol{x}, \boldsymbol{y})$, we need to find the cross-covariance of $H(\boldsymbol{x})$ and $\Phi(\boldsymbol{y})$, $\langle H'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle$. This can be derived upon multiplying (A-11) by $\Phi'(\boldsymbol{y})$ and taking conditional ensemble mean

$$
\begin{aligned}
&\langle\alpha\rangle^3 \langle H'(x)\Phi'(y)\rangle \\
&\quad = e^{\alpha_G\langle\Psi(x)\rangle}\Bigg[\alpha_G \langle\alpha\rangle^2 \langle\Psi'(x)\Phi'(y)\rangle + \frac{1}{2}\alpha_G^2 \langle\alpha\rangle^2 \langle\Psi'^2(x)\Phi'(y)\rangle \\
&\qquad + \alpha_G \langle\alpha\rangle^2 \left(1+\alpha_G \langle\Psi(x)\rangle\right)\langle\beta'\Psi'(x)\Phi'(y)\rangle - \alpha_G \langle\alpha\rangle\langle\alpha'\Psi'(x)\Phi'(y)\rangle \\
&\qquad + \frac{1}{2}\alpha_G \langle\alpha\rangle^2 \left(1+3\alpha_G \langle\Psi(x)\rangle + \alpha_G^2 \langle\Psi(x)\rangle^2\right)\langle\beta'^2\Psi'(x)\Phi'(y)\rangle \\
&\qquad - \alpha_G \langle\alpha\rangle\left(1+\alpha_G \langle\Psi(x)\rangle\right)\langle\alpha'\beta'\Psi'(x)\Phi'(y)\rangle + \alpha_G \langle\alpha'^2\Psi'(x)\Phi'(y)\rangle \\
&\qquad + \alpha_G^2 \langle\alpha\rangle^2\left(1+\frac{1}{2}\alpha_G \langle\Psi(x)\rangle\right)\langle\beta'\Psi'^2(x)\Phi'(y)\rangle - \frac{1}{2}\alpha_G^2 \langle\alpha\rangle\langle\alpha'\Psi'^2(x)\Phi'(y)\rangle \\
&\qquad + \frac{1}{4}\alpha_G^2 \langle\alpha\rangle^2 \left(4+5\alpha_G \langle\Psi(x)\rangle + \alpha_G^2 \langle\Psi(x)\rangle^2\right)\langle\beta'^2\Psi'^2(x)\Phi'(y)\rangle \\
&\qquad - \alpha_G^2 \langle\alpha\rangle\left(1+\frac{1}{2}\alpha_G \langle\Psi(x)\rangle\right)\langle\alpha'\beta'\Psi'^2(x)\Phi'(y)\rangle + \frac{1}{2}\alpha_G^2 \langle\alpha\rangle\langle\alpha'^2\Psi'^2(x)\Phi'(y)\rangle \\
&\qquad + \alpha_G \langle\alpha\rangle\left(\langle\alpha\rangle\langle\Psi(x)\rangle - 1\right)\langle\beta'\Phi'(y)\rangle \\
&\qquad + \alpha_G\left(\frac{1}{2}\langle\alpha\rangle^2 \langle\Psi(x)\rangle\left(1+\alpha_G \langle\Psi(x)\rangle\right) - \frac{1}{2}\langle\alpha\rangle - \alpha_G \langle\alpha\rangle\langle\Psi(x)\rangle + \alpha_G\right)\langle\beta'^2\Phi'(y)\rangle\Bigg]
\end{aligned}
\tag{A-13}
$$

where terms that are obviously higher than second order in σ_β and σ_Ψ, such as terms containing β'^3 or Ψ'^3, have been dropped from (A-13). Evaluating (A-13) is complicated, because it contains cross-moments associated with both perturbations $\Psi'(x)$ and Φ', such as $\langle\beta'^2\Psi'(x)\Phi'(y)\rangle$. To evaluate latter, it requires employing an eqaution for Φ', either (2-17) or (2-19). Using (2-17) to evaluate $\langle\beta'^2\Psi'(x)\Phi'(y)\rangle$, for example, requires to solve equation for $\langle\beta'^2\Psi'(x)\Phi'(y)\rangle$ with Dirichlet boundary condition of $\langle\beta'^2\Psi'(x)H'(y)\rangle$. The latter can be obtained upon multiplying (A-11) by $\langle\beta'^2\Psi'(x)\rangle$, which leads to an equation similar to (A-13). This procedure continues until the derived terms become higher orders, and thus are beyond our concern. As an example, we will show the detailed procedure in evaluating the first term in (A-13). The term $\langle\Psi'(x)\Phi'(y)\rangle$ can be obtained upon multiplying (2-19) in terms of y by $\Psi'(x)$, $x\in\Gamma_D$, taking conditional ensemble mean, and using the assumption that $\Psi'(\boldsymbol{x})$ is (statistically) independent of K_s and α and thus is independent of $G(\boldsymbol{y},\boldsymbol{x})$,

$$\left\langle \Psi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle = -\int_{\Gamma_D} \left\langle \Psi'(\boldsymbol{x})H'(z)K_s(z)\nabla_z G(z,y)\right\rangle \cdot \boldsymbol{n}(z)d\Gamma \tag{A-14}$$

The integrand contains $H'\Psi'$ which has to be evalauted using (A-11) again

$$\begin{aligned}
&\langle\alpha\rangle^3 \left\langle \Psi'(\boldsymbol{x})H'(z)K_s(z)\nabla_z G(z,\boldsymbol{y})\right\rangle \\
&= C_\Psi(\boldsymbol{x},z)\, e^{\alpha_G\langle\Psi(z)\rangle}\Big[\alpha_G\langle\alpha\rangle^2\left\langle K_s(z)\nabla_z G(z,\boldsymbol{y})\right\rangle + \alpha_G\langle\alpha\rangle^2\left(1+\alpha_G\left\langle\Psi(z)\right\rangle\right)\left\langle\beta' K_s(z)\nabla_z G(z,\boldsymbol{y})\right\rangle \\
&\qquad -\alpha_G\langle\alpha\rangle\left\langle\alpha' K_s(z)\nabla_z G(z,\boldsymbol{y})\right\rangle - \alpha_G\langle\alpha\rangle\left(1+\alpha_G\left\langle\Psi(z)\right\rangle\right)\left\langle\alpha'\beta' K_s(z)\nabla_z G(z,\boldsymbol{y})\right\rangle \\
&\qquad +\frac{1}{2}\alpha_G\langle\alpha\rangle^2\left\langle 1+3\alpha_G\left\langle\Psi(z)\right\rangle + \alpha_G^2\left\langle\Psi(z)\right\rangle^2\right\rangle\left\langle\beta'^2 K_s(z)\nabla_z G(z,\boldsymbol{y})\right\rangle \\
&\qquad +\alpha_G\left\langle\alpha'^2 K_s(z)\nabla_z G(z,\boldsymbol{y})\right\rangle\Big]
\end{aligned} \tag{A-15}$$

Terms that are obviously higher than second order have been dropped, and all terms in the right hand side of (A-15) are known (see Appendix B for details). Similarly, expressions for other terms in (A-13) are

$$\left\langle \Psi'^2(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle = -\int_{\Gamma_D} \left\langle \Psi'^2(\boldsymbol{x})H'(z)K_s(z)\nabla_z G(z,y)\right\rangle \cdot \boldsymbol{n}(z)d\Gamma \tag{A-16}$$

$$\left\langle \beta'\Psi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle = -\int_{\Gamma_D} \left\langle \beta'\Psi'(\boldsymbol{x})H'(z)K_s(z)\nabla_z G(z,\boldsymbol{y})\right\rangle \cdot \boldsymbol{n}(z)d\Gamma \tag{A-17}$$

$$\left\langle \beta'^2\Psi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle = -\int_{\Gamma_D} \left\langle \beta'^2\Psi'(\boldsymbol{x})H'(z)K_s'(z)\nabla_z G(z,\boldsymbol{y})\right\rangle \cdot \boldsymbol{n}(z)d\Gamma \tag{A-18}$$

$$\left\langle \beta'\Psi'^2(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle = -\int_{\Gamma_D} \left\langle \beta'\Psi'^2(\boldsymbol{x})H'(z)K_s(z)\nabla_z G(z,\boldsymbol{y})\right\rangle \cdot \boldsymbol{n}(z)d\Gamma \tag{A-19}$$

$$\left\langle \beta'^2\Psi'^2(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle = -\int_{\Gamma_D} \left\langle \beta'^2\Psi'^2(\boldsymbol{x})H'(z)K_s(z)\nabla_z G(z,\boldsymbol{y})\right\rangle \cdot \boldsymbol{n}(z)d\Gamma \tag{A-20}$$

where the integrands are

$$\begin{aligned}
&\langle\alpha\rangle^3\left\langle\Psi'^2(\boldsymbol{x})H'(z)K_s(z)\nabla_z G(z,\boldsymbol{y})\right\rangle \\
&=\sigma_\Psi^2(\boldsymbol{x})\,e^{\alpha_G\langle\Psi(z)\rangle}\Big[\langle\alpha\rangle^2\langle K_s(z)\nabla_z G(z,\boldsymbol{y})\rangle+\alpha_G\langle\alpha\rangle^2\langle\Psi(z)\rangle\langle\beta' K_s(z)\nabla_z G(z,\boldsymbol{y})\rangle \\
&\qquad -\langle\alpha\rangle\langle\alpha' K_s(z)\nabla_z G(z,\boldsymbol{y})\rangle-\alpha_G\langle\alpha\rangle\langle\Psi(z)\rangle\langle\alpha'\beta' K_s(z)\nabla_z G(z,\boldsymbol{y})\rangle \\
&\qquad +\frac{1}{2}\alpha_G\langle\alpha\rangle^2\langle\Psi(z)\rangle\left(1+\alpha_G\langle\Psi(z)\rangle\right)\left\langle\beta'^2 K_s(z)\nabla_z G(z,\boldsymbol{y})\right\rangle \\
&\qquad +\left\langle\alpha'^2 K_s(z)\nabla_z G(z,\boldsymbol{y})\right\rangle\Big] \\
&\quad -\langle\alpha\rangle^3\langle H(z)\rangle\sigma_\Psi^2(\boldsymbol{x})\langle K_s(z)\nabla_z G(z,\boldsymbol{y})\rangle
\end{aligned} \tag{A-21}$$

$$\begin{aligned}
\langle\alpha\rangle^2\langle\beta'\Psi'(\boldsymbol{x})H'(z)K_s(z)\nabla_z G(z,\boldsymbol{y})\rangle &= C_\Psi(\boldsymbol{x},z)\,e^{\alpha_G\langle\Psi(z)\rangle}\Big[\alpha_G\langle\alpha\rangle\left(1+\alpha_G\langle\Psi(z)\rangle\right)\left\langle\beta'^2 K_s(z)\nabla_z G(z,\boldsymbol{y})\right\rangle \\
&\quad +\alpha_G\langle\alpha\rangle\langle\beta' K_s(z)\nabla_z G(z,\boldsymbol{y})\rangle-\alpha_G\left\langle\alpha'\beta' K_s(z)\nabla_z G(z,\boldsymbol{y})\right\rangle\Big]
\end{aligned} \tag{A-22}$$

$$\begin{aligned}
&\langle\alpha\rangle^3\left\langle\beta'\Psi'^2(\boldsymbol{x})H'(z)K_s(z)\nabla_z G(z,\boldsymbol{y})\right\rangle \\
&=\sigma_\Psi^2(\boldsymbol{x})\,e^{\alpha_G\langle\Psi(z)\rangle}\Big[\langle\alpha\rangle^2\langle\beta' K_s(z)\nabla_z G(z,\boldsymbol{y})\rangle+\alpha_G\langle\alpha\rangle^2\langle\Psi(z)\rangle\left\langle\beta'^2 K_s(z)\nabla_z G(z,\boldsymbol{y})\right\rangle \\
&\qquad -\langle\alpha\rangle\langle\alpha'\beta' K_s(z)\nabla_z G(z,\boldsymbol{y})\rangle\Big] \\
&\quad -\langle\alpha\rangle^3\sigma_\Psi^2(\boldsymbol{x})\langle H(z)\rangle\langle\beta' K_s(z)\nabla_z G(z,\boldsymbol{y})\rangle
\end{aligned} \tag{A-23}$$

$$\langle\alpha\rangle\left\langle\beta'^2\Psi'(\boldsymbol{x})H'(z)K_s(z)\nabla_z G(z,\boldsymbol{y})\right\rangle=\alpha_G C_\Psi(\boldsymbol{x},z)\,e^{\alpha_G\langle\Psi(z)\rangle}\left\langle\beta'^2 K_s(z)\nabla_z G(z,\boldsymbol{y})\right\rangle \tag{A-24}$$

$$\langle\alpha\rangle\left\langle\beta'^2\Psi'^2(\boldsymbol{x})H'(z)K_s(z)\nabla_z G(z,\boldsymbol{y})\right\rangle=\sigma_\Psi^2(\boldsymbol{x})\left(e^{\alpha_G\langle\Psi(z)\rangle}-\langle\alpha\rangle\langle H(z)\rangle\right)\left\langle\beta'^2 K_s(z)\nabla_z G(z,\boldsymbol{y})\right\rangle \tag{A-25}$$

After evaluating (A-14) to (A-25) to second order in σ_Ψ, σ_Y, and σ_β, and combining all terms, we obtain

$$\langle H'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle^{(0,0)}=-e^{\alpha_G\langle\Psi(\boldsymbol{x})\rangle}\int_{\Gamma_D} e^{\alpha_G\langle\Psi(z)\rangle}C_\Psi(\boldsymbol{x},z)K_G(z)\nabla_z G^{(0,0)}(z,\boldsymbol{y})\cdot\boldsymbol{n}(z)d\Gamma \tag{A-26}$$

$$
\begin{aligned}
&\left\langle H'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle^{(0,2)} \\
&= -\frac{1}{2}\left(\alpha_G\left\langle\Psi(\boldsymbol{x})\right\rangle - 1\right)\sigma_\Psi^2(\boldsymbol{x})e^{\alpha_G\langle\Psi(\boldsymbol{x})\rangle}\int_{\Gamma_D} e^{\alpha_G\langle\Psi(z)\rangle}K_G(z)\left\langle\beta'\nabla_z G^{(0,1)}(z,\boldsymbol{y})\right\rangle\cdot\boldsymbol{n}(z)d\Gamma \\
&\quad - e^{\alpha_G\langle\Psi(\boldsymbol{x})\rangle}\int_{\Gamma_D} e^{\alpha_G\langle\Psi(z)\rangle}\, C_\Psi(\boldsymbol{x},z)\, K_G(z)\Big[\left\langle\nabla_z G^{(0,2)}(z,\boldsymbol{y})\right\rangle + \alpha_G\left(\left\langle\Psi(\boldsymbol{x})\right\rangle + \left\langle\Psi(z)\right\rangle\right)\left\langle\beta'\,\nabla_z G^{(0,1)}(z,\boldsymbol{y})\right\rangle \\
&\qquad + \frac{1}{2}\sigma_\beta^2\alpha_G\left(\left\langle\Psi(\boldsymbol{x})\right\rangle + \left\langle\Psi(z)\right\rangle\right)\left(\alpha_G\left\langle\Psi(\boldsymbol{x})\right\rangle + \alpha_G\left\langle\Psi(z)\right\rangle + 1\right)\nabla_z G^{(0,0)}(z,\boldsymbol{y})\Big]\cdot\boldsymbol{n}(z)d\Gamma \\
&\quad + \frac{1}{\alpha_G}e^{\alpha_G\langle\Psi(\boldsymbol{x})\rangle}\left[\alpha_G\left\langle\Psi(\boldsymbol{x})\right\rangle C_{\beta\Phi}^{(0,2)}(\boldsymbol{y}) + \frac{1}{2}\left(1 - \alpha_G\left\langle\Psi(\boldsymbol{x})\right\rangle + \alpha_G^2\left\langle\Psi(\boldsymbol{x})\right\rangle^2\right)\left\langle\beta'^2\Phi'(\boldsymbol{y})\right\rangle^{(0,2)}\right]
\end{aligned}
\tag{A-27}
$$

$$
\begin{aligned}
\left\langle H'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle^{(2,0)} &= -e^{\alpha_G\langle\Psi(\boldsymbol{x})\rangle}\int_{\Gamma_D} e^{\alpha_G\langle\Psi(z)\rangle}C_\Psi(\boldsymbol{x},z)K_G(z) \\
&\quad *\left[\nabla_z\left\langle G^{(2,0)}(z,\boldsymbol{y})\right\rangle + \left\langle Y'(z)\nabla_z G^{(1,0)}(z,\boldsymbol{y})\right\rangle + \frac{1}{2}\sigma_Y^2(z)\nabla_z G^{(0,0)}(z,\boldsymbol{y})\right]\cdot\boldsymbol{n}(z)d\Gamma
\end{aligned}
\tag{A-28}
$$

$$
\begin{aligned}
&\left\langle H'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle^{(2,2)} \\
&= -\frac{1}{2}\left\langle\alpha_G\left\langle\Psi(\boldsymbol{x})\right\rangle - 1\right\rangle\sigma_\Psi^2(\boldsymbol{x})e^{\alpha_G\langle\Psi(\boldsymbol{x})\rangle}\int_{\Gamma_D} e^{\alpha_G\langle\Psi(z)\rangle}K_G(z) \\
&\qquad *\left[\left\langle\beta'\nabla_z G^{(2,1)}(z,\boldsymbol{y})\right\rangle + \left\langle\beta' Y'(z)\nabla_z G^{(1,1)}(z,\boldsymbol{y})\right\rangle + 0.5\sigma_Y^2(z)\nabla_z\left\langle\beta' G^{(0,1)}(z,\boldsymbol{y})\right\rangle\right]\cdot\boldsymbol{n}(z)d\Gamma \\
&\quad - e^{\alpha_G\langle\Psi(\boldsymbol{x})\rangle}\int_{\Gamma_D} e^{\alpha_G\langle\Psi(z)\rangle}C_\Psi(\boldsymbol{x},z)K_G(z)\Big[\left\langle\nabla_z G^{(2,2)}(z,\boldsymbol{y})\right\rangle + \left\langle Y'(z)\nabla_z G^{(1,2)}(z,\boldsymbol{y})\right\rangle + 0.5\sigma_Y^2(z)\nabla_z\left\langle G^{(0,2)}(z,\boldsymbol{y})\right\rangle \\
&\qquad + \alpha_G\left(\left\langle\Psi(\boldsymbol{x})\right\rangle + \left\langle\Psi(z)\right\rangle\right)\left(\left\langle\beta'\nabla_z G^{(2,1)}(z,\boldsymbol{y})\right\rangle + \left\langle\beta' Y'(z)\nabla_z G^{(1,1)}(z,\boldsymbol{y})\right\rangle + 0.5\sigma_Y^2(z)\nabla_z\left\langle\beta' G^{(0,1)}(z,\boldsymbol{y})\right\rangle\right) \\
&\qquad + 0.5\sigma_\beta^2\alpha_G\left(\left\langle\Psi(\boldsymbol{x})\right\rangle + \left\langle\Psi(z)\right\rangle\right)\left(\alpha_G\left\langle\Psi(\boldsymbol{x})\right\rangle + \alpha_G\left\langle\Psi(z)\right\rangle + 1\right) \\
&\qquad *\left(\left\langle\beta'\nabla_z G^{(2,1)}(z,\boldsymbol{y})\right\rangle + \left\langle\beta' Y'(z)\nabla_z G^{(1,1)}(z,\boldsymbol{y})\right\rangle + 0.5\sigma_Y^2(z)\nabla_z\left\langle\beta' G^{(0,1)}(z,\boldsymbol{y})\right\rangle\right)\Big]\cdot\boldsymbol{n}(z)d\Gamma \\
&\quad + \frac{1}{\alpha_G}e^{\alpha_G\langle\Psi(\boldsymbol{x})\rangle}\left[\alpha_G\left\langle\Psi(\boldsymbol{x})\right\rangle C_{\beta\Phi}^{(2,2)}(\boldsymbol{y}) + \frac{1}{2}\left(1 - \alpha_G\left\langle\Psi(\boldsymbol{x})\right\rangle + \alpha_G^2\left\langle\Psi(\boldsymbol{x})\right\rangle^2\right)\left\langle\beta'^2\Phi'(\boldsymbol{y})\right\rangle^{(2,2)}\right]
\end{aligned}
\tag{A-29}
$$

For the deterministic pressure head boundary condition, i.e., $C_\Psi(\boldsymbol{x},z)\equiv 0$, (A-26)-(A-29) simplify to

$$C_{H\Phi}^{(0,0)}(x,y)=0$$
$$C_{H\Phi}^{(2,0)}(x,y)=0$$
$$C_{H\Phi}^{(0,2)}(x,y)=\frac{1}{\alpha_G}e^{\alpha_G\langle\Psi(x)\rangle}\left[\left(\alpha_G\langle\Psi(x)\rangle-1\right)\ C_{\beta\Phi}^{(0,2)}(y)+0.5\left(1-\alpha_G\langle\Psi(x)\rangle+\alpha_G^2\langle\Psi(x)\rangle^2\right)\left\langle\beta'^2\Phi'(y)\right\rangle^{(0,2)}\right] \quad \text{(A-30)}$$
$$C_{H\Phi}^{(2,2)}(x,y)=\frac{1}{\alpha_G}e^{\alpha_G\langle\Psi(x)\rangle}\left[\left(\alpha_G\langle\Psi(x)\rangle-1\right)\ C_{\beta\Phi}^{(2,2)}(y)+0.5\left(1-\alpha_G\langle\Psi(x)\rangle+\alpha_G^2\langle\Psi(x)\rangle^2\right)\left\langle\beta'^2\Phi'(y)\right\rangle^{(2,2)}\right]$$

Note that, for deterministic α and pressure head boundary, $C_{H\Phi}^{(2,0)}(x,y)=0$. This explains why the exact equation for the conditional covariance function C_Φ, (A7) of *Tartakovsky et al.* [1999], should have a term $\langle H'(x)\Phi'(y)\rangle$ on the Dirichlet boundary condition, but the corresponding Dirichlet boundary condition for their second order approximation, (42) of the above authors, is still valid and their numerical results are correct. The missing term is generally non-zero, but it is zero under the assumptions that α is a deterministic constant and that the boundary condition for pressure head is also deterministic on the Dirichlet boundary.

A.4.2 Cross-covariance $\langle\alpha' H'(x)\rangle$ and $\langle\alpha'^2 H'(x)\rangle$

Multiplying (A-9) by α' and noting that, to second order in σ_β, $\langle\alpha'\beta'\rangle = \alpha_G\sigma_\beta^2$, and $\langle\alpha'^2\rangle = \alpha_G^2\sigma_\beta^2$, yields

$$\langle\alpha\rangle^2\langle\alpha' H'(x)\rangle=\alpha_G^2 e^{\alpha_G\langle\Psi(x)\rangle}\left[\alpha_G\langle\Psi(x)\rangle-1+\left(\alpha_G\langle\alpha\rangle+\frac{1}{2}\alpha_G^2\langle\alpha\rangle\langle\Psi(x)\rangle-\frac{1}{2}\alpha_G^2\right)\sigma_\Psi^2(x)\right] \quad \text{(A-31)}$$

which gives

$$\langle\alpha' H'(x)\rangle^{(0,2)}=\sigma_\beta^2 e^{\alpha_G\langle\Psi(x)\rangle}\left[\alpha_G\langle\Psi(x)\rangle-1+\frac{1}{2}\alpha_G^2\left(\alpha_G\langle\Psi(x)\rangle+1\right)\sigma_\Psi^2(x)\right] \quad \text{(A-32)}$$

For the deterministic Dirichlet boundary condition, we have

$$\left\langle \alpha' H'(\boldsymbol{x}) \right\rangle^{(0,2)} = \sigma_\beta^2 \, e^{\alpha_G \langle \Psi(\boldsymbol{x}) \rangle} \left(\alpha_G \left\langle \Psi(\boldsymbol{x}) \right\rangle - 1 \right) \tag{A-33}$$

Similarly, for $\langle \alpha'^2 H'(\boldsymbol{x}) \rangle$, we have

$$\left\langle \alpha \right\rangle \left\langle \alpha'^2 H'(\boldsymbol{x}) \right\rangle = e^{\alpha_G \langle \Psi(\boldsymbol{x}) \rangle} \left(1 + \frac{1}{2} \alpha_G^2 \sigma_\Psi^2(\boldsymbol{x}) \right) \left\langle \alpha'^2 \right\rangle - \left\langle \alpha \right\rangle \left\langle H(\boldsymbol{x}) \right\rangle \left\langle \alpha'^2 \right\rangle \tag{A-34}$$

which results in $\left\langle \alpha'^2 H'(\boldsymbol{x}) \right\rangle^{(0,2)} = 0$.

A.4.3 $\langle \alpha' \Phi'(x) H'(y) \rangle$

Similar to (A-13), for $\langle \alpha' \Phi'(\boldsymbol{x}) H'(\boldsymbol{y}) \rangle$ we have

$$\begin{aligned}
&\left\langle \alpha \right\rangle^3 \left\langle \alpha' \Phi'(\boldsymbol{x}) H'(\boldsymbol{y})) \right\rangle \\
&\quad = e^{\alpha_G \langle \Psi(\boldsymbol{y}) \rangle} \Big[\alpha_G \left\langle \alpha \right\rangle^2 \left\langle \alpha' \Psi'(\boldsymbol{y}) \Phi'(\boldsymbol{x}) \right\rangle + \frac{1}{2} \alpha_G^2 \left\langle \alpha \right\rangle^2 \left\langle \alpha' \Psi'^2(\boldsymbol{y}) \Phi'(\boldsymbol{x}) \right\rangle \\
&\qquad + \alpha_G \left\langle \alpha \right\rangle^2 \left(1 + \alpha_G \left\langle \Psi(\boldsymbol{y}) \right\rangle \right) \left\langle \alpha' \beta' \Psi'(\boldsymbol{y}) \Phi'(\boldsymbol{x}) \right\rangle - \alpha_G \left\langle \alpha \right\rangle \left\langle \alpha'^2 \Psi'(\boldsymbol{y}) \Phi'(\boldsymbol{x}) \right\rangle \\
&\qquad + \alpha_G^2 \left\langle \alpha \right\rangle^2 \left(1 + \frac{1}{2} \alpha_G \left\langle \Psi(\boldsymbol{y}) \right\rangle \right) \left\langle \alpha' \beta' \Psi'^2(\boldsymbol{y}) \Phi'(\boldsymbol{x}) \right\rangle - \frac{1}{2} \alpha_G^2 \left\langle \alpha \right\rangle \left\langle \alpha'^2 \Psi'^2(\boldsymbol{y}) \Phi'(\boldsymbol{x}) \right\rangle \\
&\qquad + \alpha_G \left\langle \alpha \right\rangle \left(\left\langle \alpha \right\rangle \left\langle \Psi(\boldsymbol{y}) \right\rangle - 1 \right) \left\langle \alpha' \beta' \Phi'(\boldsymbol{x}) \right\rangle \Big] \\
&\quad - \left\langle \alpha \right\rangle^3 \left\langle H(\boldsymbol{y}) \right\rangle \left\langle \alpha' \Phi'(\boldsymbol{x}) \right\rangle
\end{aligned} \tag{A-35}$$

and its approximations to second order

$$\begin{aligned}
&\left\langle \alpha' \Phi'(\boldsymbol{x}) H'(\boldsymbol{y})) \right\rangle^{(0,2)} \\
&= -\frac{1}{2} \alpha_G^2 \sigma_\Psi^2(\boldsymbol{y}) R_{\beta\Phi}^{(0,2)}(\boldsymbol{x}) e^{\alpha_G \langle \Psi(\boldsymbol{y}) \rangle} \\
&\quad - \alpha_G^2 e^{\alpha_G \langle \Psi(\boldsymbol{y}) \rangle} \int_{\Gamma_D} e^{\alpha_G \langle \Psi(\boldsymbol{z}) \rangle} C_\Psi(\boldsymbol{y}, \boldsymbol{z}) \, K_G(\boldsymbol{z}) \left[\left\langle \beta' \nabla_z G^{(0,1)}(\boldsymbol{z}, \boldsymbol{x}) \right\rangle + \sigma_\beta^2 \alpha_G \left\langle \Psi(\boldsymbol{z}) \right\rangle \left\langle \nabla_z G^{(0,0)}(\boldsymbol{z}, \boldsymbol{x}) \right\rangle \right] \cdot \boldsymbol{n}(\boldsymbol{z}) d\Gamma \\
&\quad - \sigma_\beta^2 \alpha_G^2 \left\langle \Psi(\boldsymbol{y}) \right\rangle e^{\alpha_G \langle \Psi(\boldsymbol{y}) \rangle} \int_{\Gamma_D} e^{\alpha_G \langle \Psi(\boldsymbol{z}) \rangle} C_\Psi(\boldsymbol{y}, \boldsymbol{z}) \, K_G(\boldsymbol{z}) \left\langle \nabla_z G^{(0,0)}(\boldsymbol{z}, \boldsymbol{x}) \right\rangle \cdot \boldsymbol{n}(\boldsymbol{z}) d\Gamma
\end{aligned} \tag{A-36}$$

$$
\begin{aligned}
&\left\langle \alpha'\Phi'(\boldsymbol{x})H'(\boldsymbol{y})\right\rangle^{(2,2)} \\
&= e^{\alpha_G\langle\Psi(\boldsymbol{y})\rangle}\left[-\frac{1}{2}\alpha_G^2\sigma_\Psi^2(\boldsymbol{y})C_{\beta\Phi}^{(2,2)}(\boldsymbol{x})+\left(\alpha_G\left\langle\Psi(\boldsymbol{y})\right\rangle-1\right)\left\langle\beta'^2\Phi'(\boldsymbol{x})\right\rangle^{(2,2)}\right] \\
&\quad -\alpha_G^2 e^{\alpha_G\langle\Psi(\boldsymbol{y})\rangle}\int_{\Gamma_D} e^{\alpha_G\langle\Psi(\boldsymbol{z})\rangle}C_\Psi(\boldsymbol{y},\boldsymbol{z})\,K_G(\boldsymbol{z})\Big[\left\langle\beta'\nabla_z G^{(2,1)}(\boldsymbol{z},\boldsymbol{x})\right\rangle+\left\langle\beta'Y'(\boldsymbol{z})\nabla_z G^{(0,1)}(\boldsymbol{z},\boldsymbol{x})\right\rangle \\
&\qquad\qquad +\frac{1}{2}\sigma_Y^2(\boldsymbol{z})\left\langle\beta'\nabla_z G^{(0,1)}(\boldsymbol{z},\boldsymbol{x})\right\rangle\Big]\cdot\boldsymbol{n}(\boldsymbol{z})d\Gamma \\
&\quad -\sigma_\beta^2\alpha_G^2\left\langle\Psi(\boldsymbol{y})\right\rangle e^{\alpha_G\langle\Psi(\boldsymbol{y})\rangle}\int_{\Gamma_D} e^{\alpha_G\langle\Psi(\boldsymbol{z})\rangle}C_\Psi(\boldsymbol{y},\boldsymbol{z})\,K_G(\boldsymbol{z})\Big[\left\langle\nabla_z G^{(2,0)}(\boldsymbol{z},\boldsymbol{x})\right\rangle+\left\langle Y'(\boldsymbol{z})\nabla_z G^{(1,0)}(\boldsymbol{z},\boldsymbol{x})\right\rangle \\
&\qquad\qquad +\frac{1}{2}\sigma_Y^2(\boldsymbol{z})\left\langle\nabla_z G^{(0,0)}(\boldsymbol{z},\boldsymbol{x})\right\rangle\Big]\cdot\boldsymbol{n}(\boldsymbol{z})d\Gamma
\end{aligned}
\tag{A-37}
$$

A.4.4 $\langle\alpha'^2\Phi'(\mathrm{x})\mathrm{H}'(\mathrm{y})\rangle$

Rewriting (A-11) in terms of $\boldsymbol{y}$, multiplying by $\alpha'^2\Phi'(\boldsymbol{x})$, and taking conditional ensemble mean yields

$$
\begin{aligned}
&\left\langle\alpha\right\rangle\left\langle\alpha'^2\Phi'(\boldsymbol{x})H'(\boldsymbol{y})\right\rangle \\
&= e^{\alpha_G\langle\Psi(\boldsymbol{y})\rangle}\left[\left\langle\alpha'^2\Phi'(\boldsymbol{x})\right\rangle+\alpha_G\left\langle\alpha'^2\Psi'(\boldsymbol{y})\Phi'(\boldsymbol{x})\right\rangle+\frac{1}{2}\alpha_G^2\left\langle\alpha'^2\Psi'^2(\boldsymbol{y})\Phi'(\boldsymbol{x})\right\rangle\right]-\left\langle\alpha\right\rangle\left\langle H(\boldsymbol{y})\right\rangle\left\langle\alpha'^2\Phi'(\boldsymbol{x})\right\rangle
\end{aligned}
\tag{A-38}
$$

Here again, terms of higher than second order have been omitted. Expanding (A-38) in powers of σ_Y and σ_β leads to the following second order approximations

$$
\begin{aligned}
\left\langle\alpha'^2\Phi'(\boldsymbol{x})H'(\boldsymbol{y})\right\rangle^{(0,2)} &= -\frac{1}{2}\alpha_G^3\sigma_\Psi^2(\boldsymbol{y})e^{\alpha_G\langle\Psi(\boldsymbol{y})\rangle}\left\langle\beta'^2\Phi'(\boldsymbol{x})\right\rangle^{(0,2)} \\
&\quad -\sigma_\beta^2\alpha_G^2 e^{\alpha_G\langle\Psi(\boldsymbol{y})\rangle}\int_{\Gamma_D} e^{\alpha_G\langle\Psi(\boldsymbol{z})\rangle}C_\Psi(\boldsymbol{y},\boldsymbol{z})\,K_G(\boldsymbol{z})\left\langle\nabla_z G^{(0,0)}(\boldsymbol{z},\boldsymbol{x})\right\rangle\cdot\boldsymbol{n}(\boldsymbol{z})d\Gamma
\end{aligned}
\tag{A-39}
$$

$$
\begin{aligned}
\left\langle\alpha'^2\Phi'(\boldsymbol{x})H'(\boldsymbol{y})\right\rangle^{(2,2)} &= -\frac{1}{2}\alpha_G^3\sigma_\Psi^2(\boldsymbol{y})e^{\alpha_G\langle\Psi(\boldsymbol{y})\rangle}\left\langle\beta'^2\Phi'(\boldsymbol{x})\right\rangle^{(2,2)} \\
&\quad -\sigma_\beta^2\alpha_G^2 e^{\alpha_G\langle\Psi(\boldsymbol{y})\rangle}\int_{\Gamma_D} e^{\alpha_G\langle\Psi(\boldsymbol{z})\rangle}C_\Psi(\boldsymbol{y},\boldsymbol{z})\,K_G(\boldsymbol{z})\Big[\left\langle\nabla_z G^{(2,0)}(\boldsymbol{z},\boldsymbol{x})\right\rangle \\
&\qquad +\left\langle Y'(\boldsymbol{z})\nabla_z G^{(1,0)}(\boldsymbol{z},\boldsymbol{x})\right\rangle+\frac{1}{2}\sigma_Y^2(\boldsymbol{z})\left\langle\nabla_z G^{(0,0)}(\boldsymbol{z},\boldsymbol{x})\right\rangle\Big]\cdot\boldsymbol{n}(\boldsymbol{z})d\Gamma
\end{aligned}
\tag{A-40}
$$

A.4.5 $\langle Y'(x)\Phi'(y)H'(z)\rangle$

Multiplying (A-9) by $Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})$ and taking conditional mean gives

$$
\begin{aligned}
&\langle\alpha\rangle^3\langle Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})H'(z)\rangle \\
&= e^{\alpha_G\langle\Psi(z)\rangle}\Big[\langle\alpha\rangle^2\langle Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle+\alpha_G\langle\alpha\rangle^2\langle Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Psi'(z)\rangle+\alpha_G\langle\alpha\rangle^2\langle\Psi(z)\rangle\langle\beta'Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle \\
&\quad -\langle\alpha\rangle\langle\alpha'Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle+\frac{1}{2}\alpha_G^2\langle\alpha\rangle^2\langle Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Psi'^2(z)\rangle \\
&\quad +\frac{1}{2}\alpha_G\langle\alpha\rangle^2\langle\Psi(z)\rangle\left(1+\alpha_G\langle\Psi(z)\rangle\right)\langle\beta'^2Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle-\alpha_G\langle\alpha\rangle\langle\Psi(z)\rangle\langle\alpha'\beta'Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle \\
&\quad +\langle\alpha'^2Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle+\alpha_G\langle\alpha\rangle^2\left(1+\alpha_G\langle\Psi(z)\rangle\right)\langle\beta'Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Psi'(z)\rangle-\alpha_G\langle\alpha\rangle\langle\alpha'Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Psi'(z)\rangle \\
&\quad +\frac{1}{2}\alpha_G\langle\alpha\rangle^2\left(1+3\alpha_G\langle\Psi(z)\rangle+\alpha_G^2\langle\Psi(z)\rangle^2\right)\langle\beta'^2Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Psi'(z)\rangle \\
&\quad -\alpha_G\langle\alpha\rangle\left(1+\alpha_G\langle\Psi(z)\rangle\right)\langle\alpha'\beta'Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Psi'(z)\rangle+\alpha_G\langle\alpha'^2Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Psi'(z)\rangle \\
&\quad +\alpha_G^2\langle\alpha\rangle^2\left(1+\frac{1}{2}\alpha_G\langle\Psi(z)\rangle\right)\langle\beta'Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Psi'^2(z)\rangle-\frac{1}{2}\alpha_G^2\langle\alpha\rangle\langle\alpha'Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Psi'^2(z)\rangle \\
&\quad +\frac{1}{4}\alpha_G^2\langle\alpha\rangle^2\left(4+5\alpha_G\langle\Psi(z)\rangle+\alpha_G^2\langle\Psi(z)\rangle^2\right)\langle\beta'^2Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Psi'^2(z)\rangle \\
&\quad -\alpha_G^2\langle\alpha\rangle\left(1+\frac{1}{2}\alpha_G\langle\Psi(z)\rangle\right)\langle\alpha'\beta'Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Psi'^2(z)\rangle+\frac{1}{2}\alpha_G^2\langle\alpha\rangle\langle\alpha'^2Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Psi'^2(z)\rangle\Big] \\
&\quad -\langle\alpha\rangle^3\langle H(z)\rangle\langle Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle+HO
\end{aligned}
\tag{A-41}
$$

Similar to the procedure we used in evaluating (A-13), evaluating all terms in (A-41) in powers of σ_Y and σ_β leads to following approximations

$$
\begin{aligned}
&\langle Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})H'(z)\rangle^{(2,0)} \\
&= -\frac{e^{\alpha_G\langle\Psi(z)\rangle}}{\alpha_G}\int_{\Gamma_D}C_\Psi(z,\boldsymbol{u})e^{\alpha_G\langle\Psi(\boldsymbol{u})\rangle}\left[\langle Y'(\boldsymbol{x})\nabla_u^T G^{(1,0)}(\boldsymbol{u},\boldsymbol{y})\rangle+C_Y(\boldsymbol{x},\boldsymbol{u})\langle\nabla_u^T G^{(0,0)}(\boldsymbol{u},\boldsymbol{y})\rangle\right]K_G(\boldsymbol{u})n(\boldsymbol{u})d\Gamma
\end{aligned}
\tag{A-42}
$$

$$
\begin{aligned}
&\left\langle Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})H'(\boldsymbol{z})\right\rangle^{(2,2)} \\
&= \frac{e^{\alpha_G\langle\Psi(z)\rangle}}{\alpha_G}\Bigg\{-\frac{1}{2}\alpha_G^2\sigma_\Psi^2(z)\left\langle Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle^{(2,2)} \\
&\qquad -\frac{\sigma_\beta^2}{2}\left[2+\alpha_G\left\langle\Psi(z)\right\rangle\left(\alpha_G\left\langle\Psi(z)\right\rangle-1\right)+\frac{1}{2}\alpha_G^2(1+3\alpha_G\left\langle\Psi(z)\right\rangle+\alpha_G^2\left\langle\Psi(z)\right\rangle^2\right]\sigma_\Psi^2(z)\left\langle Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle^{(2,2)} \\
&\qquad +\left(\alpha_G\left\langle\Psi(z)\right\rangle-1\right)\left\langle\beta'Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle^{(2,2)}+\left[1+\frac{1}{2}\alpha_G\left\langle\Psi(z)\right\rangle\left(\alpha_G\left\langle\Psi(z)\right\rangle-1\right)\right]\left\langle\beta'^2Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle^{(2,2)} \\
&\qquad +\alpha_G\left\langle Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Psi'(z)\right\rangle^{(2,2)}-\frac{1}{2}\sigma_\beta^2\alpha_G\left\langle Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Psi'(z)\right\rangle^{(2,0)} \\
&\qquad +\alpha_G^2\left\langle\Psi(z)\right\rangle\left\langle\beta'Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Psi'(z)\right\rangle^{(2,2)}+\frac{1}{2}\alpha_G\left(1+5\alpha_G\left\langle\Psi(z)\right\rangle+\alpha_G^2\left\langle\Psi(z)\right\rangle^2\right)\left\langle\beta'^2Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Psi'(z)\right\rangle^{(2,2)} \\
&\qquad +\frac{1}{2}\alpha_G^2\left(1+\alpha_G\left\langle\Psi(z)\right\rangle\right)\left\langle\beta'Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Psi'^2(z)\right\rangle^{(2,2)}+\frac{1}{2}\alpha_G^2\left\langle Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Psi'^2(z)\right\rangle^{(2,2)}\Bigg\}
\end{aligned}
\tag{A-43}
$$

where terms related to Ψ' are given by the following equations

$$
\left\langle Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Psi'(z)\right\rangle^{(2,0)} = -\int_{\Gamma_D} C_\Psi(z,\boldsymbol{u})\, e^{\alpha_G\langle\Psi(\boldsymbol{u})\rangle}\left[\left\langle Y'(\boldsymbol{x})\nabla_u^T G^{(1,0)}(\boldsymbol{u},\boldsymbol{y})\right\rangle + C_Y(\boldsymbol{x},\boldsymbol{u})\left\langle\nabla_u^T G^{(0,0)}(\boldsymbol{u},\boldsymbol{y})\right\rangle\right]K_G(\boldsymbol{u})\, \boldsymbol{n}(\boldsymbol{u})d\Gamma
\tag{A-44}
$$

$$
\begin{aligned}
&\left\langle Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Psi'(z)\right\rangle^{(2,2)} \\
&= -\int_{\Gamma_D} C_\Psi(z,\boldsymbol{u})e^{\alpha_G\langle\Psi(\boldsymbol{u})\rangle}\Big[\left\langle Y'(\boldsymbol{x})\nabla_u^T G^{(1,2)}(\boldsymbol{u},\boldsymbol{y})\right\rangle + C_Y(\boldsymbol{x},\boldsymbol{u})\left\langle\nabla_u^T G^{(0,2)}(\boldsymbol{u},\boldsymbol{y})\right\rangle \\
&\qquad +\frac{1}{2}\sigma_\beta^2\alpha_G\left\langle\Psi(\boldsymbol{u})\right\rangle\left(\alpha_G\left\langle\Psi(\boldsymbol{u})\right\rangle+1\right)\left(\left\langle Y'(\boldsymbol{x})\nabla_u^T G^{(1,0)}(\boldsymbol{u},\boldsymbol{y})\right\rangle + C_Y(\boldsymbol{x},\boldsymbol{u})\left\langle\nabla_u^T G^{(0,0)}(\boldsymbol{u},\boldsymbol{y})\right\rangle\right) \\
&\qquad +\alpha_G\left\langle\Psi(\boldsymbol{u})\right\rangle\left(\left\langle\beta'Y'(\boldsymbol{x})\nabla_u^T G^{(1,1)}(\boldsymbol{u},\boldsymbol{y})\right\rangle + C_Y(\boldsymbol{x},\boldsymbol{u})\left\langle\beta'\nabla_u^T G^{(0,1)}(\boldsymbol{u},\boldsymbol{y})\right\rangle\right)\Big]K_G(\boldsymbol{u})\boldsymbol{n}(\boldsymbol{u})d\Gamma
\end{aligned}
\tag{A-45}
$$

$$
\begin{aligned}
&\left\langle Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Psi'^2(z)\right\rangle^{(2,2)} \\
&= -\sigma_\Psi^2(z)\int_{\Gamma_D}\frac{e^{\alpha_G\langle\Psi(\boldsymbol{u})\rangle}}{\alpha_G}\Big[-\frac{1}{2}\sigma_\beta^2\alpha_G\left\langle\Psi(\boldsymbol{u})\right\rangle\left\langle Y'(\boldsymbol{x})\nabla_u^T G^{(1,0)}(\boldsymbol{u},\boldsymbol{y})\right\rangle + C_Y(\boldsymbol{x},\boldsymbol{u})\left\langle\nabla_u^T G^{(0,0)}(\boldsymbol{u},\boldsymbol{y})\right\rangle \\
&\qquad +\left(\alpha_G\left\langle\Psi(\boldsymbol{u})\right\rangle-1\right)\left(\left\langle\beta'Y'(\boldsymbol{x})\nabla_u^T G^{(1,1)}(\boldsymbol{u},\boldsymbol{y})\right\rangle + C_Y(\boldsymbol{x},\boldsymbol{u})\left\langle\beta'\nabla_u^T G^{(0,1)}(\boldsymbol{u},\boldsymbol{y})\right\rangle\right)\Big]K_G(\boldsymbol{u})\boldsymbol{n}(\boldsymbol{u})d\Gamma
\end{aligned}
\tag{A-46}
$$

$$
\begin{aligned}
&\left\langle\beta'Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Psi'(z)\right\rangle^{(2,2)} \\
&= -\int_{\Gamma_D} C_\Psi(z,\boldsymbol{u})e^{\alpha_G\langle\Psi(\boldsymbol{u})\rangle}\Big[\left\langle\beta'Y'(\boldsymbol{x})\nabla_u^T G^{(1,1)}(\boldsymbol{u},\boldsymbol{y})\right\rangle + C_Y(\boldsymbol{x},\boldsymbol{u})\left\langle\beta'\nabla_u^T G^{(0,1)}(\boldsymbol{u},\boldsymbol{y})\right\rangle \\
&\qquad +\sigma_\beta^2\alpha_G\left\langle\Psi(\boldsymbol{u})\right\rangle\left(\left\langle Y'(\boldsymbol{x})\nabla_u^T G^{(1,0)}(\boldsymbol{u},\boldsymbol{y})\right\rangle + C_Y(\boldsymbol{x},\boldsymbol{u})\left\langle\nabla_u^T G^{(0,0)}(\boldsymbol{u},\boldsymbol{y})\right\rangle\right)\Big]K_G(\boldsymbol{u})\boldsymbol{n}(\boldsymbol{u})d\Gamma
\end{aligned}
\tag{A-47}
$$

$$
\begin{aligned}
&\left\langle \beta'^2 Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Psi'(z)\right\rangle^{(2,2)} \\
&\quad = -\sigma_\beta^2 \int_{\Gamma_D} C_\Psi(z,\boldsymbol{u}) e^{\alpha_G\langle\Psi(\boldsymbol{u})\rangle} \left[\left\langle Y'(\boldsymbol{x})\nabla_u^T G^{(1,0)}(\boldsymbol{u},\boldsymbol{y})\right\rangle + C_Y(\boldsymbol{x},\boldsymbol{u})\left\langle \nabla_u^T G^{(0,0)}(\boldsymbol{u},\boldsymbol{y})\right\rangle\right] K_G(\boldsymbol{u}) n(\boldsymbol{u}) d\Gamma
\end{aligned} \tag{A-48}
$$

$$
\begin{aligned}
&\left\langle \beta' Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Psi'^2(z)\right\rangle^{(2,2)} \\
&\quad = -\sigma_\Psi^2(z) \int_{\Gamma_D} \frac{e^{\alpha_G\langle\Psi(\boldsymbol{u})\rangle}}{\alpha_G} \left(\alpha_G \langle\Psi(\boldsymbol{u})\rangle - 1\right)\left[\left\langle Y'(\boldsymbol{x})\nabla_u^T G^{(1,0)}(\boldsymbol{u},\boldsymbol{y})\right\rangle + C_Y(\boldsymbol{x},\boldsymbol{u})\left\langle \nabla_u^T G^{(0,0)}(\boldsymbol{u},\boldsymbol{y})\right\rangle\right] K_G(\boldsymbol{u}) n(\boldsymbol{u}) d\Gamma
\end{aligned} \tag{A-49}
$$

A.4.6 $\langle\alpha' Y'(x)\Phi'(y)H'(z)\rangle$

From (A-11) we have

$$
\begin{aligned}
&\langle\alpha\rangle^3 \langle\alpha' Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})H'(z)\rangle \\
&\quad = e^{\alpha_G\langle\Psi(z)\rangle}\Big[\langle\alpha\rangle^2 \langle\alpha' Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle + \alpha_G\langle\alpha\rangle^2\langle\alpha' Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Psi'(z)\rangle + \alpha_G\langle\alpha\rangle^2\langle\Psi(z)\rangle\langle\alpha'\beta' Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle \\
&\qquad - \langle\alpha\rangle\left\langle\alpha'^2 Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle + \frac{1}{2}\alpha_G^2\langle\alpha\rangle^2\left\langle\alpha' Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Psi'^2(z)\right\rangle \\
&\qquad + \alpha_G\langle\alpha\rangle^2\left(1+\alpha_G\langle\Psi(z)\rangle\right)\langle\alpha'\beta' Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Psi'(z)\rangle - \alpha_G\langle\alpha\rangle\left\langle\alpha'^2 Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Psi'(z)\right\rangle \\
&\qquad + \alpha_G^2\langle\alpha\rangle^2\left(1+\frac{1}{2}\alpha_G\langle\Psi(z)\rangle\right)\left\langle\alpha'\beta' Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Psi'^2(z)\right\rangle - \frac{1}{2}\alpha_G^2\langle\alpha\rangle\left\langle\alpha'^2 Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Psi'^2(z)\right\rangle\Big] \\
&\quad - \langle\alpha\rangle^3\langle H(z)\rangle\langle\alpha' Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle + HO
\end{aligned} \tag{A-50}
$$

To second order,

$$
\begin{aligned}
&\langle\alpha' Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})H'(z)\rangle^{(2,2)} \\
&\quad = e^{\alpha_G\langle\Psi(z)\rangle}\left[-\frac{1}{2}\alpha_G^2\sigma_\Psi^2(z)\langle\beta' Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle^{(2,2)} + +\left(\alpha_G\langle\Psi(z)\rangle - 1\right)\left\langle\beta'^2 Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle^{(2,2)}\right. \\
&\qquad \left. + \alpha_G\langle\beta' Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Psi'(z)\rangle^{(2,2)} + \alpha_G^2\langle\Psi(z)\rangle\left\langle\beta'^2 Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Psi'(z)\right\rangle^{(2,2)}\right]
\end{aligned} \tag{A-51}
$$

A.4.7 $\langle\alpha'^2 Y'(x)\Phi'(y)H'(z)\rangle$

From (A-11) we have

$$
\begin{aligned}
&\langle\alpha\rangle^3\langle\alpha'^2Y'(x)\Phi'(y)H'(z)\rangle\\
&\quad=e^{\alpha_G\langle\Psi(z)\rangle}\left[\langle\alpha\rangle^2\langle\alpha'^2Y'(x)\Phi'(y)\rangle+\alpha_G\langle\alpha\rangle^2\langle\alpha'^2Y'(x)\Phi'(y)\Psi'(z)\rangle+\frac{1}{2}\alpha_G^2\langle\alpha\rangle^2\langle\alpha'^2Y'(x)\Phi'(y)\Psi'^2(z)\rangle\right]\\
&\qquad-\langle\alpha\rangle^3\langle H(z)\rangle\langle\alpha'^2Y'(x)\Phi'(y)\rangle+HO
\end{aligned}\tag{A-52}
$$

To second order,

$$
\begin{aligned}
&\langle\alpha'^2Y'(x)\Phi'(y)H'(z)\rangle^{(2,2)}\\
&\quad=-\alpha_G e^{\alpha_G\langle\Psi(z)\rangle}\left[\frac{1}{2}\alpha_G^2\sigma_\Psi^2(z)\langle\beta'^2Y'(x)\Phi'(y)\rangle^{(2,2)}+\alpha_G^2\sigma_\beta^2\int_{\Gamma_D}e^{\alpha_G\langle\Psi(u)\rangle}C_Y(x,u)\langle Y'(x)\nabla_u^TG^{(1,0)}(u,y)\rangle K_G(u)n(u)d\Gamma\right]
\end{aligned}\tag{A-53}
$$

A.4.8 $\langle Y'(x)Y'(y)\Phi'(x)H'(z)\rangle$

Multiplying (A-11) in terms of z by $Y'(x)Y'(y)\Phi'(x)$ and taking conditional mean yields

$$
\begin{aligned}
&\langle\alpha\rangle^3\langle Y'(x)Y'(y)\Phi'(x)H'(z)\rangle\\
&=e^{\alpha_G\langle\Psi(z)\rangle}\Big[\langle\alpha\rangle^2\langle Y'(x)Y'(y)\Phi'(x)\rangle+\alpha_G\langle\alpha\rangle^2\langle Y'(x)Y'(y)\Phi'(x)\Psi'(z)\rangle+\alpha_G\langle\alpha\rangle^2\langle\Psi(z)\rangle\langle\beta'Y'(x)Y'(y)\Phi'(x)\rangle\\
&\qquad-\langle\alpha\rangle\langle\alpha'Y'(x)Y'(y)\Phi'(x)\rangle+\frac{1}{2}\alpha_G^2\langle\alpha\rangle^2\langle Y'(x)Y'(y)\Phi'(x)\Psi'^2(z)\rangle\\
&\qquad+\frac{1}{2}\alpha_G\langle\alpha\rangle^2\langle\Psi(z)\rangle(1+\alpha_G\langle\Psi(z)\rangle)\langle\beta'^2Y'(x)Y'(y)\Phi'(x)\rangle-\alpha_G\langle\alpha\rangle\langle\Psi(z)\rangle\langle\alpha'\beta'Y'(x)Y'(y)\Phi'(x)\rangle\\
&\qquad+\alpha_G\langle\alpha\rangle^2(1+\alpha_G\langle\Psi(z)\rangle)\langle\beta'Y'(x)Y'(y)\Phi'(x)\Psi'(z)\rangle-\alpha_G\langle\alpha\rangle\langle\alpha'Y'(x)Y'(y)\Phi'(x)\Psi'(z)\rangle\\
&\qquad+\langle\alpha'^2Y'(x)\Phi'(x)\rangle+\frac{1}{2}\alpha_G\langle\alpha\rangle^2\left(1+3\alpha_G\langle\Psi(z)\rangle+\alpha_G^2\langle\Psi(z)\rangle^2\right)\langle\beta'^2Y'(x)Y'(y)\Phi'(x)\Psi'(z)\rangle\\
&\qquad-\alpha_G\langle\alpha\rangle(1+\alpha_G\langle\Psi(z)\rangle)\langle\alpha'\beta'Y'(x)Y'(y)\Phi'(x)\Psi'(z)\rangle+\alpha_G\langle\alpha'^2Y'(x)Y'(y)\Phi'(x)\Psi'(z)\rangle\\
&\qquad+\alpha_G^2\langle\alpha\rangle^2\left(1+\frac{1}{2}\alpha_G\langle\Psi(z)\rangle\right)\langle\beta'Y'(x)Y'(y)\Phi'(x)\Psi'^2(z)\rangle-\frac{1}{2}\alpha_G^2\langle\alpha\rangle\langle\alpha'Y'(x)Y'(y)\Phi'(x)\Psi'^2(z)\rangle\\
&\qquad+\frac{1}{4}\alpha_G^2\langle\alpha\rangle^2\left(4+5\alpha_G\langle\Psi(z)\rangle+\alpha_G^2\langle\Psi(z)\rangle^2\right)\langle\beta'^2Y'(x)Y'(y)\Phi'(x)\Psi'^2(z)\rangle\\
&\qquad-\alpha_G^2\langle\alpha\rangle\left(1+\frac{1}{2}\alpha_G\langle\Psi(z)\rangle\right)\langle\alpha'\beta'Y'(x)Y'(y)\Phi'(x)\Psi'^2(z)\rangle+\frac{1}{2}\alpha_G^2\langle\alpha\rangle\langle\alpha'^2Y'(x)Y'(y)\Phi'(x)\Psi'^2(z)\rangle\Big]\\
&\quad-\langle\alpha\rangle^3\langle H(z)\rangle\langle Y'(x)Y'(y)\Phi'(x)\rangle+HO
\end{aligned}\tag{A-54}
$$

Evaluating all terms in second order gives the following approximations,

$$\left\langle Y'(\boldsymbol{x})Y'(\boldsymbol{y})\Phi'(\boldsymbol{x})H'(z)\right\rangle^{(2,0)} = e^{\alpha_G\langle\Psi(z)\rangle}\left[-\frac{1}{2}\alpha_G\sigma_\Psi^2(z)\left\langle Y'(\boldsymbol{x})Y'(\boldsymbol{y})\Phi'(\boldsymbol{x})\right\rangle^{(2,0)} + \left\langle Y'(\boldsymbol{x})Y'(\boldsymbol{y})\Phi'(\boldsymbol{x})\Psi'(z)\right\rangle^{(2,0)} + \frac{1}{2}\alpha_G\left\langle Y'(\boldsymbol{x})Y'(\boldsymbol{y})\Phi'(\boldsymbol{x})\Psi'^2(z)\right\rangle^{(2,0)}\right] \tag{A-55}$$

$$\begin{aligned}
&\left\langle Y'(\boldsymbol{x})Y'(\boldsymbol{y})\Phi'(\boldsymbol{x})H'(z)\right\rangle^{(2,2)} \\
&= \frac{e^{\alpha_G\langle\Psi(z)\rangle}}{\alpha_G}\Bigg[-\frac{1}{2}\alpha_G^2\sigma_\Psi^2(z)\left\langle Y'(\boldsymbol{x})Y'(\boldsymbol{y})\Phi'(\boldsymbol{x})\right\rangle^{(2,2)} \\
&\quad -\frac{1}{2}\sigma_\beta^2\left(\alpha_G^2\left\langle\Psi(z)\right\rangle^2 - 1 + \frac{1}{2}\alpha_G^3\left\langle\Psi(z)\right\rangle\left(\alpha_G\left\langle\Psi(z)\right\rangle + 3\right)\sigma_\Psi^2(z)\right)\left\langle Y'(\boldsymbol{x})Y'(\boldsymbol{y})\Phi'(\boldsymbol{x})\right\rangle^{(2,0)} \\
&\quad +\frac{1}{2}\left(\alpha_G^2\left\langle\Psi(z)\right\rangle^2 + 3\alpha_G\left\langle\Psi(z)\right\rangle - 2\right)\left\langle\beta' Y'(\boldsymbol{x})Y'(\boldsymbol{y})\Phi'(\boldsymbol{x})\right\rangle^{(2,2)} \\
&\quad +\left(\alpha_G\left\langle\Psi(z)\right\rangle - 1\right)\left\langle\beta'^2 Y'(\boldsymbol{x})Y'(\boldsymbol{y})\Phi'(\boldsymbol{x})\right\rangle^{(2,2)} \\
&\quad +\alpha_G\left(\left\langle Y'(\boldsymbol{x})Y'(\boldsymbol{y})\Phi'(\boldsymbol{x})\Psi'(z)\right\rangle^{(2,2)} - \frac{1}{2}\sigma_\beta^2\left\langle Y'(\boldsymbol{x})Y'(\boldsymbol{y})\Phi'(\boldsymbol{x})\Psi'(z)\right\rangle^{(2,0)}\right) \\
&\quad +\frac{1}{2}\alpha_G^2\left(\left\langle Y'(\boldsymbol{x})Y'(\boldsymbol{y})\Phi'(\boldsymbol{x})\Psi'^2(z)\right\rangle^{(2,2)} - \frac{1}{2}\sigma_\beta^2\left\langle Y'(\boldsymbol{x})Y'(\boldsymbol{y})\Phi'(\boldsymbol{x})\Psi'^2(z)\right\rangle^{(2,0)}\right) \\
&\quad +\alpha_G^2\left\langle\Psi(z)\right\rangle\left\langle\beta' Y'(\boldsymbol{x})Y'(\boldsymbol{y})\Phi'(\boldsymbol{x})\Psi'(z)\right\rangle^{(2,2)} \\
&\quad +\frac{1}{2}\alpha_G\left(1 + \alpha_G\left\langle\Psi(z)\right\rangle + \alpha_G^2\left\langle\Psi(z)\right\rangle^2\right)\left\langle\beta'^2 Y'(\boldsymbol{x})Y'(\boldsymbol{y})\Phi'(\boldsymbol{x})\Psi'(z)\right\rangle^{(2,2)} \\
&\quad +\frac{1}{4}\alpha_G^2\left(6 + 7\alpha_G\left\langle\Psi(z)\right\rangle + \alpha_G^2\left\langle\Psi(z)\right\rangle^2\right)\left\langle\beta' Y'(\boldsymbol{x})Y'(\boldsymbol{y})\Phi'(\boldsymbol{x})\Psi'^2(z)\right\rangle^{(2,2)} \\
&\quad -\frac{1}{2}\alpha_G^2\left(1 + \alpha_G\left\langle\Psi(z)\right\rangle\right)\left\langle\beta'^2 Y'(\boldsymbol{x})Y'(\boldsymbol{y})\Phi'(\boldsymbol{x})\Psi'^2(z)\right\rangle^{(2,2)}\Bigg]
\end{aligned} \tag{A-56}$$

where terms in (A-53)-(A-54) are given by

$$\left\langle Y'(\boldsymbol{x})Y'(\boldsymbol{y})\Phi'(\boldsymbol{x})\Psi'(z)\right\rangle^{(2,0)} = -C_Y(\boldsymbol{x},\boldsymbol{y})\int_{\Gamma_D} C_\Psi(z,\boldsymbol{u})e^{\alpha_G\langle\Psi(\boldsymbol{u})\rangle}\left\langle\nabla_u^T G^{(0,0)}(\boldsymbol{u},z)\right\rangle K_G(\boldsymbol{u})\boldsymbol{n}(\boldsymbol{u})d\Gamma \tag{A-57}$$

$$\begin{aligned}
&\left\langle Y'(\boldsymbol{x})Y'(\boldsymbol{y})\Phi'(\boldsymbol{x})\Psi'(z)\right\rangle^{(2,2)} \\
&= -C_Y(\boldsymbol{x},\boldsymbol{y})\int_{\Gamma_D} C_\Psi(z,\boldsymbol{u})e^{\alpha_G\langle\Psi(\boldsymbol{u})\rangle}\Big[\left\langle\nabla_u^T G^{(0,2)}(\boldsymbol{u},z)\right\rangle + \alpha_G\left\langle\Psi(\boldsymbol{u})\right\rangle\left\langle\beta'\nabla_u^T G^{(0,1)}(\boldsymbol{u},z)\right\rangle \\
&\qquad + \frac{1}{2}\sigma_\beta^2\left(\alpha_G^2\left\langle\Psi(\boldsymbol{u})\right\rangle^2 + \alpha_G\left\langle\Psi(\boldsymbol{u})\right\rangle - 1\right)\left\langle\nabla_u^T G^{(0,0)}(\boldsymbol{u},z)\right\rangle\Big]K_G(\boldsymbol{u})\boldsymbol{n}(\boldsymbol{u})d\Gamma
\end{aligned} \tag{A-58}$$

$$\left\langle Y'(\boldsymbol{x})Y'(\boldsymbol{y})\Phi'(\boldsymbol{x})\Psi'^2(z)\right\rangle^{(2,0)} = 0 \tag{A-59}$$

$$\left\langle Y'(\mathbf{x})Y'(\mathbf{y})\Phi'(\mathbf{x})\Psi'^2(\mathbf{z})\right\rangle^{(2,2)} = -C_Y(\mathbf{x},\mathbf{y})\sigma_\Psi^2(\mathbf{z})\int_{\Gamma_D} e^{\alpha_G\langle\Psi(\mathbf{u})\rangle}\left\langle\Psi(\mathbf{u})\right\rangle\left\langle\beta'\nabla_u^T G^{(0,1)}(\mathbf{u},\mathbf{z})\right\rangle K_G(\mathbf{u})\mathbf{n}(\mathbf{u})d\Gamma \tag{A-60}$$

$$\left\langle\beta' Y'(\mathbf{x})Y'(\mathbf{y})\Phi'(\mathbf{x})\Psi'(\mathbf{z})\right\rangle^{(2,2)} = -C_Y(\mathbf{x},\mathbf{y})\int_{\Gamma_D} C_\Psi(\mathbf{z},\mathbf{u})e^{\alpha_G\langle\Psi(\mathbf{u})\rangle}\left[\left\langle\beta'\nabla_u^T G^{(0,1)}(\mathbf{u},\mathbf{x})\right\rangle + \alpha_G\left\langle\Psi(\mathbf{u})\right\rangle\sigma_\beta^2\left\langle\nabla_u^T G^{(0,0)}(\mathbf{u},\mathbf{x})\right\rangle\right]K_G(\mathbf{u})\mathbf{n}(\mathbf{u})d\Gamma \tag{A-61}$$

$$\left\langle\beta' Y'(\mathbf{x})Y'(\mathbf{y})\Phi'(\mathbf{x})\Psi'^2(\mathbf{z})\right\rangle^{(2,2)} = -\frac{1}{\alpha_G}\sigma_\beta^2 C_Y(\mathbf{x},\mathbf{y})\sigma_\Psi^2(\mathbf{z})\int_{\Gamma_D} e^{\alpha_G\langle\Psi(\mathbf{u})\rangle}\left(\alpha_G\left\langle\Psi(\mathbf{u})\right\rangle - 1\right)\left\langle\nabla_u^T G^{(0,0)}(\mathbf{u},\mathbf{x})\right\rangle K_G(\mathbf{u})\mathbf{n}(\mathbf{u})d\Gamma \tag{A-62}$$

$$\left\langle\beta'^2 Y'(\mathbf{x})Y'(\mathbf{y})\Phi'(\mathbf{x})\Psi'(\mathbf{z})\right\rangle^{(2,2)} = -\sigma_\beta^2 C_Y(\mathbf{x},\mathbf{y})\int_{\Gamma_D} C_\Psi(\mathbf{u},\mathbf{z})e^{\alpha_G\langle\Psi(\mathbf{u})\rangle}\left\langle\nabla_u^T G^{(0,0)}(\mathbf{u},\mathbf{x})\right\rangle K_G(\mathbf{u})\mathbf{n}(\mathbf{u})d\Gamma \tag{A-63}$$

$$\left\langle\beta'^2 Y'(\mathbf{x})Y'(\mathbf{y})\Phi'(\mathbf{x})\Psi'^2(\mathbf{z})\right\rangle^{(2,2)} = 0 \tag{A-64}$$

A.5 *H′*-RELATED TERMS AS BOUNDARY INTEGRALS

The explicit expression for Φ', (2-19), includes an integral over the Dirichlet boundary,

$$\begin{aligned}\Phi'(\mathbf{y}) = &-\int_\Omega \nabla_z^T\, G(\mathbf{z},\mathbf{y})\Big[K_s'(\mathbf{z})\,\nabla\left\langle\Phi(\mathbf{z})\right\rangle + \mathbf{r}(\mathbf{z}) + g\left(\alpha' K_s(\mathbf{z})\left\langle\Phi(\mathbf{z})\right\rangle + \left\langle\alpha\right\rangle K_s'(\mathbf{z})\left\langle\Phi(\mathbf{z})\right\rangle\right.\\ &\qquad\left. - \left\langle\alpha\right\rangle R_{K\Phi}(\mathbf{z}) - \left\langle K_s(\mathbf{z})\right\rangle R_{\alpha\Phi}(\mathbf{z}) - R_{\alpha K\Phi}(\mathbf{z})\right)\mathbf{e}_3\Big]\mathrm{d}\Omega\\ &+\int_\Omega f'(\mathbf{z})\, G(\mathbf{z},\mathbf{y})\,\mathrm{d}\Omega\\ &+\int_{\Gamma_N} G(\mathbf{z},\mathbf{y})Q'(\mathbf{z})\,\mathrm{d}\Gamma\\ &-\int_{\Gamma_D} H'(\mathbf{z})K_s(\mathbf{z})\,\nabla_z \mathrm{G}(\mathbf{z},\mathbf{y})\cdot\mathbf{n}(\mathbf{z})\,\mathrm{d}\Gamma\end{aligned} \tag{A-65}$$

as a result, (cross-)covariance functions associated with Φ' also include a boundary integral over the Dirichlet boundary. In this section, all terms related to these boundary integrals are formulated.

A.5.1 $\langle\alpha'\Phi'(y)\rangle$

Multiplying (A-65) by α' and taking conditional mean yields an explicit expression for $\langle\alpha'\Phi'(\mathbf{y})\rangle$, but for the moment we only concern the term related to H', the integral over the Dirichlet boundary,

$$\langle\alpha'\Phi'(y)\rangle_{\Gamma_D} = -\int_{\Gamma_D}\left\langle\alpha' H'(z)\nabla_z^T G(z,y)K_s(z)\right\rangle n(z)d\Gamma \tag{A-66}$$

where $\langle\alpha'\Phi'(\mathbf{y})\rangle_{\Gamma D}$ denotes the term related to the Dirichlet boundary in cross-covariance $\langle\alpha'\Phi'(\mathbf{y})\rangle$. Expressing (A-11) in terms of $\mathbf{y}$, multiplying by $\alpha'\nabla_z^T G(z,y)K_s(z)$, taking conditional mean, and ignoring terms that are obviously higher than second order, such as those containing α'^3 or $\alpha'\beta'^2$, we have

$$\begin{aligned}
&\langle\alpha\rangle^3\left\langle\alpha' H'(z)\nabla_z^T G(z,y)K_s(z)\right\rangle \\
&\quad = e^{\alpha_G\langle\Psi(x)\rangle}\Big[\left(1+0.5\alpha_G^2\sigma_\Psi^2\right)\langle\alpha\rangle^2\left\langle\alpha'\nabla_z^T G(z,y)K_s(z)\right\rangle \\
&\qquad + \left[\alpha_G\langle\Psi(x)\rangle + \left(1+0.5\alpha_G\langle\Psi(x)\rangle\right)\alpha_G^2\sigma_\Psi^2\right]\langle\alpha\rangle^2\left\langle\alpha'\beta'\nabla_z^T G(z,y)K_s(z)\right\rangle \\
&\qquad - \left(1+0.5\alpha_G^2\sigma_\Psi^2\right)\langle\alpha\rangle\left\langle\alpha'^2\nabla_z^T G(z,y)K_s(z)\right\rangle\Big] \\
&\quad - \langle\alpha\rangle^3\langle H(x)\rangle\left\langle\alpha'\nabla_z^T G(z,y)K_s(z)\right\rangle
\end{aligned} \tag{A-67}$$

All unknown terms in (A-67) can be evaluated as follows

$$\begin{aligned}
&\left\langle\alpha'\nabla_z^T G(z,y)K_s(z)\right\rangle^{(0,2)} = \alpha_G\left\langle\beta'\nabla_z^T G^{(0,1)}(z,y)\right\rangle K_G(z) \\
&\left\langle\alpha'\nabla_z^T G(z,y)K_s(z)\right\rangle^{(2,2)} \\
&\quad = \alpha_G\left[\left\langle\beta'\nabla_z^T G^{(2,1)}(z,y)\right\rangle + \left\langle\beta' Y'(z)\nabla_z^T G^{(1,1)}(z,y)\right\rangle + 0.5\sigma_Y^2(z)\left\langle\beta'\nabla_z^T G^{(0,1)}(z,y)\right\rangle\right]K_G(z)
\end{aligned} \tag{A-68}$$

$$\left\langle \alpha'^2 \nabla_z^T G(z,y) K_s(z) \right\rangle^{(0,2)} = \alpha_G^2 \sigma_\beta^2 \left\langle \nabla_z^T G^{(0,0)}(z,y) \right\rangle K_G(z)$$
$$\left\langle \alpha'^2 \nabla_z^T G(z,y) K_s(z) \right\rangle^{(2,2)} \tag{A-69}$$
$$= \alpha_G^2 \sigma_\beta^2 \left[\left\langle \nabla_z^T G^{(2,0)}(z,y) \right\rangle + \left\langle Y'(z) \nabla_z^T G^{(1,0)}(z,y) \right\rangle + 0.5\sigma_Y^2(z) \left\langle \nabla_z^T G^{(0,0)}(z,y) \right\rangle \right] K_G(z)$$

and

$$\left\langle \alpha'\beta' \nabla_z^T G(z,y) K_s(z) \right\rangle^{(0,2)} = \alpha_G \sigma_\beta^2 \left\langle \nabla_z^T G^{(0,0)}(z,y) \right\rangle K_G(z)$$
$$\left\langle \alpha'\beta' \nabla_z^T G(z,y) K_s(z) \right\rangle^{(2,2)} \tag{A-70}$$
$$= \alpha_G \sigma_\beta^2 \left[\left\langle \nabla_z^T G^{(2,0)}(z,y) \right\rangle + \left\langle Y'(z) \nabla_z^T G^{(1,0)}(z,y) \right\rangle + 0.5\sigma_Y^2(z) \left\langle \nabla_z^T G^{(0,0)}(z,y) \right\rangle \right] K_G(z)$$

where terms related to G are determined in Appendix B. Expanding (A-64) in terms of σ_β and σ_Y, substituting (A-68)-(A-70) into it, and collecting terms of same order, we find the integrand of (A-66) to be

$$\left\langle \alpha' H'(z) \nabla_z^T G(z,y) K_s(z) \right\rangle^{(0,2)}$$
$$= e^{\alpha_G \langle \Psi(z) \rangle} \left[\alpha_G \left\langle \Psi(z) \right\rangle - 1 + \frac{1}{2} \left(\alpha_G \left\langle \Psi(z) \right\rangle + 1 \right) \alpha_G^2 \sigma_\Psi^2(z) \right] \sigma_\beta^2 \nabla_z^T G^{(0,0)}(z,y) K_G(z) \tag{A-71}$$

$$\left\langle \alpha' H'(z) \nabla_z^T G(z,y) K_s(z) \right\rangle^{(2,2)} = \sigma_\beta^2 e^{\alpha_G \langle \Psi(z) \rangle} \left[\alpha_G \left\langle \Psi(z) \right\rangle - 1 + \frac{1}{2} \left(\alpha_G \left\langle \Psi(z) \right\rangle + 1 \right) \alpha_G^2 \sigma_\Psi^2(z) \right]$$
$$* \left[\left\langle \nabla_z^T G^{(2,0)}(z,y) \right\rangle + \left\langle Y'(z) \nabla_z^T G^{(1,0)}(z,y) \right\rangle + 0.5\sigma_Y^2(z) \left\langle \nabla_z^T G^{(0,0)}(z,y) \right\rangle \right] K_G(z) \tag{A-72}$$

The integral in (A-66) must be calculated numerically.

A.5.2 $\langle Y'(x)\Phi'(y) \rangle$

Similarly, for covariance function $\langle Y'(\boldsymbol{x})\Phi'(\boldsymbol{y}) \rangle$, the term related to H' is

$$\left\langle Y'(\boldsymbol{x}) \Phi'(\boldsymbol{y}) \right\rangle_{\Gamma_D} = -\int_{\Gamma_D} \left\langle Y'(\boldsymbol{x}) H'(z) \nabla_z^T G(z,y) K_s(z) \right\rangle n(z) d\Gamma \tag{A-73}$$

and its integrand can be approximated by multiplying (A-11) by $Y'(x)\nabla_z^T G(z,y)K_s(z)$, taking conditional mean, and collect terms of same order,

$$\left\langle Y'(x)H'(z)\nabla_z^T G(z,y)K_s(z)\right\rangle^{(2,0)} = 0$$

$$\left\langle Y'(x)H'(z)\nabla_z^T G(z,y)K_s(z)\right\rangle^{(2,2)} = \frac{e^{\alpha_G\langle\Psi(z)\rangle}}{\alpha_G}\left[\alpha_G\langle\Psi(z)\rangle - 1 + \frac{1}{2}\left(\alpha_G\langle\Psi(z)\rangle + 1\right)\alpha_G^2\sigma_\Psi^2(z)\right] * \left[\left\langle\beta' Y'(x)\nabla_z^T G^{(1,1)}(z,y)\right\rangle + C_Y(x,z)\left\langle\beta'\nabla_z^T G^{(0,1)}(z,y)\right\rangle\right]K_G(z) \quad \text{(A-74)}$$

A.5.3 ⟨α′Y′(x)Φ′(y)⟩

Multiplying (A-65) by $\alpha' Y'(x)$, taking conditional mean, and retaining only the term related to H', gives

$$\left\langle\alpha' Y'(x)\Phi'(y)\right\rangle_{\Gamma_D} = -\int_{\Gamma_D}\left\langle\alpha' Y'(x)H'(z)\nabla_z^T G(z,y)K_s(z)\right\rangle n(z)d\Gamma \quad \text{(A-75)}$$

Its second order approximation of the integrand is

$$\left\langle\alpha' Y'(x)H'(z)\nabla_z^T G(z,y)K_s(z)\right\rangle^{(2,2)} = \sigma_\beta^2 e^{\alpha_G\langle\Psi(z)\rangle}\left[\alpha_G\langle\Psi(z)\rangle - 1 + \frac{1}{2}\left(\alpha_G\langle\Psi(z)\rangle + 1\right)\alpha_G^2\sigma_\Psi^2(z)\right] * \left[\left\langle Y'(x)\nabla_z^T G^{(0,1)}(z,y)\right\rangle + C_Y(x,z)\left\langle\nabla_z^T G^{(0,0)}(z,y)\right\rangle\right]K_G(z) \quad \text{(A-76)}$$

A.5.4 ⟨Y′(x)Y′(y)Φ′(y)⟩

Multiplying (A-65) by $Y'(x)Y'(y)$, taking conditional mean, and retaining only the term related to H', gives

$$\left\langle Y'(x)Y'(y)\Phi'(y)\right\rangle_{\Gamma_D} = -\int_{\Gamma_D}\left\langle Y'(x)Y'(y)H'(z)\nabla_z^T G(z,y)K_s(z)\right\rangle n(z)d\Gamma \quad \text{(A-77)}$$

The second order approximation of the integrand can be obtained upon multiplying (A-11) by $Y'(x)Y'(y)\nabla_z^T G(z,y)K_s(z)$, and evaluate it to second order

$$\begin{aligned}
&\left\langle Y'(\boldsymbol{x})Y'(\boldsymbol{y})H'(z)\nabla_z^T G(z,\boldsymbol{y})K_s(z)\right\rangle^{(2,2)} \\
&= \frac{e^{\alpha_G\langle\Psi(z)\rangle}}{\alpha_G}\left[\alpha_G\left\langle\Psi(z)\right\rangle - 1 + \frac{1}{2}\left(\alpha_G\left\langle\Psi(z)\right\rangle + 1\right)\alpha_G^2\sigma_\Psi^2(z)\right]C_Y(\boldsymbol{x},\boldsymbol{y})\left\langle\beta'\nabla_z^T G^{(0,1)}(z,\boldsymbol{y})\right\rangle K_G(z) \\
&\quad + \frac{\sigma_\beta^2}{2}\frac{e^{\alpha_G\langle\Psi(z)\rangle}}{\alpha_G}\left[3 + \alpha_G\left\langle\Psi(z)\right\rangle\left(\alpha_G\left\langle\Psi(z)\right\rangle + 1\right) - \frac{1}{2}\alpha_G\left\langle\Psi(z)\right\rangle\left(4\alpha_G\left\langle\Psi(z)\right\rangle - 3\right)\alpha_G^2\sigma_\Psi^2(z)\right] \\
&\quad * C_Y(\boldsymbol{x},\boldsymbol{y})\left\langle\nabla_z^T G^{(0,0)}(z,\boldsymbol{y})\right\rangle K_G(z)
\end{aligned} \tag{A-78}$$

Again, (A-77) must be integrated numerically.

A.5.5 $\langle\alpha' Y'(x)Y'(y)\Phi'(z)\rangle$

Multiplying (A-65) by $\alpha' Y'(\boldsymbol{x})Y'(\boldsymbol{y})$, taking conditional mean, and retaining only the term related to H', gives

$$\left\langle\alpha' Y'(\boldsymbol{x})Y'(\boldsymbol{y})\Phi'(z)\right\rangle_{\Gamma_D} = -\int_{\Gamma_D}\left\langle\alpha' Y'(\boldsymbol{x})Y'(\boldsymbol{y})H'(\boldsymbol{u})\nabla_u^T G(\boldsymbol{u},z)K_s(\boldsymbol{u})\right\rangle n(\boldsymbol{u})d\Gamma \tag{A-79}$$

$$\begin{aligned}
&\left\langle\alpha' Y'(\boldsymbol{x})Y'(\boldsymbol{y})H'(\boldsymbol{u})\nabla_u^T G(\boldsymbol{u},z)K_s(\boldsymbol{u})\right\rangle^{(2,2)} \\
&= \sigma_\beta^2\, e^{\alpha_G\langle\Psi(\boldsymbol{u})\rangle}C_Y(\boldsymbol{x},\boldsymbol{y})\left[\alpha_G\left\langle\Psi(\boldsymbol{u})\right\rangle - 1 + \frac{1}{2}\left(\alpha_G\left\langle\Psi(\boldsymbol{u})\right\rangle + 1\right)\alpha_G^2\sigma_\Psi^2(\boldsymbol{u})\right]\left\langle\nabla_u^T G^{(0,0)}(\boldsymbol{u},z)\right\rangle K_G(\boldsymbol{u})
\end{aligned} \tag{A-80}$$

A.5.6 $\langle\alpha'^2\Phi'(y)\rangle$

Multiplying (A-65) by α'^2, taking conditional mean, and retaining only the integral over the Dirichlet boundary gives

$$\left\langle\alpha'^2\Phi'(\boldsymbol{y})\right\rangle_{\Gamma_D} = -\int_{\Gamma_D}\left\langle\alpha'^2 H'(z)\nabla_z^T G(z,\boldsymbol{y})K_s(z)\right\rangle n(z)d\Gamma \tag{A-81}$$

The corresponding integrand to second order in σ_β and σ_Y is

$$\left\langle \alpha'^2 H'(z)\nabla_z^T G(z,y)K_s(z)\right\rangle^{(0,2)} = 0$$
$$\left\langle \alpha'^2 H'(z)\nabla_z^T G(z,y)K_s(z)\right\rangle^{(2,2)} = 0 \tag{A-82}$$

A.5.7 $\langle \alpha'^2 \mathbf{Y}'(\mathrm{x})\Phi'(\mathrm{y})\rangle$

Multiplying (A-65) by $\alpha'^2 Y'(\boldsymbol{x})$, taking conditional mean, the integral over the Dirichlet boundary is

$$\left\langle \alpha'^2 Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle_{\Gamma_D} = -\int_{\Gamma_D} \left\langle \alpha'^2 Y'(\boldsymbol{x}) H'(z)\nabla_z^T G(z,\boldsymbol{y})K_s(z)\right\rangle n(z)d\Gamma \tag{A-83}$$

The corresponding integrand to second order in σ_β and σ_Y is

$$\left\langle \alpha'^2 Y'(\boldsymbol{x}) H'(z)\nabla_z^T G(z,\boldsymbol{y})K_s(z)\right\rangle^{(2,2)} = 0 \tag{A-84}$$

A.5.8 $\langle \alpha' \mathbf{Y}'(\mathrm{x})\mathbf{Y}'(\mathrm{y})\Phi'(\mathrm{z})\rangle$

Expressing (A-65) in terms of z, multiplying by $\alpha' Y'(\boldsymbol{x})Y'(\boldsymbol{y})$, and taking conditional mean, the integral over the Dirichlet boundary is

$$\left\langle \alpha' Y'(\boldsymbol{x})Y'(\boldsymbol{y})\Phi'(z)\right\rangle_{\Gamma_D} = -\int_{\Gamma_D} \left\langle \alpha' Y'(\boldsymbol{x})Y'(\boldsymbol{y}) H'(\boldsymbol{u})\nabla_u^T G(\boldsymbol{u},z)K_s(\boldsymbol{u})\right\rangle n(\boldsymbol{u})d\Gamma \tag{A-85}$$

Its integrand to second order in σ_β and σ_Y can be obtained by multiplying (A-11) by $\alpha' Y'(\boldsymbol{x})Y'(\boldsymbol{y})\nabla_u^T G(\boldsymbol{u},z)K_s(\boldsymbol{u})$, taking conditional mean, and collecting terms of same order

$$\begin{aligned}&\left\langle \alpha' Y'(\boldsymbol{x})Y'(\boldsymbol{y}) H'(\boldsymbol{u})\nabla_u^T G(\boldsymbol{u},z)K_s(\boldsymbol{u})\right\rangle^{(2,2)} \\ &\qquad = \sigma_\beta^2 e^{\alpha_G\langle\Psi(\boldsymbol{u})\rangle}\left(\alpha_G\left\langle\Psi(\boldsymbol{u})\right\rangle - 1 + \frac{1}{2}\left(\alpha_G\left\langle\Psi(\boldsymbol{u})\right\rangle\right)\sigma_\Psi^2(\boldsymbol{u})\right) C_Y(\boldsymbol{x},\boldsymbol{y})\nabla_u^T G^{(0,0)}(\boldsymbol{u},z)K_s(\boldsymbol{u})\end{aligned} \tag{A-86}$$

A.5.9 $\langle \alpha'^2 Y'(x) Y'(y) \Phi'(z) \rangle$

Rewriting (A-65) in terms of z and multiplying it by $\alpha'^2 Y'(\boldsymbol{x}) Y'(\boldsymbol{y})$, and taking conditional mean yield

$$\left\langle \alpha'^2 Y'(\boldsymbol{x}) Y'(\boldsymbol{y}) \Phi'(z) \right\rangle_{\Gamma_D} = -\int_{\Gamma_D} \left\langle \alpha'^2 Y'(\boldsymbol{x}) Y'(\boldsymbol{y}) H'(\boldsymbol{u}) \nabla_u^T G(\boldsymbol{u}, z) K_s(\boldsymbol{u}) \right\rangle n(\boldsymbol{u}) d\Gamma \tag{A-87}$$

Using (A-11), we have

$$\begin{aligned} &\langle \alpha \rangle^3 \left\langle \alpha'^2 Y'(\boldsymbol{x}) Y'(\boldsymbol{y}) H'(\boldsymbol{u}) \nabla_u^T G(\boldsymbol{u}, z) K_s(\boldsymbol{u}) \right\rangle \\ &\qquad = e^{\alpha_G \langle \Psi(\boldsymbol{u}) \rangle} \left(1 + \frac{1}{2} \alpha_G^2 \sigma_\Psi^2(\boldsymbol{u}) \right) \langle \alpha \rangle^2 \left\langle \alpha'^2 Y'(\boldsymbol{x}) Y'(\boldsymbol{y}) \nabla_u^T G(\boldsymbol{u}, z) K_s(\boldsymbol{u}) \right\rangle \\ &\qquad - \langle \alpha \rangle^3 \langle H(\boldsymbol{u}) \rangle \left\langle \alpha'^2 Y'(\boldsymbol{x}) Y'(\boldsymbol{y}) \nabla_u^T G(\boldsymbol{u}, z) K_s(\boldsymbol{u}) \right\rangle \end{aligned} \tag{A-88}$$

Expanding all terms in powers of σ_Y and σ_β results in

$$\left\langle \alpha'^2 Y'(\boldsymbol{x}) Y'(\boldsymbol{y}) H'(\boldsymbol{u}) \nabla_u^T G(\boldsymbol{u}, z) K_s(\boldsymbol{u}) \right\rangle^{(n,m)} = 0 \qquad n,\ m \le 2 \tag{A-89}$$

APPENDIX B

RECURSIVE EQUATIONS FOR THE AUXILIARY FUNCTION

B.1 INTRODUCTION

From Appendix A we note that solving the first and second conditional moment equations to second order in σ_Y and σ_β requires not only the mean auxiliary approximations $\langle G^{(0,0)}(y, x)\rangle$, $\langle G^{(0,2)}(y, x)\rangle$, $\langle G^{(2,0)}(y, x)\rangle$ and $\langle G^{(2,2)}(y, x)\rangle$, but also mixed moments that include combinations of $Y'(x)$, β' and lower-order approximations of the auxiliary functions, for instance, $\langle \beta' Y'(z)\nabla_x\nabla_y^T G^{(1,1)}(y,x)\rangle$. Quantities containing derivatives, such as $\langle \beta' Y'(z)\nabla_x\nabla_y^T G^{(1,1)}(y,x)\rangle$, can be obtained by formulating their corresponding terms without derivatives, like $\langle \beta' Y'(z) G^{(1,1)}(y,x)\rangle$, and then taking their derivatives. In this appendix, we derive recursive equations for all terms related to the auxiliary function G defined through

$$\begin{cases} \nabla_y \cdot \left[K_s(y)\nabla_y G(y,x)\right] - g\alpha e_3^T\, K_s(y)\nabla_y G(y,x) + \delta(x-y) = 0 & x, y \in \Omega \\ \mathrm{G}(y,x) = 0 & x \in \Omega,\ \ y \in \Gamma_D \\ \nabla_y G(y,x)\cdot n(y) = 0 & x \in \Omega,\ \ y \in \Gamma_N \end{cases} \tag{B-1}$$

Expanding $K_s(x)$, α and G as

$$K_s(x) = e^{Y(x)} = e^{\langle Y(x)\rangle + Y'(x)E} = K_G(x)\sum_{n=0}^{\infty}\frac{[Y'(x)]^n}{n!} \tag{B-2}$$

$$\alpha = e^{\beta} = e^{\langle\beta\rangle+\beta'} = \alpha_G \sum_{m=0}^{\infty}\frac{\beta'^m}{m!} \tag{B-3}$$

$$G(\boldsymbol{y},\boldsymbol{x}) = \sum_{n,m=0}^{\infty} G^{(n,m)}(\boldsymbol{y},\boldsymbol{x}) \tag{B-4}$$

where n and m designates terms including n^{th} power of σ_Y and m^{th} power of σ_β.

Substituting (B-2)-(B-4) into (B-1) yields

$$\begin{cases} \displaystyle\sum_{n=0}^{\infty}\sum_{m=0}^{\infty}\Bigg\{\nabla_y\cdot\left[K_G(\boldsymbol{y})\sum_{k=0}^{n}\frac{[Y'(\boldsymbol{y})]^k}{k!}\nabla_y G^{(n-k,m)}(\boldsymbol{y},\boldsymbol{x})\right] & \\ \displaystyle\quad -g\alpha_G\boldsymbol{e}_3^T K_G(\boldsymbol{y})\sum_{k=0}^{n}\frac{[Y'(\boldsymbol{y})]^k}{k!}\sum_{p=0}^{m}\frac{(\beta')^p}{p!}\nabla_y G^{(n-k,m-p)}(\boldsymbol{y},\boldsymbol{x})\Bigg\} + \delta(\boldsymbol{x}-\boldsymbol{y}) = 0 & \boldsymbol{x},\ \boldsymbol{y}\in\Omega \\ \displaystyle\sum_{n=0}^{\infty}\sum_{m=0}^{\infty} G^{(n,m)}(\boldsymbol{y},\boldsymbol{x}) = 0 & \boldsymbol{x}\in\Omega,\ \boldsymbol{y}\in\Gamma_D \\ \displaystyle\sum_{n=0}^{\infty}\sum_{m=0}^{\infty}\left[\nabla_y G^{(n,m)}(\boldsymbol{y},\boldsymbol{x})\right]\cdot\boldsymbol{n}(\boldsymbol{y}) = 0 & \boldsymbol{x}\in\Omega,\ \boldsymbol{y}\in\Gamma_N \end{cases} \tag{B-5}$$

The deterministic solution $\langle G^{(0,0)}(\boldsymbol{y},\boldsymbol{x})\rangle = G^{(0,0)}(\boldsymbol{y},\boldsymbol{x})$ can be obtained by solving

$$\begin{cases} \nabla_y\cdot\left[K_G(\boldsymbol{y})\nabla_y G^{(0,0)}(\boldsymbol{y},\boldsymbol{x})\right] - g\alpha_G\boldsymbol{e}_3^T K_G(\boldsymbol{y})\nabla_y G^{(0,0)}(\boldsymbol{y},\boldsymbol{x}) + \delta(\boldsymbol{x}-\boldsymbol{y}) = 0 & \boldsymbol{x},\boldsymbol{y}\in\Omega \\ G^{(0,0)}(\boldsymbol{y},\boldsymbol{x}) = 0 & \boldsymbol{x}\in\Omega,\ \boldsymbol{y}\in\Gamma_D \\ \nabla_y G^{(0,0)}(\boldsymbol{y},\boldsymbol{x})\cdot\boldsymbol{n}(\boldsymbol{y}) = 0 & \boldsymbol{x}\in\Omega,\ \boldsymbol{y}\in\Gamma_N \end{cases} \tag{B-6}$$

In general, for $\mathrm{n}+\mathrm{m}\geq 1$, we have

$$\begin{cases} \displaystyle\nabla_y\cdot\left[K_G(\boldsymbol{y})\sum_{k=0}^{n}\frac{[Y'(\boldsymbol{y})]^k}{k!}\nabla_y G^{(n-k,m)}(\boldsymbol{y},\boldsymbol{x})\right] & \\ \displaystyle\quad - g\alpha_G\boldsymbol{e}_3^T K_G(\boldsymbol{y})\sum_{k=0}^{n}\frac{[Y'(\boldsymbol{y})]^k}{k!}\sum_{p=0}^{m}\frac{(\beta')^p}{p!}\nabla_y G^{(n-k,m-p)}(\boldsymbol{y},\boldsymbol{x}) = 0 & \boldsymbol{x},\ \boldsymbol{y}\in\Omega \\ G^{(n,m)}(\boldsymbol{y},\boldsymbol{x}) = 0 & \boldsymbol{x}\in\Omega,\ \boldsymbol{y}\in\Gamma_D \\ \nabla_y G^{(n,m)}(\boldsymbol{y},\boldsymbol{x})\cdot\boldsymbol{n}(\boldsymbol{y}) = 0 & \boldsymbol{x}\in\Omega,\ \boldsymbol{y}\in\Gamma_N \end{cases} \tag{B-7}$$

(B-7) constitute recursive equations for $\langle G^{(n,m)}(\boldsymbol{y},\boldsymbol{x})\rangle$. Here we devolop equations for those approximations that are required to obtain the conditional first and second moment equations to second order in σ_Y and σ_β.

B.2 TERMS RELATED TO $G^{(1,0)}(y,x)$

Setting n=1 and m=0 in (B-7) yields

$$\begin{cases} \nabla_y \cdot \left[K_G(y) \left(\nabla_y G^{(1,0)}(y,x) + Y'(y) \nabla_y G^{(0,0)}(y,x) \right) \right] & \\ \quad - g\alpha_G e_3^T K_G(y) \left(\nabla_y G^{(1,0)}(y,x) + Y'(y) \nabla_y G^{(0,0)}(y,x) \right) = 0 & x,\ y \in \Omega \\ G^{(1,0)}(y,x) = 0 & x \in \Omega,\ y \in \Gamma_D \\ \nabla_y G^{(1,0)}(y,x) \cdot n(y) = 0 & x \in \Omega,\ y \in \Gamma_N \end{cases} \tag{B-8}$$

Taking ensemble mean of equation (B-8), and noting that $\langle Y'(y) \rangle = 0$ while $G^{(0,0)}(y,x)$ is deterministic, we have

$$\begin{cases} \nabla_y \cdot \left[K_G(y)\, \nabla_y \left\langle G^{(1,0)}(y,x) \right\rangle \right] - g\alpha_G e_3^T K_G(y) \nabla_y \left\langle G^{(1,0)}(y,x) \right\rangle = 0 & x, y \in \Omega \\ \left\langle G^{(1,0)}(y,x) \right\rangle = 0 & x \in \Omega,\ y \in \Gamma_D \\ \nabla_y \left\langle G^{(1,0)}(y,x) \right\rangle \cdot n(y) = 0 & x \in \Omega,\ y \in \Gamma_N \end{cases} \tag{B-9}$$

(B-9) has a trivil solution:

$$\left\langle G^{(1,0)}(y,x) \right\rangle \equiv 0 \qquad x, y \in \Omega \tag{B-10}$$

Uniqueness of the solution implies that (B-10) is the solution of (B-9). Multiplying (B-8) by $Y'(z)$ and taking conditional ensemble mean, we get the equations for $\langle Y'(z) G^{(1,0)}(y,x) \rangle$

$$\begin{cases} \nabla_y \cdot \left[K_G(y) \left(\nabla_y \left\langle Y'(z) G^{(1,0)}(y,x) \right\rangle + C_Y(y,z) \nabla_y \left\langle G^{(0,0)}(y,x) \right\rangle \right) \right] & \\ \quad - g\alpha_G e_3^T K_G(y) \left(\nabla_y \left\langle Y'(z) G^{(1,0)}(y,x) \right\rangle + C_Y(y,z) \nabla_y \left\langle G^{(0,0)}(y,x) \right\rangle \right) = 0 & x, y, z \in \Omega \\ \left\langle Y'(z) G^{(1,0)}(y,x) \right\rangle = 0 & x, z \in \Omega,\ y \in \Gamma_D \\ \nabla_y \left\langle Y'(z) G^{(1,0)}(y,x) \right\rangle \cdot n(y) = 0 & x, z \in \Omega,\ y \in \Gamma_N \end{cases} \tag{B-11}$$

where $C_Y(x, y)$ is the conditional auto-covariance of Y between point x and y. Once (B-11) is solved, the terms $\langle Y'(x) G^{(1,0)}(y,x) \rangle$ and $\langle Y'(y) G^{(1,0)}(y,x) \rangle$ can be derived by setting z

$= \boldsymbol{x}$ and $z = \boldsymbol{y}$, respectively, in $\langle Y'(z)G^{(1,0)}(\boldsymbol{y},\boldsymbol{x})\rangle$, and $\langle Y'(\boldsymbol{y})\nabla_y G^{(1,0)}(\boldsymbol{y},\boldsymbol{x})\rangle$ can be evaluated by taking the derivative of $\langle Y'(z)G^{(1,0)}(\boldsymbol{y},\boldsymbol{x})\rangle$ with respect to $\boldsymbol{y}$, then evaluating it at $z = \boldsymbol{y}$.

Multiplying (B-8) by $\beta' Y'(z)$, taking conditional ensemble mean, and recalling that we consider β' and Y' to be uncorrelated, we get the solution for $\langle \beta' Y'(z)G^{(1,0)}(\boldsymbol{y},\boldsymbol{x})\rangle$

$$\left\langle \beta' Y'(z) G^{(1,0)}(\boldsymbol{y},\boldsymbol{x})\right\rangle \equiv 0 \qquad \boldsymbol{x},\, \boldsymbol{y},\, z \in \Omega \tag{B-12}$$

B.3 TERMS RELATED TO $G^{(0,1)}(\boldsymbol{y},\boldsymbol{x})$

From (B-7) we have

$$\begin{cases} \nabla_y \cdot \left[K_G(\boldsymbol{y})\nabla_y G^{(0,1)}(\boldsymbol{y},\boldsymbol{x})\right] - \mathrm{g}\,\alpha_G \boldsymbol{e}_3^T K_G(\boldsymbol{y})\left(\nabla_y G^{(0,1)}(\boldsymbol{y},\boldsymbol{x}) + \beta' \nabla_y G^{(0,0)}(\boldsymbol{y},\boldsymbol{x})\right) = 0 & \boldsymbol{x},\boldsymbol{y} \in \Omega \\ G^{(0,1)}(\boldsymbol{y},\boldsymbol{x}) = 0 & \boldsymbol{x} \in \Omega\,,\ \boldsymbol{y} \in \Gamma_D \\ \nabla_y G^{(0,1)}(\boldsymbol{y},\boldsymbol{x}) \cdot \boldsymbol{n}(\boldsymbol{y}) = 0 & \boldsymbol{x} \in \Omega\,, \boldsymbol{y} \in \Gamma_N \end{cases} \tag{B-13}$$

Taking ensemble mean of (B-13) and noting that $\langle \beta' \rangle = 0$, we get equations for $\langle G^{(0,1)}(\boldsymbol{y},\boldsymbol{x})\rangle$,

$$\begin{cases} \nabla_y \cdot \left[K_G(\boldsymbol{y})\nabla_y \left\langle G^{(0,1)}(\boldsymbol{y},\boldsymbol{x})\right\rangle\right] - \mathrm{g}\alpha_G \boldsymbol{e}_3^T K_G(\boldsymbol{y})\nabla_y \left\langle G^{(0,1)}(\boldsymbol{y},\boldsymbol{x})\right\rangle = 0 & \boldsymbol{x},\boldsymbol{y} \in \Omega \\ \left\langle G^{(0,1)}(\boldsymbol{y},\boldsymbol{x})\right\rangle = 0 & \boldsymbol{x} \in \Omega,\ \ \boldsymbol{y} \in \Gamma_D \\ \nabla_y \left\langle G^{(0,1)}(\boldsymbol{y},\boldsymbol{x})\right\rangle \cdot \boldsymbol{n}(\boldsymbol{y}) = 0 & \boldsymbol{x} \in \Omega,\ \ \boldsymbol{y} \in \Gamma_N \end{cases} \tag{B-14}$$

which have the solution

$$\left\langle G^{(0,1)}(\boldsymbol{y},\boldsymbol{x})\right\rangle \equiv 0 \qquad \boldsymbol{x},\, \boldsymbol{y} \in \Omega \tag{B-15}$$

To formulate equations for $\langle \beta' G^{(0,1)}(\boldsymbol{y},\boldsymbol{x})\rangle$, we multiply (B-13) by β' and take conditional ensemble mean,

$$\begin{cases} \nabla_y \cdot \left[K_G(y) \nabla_y \left\langle \beta' G^{(0,1)}(y,x) \right\rangle \right] & \\ \qquad - g\alpha_G e_3^T K_G(y) \left(\nabla_y \left\langle \beta' G^{(0,1)}(y,x) \right\rangle + \sigma_\beta^2 \nabla_y \left\langle G^{(0,0)}(y,x) \right\rangle \right) = 0 & x,\ y \in \Omega \\ \left\langle \beta' G^{(0,1)}(y,x) \right\rangle = 0 & x, \in \Omega \quad y \in \Gamma_D \\ \nabla_y \left\langle \beta' G^{(0,1)}(y,x) \right\rangle \cdot n(y) = 0 & x \in \Omega, \quad y \in \Gamma_N \end{cases} \tag{B-16}$$

The term $\langle \beta' \nabla_y G^{(0,1)}(y,x) \rangle$ can be derived by taking the derivative of $\langle \beta' G^{(0,1)}(y,x) \rangle$ with respect to y, after (B-16) has been solved.

B.4 TERMS RELATED TO $G^{(1,1)}(y,x)$

Setting n=1 and m=1 in (B-7) gives

$$\begin{cases} \nabla_y \cdot \left[K_G(y) \left(\nabla_y G^{(1,1)}(y,x) + Y'(y) \nabla_y G^{(0,1)}(y,x) \right) \right] - g\alpha_G e_3^T K_G(y) \left[\nabla_y G^{(1,1)}(y,x) \right. & \\ \qquad \left. + Y'(y) \nabla_y G^{(0,1)}(y,x) + \beta' \nabla_y G^{(1,0)}(y,x) + \beta' Y'(y) \nabla_y G^{(0,0)}(y,x) \right] = 0 & x,\ y \in \Omega \\ G^{(1,1)}(y,x) = 0 & x \in \Omega, \ y \in \Gamma_D \\ \nabla_y G^{(1,1)}(y,x) \cdot n(y) = 0 & x \in \Omega, \ y \in \Gamma_N \end{cases} \tag{B-17}$$

Taking conditional mean of this equation, using (B-10) and (B-15), and recalling our assumption that $Y'(y)$ and β' are uncorrelated leads to

$$\begin{cases} \nabla_y \cdot \left[K_G(y) \nabla_y \left\langle G^{(1,1)}(y,x) \right\rangle \right] - g\alpha_G e_3^T K_G(y) \nabla_y \left\langle G^{(1,1)}(y,x) \right\rangle = 0 & x,\ y \in \Omega \\ \left\langle G^{(1,1)}(y,x) \right\rangle = 0 & x,\ y \in \Omega,\ y \in \Gamma_D \\ \nabla_y \left\langle G^{(1,1)}(y,x) \right\rangle \cdot n(y) = 0 & x,\ y \in \Omega,\ y \in \Gamma_N \end{cases} \tag{B-18}$$

which has the solution

$$\left\langle G^{(1,1)}(y,x) \right\rangle \equiv 0 \qquad x,\ y \in \Omega \tag{B-19}$$

Multiplying (B-17) by β' and taking conditional mean yield

$$\begin{cases} \nabla_y \cdot \left[K_G(y) \nabla_y \left\langle \beta' G^{(1,1)}(y,x) \right\rangle \right] - g\alpha_G e_3^T K_G(y) \left(\nabla_y \left\langle \beta' G^{(1,1)}(y,x) \right\rangle + \sigma_\beta^2 \nabla_y \left\langle G^{(1,0)}(y,x) \right\rangle \right) = 0 & x,\, y \in \Omega \\ \left\langle \beta' G^{(1,1)}(y,x) \right\rangle = 0 & x,\, y \in \Omega\,, y \in \Gamma_D \\ \nabla_y \left\langle \beta' G^{(1,1)}(y,x) \right\rangle \cdot n(y) = 0 & x,\, y \in \Omega\,,\; y \in \Gamma_N \end{cases} \quad \text{(B-20)}$$

where $\langle G^{(1,0)} \rangle = 0$, according to (B-10). Therefore, (B-20) has the solution

$$\left\langle \beta' G^{(1,1)}(y,x) \right\rangle \equiv 0 \qquad x,\, y \in \Omega \qquad \text{(B-21)}$$

Similarly, we have

$$\left\langle Y'(z) \nabla_y G^{(1,1)}(y,x) \right\rangle \equiv 0 \qquad x,\, y, z \in \Omega \qquad \text{(B-22)}$$

An equation for $\langle \beta' Y'(z) G^{(1,1)} \rangle$ can be derived upon multiplying (B-17) by $\beta' Y'(z)$ and taking conditional mean,

$$\begin{cases} \nabla_y \cdot \left[K_G(y) \left(\nabla_y \left\langle \beta' Y'(z)\, G^{(1,1)}(y,x) \right\rangle + C_Y(y,z) \nabla_y \left\langle \beta' G^{(0,1)}(y,x) \right\rangle \right) \right] & \\ \quad - g\alpha_G e_3^T K_G(y) \left(\nabla_y \left\langle \beta' Y'(z)\, G^{(1,1)}(y,x) \right\rangle + C_Y(y,z) \left\langle \beta' G^{(0,1)}(y,x) \right\rangle \right. & \\ \quad \left. + \sigma_\beta^2 C_Y(y,z) \nabla_y G^{(0,0)}(y,x) \right) = 0 & x,\; y, z \in \Omega \\ \left\langle \beta' Y'(z)\, G^{(1,1)}(y,x) \right\rangle = 0 & x, z \in \Omega \quad y \in \Gamma_D \\ \nabla_y \left\langle \beta' Y'(z)\, G^{(1,1)}(y,x) \right\rangle \cdot n(y) = 0 & x, z \in \Omega, \;\; y \in \Gamma_N \end{cases} \quad \text{(B-23)}$$

Its related terms such as $\langle \beta' Y'(z) \nabla_y G^{(1,1)}(y, x) \rangle$ can be obtained numerically by taking the derivative of $\langle \beta' Y'(z) G^{(1,1)}(y, x) \rangle$ with respect to y.

B.5 TERMS RELATED TO $G^{(0,2)}(y,x)$

Equations for $G^{(0,2)}(y, x)$ can be formulated from (B-7) by setting n=0 and m=2,

$$\begin{cases} \nabla_y \cdot \left[K_G(y) \nabla_y G^{(0,2)}(y,x) \right] \\ \quad - g\alpha_G e_3^T K_G(y) \left[\nabla_y G^{(0,2)}(y,x) + \beta' \nabla_y G^{(0,1)}(y,x) + \frac{\beta'^2}{2} \nabla_y G^{(0,0)}(y,x) \right] = 0 & x,\ y \in \Omega \\ \mathrm{G}^{(0,2)}(y,x) = 0 & x,\ y \in \Omega,\ y \in \Gamma_\mathrm{D} \\ \nabla_y G^{(0,2)}(y,x) \cdot n(y) = 0 & x,\ y \in \Omega,\ y \in \Gamma_\mathrm{N} \end{cases} \tag{B-24}$$

Taking ensemble mean of (B-24) leads to

$$\begin{cases} \nabla_y \cdot \left[K_G(y) \nabla_y \left\langle G^{(0,2)}(y,x) \right\rangle \right] \\ \quad - g\alpha_G e_3^T K_G(y) \left[\nabla_y \left\langle G^{(0,2)}(y,x) \right\rangle + \nabla_y \left\langle \beta' G^{(0,1)}(y,x) \right\rangle + \frac{\sigma_\beta^2}{2} \nabla_y G^{(0,0)}(y,x) \right] = 0 & x,\ y \in \Omega \\ \left\langle G^{(0,2)}(y,x) \right\rangle = 0 & x \in \Omega,\ y \in \Gamma_\mathrm{D} \\ \nabla_y \left\langle G^{(0,2)}(y,x) \right\rangle \cdot n(y) = 0 & x \in \Omega,\ y \in \Gamma_\mathrm{N} \end{cases} \tag{B-25}$$

Due to the assumption that Y' and β' are uncorrelated, it is easy to see from (B-24) that $\langle Y'(\mathrm{z}) G^{(0,2)}(y,x) \rangle = 0$.

B.6 TERMS RELATED TO $\mathbf{G^{(2,0)}(y,x)}$

Setting n=2 and m=0 in (B-7) gives

$$\begin{cases} \nabla_y \cdot \left[K_G(y) \left(\nabla_y G^{(2,0)}(y,x) + Y'(y) \nabla_y G^{(1,0)}(y,x) + \frac{1}{2} Y'^2(y) \nabla_y G^{(0,0)}(y,x) \right) \right] \\ \quad + g\alpha_G e_3^T K_G(y) \left[\nabla_y G^{(2,0)}(y,x) + \frac{1}{2} Y'(y) \nabla_y G^{(1,0)}(y,x) + \frac{1}{2} Y'^2(y) \nabla_y G^{(0,0)}(y,x) \right] = 0 & x, y \in \Omega \\ G^{(2,1)}(y,x) = 0 & x \in \Omega,\ y \in \Gamma_\mathrm{D} \\ \nabla_y G^{(2,1)}(y,x) \cdot n(y) = 0 & x \in \Omega,\ y \in \Gamma_\mathrm{N} \end{cases} \tag{B-26}$$

Taking conditional mean of (B-26) gives

$$\begin{cases} \nabla_y \cdot \left[K_G(y) \left(\nabla_y \left\langle G^{(2,0)}(y,x) \right\rangle + \left\langle Y'(y) \nabla_y G^{(1,0)}(y,x) \right\rangle + \frac{\sigma_Y^2(y)}{2} \nabla_y G^{(0,0)}(y,x) \right) \right] \\ \quad - g\alpha_G e_3^T K_G(y) \left(\nabla_y \left\langle G^{(2,0)}(y,x) \right\rangle + \left\langle Y'(y) G^{(1,0)}(y,x) \right\rangle + \frac{\sigma_Y^2(y)}{2} \nabla_y G^{(0,0)}(y,x) \right) = 0 & x, y \in \Omega \\ \left\langle G^{(2,0)}(y,x) \right\rangle = 0 & x \in \Omega,\ y \in \Gamma_D \\ \nabla_y \left\langle G^{(2,0)}(y,x) \right\rangle \cdot n(y) = 0 & x \in \Omega,\ y \in \Gamma_N \end{cases} \tag{B-27}$$

It is obvious from (B-26) that $\langle \beta' G^{(2,0)}(y, x) \rangle = 0$.

B.7 TERMS RELATED TO $G^{(1,2)}(y, x)$

Again, from (B-7) we have

$$\begin{cases} \nabla_y \cdot \left[K_G(y) \left(\nabla_y G^{(1,2)}(y,x) + Y'(y) \nabla_y G^{(0,2)}(y,x) \right) \right] \\ \quad - g\alpha_G e_3^T K_G(y) \left[\nabla_y G^{(1,2)}(y,x) + \beta' \nabla_y G^{(1,1)}(y,x) + 0.5\beta'^2 \nabla_y G^{(1,0)}(y,x) \right. \\ \quad \left. + Y'(y) \nabla_y G^{(0,2)}(y,x) + \beta' Y'(y) \nabla_y G^{(0,1)}(y,x) + 0.5\beta'^2 Y'(y) \nabla_y G^{(0,0)}(y,x) \right] = 0 & x, y \in \Omega \\ G^{(1,2)}(y,x) = 0 & x, y \in \Omega,\ y \in \Gamma_D \\ \nabla_y G^{(1,2)}(y,x) \cdot n(y) = 0 & x, y \in \Omega,\ y \in \Gamma_N \end{cases} \tag{B-28}$$

Taking the conditional mean of (B-28) yields

$$\left\langle G^{(1,2)}(y,x) \right\rangle \equiv 0 \qquad x, y \in \Omega \tag{B-29}$$

Multiplying (B-28) by $Y'(z)$ and taking conditional mean yields equations for $\langle Y'(z) G^{(1,2)}(y, x) \rangle$:

$$\begin{cases} \nabla_y \cdot \left[K_G(y) \left(\nabla_y \left\langle Y'(z) G^{(1,2)}(y,x) \right\rangle + C_Y(y,z) \nabla_y \left\langle G^{(0,2)}(y,x) \right\rangle \right) \right] \\ \quad - g\alpha_G e_3^T K_G(y) \left[\nabla_y \left\langle Y'(z) G^{(1,2)}(y,x) \right\rangle + \left\langle \beta' Y'(z) \nabla_y G^{(1,1)}(y,x) \right\rangle + 0.5\sigma_\beta^2 \left\langle Y'(z) \nabla_y G^{(1,0)}(y,x) \right\rangle \right. \\ \quad \left. + C_Y(y,z) \left(\nabla_y \left\langle G^{(0,2)}(y,x) \right\rangle + \nabla_y \left\langle \beta' G^{(0,1)}(y,x) \right\rangle + 0.5\sigma_\beta^2 \nabla_y G^{(0,0)}(y,x) \right) \right] = 0 & x, y \in \Omega \\ \left\langle Y'(z) G^{(1,2)}(y,x) \right\rangle = 0 & x, y \in \Omega,\ y \in \Gamma_D \\ \nabla_y \left\langle Y'(z) G^{(1,2)}(y,x) \right\rangle \cdot n(y) = 0 & x, y \in \Omega,\ y \in \Gamma_N \end{cases} \tag{B-30}$$

B.8 TERMS RELATED TO $G^{(2,1)}$ (*y*,*x*)

From (B-7), the equation for $G^{(2,1)}(y, x)$ reads

$$\begin{cases} \nabla_y \cdot \left[K_G(y)\left(\nabla_y G^{(2,1)}(y,x) + Y'(y)\nabla_y G^{(1,1)}(y,x) + 0.5Y'^2(y)\nabla_y G^{(0,1)}(y,x)\right)\right] \\ \quad + g\alpha_G e_3^T K_G(y)\left[\nabla_y G^{(2,1)}(y,x) + \beta'\nabla_y G^{(2,0)}(y,x) + 0.5Y'(y)\nabla_y G^{(1,1)}(y,x)\right. \\ \quad \left. +\beta' Y'(y)\nabla_y G^{(1,0)}(y,x) + 0.5Y'^2(y)\nabla_y G^{(0,1)}(y,x) + 0.5\beta' Y'^2(y)\nabla_y G^{(0,0)}(y,x)\right] = 0 & x, y \in \Omega \\ G^{(2,1)}(y,x) = 0 & x \in \Omega,\ y \in \Gamma_D \\ \nabla_y G^{(2,1)}(y,x)\cdot n(y) = 0 & x \in \Omega,\ y \in \Gamma_N \end{cases} \quad \text{(B-31)}$$

Taking conditional mean of (B-30) leads to

$$\begin{cases} \nabla_y \cdot \left[K_G(y)\left(\nabla_y \left\langle G^{(2,1)}(y,x)\right\rangle + \left\langle Y'(y)\nabla_y G^{(1,1)}(y,x)\right\rangle + 0.5\sigma_Y^2(y)\left\langle \nabla_y G^{(0,1)}(y,x)\right\rangle\right)\right] \\ \quad - g\alpha_G e_3^T K_G(y)\left[\nabla_y \left\langle G^{(2,1)}(y,x)\right\rangle + 0.5\left\langle Y'(y)\nabla_y G^{(1,1)}(y,x)\right\rangle\right. \\ \quad \left. +\left\langle \beta' Y'(y)\nabla_y G^{(1,0)}(y,x)\right\rangle + 0.5\sigma_Y^2(y)\left\langle \nabla_y G^{(0,1)}(y,x)\right\rangle\right] = 0 & x, y \in \Omega \\ \left\langle G^{(2,1)}(y,x)\right\rangle = 0 & x \in \Omega,\ y \in \Gamma_D \\ \nabla_y \left\langle G^{(2,1)}(y,x)\right\rangle \cdot n(y) = 0 & x \in \Omega,\ y \in \Gamma_N \end{cases} \quad \text{(B-32)}$$

It can be shown that (B-32) has a trivial solution. Equations for $\langle \beta' G^{(2,1)}(y, x)\rangle$ can be obtained upon multiplying (B-31) by β' and taking conditional mean,

$$\begin{cases} \nabla_y \cdot \left[K_G(y)\left(\left\langle \beta'\nabla_y G^{(2,1)}(y,x)\right\rangle + \left\langle \beta' Y'(y)\nabla_y G^{(1,1)}(y,x)\right\rangle + \dfrac{\sigma_Y^2(y)}{2}\left\langle \beta'\nabla_y G^{(0,1)}(y,x)\right\rangle\right)\right] \\ \quad - g\alpha_G e_3^T K_G(y)\left[\left\langle \beta'\nabla_y G^{(2,1)}(y,x)\right\rangle + \sigma_\beta^2\left\langle \nabla_y G^{(2,0)}(y,x)\right\rangle + \left\langle \beta' Y'(y)\nabla_y G^{(1,1)}(y,x)\right\rangle\right. \\ \quad \left. +\sigma_\beta^2\left\langle Y'(y)\nabla_y G^{(1,0)}(y,x)\right\rangle + \dfrac{\sigma_Y^2(y)}{2}\left\langle \beta'\nabla_y G^{(0,1)}(y,x)\right\rangle + \dfrac{1}{2}\sigma_\beta^2\sigma_Y^2(y)\nabla_y G^{(0,0)}(y,x)\right] = 0 & x, y \in \Omega \\ \left\langle \beta' G^{(2,1)}(y,x)\right\rangle = 0 & x \in \Omega,\ y \in \Gamma_D \\ \left\langle \beta'\nabla_y G^{(2,1)}(y,x)\right\rangle \cdot n(y) = 0 & x \in \Omega,\ y \in \Gamma_N \end{cases} \quad \text{(B-33)}$$

B.9 TERMS RELATED TO $G^{(2,2)}(y,x)$

Finally, setting n, m=2 in (B-7) and taking conditional mean gives

$$\begin{cases}\nabla_y\cdot\Big[K_G(y)\Big(\nabla_y\big\langle G^{(2,2)}(y,x)\big\rangle+\big\langle Y'(y)\nabla_y G^{(1,2)}(y,x)\big\rangle+0.5\sigma_Y^2(y)\nabla_y\big\langle G^{(0,2)}(y,x)\big\rangle\Big)\Big] & \\ \quad -g\alpha_G e_3^T K_G(y)\Big[\nabla_y\big\langle G^{(2,2)}(y,x)\big\rangle+\big\langle\beta'\nabla_y G^{(2,1)}(y,x)\big\rangle+0.5\sigma_\beta^2\nabla_y\big\langle G^{(2,0)}(y,x)\big\rangle & \\ \quad +\big\langle Y'(y)\nabla_y G^{(1,2)}(y,x)\big\rangle+\big\langle\beta' Y'(y)\nabla_y G^{(1,1)}(y,x)\big\rangle+0.5\sigma_\beta^2\big\langle Y'(y)\nabla_y G^{(1,0)}(y,x)\big\rangle & \\ \quad +0.5\sigma_Y^2(y)\Big(\nabla_y\big\langle G^{(0,2)}(y,x)\big\rangle+\nabla_y\big\langle\beta' G^{(0,1)}(y,x)\big\rangle+0.5\sigma_\beta^2\nabla_y G^{(0,0)}(y,x)\Big)\Big]=0 & x,y\in\Omega \\ \big\langle G^{(2,2)}(y,x)\big\rangle = 0 & x,\ y\in\Omega,\ \ y\in\Gamma_D \\ \nabla_y\big\langle G^{(2,2)}(y,x)\big\rangle\cdot n(y)=0 & x,\ y\in\Omega,\ \ y\in\Gamma_N\end{cases}\tag{B-34}$$

APPENDIX C
DERIVATION OF RECURSIVE MOMENT EQUATIONS

As we have seen from Chapter 3, solving conditional first moment euquations (mean equations) for the transformed variable and flux, and second moment equations (their associated (co)variance and cross-covariance) involve some other terms that must be solved first. In this section, we will derive all terms required in solving the first and second moment equations.

C.1 $\langle K'(X)\Phi'(Y)\rangle$ AND $\langle K'(X)\nabla\Phi'(Y)\rangle$

Expressing the explicit expression for Φ', (2-19), in terms of $\boldsymbol{y}$, multiplying it by $Y'(\boldsymbol{x})$, and taking conditional ensemble mean, gives

$$\begin{aligned}
\langle Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle = &-\int_\Omega \langle Y'(\boldsymbol{x})\nabla_z^T G(\boldsymbol{z},\boldsymbol{y})K_s'(\boldsymbol{z})\rangle\left[\nabla\langle\Phi(\boldsymbol{z})\rangle + g\langle\alpha\rangle\langle\Phi(\boldsymbol{z})\rangle\boldsymbol{e}_3\right]\mathrm{d}\Omega \\
&-\int_\Omega \langle Y'(\boldsymbol{x})\nabla_z^T G(\boldsymbol{z},\boldsymbol{y})\rangle\, \boldsymbol{r}(\boldsymbol{z})\mathrm{d}\Omega \\
&-\mathrm{g}\int_\Omega \langle \alpha' Y'(\boldsymbol{x})\nabla_z^T G(\boldsymbol{z},\boldsymbol{y})K_s(\boldsymbol{z})\rangle\langle\Phi(\boldsymbol{z})\rangle\boldsymbol{e}_3\ \mathrm{d}\Omega \\
&+g\int_\Omega \langle Y'(\boldsymbol{x})\nabla_z^T G(\boldsymbol{z},\boldsymbol{y})\rangle\left(\langle\alpha\rangle R_{K\Phi}(\boldsymbol{z}) + \langle K_s(\boldsymbol{z})\rangle R_{\alpha\Phi}(\boldsymbol{z}) + R_{\alpha K\Phi}(\boldsymbol{z})\right)\boldsymbol{e}_3\mathrm{d}\Omega \\
&-\int_{\Gamma_D} \langle Y'(\boldsymbol{x})H'(\boldsymbol{z})\nabla_z^T G(\boldsymbol{z},\boldsymbol{y})K_s(\boldsymbol{z})\rangle\, \boldsymbol{n}(\boldsymbol{z})d\Gamma
\end{aligned} \tag{C-1}$$

where

$$\begin{aligned}
\boldsymbol{r}(\boldsymbol{z}) &= -\langle K_s'(\boldsymbol{z})\nabla\Phi'(\boldsymbol{z})\rangle \\
R_{K\Phi}(\boldsymbol{z}) &= \langle K_s'(\boldsymbol{z})\Phi'(\boldsymbol{z})\rangle \\
R_{\alpha\Phi}(\boldsymbol{z}) &= \langle \alpha'\Phi'(\boldsymbol{z})\rangle \\
R_{\alpha K\Phi}(\boldsymbol{z}) &= \langle \alpha' K'(\boldsymbol{z})\ \Phi'(\boldsymbol{z})\rangle
\end{aligned} \tag{C-2}$$

The integral over the Neumann boundary in (C-1) has been dropped due to the fact that both Y' and G are independent of perturbations of prescribed influx Q' on this boundary. The integral over the low domain that contains fluctuation f' is also vanished because Y' and G are independent of f'. The integrand of the integral over Dirichlet boundary was evaluated in (A-74) of Appendix A.

As stated in Chapter 4, exact equations are not workable because they are not closed. Expanding (C-1) in powers of σ_Y and σ_β using (3-1) and (3-2), we can obtain recursive solutions to any order. The second term in the first integral of (C-1), for example, can be expressed

$$\begin{aligned} & g\int_\Omega \left\langle Y'(x)\nabla_z^T G(z,y)K_s'(z)\right\rangle\langle\alpha\rangle\langle\Phi(z)\rangle e_3 \mathrm{d}\Omega \\ & \quad = g\alpha_G\int_\Omega \sum_{n,m=0}^{\infty}\left\langle Y'(x)\nabla_z^T G(z,y)K_s'(z)\right\rangle^{(n,m)} \sum_{m=0}^{\infty}\frac{\left\langle\beta'^m\right\rangle}{m!}\sum_{n,m=0}^{\infty}\left\langle\Phi^{(n,m)}(z)\right\rangle e_3 \mathrm{d}\Omega \\ & \quad = g\alpha_G \sum_{n,m=0}^{\infty}\sum_{i=0}^{n}\sum_{j+k+l=m}\frac{\left\langle\beta'^j\right\rangle}{j!}\int_\Omega \left\langle Y'(x)\nabla_z^T G(z,y)K_s'(z)\right\rangle^{(i,k)}\left\langle\Phi^{(n-i,l)}(z)\right\rangle e_3 \mathrm{d}\Omega \end{aligned} \tag{C-3}$$

Similarly, expanding all terms in (C-1) and equating terms of same order, we have

$$C_{Y\Phi}^{(2,0)}(x,y) = -\int_\Omega C_Y(x,z)\,\nabla_z^T\left\langle G^{(0,0)}(z,y)\right\rangle K_G(z)\,\left[\nabla\left\langle\Phi^{(0,0)}(z)\right\rangle + g\alpha_G\left\langle\Phi^{(0,0)}(z)\right\rangle e_3\right]d\Omega \tag{C-4}$$

$$\begin{aligned} C_{Y\Phi}^{(2,2)}(x,y) &= \left\langle Y'(x)\Phi'(y)\right\rangle \\ &= -\int_\Omega C_Y(x,z)\,\nabla_z^T\left\langle G^{(0,2)}(z,y)\right\rangle K_G(z)\,\left[\nabla\left\langle\Phi^{(0,0)}(z)\right\rangle + g\alpha_G\left\langle\Phi^{(0,0)}(z)\right\rangle e_3\right]d\Omega \\ &\quad -\int_\Omega C_Y(x,z)\nabla_z^T\left\langle G^{(0,0)}(z,y)\right\rangle K_G(z)\left[\nabla\left\langle\Phi^{(0,2)}(z)\right\rangle + g\alpha_G\left(\left\langle\Phi^{(0,2)}(z)\right\rangle + \frac{\sigma_\beta^2}{2}\left\langle\Phi^{(0,0)}(z)\right\rangle\right)e_3\right]d\Omega \\ &\quad - g\,\alpha_G\int_\Omega\left[C_Y(x,z)\,\left\langle\beta'\nabla_z^T G^{(0,1)}(z,y)\right\rangle + \left\langle\beta' Y'(x)\nabla_z^T G^{(1,1)}(z,y)\right\rangle\right]K_G(z)\left\langle\Phi^{(0,0)}(z)\right\rangle e_3 d\Omega \\ &\quad + g\int_\Omega\left\langle Y'(x)\,\nabla_z^T G^{(1,0)}(z,y)\right\rangle K_G(z)\,R_{\alpha\Phi}^{(0,2)}(z)e_3 d\Omega \\ &\quad -\int_{\Gamma_D}\left\langle Y'(x)H'(z)\nabla_z^T G(z,y)K_s(z)\right\rangle^{(2,2)} n(z)d\Gamma \end{aligned} \tag{C-5}$$

Here the definitions of terms, such as K_G *and* σ_β^2, can be found in Chapter 4. The terms related to G have been evaluated in Appendix B. All omitted lower-order terms, such as $\langle Y'(\mathbf{x})\Phi'(\mathbf{y})\rangle^{(0,0)}$, $\langle Y'(\mathbf{x})\Phi'(\mathbf{y})\rangle^{(0,1)}$, are zero. Approximations of the cross-covariance function $\langle K'(\mathbf{x})\Phi'(\mathbf{y})\rangle$ can be obtained to second order, using (C-4)-(C-5),

$$\begin{aligned}\left\langle K_s'(\mathbf{x})\Phi'(\mathbf{y})\right\rangle^{(2,0)} &= K_G(\mathbf{x})\left\langle Y'(\mathbf{x})\Phi'(\mathbf{y})\right\rangle^{(2,0)}\\ \left\langle K_s'(\mathbf{x})\Phi'(\mathbf{y})\right\rangle^{(2,2)} &= K_G(\mathbf{x})\left\langle Y'(\mathbf{x})\Phi'(\mathbf{y})\right\rangle^{(2,2)}\end{aligned} \tag{C-6}$$

Equations (C-5) and (C-6) show that $\langle K'(\mathbf{x})\Phi'(\mathbf{y})\rangle^{(2,0)}$ does not include any term related to the boundary integral over the Dirichlet boundary. This is why the second order approximation (44) is still valid in *Tartakovsky et al* [1999], though in their exact equation, (A9), the integral over Dirichlet boundary has been mistakenly dropped. The same applies to some other terms, such as $\langle K'(\mathbf{x})\nabla\Phi'(\mathbf{y})\rangle$.

Taking the derivative of (C-1) with respect to $\mathbf{y}$ yields an explicit expression for $\langle Y'(\mathbf{x})\nabla\Phi'(\mathbf{y})\rangle$,

$$\begin{aligned}\left\langle Y'(\mathbf{x})\nabla\Phi'(\mathbf{y})\right\rangle = &-\int_\Omega \left\langle Y'(\mathbf{x})\nabla_y\nabla_z^T G(\mathbf{z},\mathbf{y})K_s'(\mathbf{z})\right\rangle\left[\nabla\left\langle\Phi(\mathbf{z})\right\rangle + g\left\langle\alpha\right\rangle\left\langle\Phi(\mathbf{z})\right\rangle\mathbf{e}_3\right]\mathrm{d}\Omega\\ &-\int_\Omega \left\langle Y'(\mathbf{x})\nabla_y\nabla_z^T G(\mathbf{z},\mathbf{y})\right\rangle r(\mathbf{z})\mathrm{d}\Omega\\ &-\mathrm{g}\int_\Omega \left\langle \alpha' Y'(\mathbf{x})\nabla_y\nabla_z^T G(\mathbf{z},\mathbf{y})K_s(\mathbf{z})\right\rangle\left\langle\Phi(\mathbf{z})\right\rangle\mathbf{e}_3\,\mathrm{d}\Omega\\ &+g\int_\Omega \left\langle Y'(\mathbf{x})\nabla_y\nabla_z^T G(\mathbf{z},\mathbf{y})\right\rangle\left(\left\langle\alpha\right\rangle R_{K\Phi}(\mathbf{z}) + \left\langle K_s(\mathbf{z})\right\rangle R_{\alpha\Phi}(\mathbf{z}) + R_{\alpha K\Phi}(\mathbf{z})\right)\mathbf{e}_3\mathrm{d}\Omega\\ &-\int_{\Gamma_D} \left\langle Y'(\mathbf{x})H'(\mathbf{z})\nabla_y\nabla_z^T G(\mathbf{z},\mathbf{y})K_s(\mathbf{z})\right\rangle\mathbf{n}(\mathbf{z})d\Gamma\end{aligned} \tag{C-7}$$

Corresponding second order approximations are:

$$\left\langle Y'(\mathbf{x})\nabla\Phi'(\mathbf{y})\right\rangle^{(2,0)} = -\int_\Omega C_Y(\mathbf{x},\mathbf{z})\nabla_y\nabla_z^T G^{(0,0)}(\mathbf{z},\mathbf{y})K_G(\mathbf{z})\left(\nabla\left\langle\Phi^{(0,0)}(\mathbf{z})\right\rangle + \mathrm{g}\alpha_G\left\langle\Phi^{(0,0)}(\mathbf{z})\right\rangle\mathbf{e}_3\right)d\Omega \tag{C-8}$$

$$\begin{aligned}\left\langle Y'(x)\nabla\Phi'(y)\right\rangle^{(2,2)} = &-\int_{\Omega} C_Y(x,z)\nabla_y\nabla_z^T\left\langle G^{(0,2)}(z,y)\right\rangle K_G(z)\left[\nabla\left\langle\Phi^{(0,0)}(z)\right\rangle + \mathrm{g}\,\alpha_G\left\langle\Phi^{(0,0)}(z)\right\rangle e_3\right]d\Omega \\ &-\int_{\Omega} C_Y(x,z)\nabla_y\nabla_z^T G^{(0,0)}(z,y)K_G(z)\left[\nabla\left\langle\Phi^{(0,2)}(z)\right\rangle + \mathrm{g}\,\alpha_G\left(\left\langle\Phi^{(0,2)}(z)\right\rangle + \frac{\sigma_\beta^2}{2}\left\langle\Phi^{(0,0)}(z)\right\rangle\right)e_3\right]d\Omega \\ &-\mathrm{g}\,\alpha_G\int_{\Omega}\left[C_Y(x,z)\left\langle\beta'\nabla_y\nabla_z^T G^{(0,1)}(z,y)\right\rangle + \left\langle\beta' Y'(x)\nabla_y\nabla_z^T G^{(1,1)}(z,y)\right\rangle\right]K_G(z)\left\langle\Phi^{(0,0)}(z)\right\rangle e_3 d\Omega \\ &+\mathrm{g}\int_{\Omega}\left\langle Y'(x)\nabla_y\nabla_z^T G^{(1,0)}(z,y)\right\rangle K_G(z)\, R_{\alpha\Phi}^{(0,2)}(z)e_3 d\Omega \\ &-\int_{\Gamma_D}\left\langle Y'(x)H'(z)\nabla_y\nabla_z^T G(z,y)K_s(z)\right\rangle^{(2,2)} n(z)d\Gamma\end{aligned} \tag{C-9}$$

The integrand of the intergal over the Dirichlet boundary can be obtained from (A-74) of Appendix A by taking the derivative with respect to $\boldsymbol{y}$. Once (C-8) and (C-9) are solved, $\boldsymbol{R}^{(2,0)}(\boldsymbol{x},\boldsymbol{y})=\langle K'(\boldsymbol{x})\nabla\Phi'(\boldsymbol{y})\rangle^{(2,0)}$ and $\boldsymbol{R}^{(2,2)}(\boldsymbol{x},\boldsymbol{y})=\langle K'(\boldsymbol{x})\nabla\Phi'(\boldsymbol{y})\rangle^{(2,2)}$ can be evaluated simply upon multiplying (C-8) and (C-9) by $K_G(\boldsymbol{x})$. "Residual flux" $\boldsymbol{r}^{(2,0)}(\boldsymbol{x})=\boldsymbol{R}^{(2,0)}(\boldsymbol{x},\boldsymbol{x})$ and $\boldsymbol{r}^{(2,2)}(\boldsymbol{x})=\boldsymbol{R}^{(2,2)}(\boldsymbol{x},\boldsymbol{x})$ can be calculated.

C.2 $\langle\alpha'\Phi'(y)\rangle$ AND $\langle\alpha'^2\Phi'(y)\rangle$

Multiplying (2-19) by α' and taking conditional ensemble mean yields an expression for the cross-covariance function $R_{\alpha\Phi}(\boldsymbol{x})$,

$$\begin{aligned}R_{\alpha\Phi}(x) = \left\langle\alpha'\Phi'(x)\right\rangle = &-\int_{\Omega}\left\langle\alpha'\nabla_z^T G(z,x)\, K_s'(z)\right\rangle\left[\nabla\left\langle\Phi(z)\right\rangle + g\left\langle\alpha\right\rangle\left\langle\Phi(z)\right\rangle e_3\right]\mathrm{d}\Omega \\ &-\int_{\Omega}\left\langle\alpha'\nabla_z^T G(z,x)\right\rangle r(z)\mathrm{d}\Omega \\ &-\mathrm{g}\int_{\Omega}\left\langle\alpha'^2\nabla_z^T G(z,x)\, K_s(z)\right\rangle\left\langle\Phi(z)\right\rangle e_3\mathrm{d}\Omega \\ &+g\int_{\Omega}\left\langle\alpha'\,\nabla_z^T G(z,x)\right\rangle\left(\left\langle\alpha\right\rangle R_{K\Phi}(z) + \left\langle K_s(z)\right\rangle R_{\alpha\Phi}(z) + R_{\alpha K\Phi}(z)\right)e_3\mathrm{d}\Omega \\ &-\int_{\Gamma_D}\left\langle\alpha' H'(z)\nabla_z^T G(z,x)K_s(z)\right\rangle n(z)d\Gamma\end{aligned} \tag{C-10}$$

The boundary integral over the Neumann boundary has been dropped because α' is uncorrelated with Q' and G, and so has the volume integral containing f'. Approximations to second order can be obtained in a manner similar that described earlier,

$$R_{\alpha\Phi}^{(0,2)}(x) = -g\alpha_G^2\sigma_\beta^2\int_\Omega \nabla_y^T G^{(0,0)}(y,x)\, K_G(y)\left\langle \Phi^{(0,0)}(y)\right\rangle e_3 d\Omega - \int_{\Gamma_D}\left\langle \alpha' H'(y)\nabla_y^T G(y,x) K_s(y)\right\rangle^{(0,2)} n(y) d\Gamma \tag{C-11}$$

$$\begin{aligned} R_{\alpha\Phi}^{(2,2)}(x) = &-\alpha_G\int_\Omega\left\langle Y'(y)\beta'\nabla_y^T G^{(1,1)}(y,x)\right\rangle K_G(y)\,\left(\nabla\left\langle \Phi^{(0,0)}(y)\right\rangle + g\alpha_G\left\langle \Phi^{(0,0)}(y)\right\rangle e_3\right) d\Omega \\ &- \alpha_G\int_\Omega\left\langle \beta'\nabla_y^T G^{(0,1)}(y,x)\right\rangle\, r^{(2,0)}(y) d\Omega \\ &- g\,\alpha_G^2\sigma_\beta^2\int_\Omega\Big[\left(0.5\sigma_Y^2(y)\nabla_y^T G^{(0,0)}(y,x) + \left\langle Y'(y)\nabla_y^T G^{(1,0)}(y,x)\right\rangle\right)\left\langle \Phi^{(0,0)}(y)\right\rangle \\ &\qquad + \nabla_y^T\left\langle G^{(2,0)}(y,x)\right\rangle\left\langle \Phi^{(0,0)}(y)\right\rangle + \nabla_y^T G^{(0,0)}(y,x)\left\langle \Phi^{(2,0)}(y)\right\rangle\Big] K_G(y)\, e_3 d\Omega \\ &- g\alpha_G^2\int_\Omega\left\langle \beta'\nabla_y^T G^{(0,1)}(y,x)\right\rangle R_{K\Phi}^{(2,0)}(y)\, e_3 d\Omega \\ &- \int_{\Gamma_D}\left\langle \alpha' H'(y)\nabla_y^T G(y,x) K_s(y)\right\rangle^{(2,2)} n(y) d\Gamma \end{aligned} \tag{C-12}$$

The integrands of integrals over the Dirichlet boundary are as shown in (A-71) and (A-72) of Appendix A.

Multiplying (2-19) by α'^2 and taking conditional ensemble mean yields an explicit expression for $\langle \alpha'^2\Phi'(y)\rangle$,

$$\begin{aligned} \left\langle \alpha'^2\Phi'(x)\right\rangle = &-\int_\Omega\left\langle \alpha'^2\nabla_z^T G(z,x)\, K_s'(z)\right\rangle\left[\nabla\left\langle \Phi(z)\right\rangle + g\left\langle \alpha\right\rangle\left\langle \Phi(z)\right\rangle e_3\right] d\Omega \\ &- \int_\Omega\left\langle \alpha'^2\nabla_z^T G(z,x)\right\rangle R(z,z) d\Omega \\ &+ g\int_\Omega\left\langle \alpha'^2\nabla_z^T G(z,x)\right\rangle\left(\left\langle \alpha\right\rangle R_{K\Phi}(z) + \left\langle K_s(z)\right\rangle R_{\alpha\Phi}(z) + R_{\alpha K\Phi}(z)\right) e_3 d\Omega \\ &- \int_{\Gamma_D}\left\langle \alpha'^2 H'(z)\nabla_z^T G(z,x) K_s(z)\right\rangle n(z) d\Gamma \end{aligned} \tag{C-13}$$

Its approximations to second order are

$$\left\langle \alpha'^2\Phi'(x)\right\rangle^{(0,2)} = 0 \tag{C-14}$$

$$\begin{aligned} &\left\langle \alpha'^2\Phi'(x)\right\rangle^{(2,2)} \\ &= -\alpha_G^2\sigma_\beta^2\int_\Omega\Big[\nabla_z^T\left\langle G^{(2,0)}(z,x)\right\rangle + \left\langle Y'(z)\nabla_z^T G^{(1,0)}(z,x)\right\rangle\Big] K_G(z)\left[\nabla\left\langle \Phi^{(0,0)}(z)\right\rangle + g\alpha_G\left\langle \Phi^{(0,0)}(z)\right\rangle e_3\right] \\ &\qquad + \nabla_z^T\left\langle G^{(0,0)}(z,x)\right\rangle K_G(z)\left[\nabla\left\langle \Phi^{(2,0)}(z)\right\rangle + g\alpha_G\left\langle \Phi^{(2,0)}(z)\right\rangle e_3\right] d\Omega \\ &\quad - \alpha_G^2\sigma_\beta^2\int_\Omega \nabla_z^T\left\langle G^{(0,0)}(z,x)\right\rangle r^{(2,0)}(z) d\Omega \\ &\quad + g\alpha_G^3\sigma_\beta^2\int_\Omega \nabla_z^T\left\langle G^{(0,0)}(z,x)\right\rangle R_{K\Phi}^{(2,0)}(z)\, e_3 d\Omega \end{aligned} \tag{C-15}$$

where boundary integrals over the Dirichlet boundary in (C-14) and (C-15), as evaluated in (A-82) of Appendix A, are zero and have been dropped.

C.3 $\langle \alpha' Y'(X)\Phi'(Y)\rangle$

Rewriting (2-19) in terms of y, multiplying by $\alpha' Y'(x)$, and taking conditional ensemble mean yields

$$\begin{aligned}
C_{\alpha Y\Phi}(x,y) &= \langle \alpha' Y'(x)\ \Phi'(y)\rangle \\
&= -\int_\Omega \langle \alpha' Y'(x)\nabla_z^T G(z,y)\ K_s'(z)\rangle\left[\nabla\langle \Phi(z)\rangle + g\langle\alpha\rangle\langle\Phi(z)\rangle e_3\right]d\Omega \\
&\quad -\int_\Omega \langle \alpha' Y'(x)\nabla_z^T G(z,y)\rangle r(z)d\Omega \\
&\quad -g\int_\Omega \langle \alpha'^2 Y'(x)\nabla_z^T G(z,y)\ K_s(z)\rangle\ \langle\Phi(z)\rangle e_3\ d\Omega \\
&\quad +g\int_\Omega \langle \alpha' Y'(x)\nabla_z^T G(z,y)\rangle\ \left(\langle\alpha\rangle R_{K\Phi}(z) + \langle K_s(z)\rangle\ R_{\alpha\Phi}(z) + R_{\alpha K\Phi}(z)\right)e_3 d\Omega \\
&\quad -\int_{\Gamma_D} \langle \alpha' Y'(x)H'(z)\nabla_z^T G(z,y)K_s(z)\rangle n(z)d\Gamma
\end{aligned} \tag{C-16}$$

Expanding (C-16) and collecting terms of like order gives the following approximation,

$$\begin{aligned}
C_{\alpha K\Phi}^{(2,2)}(x,y) &= \langle \alpha' K_s'(x)\Phi'(y)\rangle^{(2,2)} \\
&= -\alpha_G K_G(x)\int_\Omega C_Y(x,z)\langle \beta'\nabla_z^T G^{(0,1)}(z,y)\rangle K_G(z)\left[\nabla\langle\Phi^{(0,0)}(z)\rangle + g\alpha_G\langle\Phi^{(0,0)}(z)\rangle e_3\right]d\Omega \\
&\quad -g\ \alpha_G^2\sigma_\beta^2 K_G(x)\int_\Omega \langle Y'(z)\nabla_z^T G^{(1,0)}(z,y)\rangle K_G(z)\langle\Phi^{(0,0)}(z)\rangle\ e_3 d\Omega \\
&\quad -K_G(x)\int_{\Gamma_D} \langle \alpha' Y'(x)H'(z)\nabla_z^T G(z,y)K_s(z)\rangle^{(2,2)} n(z)d\Gamma
\end{aligned} \tag{C-17}$$

where the integrand of the boundary integral has been evaluated in (A-76).

C.4 $\langle \alpha'^2 Y'(x)\Phi'(y)\rangle$

Rewriting (2-19) in terms of y, multiplying by $\alpha'^2 Y'(x)$, and taking conditional ensemble mean gives

$$\left\langle \alpha'^2 Y'(x)\ \Phi'(y)\right\rangle = -\int_\Omega \left\langle \alpha'^2 Y'(x)\nabla_z^T G(z,y)\ K_s'(z)\right\rangle \left[\nabla\left\langle \Phi(z)\right\rangle + g\left\langle \alpha\right\rangle \left\langle \Phi(z)\right\rangle e_3\right] d\Omega \\ - \int_{\Gamma_D} \left\langle \alpha'^2 Y'(x) H'(z)\nabla_z^T G(z,y) K_s(z)\right\rangle n(z)\, d\Gamma \tag{C-18}$$

The approximation to second order is

$$\left\langle \alpha'^2 Y'(x)\ \Phi'(y)\right\rangle^{(2,2)} = -\alpha_G^2 \sigma_\beta^2 \int_\Omega C_Y(x,z)\left\langle \nabla_z^T G^{(0,0)}(z,y)\right\rangle K_G(z)\left[\nabla\left\langle \Phi^{(0,0)}(z)\right\rangle + g\alpha_G\left\langle \Phi^{(0,0)}(z)\right\rangle e_3\right] d\Omega \tag{C-19}$$

The integral over the Dirichlet boundary has been dropped, because, according to (A-84), the integrand $\left\langle \alpha'^2 Y'(x) H'(z)\nabla_z^T G(z,y) K_s(z)\right\rangle$ is higher than second order.

C.5 $\langle \alpha'\Phi'(x)\Phi'(y)\rangle$ AND $\langle \alpha'^2\Phi'(x)\Phi'(y)\rangle$

When there is more than one perturbation Φ' appearing in one term, it is more convenient to use the implicit equations for Φ', i.e., (2-17). Rewriting it in terms of y, multiplying by $\alpha'\Phi'(x)$, and taking conditional mean yields

$$\begin{cases} \nabla_y \cdot \Big[\left\langle K_s(y)\right\rangle \nabla_y \left\langle \alpha'\Phi'(x)\Phi'(y)\right\rangle + \left\langle \alpha' K_s'(y)\Phi'(x)\nabla\Phi'(y)\right\rangle + \left\langle \alpha' K_s'(y)\Phi'(x)\right\rangle \nabla\left\langle \Phi(y)\right\rangle + R_{\alpha\Phi}(x) r(y) \\ \quad + g\ \Big(\left\langle \alpha\right\rangle \left\langle K_s(y)\right\rangle \left\langle \alpha'\Phi'(x)\Phi'(y)\right\rangle + \left\langle \alpha\right\rangle \left\langle \alpha'^2 K_s'(y)\Phi'(x)\Phi'(y)\right\rangle + \left\langle K_s(y)\right\rangle \left\langle \alpha'^2 \Phi'(x)\Phi'(y)\right\rangle \\ \quad + \left\langle \alpha'^2 K'(y)\Phi'(x)\Phi'(y)\right\rangle + \left\langle K_s(y)\right\rangle \left\langle \Phi(y)\right\rangle \left\langle \alpha'^2 \Phi'(x)\right\rangle + \left\langle \alpha'^2 K_s'(y)\Phi'(x)\right\rangle \left\langle \Phi(y)\right\rangle \\ \quad + \left\langle \alpha\right\rangle \left\langle \alpha' K_s'(y)\Phi'(x)\right\rangle \left\langle \Phi(y)\right\rangle - \big(\left\langle \alpha\right\rangle R_{K\Phi}(y) + \left\langle K_s(y)\right\rangle R_{\alpha\Phi}(y) + R_{\alpha K\Phi}(y) \big) R_{\alpha\Phi}(x) \Big)\ e_3 \Big] \\ \quad + \left\langle \alpha'\Phi'(x) f'(y)\right\rangle = 0 & x, y \in \Omega \\ \left\langle \alpha'\Phi'(x)\Phi'(y)\right\rangle = \left\langle \alpha'\Phi'(x) H'(y)\right\rangle & x \in \Omega, y \in \Gamma_D \\ n(z)\cdot[*] = \left\langle \alpha'\Phi'(x) Q'(y)\right\rangle & x \in \Omega, y \in \Gamma_N \end{cases} \tag{C-20}$$

where $\langle\alpha'\Phi'(\boldsymbol{x})H'(\boldsymbol{y})\rangle$ has been solved in (A-36) and (A-37) of Appendix A. $\langle\alpha'\Phi'(\boldsymbol{x})f'(\boldsymbol{y})\rangle$ and $\langle\alpha'\Phi'(\boldsymbol{x})Q'(\boldsymbol{y})\rangle$ can be obtained by multiplying (2-19), the explicit equation for $\Phi'(\boldsymbol{x})$, by $\alpha'f'(\boldsymbol{y})$ and $\alpha'Q'(\boldsymbol{y})$, respectively, and taking their conditional means,

$$\begin{aligned}
&\langle\alpha'\Phi'(\boldsymbol{x})f'(\boldsymbol{y})\rangle = \int_{\Omega}\langle f'(\boldsymbol{y})f'(\boldsymbol{u})\rangle\langle\alpha'G(\boldsymbol{u},\boldsymbol{x})\rangle\, d\Omega \\
&\langle\alpha'\Phi'(\boldsymbol{x})Q'(\boldsymbol{y})\rangle = \int_{\Gamma_N}\langle Q'(\boldsymbol{y})Q'(\boldsymbol{u})\rangle\langle\alpha'G(\boldsymbol{u},\boldsymbol{x})\rangle\, d\Gamma
\end{aligned} \tag{C-21}$$

All other terms have been dropped from (C-21) due to the assumption that f and Q are uncorrelated with K_s and α, and thus with G. All other terms in (C-20) are solved accordingly. Recursive approximations of (C-20) to second order are

$$\begin{cases}
\nabla_y\cdot\left[K_G(\boldsymbol{y})\,\nabla_y\langle\alpha'\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle^{(0,2)} + g\alpha_G K_G(\boldsymbol{y})\,\langle\alpha'\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle^{(0,2)}\boldsymbol{e}_3\right] & \\
\quad + \langle\alpha'\Phi'(\boldsymbol{x})f'(\boldsymbol{y})\rangle^{(0,2)} = 0 & \boldsymbol{x},\boldsymbol{y}\in\Omega \\
\langle\alpha'\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle^{(0,2)} = \langle\alpha'\Phi'(\boldsymbol{x})H'(\boldsymbol{y})\rangle^{(0,2)} & \boldsymbol{x}\in\Omega,\boldsymbol{y}\in\Gamma_D \\
\boldsymbol{n}(\boldsymbol{z})\cdot[*] = \langle\alpha'\Phi'(\boldsymbol{x})Q'(\boldsymbol{y})\rangle^{(0,2)} & \boldsymbol{x}\in\Omega,\boldsymbol{y}\in\Gamma_N
\end{cases} \tag{C-22}$$

$$\begin{cases}
\nabla_y\cdot\Big[K_G(\boldsymbol{y})\,\nabla_y\langle\alpha'\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle^{(2,2)} + \langle\alpha'K_s'(\boldsymbol{y})\Phi'(\boldsymbol{x})\nabla\Phi'(\boldsymbol{y})\rangle^{(2,2)} & \\
\qquad + \langle\alpha'K_s'(\boldsymbol{y})\Phi'(\boldsymbol{x})\rangle^{(2,2)}\nabla\langle\Phi^{(0,0)}(\boldsymbol{y})\rangle + \boldsymbol{R}^{(2,0)}(\boldsymbol{y},\boldsymbol{y})R_{\alpha\Phi}^{(0,2)}(\boldsymbol{x}) & \\
\quad + g\,\Big(\alpha_G K_G(\boldsymbol{y})\langle\alpha'\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle^{(2,2)} + K_G(\boldsymbol{y})\langle\alpha'^2\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle^{(2,2)} & \\
\qquad + K_G(\boldsymbol{y})\langle\Phi^{(0,0)}(\boldsymbol{y})\rangle\langle\alpha'^2\Phi'(\boldsymbol{x})\rangle^{(2,2)} + \langle\alpha'^2K_s'(\boldsymbol{y})\Phi'(\boldsymbol{x})\rangle^{(2,2)}\langle\Phi^{(0,0)}(\boldsymbol{y})\rangle & \\
\qquad + \alpha_G\langle\alpha'K_s'(\boldsymbol{y})\Phi'(\boldsymbol{x})\rangle^{(2,2)}\langle\Phi^{(0,0)}(\boldsymbol{y})\rangle - \alpha_G C_{K\Phi}^{(2,0)}(\boldsymbol{y})R_{\alpha\Phi}^{(0,2)}(\boldsymbol{x})\Big)\boldsymbol{e}_3\Big] & \\
\quad + \langle\alpha'\Phi'(\boldsymbol{x})f'(\boldsymbol{y})\rangle^{(2,2)} = 0 & \boldsymbol{x},\boldsymbol{y}\in\Omega \\
\langle\alpha'\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle^{(2,2)} = \langle\alpha'\Phi'(\boldsymbol{x})H'(\boldsymbol{y})\rangle^{(2,2)} & \boldsymbol{x}\in\Omega,\boldsymbol{y}\in\Gamma_D \\
\boldsymbol{n}(\boldsymbol{z})\cdot[*] = \langle\alpha'\Phi'(\boldsymbol{x})Q'(\boldsymbol{y})\rangle^{(2,2)} & \boldsymbol{x}\in\Omega,\boldsymbol{y}\in\Gamma_N
\end{cases} \tag{C-23}$$

where

$$\left\langle \alpha'\Phi'(\boldsymbol{x})f'(\boldsymbol{y})\right\rangle^{(0,2)} = \alpha_G \int_\Omega C_f(\boldsymbol{y},\boldsymbol{u})\left\langle \beta' G^{(0,1)}(\boldsymbol{u},\boldsymbol{x})\right\rangle d\Omega$$
$$\left\langle \alpha'\Phi'(\boldsymbol{x})Q'(\boldsymbol{y})\right\rangle^{(0,2)} = \alpha_G \int_{\Gamma_N} C_Q(\boldsymbol{y},\boldsymbol{u})\left\langle \beta' G^{(0,1)}(\boldsymbol{u},\boldsymbol{x})\right\rangle d\Gamma \tag{C-24}$$

$$\left\langle \alpha'\Phi'(\boldsymbol{x})f'(\boldsymbol{y})\right\rangle^{(2,2)} = \alpha_G \int_\Omega C_f(\boldsymbol{y},\boldsymbol{u})\left\langle \beta' G^{(2,1)}(\boldsymbol{u},\boldsymbol{x})\right\rangle d\Omega$$
$$\left\langle \alpha'\Phi'(\boldsymbol{x})Q'(\boldsymbol{y})\right\rangle^{(2,2)} = \alpha_G \int_{\Gamma_N} C_Q(\boldsymbol{y},\boldsymbol{u})\left\langle \beta' G^{(2,1)}(\boldsymbol{u},\boldsymbol{x})\right\rangle d\Gamma \tag{C-25}$$

Here C_f and C_Q are covariance functions of f and Q, respectively. For $\langle\alpha'^2\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle$, the exact equations are

$$\begin{cases}
\nabla_y\cdot\Big[\langle K_s(\boldsymbol{y})\rangle\,\nabla_y\left\langle \alpha'^2\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle + \left\langle \alpha'^2 K_s'(\boldsymbol{y})\Phi'(\boldsymbol{x})\nabla\Phi'(\boldsymbol{y})\right\rangle + \left\langle \alpha'^2 K_s'(\boldsymbol{y})\Phi'(\boldsymbol{x})\right\rangle\nabla\langle\Phi(\boldsymbol{y})\rangle \\
\quad + \boldsymbol{R}(\boldsymbol{y},\boldsymbol{y})\left\langle \alpha'^2\Phi'(\boldsymbol{x})\right\rangle \\
\quad + g\Big(\langle\alpha\rangle\langle K_s(\boldsymbol{y})\rangle\left\langle \alpha'^2\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle + \langle\alpha\rangle\left\langle \alpha'^2 K_s'(\boldsymbol{y})\Phi'(\boldsymbol{x})\right\rangle\langle\Phi(\boldsymbol{y})\rangle \\
\qquad - \big(\langle\alpha\rangle R_{K\Phi}(\boldsymbol{y}) + \langle K_s(\boldsymbol{y})\rangle R_{\alpha\Phi}(\boldsymbol{y}) + R_{\alpha K\Phi}(\boldsymbol{y})\big)\left\langle \alpha'^2\Phi'(\boldsymbol{x})\right\rangle\Big)\,\boldsymbol{e}_3\Big] \\
\quad + \left\langle \alpha'^2\Phi'(\boldsymbol{x})f'(\boldsymbol{y})\right\rangle = 0 & \boldsymbol{x},\boldsymbol{y}\in\Omega \\
\left\langle \alpha'^2\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle = \left\langle \alpha'^2\Phi'(\boldsymbol{x})H'(\boldsymbol{y})\right\rangle & \boldsymbol{x}\in\Omega,\boldsymbol{y}\in\Gamma_D \\
\boldsymbol{n}(\boldsymbol{z})\cdot[*] = \left\langle \alpha'^2\Phi'(\boldsymbol{x})Q'(\boldsymbol{y})\right\rangle & \boldsymbol{x}\in\Omega,\boldsymbol{y}\in\Gamma_N
\end{cases} \tag{C-26}$$

where

$$\left\langle \alpha'^2\Phi'(\boldsymbol{x})f'(\boldsymbol{y})\right\rangle = \int_\Omega \langle f'(\boldsymbol{y})f'(\boldsymbol{u})\rangle\left\langle \alpha'^2 G(\boldsymbol{u},\boldsymbol{x})\right\rangle d\Omega$$
$$\left\langle \alpha'^2\Phi'(\boldsymbol{x})Q'(\boldsymbol{y})\right\rangle = \int_{\Gamma_N} \langle Q'(\boldsymbol{y})Q'(\boldsymbol{u})\rangle\left\langle \alpha'^2 G(\boldsymbol{u},\boldsymbol{x})\right\rangle d\Gamma \tag{C-27}$$

Recursive approximations to second order are

$$\begin{cases}
\nabla_y\cdot\Big[K_G(\boldsymbol{y})\,\nabla_y\left\langle \alpha'^2\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle^{(0,2)} + g\alpha_G K_G(\boldsymbol{y})\left\langle \alpha'^2\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle^{(0,2)}\boldsymbol{e}_3\Big] \\
\quad + \left\langle \alpha'^2\Phi'(\boldsymbol{x})f'(\boldsymbol{y})\right\rangle^{(0,2)} = 0 & \boldsymbol{x},\boldsymbol{y}\in\Omega \\
\left\langle \alpha'^2\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle^{(0,2)} = \left\langle \alpha'^2\Phi'(\boldsymbol{x})H'(\boldsymbol{y})\right\rangle^{(0,2)} & \boldsymbol{x}\in\Omega,\boldsymbol{y}\in\Gamma_D \\
\boldsymbol{n}(\boldsymbol{z})\cdot[*] = \left\langle \alpha'^2\Phi'(\boldsymbol{x})Q'(\boldsymbol{y})\right\rangle^{(0,2)} & \boldsymbol{x}\in\Omega,\boldsymbol{y}\in\Gamma_N
\end{cases} \tag{C-28}$$

$$\begin{cases}\nabla_y \cdot \Big[K_G(y)\, \nabla_y \left\langle \alpha'^2 \Phi'(x)\Phi'(y)\right\rangle^{(2,2)} + \left\langle \alpha'^2 K_s'(y)\Phi'(x)\nabla\Phi'(y)\right\rangle^{(2,2)} + \left\langle \alpha'^2 K_s'(y)\Phi'(x)\right\rangle^{(2,2)}\, \nabla\left\langle \Phi^{(0,0)}(y)\right\rangle \\ \quad +g\left(\alpha_G K_G(y)\left\langle \alpha'^2\Phi'(x)\Phi'(y)\right\rangle^{(2,2)} + \alpha_G\left\langle \alpha'^2 K_s'(y)\Phi'(x)\right\rangle^{(2,2)}\left\langle \Phi^{(0,0)}(y)\right\rangle\right)e_3\Big] \\ \quad + \left\langle \alpha'^2\Phi'(x) f'(y)\right\rangle^{(2,2)} = 0 & x,y\in\Omega \\ \left\langle \alpha'^2\Phi'(x)\Phi'(y)\right\rangle^{(2,2)} = \left\langle \alpha'^2\Phi'(x)H'(y)\right\rangle^{(2,2)} & x\in\Omega, y\in\Gamma_D \\ n(z)\cdot[*] = \left\langle \alpha'^2\Phi'(x)Q'(y)\right\rangle^{(2,2)} & x\in\Omega, y\in\Gamma_N \end{cases} \tag{C-29}$$

where

$$\begin{aligned}\left\langle \alpha'^2\Phi'(x)f'(y)\right\rangle^{(0,2)} &= \alpha_G^2\sigma_\beta^2\int_\Omega C_f(y,u)\left\langle G^{(0,0)}(u,x)\right\rangle d\Omega \\ \left\langle \alpha'^2\Phi'(x)Q'(y)\right\rangle^{(0,2)} &= \alpha_G^2\sigma_\beta^2\int_{\Gamma_N} C_Q(y,u)\left\langle G^{(0,0)}(u,x)\right\rangle d\Gamma\end{aligned} \tag{C-30}$$

$$\begin{aligned}\left\langle \alpha'^2\Phi'(x)f'(y)\right\rangle^{(2,2)} &= \alpha_G^2\sigma_\beta^2\int_\Omega C_f(y,u)\left\langle G^{(2,0)}(u,x)\right\rangle d\Omega \\ \left\langle \alpha'^2\Phi'(x)Q'(y)\right\rangle^{(2,2)} &= \alpha_G^2\sigma_\beta^2\int_{\Gamma_N} C_Q(y,u)\left\langle G^{(2,0)}(u,x)\right\rangle d\Gamma\end{aligned} \tag{C-31}$$

$\langle\alpha'^2\Phi'(x)H'(y)\rangle^{(0,2)}$ and $\langle\alpha'^2\Phi'(x)H'(y)\rangle^{(2,2)}$ in (C-28) and (C-29) are solved in (A-39) and (A-40).

C.6 $\langle Y'(x)Y'(y)\Phi'(z)\rangle$

Multiplying (2-19) by $Y'(x)Y'(y)$ and taking conditional mean gives

$$\begin{aligned}&\left\langle Y'(x)Y'(y)\Phi'(z)\right\rangle \\ &\quad = -g\int_\Omega \left\langle Y'(x)Y'(y)\nabla_u^T G(u,z)\left\langle K_s(u)\right\rangle\left(\alpha'\left\langle\Phi(u)\right\rangle - R_{\alpha\Phi}(u)\right)e_3\right\rangle d\Omega \\ &\quad\ -\int_{\Gamma_D}\left\langle Y'(x)Y'(y)H'(u)\nabla_u^T G(u,z)K_s(u)\right\rangle n(u)\, d\Gamma \\ &\quad\ + HO\end{aligned} \tag{C-32}$$

where *HO* denotes summation of all terms that are obviously higher than second order. The corresponding approximation to second order is

$$\begin{aligned}
&\left\langle Y'(\boldsymbol{x})Y'(\boldsymbol{y})\Phi'(\boldsymbol{z})\right\rangle^{(2,2)} \\
&\quad = -gC_Y(\boldsymbol{x},\boldsymbol{y})\int_\Omega \left[\alpha_G \nabla_\tau^T \left\langle \beta' G^{(0,1)}(\tau,z)\right\rangle \left\langle \Phi^{(0,0)}(\tau)\right\rangle - \nabla_\tau^T \left\langle G^{(0,0)}(\tau,z)\right\rangle R_{\alpha\Phi}^{(0,2)}(\tau)\right] K_G(\tau)\boldsymbol{e}_3 \, \mathrm{d}\Omega \\
&\quad\quad - \int_{\Gamma_D} \left\langle Y'(\boldsymbol{x})Y'(\boldsymbol{y})H'(\tau)\nabla_\tau^T \mathrm{G}(\tau,z)K_s(\tau)\right\rangle^{(2,2)} \boldsymbol{n}(\tau)\, \mathrm{d}\Gamma
\end{aligned} \tag{C-33}$$

where the boundary integral is given in (A-77) and (A-78) of Appendix A.

C.7 $\langle Y'(x)\Phi'(y)\Phi'(z)\rangle$

Rewriting (2-17) in terms of z, multiplying by $Y'(\boldsymbol{x})\Phi'(y)$, and taking conditional gives the following equations for $\langle Y'(\boldsymbol{x})\Phi'(y)\Phi'(z)\rangle$,

$$\begin{cases}
\nabla_z \cdot \left[\left\langle K_s(z)\right\rangle \nabla_z \left\langle Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Phi'(z)\right\rangle + \left\langle Y'(x)K_s'(z)\Phi'(\boldsymbol{y})\nabla\Phi'(z)\right\rangle + \left\langle Y'(x)K_s'(z)\Phi'(\boldsymbol{y})\right\rangle \nabla \left\langle \Phi(z)\right\rangle \right. \\
\quad + \boldsymbol{R}(z,z)C_{Y\Phi}(x,\boldsymbol{y}) \\
\quad + g\left(\left\langle\alpha\right\rangle\left\langle K_s(z)\right\rangle\left\langle Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Phi'(z)\right\rangle + \left\langle\alpha\right\rangle\left\langle Y'(\boldsymbol{x})K_s'(z)\Phi'(\boldsymbol{y})\Phi'(z)\right\rangle + \left\langle K_s(z)\right\rangle\left\langle \alpha' Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Phi'(z)\right\rangle\right. \\
\quad\quad + \left\langle \alpha' Y'(\boldsymbol{x})K_s'(z)\Phi'(\boldsymbol{y})\Phi'(z)\right\rangle + \left\langle K_s(z)\right\rangle\left\langle\Phi(z)\right\rangle\left\langle \alpha' Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle + \left\langle \alpha' K_s'(z)Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\right\rangle\left\langle\Phi(z)\right\rangle \\
\quad\quad \left.\left. + \left\langle\alpha\right\rangle\left\langle Y'(x)K_s'(z)\Phi'(y)\right\rangle\left\langle\Phi(z)\right\rangle - \left(\left\langle\alpha\right\rangle R_{K\Phi}(z) + \left\langle K_s(z)\right\rangle R_{\alpha\Phi}(z) + R_{\alpha K\Phi}(z)\right)C_{Y\Phi}(x,\boldsymbol{y})\right)\boldsymbol{e}_3\right] \\
\quad + \left\langle Y'(x)\Phi'(\boldsymbol{y})f'(z)\right\rangle = 0 & \boldsymbol{x},\boldsymbol{y},\, z \in \Omega \\
\left\langle Y'(x)\Phi'(y)\Phi'(z)\right\rangle = \left\langle Y'(x)\Phi'(y)H'(z)\right\rangle & \boldsymbol{x},\boldsymbol{y}\in\Omega,\, z\in\Gamma_D \\
\boldsymbol{n}(z)\cdot[*] = \left\langle Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})Q'(z)\right\rangle & \boldsymbol{x},\boldsymbol{y}\in\Omega,\, z\in\Gamma_N
\end{cases} \tag{C-34}$$

where $\langle Y'(\boldsymbol{x})\Phi'(y)f'(z)\rangle$ and $\langle Y'(\boldsymbol{x})\Phi'(y)Q'(z)\rangle$ are derived from (2-19) upon multiplying by $Y'(\boldsymbol{x})f'(z)$ and $Y'(\boldsymbol{x})Q'(z)$, respectively, and taking their conditional means,

$$\begin{aligned}
\left\langle Y'(\boldsymbol{x})\Phi'(y)f'(z)\right\rangle &= \int_\Omega \left\langle f'(z)f'(\boldsymbol{u})\right\rangle\left\langle Y'(\boldsymbol{x})G(\boldsymbol{u},\boldsymbol{y})\right\rangle d\Omega \\
\left\langle Y'(\boldsymbol{x})\Phi'(y)Q'(z)\right\rangle &= \int_{\Gamma_N} \left\langle Q'(z)Q'(\boldsymbol{u})\right\rangle\left\langle Y'(\boldsymbol{x})G(\boldsymbol{u},\boldsymbol{y})\right\rangle d\Gamma
\end{aligned} \tag{C-35}$$

From (C-34), the approximations of $\langle Y'(x)\Phi'(y)\Phi'(z)\rangle$ satisfy the following equations,

$$
\begin{cases}
\nabla_z \cdot \Big[K_G(z)\nabla_z \langle Y'(x)\Phi'(y)\Phi'(z)\rangle^{(2,0)} + \langle Y'(x)K_s'(z)\Phi'(y)\nabla\Phi'(z)\rangle^{(2,0)} \\
\qquad + \langle Y'(x)K_s'(z)\Phi'(y)\rangle^{(2,0)} \nabla \langle \Phi^{(0,0)}(z)\rangle + \\
\qquad + g\Big(\alpha_G K_G(z)\langle Y'(x)\Phi'(y)\Phi'(z)\rangle^{(2,0)} + \alpha_G \langle Y'(x)K_s'(z)\Phi'(y)\Phi'(z)\rangle^{(2,0)} \\
\qquad\quad + \alpha_G \langle Y'(x)K_s'(z)\Phi'(y)\rangle^{(2,0)} \langle \Phi^{(0,0)}(z)\rangle\Big)e_3 \Big] \\
\quad + \langle Y'(x)\Phi'(y)f'(z)\rangle^{(2,0)} = 0 & x, y,\ z \in \Omega \\
\langle Y'(x)\Phi'(y)\Phi'(z)\rangle^{(2,0)} = \langle Y'(x)\Phi'(y)H'(z)\rangle^{(2,0)} & x, y \in \Omega,\ z \in \Gamma_D \\
n(z)\cdot[*] = \langle Y'(x)\Phi'(y)Q'(z)\rangle^{(2,0)} & x, y \in \Omega,\ z \in \Gamma_N
\end{cases}
\tag{C-36}
$$

$$
\begin{cases}
\nabla_z \cdot \Big[K_G(z)\nabla_z \langle Y'(x)\Phi'(y)\Phi'(z)\rangle^{(2,2)} + \langle Y'(x)K_s'(z)\Phi'(y)\nabla\Phi'(z)\rangle^{(2,2)} \\
\qquad + \langle Y'(x)K_s'(z)\Phi'(y)\rangle^{(2,2)} \nabla \langle \Phi^{(0,0)}(z)\rangle \\
\qquad + g\Big(\alpha_G K_G(z)\langle Y'(x)\Phi'(y)\Phi'(z)\rangle^{(2,2)} + \alpha_G \langle Y'(x)K_s'(z)\Phi'(y)\Phi'(z)\rangle^{(2,2)} \\
\qquad\quad + K_G(z)\langle \alpha' Y'(x)\Phi'(y)\Phi'(z)\rangle^{(2,2)} + \langle \alpha' Y'(x)K_s'(z)\Phi'(y)\Phi'(z)\rangle^{(2,2)} \\
\qquad\quad + K_G(z)\langle \Phi^{(0,0)}(z)\rangle \langle \alpha' Y'(x)\Phi'(y)\rangle^{(2,2)} + \langle \alpha' K_s'(z)Y'(x)\Phi'(y)\rangle^{(2,2)} \langle \Phi^{(0,0)}(z)\rangle \\
\qquad\quad + \alpha_G \langle Y'(x)K_s'(z)\Phi'(y)\rangle^{(2,2)} \langle \Phi^{(0,0)}(z)\rangle - K_G(z)R_{\alpha\Phi}^{(0,2)}(z)C_{K\Phi}^{(2,0)}(x,y)\Big)e_3 \Big] \\
\quad + \langle Y'(x)\Phi'(y)f'(z)\rangle^{(2,2)} = 0 & x, y,\ z \in \Omega \\
\langle Y'(x)\Phi'(y)\Phi'(z)\rangle^{(2,2)} = \langle Y'(x)\Phi'(y)H'(z)\rangle^{(2,2)} & x, y \in \Omega,\ z \in \Gamma_D \\
n(z)\cdot[*] = \langle Y'(x)\Phi'(y)Q'(z)\rangle^{(2,2)} & x, y \in \Omega,\ z \in \Gamma_N
\end{cases}
\tag{C-37}
$$

where

$$
\begin{aligned}
\langle Y'(x)\Phi'(y)f'(z)\rangle^{(2,0)} &= \int_\Omega C_f(z,u)\langle Y'(x)G^{(1,0)}(u,y)\rangle d\Omega \\
\langle Y'(x)\Phi'(y)Q'(z)\rangle^{(2,0)} &= \int_{\Gamma_N} C_Q(z,u)\langle Y'(x)G^{(1,0)}(u,y)\rangle d\Gamma
\end{aligned}
\tag{C-38}
$$

$$
\begin{aligned}
\langle Y'(x)\Phi'(y)f'(z)\rangle^{(2,2)} &= \int_\Omega C_f(z,u)\langle Y'(x)G^{(1,2)}(u,y)\rangle d\Omega \\
\langle Y'(x)\Phi'(y)Q'(z)\rangle^{(2,2)} &= \int_{\Gamma_N} C_Q(z,u)\langle Y'(x)G^{(1,2)}(u,y)\rangle d\Gamma
\end{aligned}
\tag{C-39}
$$

Once approximations for $\langle Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Phi'(\boldsymbol{z})\rangle$ have been evaluated by solving (C-36) and (C-37), approximations for $\langle Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\nabla\Phi'(\boldsymbol{z})\rangle$ can be obtained by taking their corresponding derivatives.

C.8 $\langle \alpha' \mathbf{Y}'(x)\mathbf{Y}'(y)\Phi'(z)\rangle$

Equation for $\langle\alpha' Y'(\boldsymbol{x})Y'(\boldsymbol{y})\Phi'(\boldsymbol{z})\rangle$ can be formulated upon rewriting (2-19) in terms of z, multiplying by $\alpha' Y'(\boldsymbol{x})Y'(\boldsymbol{y})$, and taking conditional mean,

$$\begin{aligned}\left\langle\alpha' Y'(\boldsymbol{x})Y'(\boldsymbol{y})\Phi'(\boldsymbol{z})\right\rangle &= -\mathrm{g}\int_{\Omega}\left\langle\alpha'^2 Y'(\boldsymbol{x})Y'(\boldsymbol{y})\nabla_u^T G(\boldsymbol{u},\boldsymbol{z})K_s(\boldsymbol{u})\right\rangle\left\langle\Phi(\boldsymbol{u})\right\rangle \boldsymbol{e}_3 \mathrm{d}\Omega \\ &\quad -\int_{\Gamma_D}\left\langle\alpha' Y'(\boldsymbol{x})Y'(\boldsymbol{y})H'(\boldsymbol{u})\nabla_u^T G(\boldsymbol{u},\boldsymbol{z})K_s(\boldsymbol{u})\right\rangle \boldsymbol{n}(\boldsymbol{z})d\Gamma + HO\end{aligned} \tag{C-40}$$

Expanding (C-40) in powers of σ_β and σ_Y gives an approximation to second order

$$\begin{aligned}\left\langle\alpha' Y'(\boldsymbol{x})Y'(\boldsymbol{y})\Phi'(\boldsymbol{z})\right\rangle^{(2,2)} &= -\mathrm{g}\alpha_G^2\sigma_\beta^2 C_Y(\boldsymbol{x},\boldsymbol{y})\int_{\Omega}\left\langle\nabla_u^T G^{(0,0)}(\boldsymbol{u},\boldsymbol{z})\right\rangle K_G(\boldsymbol{u})\left\langle\Phi^{(0,0)}(\boldsymbol{u})\right\rangle \boldsymbol{e}_3 \mathrm{d}\Omega \\ &\quad -\int_{\Gamma_D}\left\langle\alpha' Y'(\boldsymbol{x})Y'(\boldsymbol{y})H'(\boldsymbol{u})\nabla_u^T G(\boldsymbol{u},\boldsymbol{z})K_s(\boldsymbol{u})\right\rangle^{(2,2)} \boldsymbol{n}(\boldsymbol{z})d\Gamma\end{aligned} \tag{C-41}$$

where the integrand of the boundary integral is given in (A-86) of Appendix A.

C.9 $\langle \alpha' \mathbf{Y}'(x)\Phi'(y)\Phi'(z)\rangle$

Rewriting (2-17) in terms of z, multiplying by $\alpha' Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})$, and taking conditional mean gives

$$
\begin{cases}
\nabla_z \cdot \Big[\langle K_s(z) \rangle \, \nabla_z \langle \alpha' Y'(\boldsymbol{x}) \Phi'(\boldsymbol{y}) \Phi'(z) \rangle + \langle \alpha' Y'(\boldsymbol{x}) K_s'(z) \Phi'(\boldsymbol{y}) \nabla \Phi'(z) \rangle \\
\quad + \langle \alpha' Y'(\boldsymbol{x}) K_s'(z) \Phi'(\boldsymbol{y}) \rangle \nabla \langle \Phi(z) \rangle + \boldsymbol{R}(z,z) C_{\alpha Y \Phi}(x, \boldsymbol{y}) \\
\quad + g \Big(\langle \alpha \rangle \langle K_s(z) \rangle \langle \alpha' Y'(\boldsymbol{x}) \Phi'(\boldsymbol{y}) \Phi'(z) \rangle + \langle \alpha \rangle \langle \alpha' Y'(\boldsymbol{x}) K_s'(z) \Phi'(\boldsymbol{y}) \Phi'(z) \rangle \\
\qquad + \langle K_s(z) \rangle \langle \alpha'^2 Y'(\boldsymbol{x}) \Phi'(\boldsymbol{y}) \Phi'(z) \rangle + \langle \alpha'^2 Y'(\boldsymbol{x}) K_s'(z) \Phi'(\boldsymbol{y}) \Phi'(z) \rangle \\
\qquad + \langle K_s(z) \rangle \langle \Phi(z) \rangle \langle \alpha'^2 Y'(\boldsymbol{x}) \Phi'(\boldsymbol{y}) \rangle + \langle \alpha'^2 K_s'(z) Y'(\boldsymbol{x}) \Phi'(\boldsymbol{y}) \rangle \langle \Phi(z) \rangle \\
\qquad + \langle \alpha \rangle \langle \alpha' Y'(\boldsymbol{x}) K_s'(z) \Phi'(\boldsymbol{y}) \rangle \langle \Phi(z) \rangle \\
\qquad - \big(\langle \alpha \rangle R_{K\Phi}(z) + \langle K_s(z) \rangle R_{\alpha\Phi}(z) + R_{\alpha K \Phi}(z) \big) C_{\alpha Y \Phi}(\boldsymbol{x}, \boldsymbol{y}) \Big) \, \boldsymbol{e}_3 \Big] \\
\quad + \langle \alpha' Y'(\boldsymbol{x}) \Phi'(\boldsymbol{y}) f'(z) \rangle = 0 & \boldsymbol{x}, \boldsymbol{y}, \, z \in \Omega \\
\langle \alpha' Y'(\boldsymbol{x}) \Phi'(\boldsymbol{y}) \Phi'(z) \rangle = \langle \alpha' Y'(\boldsymbol{x}) \Phi'(\boldsymbol{y}) H'(z) \rangle & \boldsymbol{x}, \boldsymbol{y} \in \Omega, \; z \in \Gamma_D \\
\boldsymbol{n}(z) \cdot [*] = \langle \alpha' Y'(\boldsymbol{x}) \Phi'(\boldsymbol{y}) Q'(z) \rangle & \boldsymbol{x}, \boldsymbol{y} \in \Omega, \; z \in \Gamma_N
\end{cases}
\tag{C-42}
$$

where $\langle \alpha' Y'(\boldsymbol{x}) \Phi'(\boldsymbol{y}) H'(\boldsymbol{x}) \rangle$ is given by (A-50), and

$$
\begin{aligned}
\langle \alpha' Y'(\boldsymbol{x}) \Phi'(\boldsymbol{y}) f'(z) \rangle &= \int_\Omega \langle f'(z) f'(\boldsymbol{u}) \rangle \langle \alpha' Y'(\boldsymbol{x}) G(\boldsymbol{u}, \boldsymbol{y}) \rangle d\Omega \\
\langle \alpha' Y'(\boldsymbol{x}) \Phi'(\boldsymbol{y}) Q'(z) \rangle &= \int_{\Gamma_N} \langle Q'(z) Q'(\boldsymbol{u}) \rangle \langle \alpha' Y'(\boldsymbol{x}) G(\boldsymbol{u}, \boldsymbol{y}) \rangle d\Gamma
\end{aligned}
\tag{C-43}
$$

Expanding (C-42) and collecting terms of same order yields recursive equations for $\langle \alpha' Y'(\boldsymbol{x}) \Phi'(\boldsymbol{y}) \Phi'(z) \rangle$,

$$
\begin{cases}
\nabla_z \cdot \Big[K_G(z) \nabla_z \langle \alpha' Y'(\boldsymbol{x}) \Phi'(\boldsymbol{y}) \Phi'(z) \rangle^{(2,2)} + \langle \alpha' Y'(\boldsymbol{x}) K_s'(z) \Phi'(\boldsymbol{y}) \nabla \Phi'(z) \rangle^{(2,2)} \\
\quad + \langle \alpha' Y'(\boldsymbol{x}) K_s'(z) \Phi'(\boldsymbol{y}) \rangle^{(2,2)} \nabla \langle \Phi^{(0,0)}(z) \rangle \\
\quad + g \Big(\alpha_G K_G(z) \langle \alpha' Y'(\boldsymbol{x}) \Phi'(\boldsymbol{y}) \Phi'(z) \rangle^{(2,2)} + \alpha_G \langle \alpha' Y'(\boldsymbol{x}) K_s'(z) \Phi'(\boldsymbol{y}) \Phi'(z) \rangle^{(2,2)} \\
\qquad + K_G(z) \langle \alpha'^2 Y'(\boldsymbol{x}) \Phi'(\boldsymbol{y}) \Phi'(z) \rangle^{(2,2)} + \langle \alpha'^2 Y'(\boldsymbol{x}) K_s'(z) \Phi'(\boldsymbol{y}) \Phi'(z) \rangle^{(2,2)} \\
\qquad + K_G(z) \langle \Phi^{(0,0)}(z) \rangle \langle \alpha'^2 Y'(\boldsymbol{x}) \Phi'(\boldsymbol{y}) \rangle^{(2,2)} + \langle \alpha'^2 K_s'(z) Y'(\boldsymbol{x}) \Phi'(\boldsymbol{y}) \rangle^{(2,2)} \langle \Phi^{(0,0)}(z) \rangle \\
\qquad + \alpha_G \langle \alpha' Y'(\boldsymbol{x}) K_s'(z) \Phi'(\boldsymbol{y}) \rangle^{(2,2)} \langle \Phi^{(0,0)}(z) \rangle \Big) \boldsymbol{e}_3 \Big] \\
\quad + \langle \alpha' Y'(\boldsymbol{x}) \Phi'(\boldsymbol{y}) f'(z) \rangle^{(2,2)} = 0 & \boldsymbol{x}, \boldsymbol{y}, \, z \in \Omega \\
\langle \alpha' Y'(\boldsymbol{x}) \Phi'(\boldsymbol{y}) \Phi'(z) \rangle^{(2,2)} = \langle \alpha' Y'(\boldsymbol{x}) \Phi'(\boldsymbol{y}) H'(z) \rangle^{(2,2)} & \boldsymbol{x}, \boldsymbol{y} \in \Omega, \; z \in \Gamma_D \\
\boldsymbol{n}(z) \cdot [*] = \langle \alpha' Y'(\boldsymbol{x}) \Phi'(\boldsymbol{y}) Q'(z) \rangle^{(2,2)} & \boldsymbol{x}, \boldsymbol{y} \in \Omega, \; z \in \Gamma_N
\end{cases}
\tag{C-44}
$$

where $\langle \alpha' Y'(\boldsymbol{x}) \Phi'(\boldsymbol{y}) H'(z) \rangle^{(2,2)}$ is given by (A-51), and

$$
\begin{aligned}
\left\langle \alpha' Y'(x)\Phi'(y) f'(z)\right\rangle^{(2,2)} &= \int_{\Omega} C_f(z,u)\left\langle \alpha' Y'(x) G^{(1,1)}(u,y)\right\rangle d\Omega \\
\left\langle \alpha' Y'(x)\Phi'(y) Q'(z)\right\rangle^{(2,2)} &= \int_{\Gamma_N} C_Q(z,u)\left\langle \alpha' Y'(x) G^{(1,1)}(u,y)\right\rangle d\Gamma
\end{aligned}
\qquad \text{(C-45)}
$$

All other terms are can be found in this appendix.

C.10 $\langle Y'(x)Y'(y)\Phi'(x)\Phi'(z)\rangle$

Rewriting (2-17) in terms of z, multiplying by $Y'(x)Y'(y)\Phi'(x)$, and taking conditional mean gives equations for $\langle Y'(x)Y'(z)\Phi'(x)\Phi'(z)\rangle$,

$$
\begin{cases}
\nabla_z \cdot \Big[\langle K_s(z)\rangle \nabla_z \langle Y'(x)Y'(y)\Phi'(x)\Phi'(z)\rangle + \\
\quad + g\big(\langle\alpha\rangle\langle K_s(z)\rangle\langle Y'(x)Y'(y)\Phi'(x)\Phi'(z)\rangle + \langle K_s(z)\rangle\langle \alpha' Y'(x)Y'(y)\Phi'(x)\Phi'(z)\rangle \\
\qquad + \langle K_s(z)\rangle\langle \alpha' Y'(x)Y'(y)\Phi'(x)\rangle\langle\Phi(z)\rangle - \langle K_s(z)\rangle\langle Y'(x)Y'(y)\Phi'(x)\rangle R_{\alpha\Phi}(z)\big)\, e_3 \Big] \\
\quad + \langle Y'(x)Y'(y)\Phi'(x) f'(z)\rangle = 0 & x, y,\ z\in\Omega \\
\langle Y'(x)Y'(y)\Phi'(x)\Phi'(z)\rangle = \langle Y'(x)Y'(y)\Phi'(x) H'(z)\rangle & x, y\in\Omega,\ z\in\Gamma_D \\
n(z)\cdot[*] = \langle Y'(x)Y'(y)\Phi'(x) Q'(z)\rangle & x, y\in\Omega,\ z\in\Gamma_N
\end{cases}
\qquad \text{(C-46)}
$$

where terms that are higher than second order in either σ_Y or σ_β, such as $\langle Y'(x)Y'(y)K_s'(z)\Phi'(y)\Phi'(z)\rangle$ that is at least third order in σ_Y, have been dropped, and

$$
\begin{aligned}
\langle Y'(x)Y'(y)\Phi'(x) f'(z)\rangle &= \int_{\Omega} \langle f'(z) f'(u)\rangle\langle Y'(x)Y'(y) G(u,x)\rangle d\Omega \\
\langle Y'(x)Y'(y)\Phi'(x) Q'(z)\rangle &= \int_{\Gamma_N} \langle Q'(z) Q'(u)\rangle\langle Y'(x)Y'(y) G(u,x)\rangle d\Gamma
\end{aligned}
\qquad \text{(C-47)}
$$

Approximations of (C-46) to second order are

$$
\begin{cases}
\nabla_z \cdot \Big[K_G(z)\nabla_z \langle Y'(x)Y'(y)\Phi'(x)\Phi'(z)\rangle^{(2,0)} + g\alpha_G K_G(z)\langle Y'(x)Y'(y)\Phi'(x)\Phi'(z)\rangle^{(2,0)} e_3 \Big] \\
\quad + \langle Y'(x)Y'(y)\Phi'(x) f'(z)\rangle^{(2,2)} = 0 & x, y,\ z\in\Omega \\
\langle Y'(x)Y'(y)\Phi'(x)\Phi'(z)\rangle^{(2,0)} = \langle Y'(x)Y'(y)\Phi'(x) H'(z)\rangle^{(2,0)} & x, y\in\Omega,\ z\in\Gamma_D \\
n(z)\cdot[*] = \langle Y'(x)Y'(y)\Phi'(x) Q'(z)\rangle^{(2,0)} & x, y\in\Omega,\ z\in\Gamma_N
\end{cases}
\qquad \text{(C-48)}
$$

$$\begin{cases} \nabla_z \cdot \Big[K_G(z) \nabla_z \left\langle Y'(\boldsymbol{x}) Y'(\boldsymbol{y}) \Phi'(\boldsymbol{x}) \Phi'(z) \right\rangle^{(2,2)} \\ \quad + g \Big(\alpha_G K_G(z) \left\langle Y'(\boldsymbol{x}) Y'(\boldsymbol{y}) \Phi'(\boldsymbol{x}) \Phi'(z) \right\rangle^{(2,2)} + K_G(z) \left\langle \alpha' Y'(\boldsymbol{x}) Y'(\boldsymbol{y}) \Phi'(\boldsymbol{x}) \right\rangle^{(2,2)} \left\langle \Phi^{(0,0)}(z) \right\rangle \Big) \boldsymbol{e}_3 \Big] \\ \quad + \left\langle Y'(\boldsymbol{x}) Y'(\boldsymbol{y}) \Phi'(\boldsymbol{x}) f'(z) \right\rangle^{(2,2)} = 0 & \boldsymbol{x}, \boldsymbol{y}, z \in \Omega \\ \left\langle Y'(\boldsymbol{x}) Y'(\boldsymbol{y}) \Phi'(\boldsymbol{x}) \Phi'(z) \right\rangle^{(2,2)} = \left\langle Y'(\boldsymbol{x}) Y'(\boldsymbol{y}) \Phi'(\boldsymbol{x}) H'(z) \right\rangle^{(2,2)} & \boldsymbol{x}, \boldsymbol{y} \in \Omega,\ z \in \Gamma_D \\ \boldsymbol{n}(z) \cdot [*] = \left\langle Y'(\boldsymbol{x}) Y'(\boldsymbol{y}) \Phi'(\boldsymbol{x}) Q'(z) \right\rangle^{(2,2)} & \boldsymbol{x}, \boldsymbol{y} \in \Omega,\ z \in \Gamma_N \end{cases} \quad \text{(C-49)}$$

where

$$\begin{aligned} \left\langle Y'(\boldsymbol{x}) Y'(\boldsymbol{y}) \Phi'(\boldsymbol{x}) f'(z) \right\rangle^{(2,0)} &= C_Y(\boldsymbol{x},\boldsymbol{y}) \int_\Omega C_f(z,\boldsymbol{u}) \left\langle G^{(0,0)}(\boldsymbol{u},\boldsymbol{x}) \right\rangle d\Omega \\ \left\langle Y'(\boldsymbol{x}) Y'(\boldsymbol{y}) \Phi'(\boldsymbol{x}) Q'(z) \right\rangle^{(2,0)} &= C_Y(\boldsymbol{x},\boldsymbol{y}) \int_{\Gamma_N} C_Q(z,\boldsymbol{u}) \left\langle G^{(0,0)}(\boldsymbol{u},\boldsymbol{x}) \right\rangle d\Gamma \end{aligned} \quad \text{(C-50)}$$

$$\begin{aligned} \left\langle Y'(\boldsymbol{x}) Y'(\boldsymbol{y}) \Phi'(\boldsymbol{x}) f'(z) \right\rangle^{(2,2)} &= C_Y(\boldsymbol{x},\boldsymbol{y}) \int_\Omega C_f(z,\boldsymbol{u}) \left\langle G^{(0,2)}(\boldsymbol{u},\boldsymbol{x}) \right\rangle d\Omega \\ \left\langle Y'(\boldsymbol{x}) Y'(\boldsymbol{y}) \Phi'(\boldsymbol{x}) Q'(z) \right\rangle^{(2,2)} &= C_Y(\boldsymbol{x},\boldsymbol{y}) \int_{\Gamma_N} C_Q(z,\boldsymbol{u}) \left\langle G^{(0,2)}(\boldsymbol{u},\boldsymbol{x}) \right\rangle d\Gamma \end{aligned} \quad \text{(C-51)}$$

$\left\langle Y'(\boldsymbol{x}) Y'(\boldsymbol{y}) \Phi'(\boldsymbol{x}) H'(z) \right\rangle^{(2,0)}$ and $\left\langle Y'(\boldsymbol{x}) Y'(\boldsymbol{y}) \Phi'(\boldsymbol{x}) H'(z) \right\rangle^{(2,2)}$ in (C-48) and (C-49) are given by in (A-55) and (A-56) of Appendix A, respectively.

C.11 $\langle \alpha'^2 \mathbf{Y}'(x) \mathbf{Y}'(y) \mathbf{\Phi}'(z) \rangle$

Rewriting (2-19) in terms of z, multiplying by $\alpha'^2 Y'(\boldsymbol{x}) Y'(\boldsymbol{y})$, taking conditional mean, and recalling our assumption that both f' and Q' are uncorrelated with α', K_s', and thus G, yields an explicit equation for $\langle \alpha'^2 Y'(\boldsymbol{x}) Y'(\boldsymbol{y}) \Phi'(z) \rangle$,

$$\left\langle \alpha'^2 Y'(\boldsymbol{x}) Y'(\boldsymbol{y}) \Phi'(z) \right\rangle = -\int_{\Gamma_D} \left\langle \alpha'^2 Y'(\boldsymbol{x}) Y'(\boldsymbol{y}) H'(\boldsymbol{u}) \nabla_u^T G(\boldsymbol{u}, z) K_s(\boldsymbol{u}) \right\rangle \boldsymbol{n}(z) d\Gamma + HO \quad \text{(C-52)}$$

From (A-89) of Appendix A we know that the integrand in the above equation is higher than second order, therefore,

$$\left\langle \alpha'^2 Y'(\boldsymbol{x})Y'(\boldsymbol{y})\Phi'(\boldsymbol{z})\right\rangle^{(2,2)} = 0 \tag{C-53}$$

C.12 $\langle \alpha'^2 Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Phi'(\boldsymbol{z})\rangle$

Rewriting (2-17) in terms of $\boldsymbol{z}$, multiplying by $\alpha'^2 Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})$, taking conditional mean, gives

$$\begin{cases} \nabla_z \cdot \left[\left\langle K_s(\boldsymbol{z})\right\rangle \nabla_z \left\langle \alpha'^2 Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Phi'(\boldsymbol{z})\right\rangle + g\left(\langle\alpha\rangle\left\langle K_s(\boldsymbol{z})\right\rangle\left\langle \alpha'^2 Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Phi'(\boldsymbol{z})\right\rangle \boldsymbol{e}_3\right]\right. & \\ \quad + \left\langle \alpha'^2 Y'(\boldsymbol{x})\Phi'(\boldsymbol{y}) f'(\boldsymbol{z})\right\rangle = 0 & \boldsymbol{x},\boldsymbol{y},\ \boldsymbol{z}\in\Omega \\ \left\langle \alpha'^2 Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Phi'(\boldsymbol{z})\right\rangle = \left\langle \alpha'^2 Y'(\boldsymbol{x})\Phi'(\boldsymbol{y}) H'(\boldsymbol{z})\right\rangle & \boldsymbol{x},\boldsymbol{y}\in\Omega,\ \boldsymbol{z}\in\Gamma_D \\ \boldsymbol{n}(\boldsymbol{z})\cdot[*] = \left\langle \alpha'^2 Y'(\boldsymbol{x})\Phi'(\boldsymbol{y}) Q'(\boldsymbol{z})\right\rangle & \boldsymbol{x},\boldsymbol{y}\in\Omega,\ \boldsymbol{z}\in\Gamma_N \end{cases} \tag{C-55}$$

where

$$\begin{aligned} \left\langle \alpha'^2 Y'(\boldsymbol{x})\Phi'(\boldsymbol{y}) f'(\boldsymbol{z})\right\rangle &= \int_\Omega \left\langle f'(\boldsymbol{z}) f'(\boldsymbol{u})\right\rangle\left\langle \alpha'^2 Y'(\boldsymbol{x}) G(\boldsymbol{u},\boldsymbol{y})\right\rangle d\Omega \\ \left\langle \alpha'^2 Y'(\boldsymbol{x})\Phi'(\boldsymbol{y}) Q'(\boldsymbol{z})\right\rangle &= \int_{\Gamma_N} \left\langle Q'(\boldsymbol{z}) Q'(\boldsymbol{u})\right\rangle\left\langle \alpha'^2 Y'(\boldsymbol{x}) G(\boldsymbol{u},\boldsymbol{y})\right\rangle d\Gamma \end{aligned} \tag{C-55}$$

Expanding (C-54) yields

$$\begin{cases} \nabla_z \cdot \left[K_G(\boldsymbol{z})\ \nabla_z \left\langle \alpha'^2 Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Phi'(\boldsymbol{z})\right\rangle^{(2,2)} + g\alpha_G K_G(\boldsymbol{z})\left\langle \alpha'^2 Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Phi'(\boldsymbol{z})\right\rangle^{(2,2)} \boldsymbol{e}_3\right] & \\ \quad + \left\langle \alpha'^2 Y'(\boldsymbol{x})\Phi'(\boldsymbol{y}) f'(\boldsymbol{z})\right\rangle^{(2,2)} = 0 & \boldsymbol{x},\boldsymbol{y},\ \boldsymbol{z}\in\Omega \\ \left\langle \alpha'^2 Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Phi'(\boldsymbol{z})\right\rangle^{(2,2)} = \left\langle \alpha'^2 Y'(\boldsymbol{x})\Phi'(\boldsymbol{y}) H'(\boldsymbol{z})\right\rangle^{(2,2)} & \boldsymbol{x},\boldsymbol{y}\in\Omega,\ \boldsymbol{z}\in\Gamma_D \\ \boldsymbol{n}(\boldsymbol{z})\cdot[*] = \left\langle \alpha'^2 Y'(\boldsymbol{x})\Phi'(\boldsymbol{y}) Q'(\boldsymbol{z})\right\rangle^{(2,2)} & \boldsymbol{x},\boldsymbol{y}\in\Omega,\ \boldsymbol{z}\in\Gamma_N \end{cases} \tag{C-56}$$

where

$$\left\langle \alpha'^2 Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\, f'(\boldsymbol{z})\right\rangle^{(2,2)} = \alpha_G^2\sigma_\beta^2 \int_\Omega C_f(\boldsymbol{z},\boldsymbol{u})\left\langle Y'(\boldsymbol{x})G^{(1,0)}(\boldsymbol{u},\boldsymbol{y})\right\rangle d\Omega$$
$$\left\langle \alpha'^2 Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})Q'(\boldsymbol{z})\right\rangle^{(2,2)} = \alpha_G^2\sigma_\beta^2 \int_{\Gamma_N} C_Q(\boldsymbol{z},\boldsymbol{u})\left\langle Y'(\boldsymbol{x})G^{(1,0)}(\boldsymbol{u},\boldsymbol{y})\right\rangle d\Gamma \qquad \text{(C-57)}$$

and $\left\langle \alpha'^2 Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})H'(\boldsymbol{z})\right\rangle^{(2,2)}$ has been evaluated in (A-53).

APPENDIX D
DERIVATION OF FINITE ELEMENT SOLUTIONS FOR NONLOCAL CONDITIONAL MOMENT EQUATIONS

D.1 BASIC RELATIONS

Consider a rectangular element parallel to the Cartesian coordinates (x_1, x_2) with corner nodes numbered counterclockwise as shown in Figure D.1.

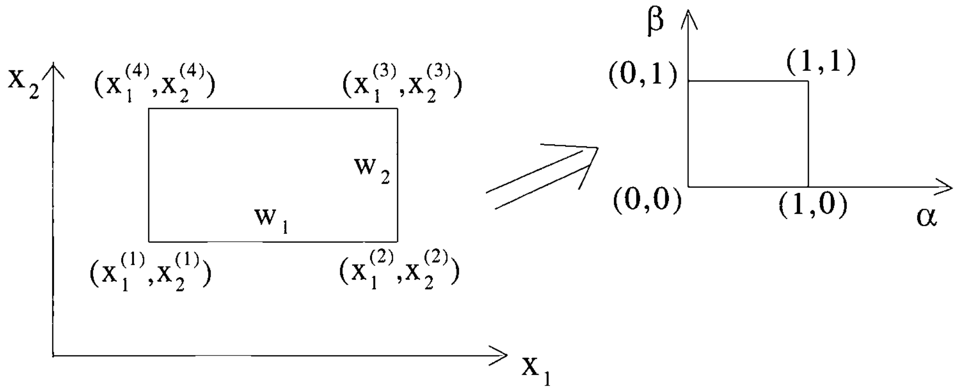


Figure D.1. Definitions of an element, local numbering and the element transformation.

Defining local coordinates

$$\alpha = \frac{x_1 - x_1^{(1)}}{w_1} \qquad \beta = \frac{x_2 - x_2^{(1)}}{w_2} \tag{D-1}$$

where w_1 and w_2 are sides of the element in the x_1 and x_2 directions, respectively (see Fig D.1), and weight functions

$$\xi_1 = (1-\alpha)(1-\beta) \qquad \xi_2 = \alpha(1-\beta)$$
$$\xi_3 = \alpha\beta \qquad \xi_4 = (1-\alpha)\beta \tag{D-2}$$

When formulating finite element equations, we will encounter integrals (either volume or boundary) that contain these weight functions. Table D.1 lists integrals over the element that have the form

$$I = \int_0^1\int_0^1 (1-\alpha)^m (1-\beta)^n \alpha^s \beta^t d\alpha d\beta \tag{D-3}$$

Based on Table D.1, element matrices that are required in formulating finite element equations in this study can be evaluated (Table D.2).

D.2 NUMERICAL SOLUTIONS OF AUXILIARY FUNCTIONS

According to Appendix B, we need to solve for nine quantities related to various orders of auxiliary functions or combinations of auxiliary functions, β', and Y'. In this section, numerical expressions for these quantities are derived.

Take $\langle G^{(0,0)}\rangle$ as an example. Consider the Galerkin orthogonalization to the zero order auxiliary function, (B-6),

$$\int_\Omega \left[\nabla_y \cdot \left[K_G(y)\nabla_y G^{(0,0)}(y,x)\right] - g\alpha_G e_3^T K_G(y)\nabla_y G^{(0,0)}(y,x) + \delta(x-y)\right] \xi_n(y) d\Omega = 0 \quad x \in \Omega \tag{D-4}$$

where $\xi_n(y)$ is the n-th weight function, n=1,2, ...NN is a global node number, and NN is the total number of nodes in the flow domain.

Table D.1. Table of Integrals

(m+n+s+t=k)

k	m	n	s	t	I	k	m	n	s	t	I
k=2	2	0	0	0	1/3	k=4	4	0	0	0	1/5
	0	2	0	0			0	4	0	0	
	0	0	2	0			0	0	4	0	
	0	0	0	2			0	0	0	4	
	1	1	0	0	1/4		3	1	0	0	1/8
	1	0	0	1			1	3	0	0	
	0	1	1	0			3	0	0	1	
	0	0	1	1			0	3	1	0	
	1	0	1	0	1/6		1	0	0	3	
	0	1	0	1			0	1	3	0	
k=3	3	0	0	0	1/4		0	0	3	1	
	0	3	0	0			2	2	0	0	1/9
	0	0	3	0			0	0	2	2	
	0	0	0	3			2	0	0	2	
	2	1	0	0	1/6		0	2	2	0	
	2	0	0	1			2	1	0	1	1/18
	1	2	0	0			1	2	1	0	
	0	2	1	0			1	0	1	2	
	0	1	2	0			0	1	2	1	
	0	0	2	1			3	0	1	0	1/20
	1	0	0	2			0	3	0	1	
	0	0	1	2			1	0	3	0	
	2	0	1	0	1/12		0	1	0	3	
	0	2	0	1			2	0	1	1	1/24
	1	0	2	0			0	2	1	1	
	0	1	0	2			1	0	2	1	
	1	1	1	0			0	1	1	2	
	1	1	0	1			1	1	2	0	
	1	0	1	1			1	1	0	2	
	0	1	1	1			2	0	2	0	1/30
							0	2	0	2	
							1	1	1	1	1/36

Table D.2. Element Matrices

Integrands	Element Matrix
ξ_n	$A_1 = \frac{w_1 w_2}{4}(1,1,1,1)^T$
$\xi_n \xi_m$	$D = \frac{w_1 w_2}{36}\begin{bmatrix} 4 & 2 & 1 & 2 \\ 2 & 4 & 2 & 1 \\ 1 & 2 & 4 & 2 \\ 2 & 1 & 2 & 4 \end{bmatrix}$
$\partial\xi_n/\partial x_1$, $\partial\xi_n/\partial x_2$	$C_1 = \frac{w_2}{8}(-1,\ 1,\ 1, -1)^T$ $\quad C_2 = \frac{w_1}{8}(-1,\ -1,\ 1,\ 1)^T$
$K\xi_n \nabla\xi_m$	$b_1 = \begin{bmatrix} -2 & 2 & 1 & -1 \\ -2 & 2 & 1 & -1 \\ -1 & 1 & 2 & -2 \\ -1 & 1 & 2 & -2 \end{bmatrix} \quad b_2 = \begin{bmatrix} -2 & -1 & 1 & 2 \\ -1 & -2 & 2 & 1 \\ -1 & -2 & 2 & 1 \\ -2 & -1 & 1 & 2 \end{bmatrix}$ $B_1 = \frac{w_1}{12}K_{11}b_1 + \frac{w_2}{12}K_{12}b_2 \quad B_2 = \frac{w_1}{12}K_{21}b_1 + \frac{w_2}{12}K_{22}b_2 \quad B=(B_1, B_2)^T$
$\nabla\xi_n * \nabla\xi_m$	$A = \frac{S_2}{6}\begin{bmatrix} 2 & -2 & -1 & 1 \\ -2 & 2 & 1 & -1 \\ -1 & 1 & 2 & -2 \\ 1 & -1 & -2 & 2 \end{bmatrix} + \frac{S_1}{6}\begin{bmatrix} 2 & 1 & -1 & -2 \\ 1 & 2 & -2 & -1 \\ -1 & -2 & 2 & 1 \\ -2 & -1 & 1 & 2 \end{bmatrix}$ where $s_1 = w_1/w_2$, $s_2 = w_2/w_1$
$K\nabla\xi_n * \nabla\xi_m$	$A = \frac{w_2 K_{11}}{6w_1}\begin{bmatrix} 2 & -2 & -1 & 1 \\ -2 & 2 & 1 & -1 \\ -1 & 1 & 2 & -2 \\ 1 & -1 & -2 & 2 \end{bmatrix} + \frac{K_{12}}{2}\begin{bmatrix} 1 & 0 & -1 & 0 \\ 0 & -1 & 0 & 1 \\ -1 & 0 & 1 & 0 \\ 0 & 1 & 0 & -1 \end{bmatrix} + \frac{w_1 K_{22}}{6w_2}\begin{bmatrix} 2 & 1 & -1 & -2 \\ 1 & 2 & -2 & -1 \\ -1 & -2 & 2 & 1 \\ -2 & -1 & 1 & 2 \end{bmatrix}$
$K\xi_n \nabla\xi_n * \nabla\xi_m$	F*

$$F = \begin{bmatrix} a & -a & b & -b \\ & a & -b & b \\ & & c & -c \\ & & & c \end{bmatrix} + \begin{bmatrix} d & e & -e & -d \\ & f & -f & -e \\ & & f & e \\ & & & d \end{bmatrix} + \frac{1}{36}*$$

$$\begin{bmatrix} 8K_{12}^{(1)} + 4K_{12}^{(2)} + 2K_{12}^{(3)} + 4K_{12}^{(4)} & -2K_{12}^{(1)} + 2K_{12}^{(2)} + K_{12}^{(3)} - K_{12}^{(4)} & -4K_{12}^{(1)} - 5K_{12}^{(2)} - 4K_{12}^{(3)} - 5K_{12}^{(4)} & -2K_{12}^{(1)} - K_{12}^{(2)} + K_{12}^{(3)} + 2K_{12}^{(4)} \\ & -4K_{12}^{(1)} - 8K_{12}^{(2)} - 4K_{12}^{(3)} - 2K_{12}^{(4)} & K_{12}^{(1)} + 2K_{12}^{(2)} - 2K_{12}^{(3)} - K_{12}^{(4)} & 5K_{12}^{(1)} + 4K_{12}^{(2)} + 5K_{12}^{(3)} + 4K_{12}^{(4)} \\ & & 2K_{12}^{(1)} + 4K_{12}^{(2)} + 8K_{12}^{(3)} + 4K_{12}^{(4)} & K_{12}^{(1)} - K_{12}^{(2)} - 2K_{12}^{(3)} + 2K_{12}^{(4)} \\ & & & -4K_{12}^{(1)} - 2K_{12}^{(2)} - 4K_{12}^{(3)} - 8K_{12}^{(4)} \end{bmatrix}$$

$$a = \frac{S_2}{24}\left(3K_{11}^{(1)} + 3K_{11}^{(2)} + K_{11}^{(3)} + K_{11}^{(4)}\right),\ b = -\frac{S_2}{24}\left(K_{11}^{(1)} + K_{11}^{(2)} + K_{11}^{(3)} + K_{11}^{(4)}\right),\ c = \frac{S_2}{24}\left(K_{11}^{(1)} + K_{11}^{(2)} + 3K_{11}^{(3)} + 3K_{11}^{(4)}\right)$$

$$d = \frac{S_1}{24}\left(3K_{22}^{(1)} + K_{22}^{(2)} + K_{22}^{(3)} + 3K_{22}^{(4)}\right),\ e = \frac{S_1}{24}\left(K_{22}^{(1)} + K_{22}^{(2)} + K_{22}^{(3)} + K_{22}^{(4)}\right),\ f = \frac{S_1}{24}\left(K_{22}^{(1)} + 3K_{22}^{(2)} + 3K_{22}^{(3)} + K_{22}^{(4)}\right)$$

Applying Green's first identity to the first term in (D-4) yields

$$\begin{aligned}&\int_{\Omega} K_G(y)\nabla_y G^{(0,0)}(\boldsymbol{y},\boldsymbol{x})\cdot\nabla_y\xi_n(\boldsymbol{y})d\Omega + g\ \alpha_G\ \boldsymbol{e}_3^T\int_{\Omega} K_G(\boldsymbol{y})\nabla_y G^{(0,0)}(\boldsymbol{y},\boldsymbol{x})\xi_n(\boldsymbol{y})\ d\Omega \\ &\quad = \int_{\Gamma_D} K_G(\boldsymbol{y})\nabla_y G^{(0,0)}(\boldsymbol{y},\boldsymbol{x})\xi_n(\boldsymbol{y})\cdot\boldsymbol{n}(\boldsymbol{y})d\Gamma + \int_{\Omega}\delta(\boldsymbol{x}-\boldsymbol{y})\xi_n(\boldsymbol{y})\ d\Omega \qquad \boldsymbol{x}\in\Omega\end{aligned} \tag{D-5}$$

This holds for all $\boldsymbol{x}\in\Omega$. For any fixed $\boldsymbol{x}$ at a global node p, let

$$G^{(0,0)}(\boldsymbol{y},\boldsymbol{x}) = \sum_{m=1}^{NN} G_{mp}^{(0,0)}\ \xi_m(\boldsymbol{y}) \tag{D-6}$$

where $G_{\mathrm{mp}}{}^{(0,0)}$ is $G^{(0,0)}(\boldsymbol{y}, \boldsymbol{x})$ evaluated at $\boldsymbol{x}$ of node p and $\boldsymbol{y}$ of node m. Substituting (D-6) into the volume integrals in (D-5), and recalling from (5-3) that

$$\begin{aligned}A_{nm} &= \sum_e A_{nm}^{(e)} = \int_{\Omega} K_G(y)\nabla_y\xi_m(\boldsymbol{y})\cdot\nabla_y\xi_n(\boldsymbol{y})d\Omega \\ \boldsymbol{B}_{nm} &= \sum_e \boldsymbol{B}_{nm}^{(e)} = \int_{\Omega} K_G(\boldsymbol{y})\nabla_y\xi_m(\boldsymbol{y})\xi_n(\boldsymbol{y})d\Omega\end{aligned} \tag{D-7}$$

gives

$$\sum_{m=1}^{NN}\left(A_{\mathrm{nm}} + g\alpha_G\boldsymbol{e}_2^T\boldsymbol{B}_{\mathrm{nm}}\right)G_{mp}^{(0,0)} = \delta_{np} + \int_{\Gamma_D} K_G(\boldsymbol{y})\nabla_y\tilde{G}^{(0,0)}(\boldsymbol{y},\boldsymbol{x})\xi_n(\boldsymbol{y})\cdot\boldsymbol{n}(\boldsymbol{y})d\Gamma \qquad \boldsymbol{x}\in\Omega \tag{D-8}$$

Here A_{nm} and $\boldsymbol{B}_{\mathrm{nm}}$ have been evaluated in Table D-2. As explained in Chapter 4, we do not need to evaluate the boundary integral in (D-8), but hereby assign the matrices as follows,

$$\tilde{A}_{nm} = \begin{cases} A_{nm} + g\alpha_G\boldsymbol{e}_2^T\boldsymbol{B}_{nm} & \text{if } n\notin\Gamma_{\mathrm{D}} \\ 1 & \text{if } n\in\Gamma_{\mathrm{D}} \text{ and } n=m \\ 0 & \text{if } n\in\Gamma_{\mathrm{D}} \text{ and } n\neq m\end{cases} \tag{D-9}$$

$$\tilde{b}_n = \begin{cases} 0 & \text{if } n \in \Gamma_D \\ \delta_{np} & \text{if } n \notin \Gamma_D \end{cases} \tag{D-10}$$

The finite element equation for the zero order auxiliary function is

$$\sum_{m=1}^{NN} \tilde{A}_{nm} \left\langle G_{mp}^{(0,0)} \right\rangle = \tilde{b}_n \qquad n, p = \overline{1, NN} \tag{D-11}$$

The derivation of numerical solutions for all other required G-related auxiliary functions can be done in a manner similar to that for $G^{(0,0)}(y, \boldsymbol{x})$ upon the following interpolation, for any fixed $\boldsymbol{x}$ at global node p, $y \in e$, and $z \in e'$,

$$\begin{aligned} \left\langle G^{(i,j)}(y,\boldsymbol{x}) \right\rangle &= \sum_{m=1}^{N} \left\langle G_{mp}^{(i,j)(e)} \right\rangle \xi_m^{(e)}(\boldsymbol{y}) \\ \left\langle \beta' G^{(i,j)}(y,\boldsymbol{x}) \right\rangle &= \sum_{m=1}^{N} \left\langle \beta' G^{(i,j)} \right\rangle_{mp}^{(e)} \xi_m^{(e)}(\boldsymbol{y}) \\ \left\langle Y'(z) G^{(i,j)}(y,\boldsymbol{x}) \right\rangle &= \sum_{m=1}^{N} \left\langle Y'(e') G^{(i,j)} \right\rangle_{mp}^{(e)} \xi_m^{(e)}(\boldsymbol{y}) \\ \left\langle Y'(y) \nabla_y G^{(i,j)}(y,\boldsymbol{x}) \right\rangle &= \sum_{m=1}^{N} \sum_{e_1 \in E_1} \frac{1}{N_{E_1}} \left\langle Y'(e_1) G^{(i,j)} \right\rangle_{mp}^{(e)} \nabla_y \xi_m^{(e)}(\boldsymbol{y}) \end{aligned} \tag{D-12}$$

These interpolations are straightforward except for the last one. Because Y' is defined in elements and $G^{(i,j)}(y,\boldsymbol{x})$ is evaluated at nodes, $\left\langle Y'(z) G^{(i,j)}(y,\boldsymbol{x}) \right\rangle$ is associate with Y' in an element and $G^{(i,j)}(y,\boldsymbol{x})$ at nodes. Therefore, $\left\langle Y'(y) G^{(i,j)}(y,\boldsymbol{x}) \right\rangle$ is not well defined. Especially, $\left\langle Y'(y) \nabla_y G^{(i,j)}(y,\boldsymbol{x}) \right\rangle$ cannot be evaluated directly from $\left\langle Y'(y) G^{(i,j)}(y,\boldsymbol{x}) \right\rangle$. Here we use an averaging scheme to evaluate $\left\langle Y'(y) \nabla_y G^{(i,j)}(y,\boldsymbol{x}) \right\rangle$, i.e., averaging all $\left\langle Y'(e_1) \nabla_y G^{(i,j)}(y,\boldsymbol{x}) \right\rangle = \nabla_y \left\langle Y'(e_1) G^{(i,j)}(y,\boldsymbol{x}) \right\rangle$, where $e_1 \in E_1$ denotes elements that are adjacent to the element e, and N_{E_1} is the number of such elements. Because equations for all required

G-related auxiliary functions have the same structure, their finite element equations have the same format as (D-11), with exactly the same $\tilde{A}$ matrix but different $\tilde{b}$. Vectors $\tilde{b}$ for all these equations have been evaluated and listed in Table D.3.

D.3 FORMULATION OF FINITE ELEMENT SOLUTION FOR CONDITIONAL HIGHER MOMENTS

In this section, we formulate finite element solutions that are required in evaluating solutions for mean and (cross-)covariance functions, as was seen in Chapter 4.

D.3.1 $\langle K'(x)\Phi'(y)\rangle$ and $\langle K'(x)\nabla\Phi'(y)\rangle$

From (D-4) and (D-5), for any $x\in e$, $y\in e'$, and $z\in e''$, let

$$\left\langle \Phi^{(0,0)(e'')}(z)\right\rangle = \sum_{p=1}^{N}\left\langle \Phi_p^{(0,0)(e'')}\right\rangle \xi_p^{(e'')}(z) \tag{D-13}$$

$$R_{\alpha\Phi}^{(2,2)}(z) = \sum_{p=1}^{N} R_{\alpha\Phi,p}^{(2,2)(e'')}(z)\, \xi_p^{(e'')}(z) \tag{D-14}$$

All symbols have been defined in Chapter 4. $G^{(i,j)}(y,x)$ are interpolated as in (D-12). Substituting (D-12)-(D-13) and (D-15) into (C-4)-(C-5), using definitions (D-7), and assuming deterministic force terms (boundary conditions and source/sink), yields

$$C_{Y\Phi}^{(2,0)}(x,y) = -\sum_{e''} C_Y(e,e'') \sum_{j,k,p=1}^{N} G_{jk}^{(0,0)(e'',e')}\left\langle \Phi_p^{(0,0)(e'')}\right\rangle\left(A_{pj}^{(e'')} + g\alpha_G e_2^T B_{pj}^{(e'')}\right)\xi_k^{(e')}(y) \tag{D-15}$$

and

Table D.3. Finite Element Equations for Auxiliary Functions*

X_{mp}	$\tilde{b}_n$ ***for*** $n \notin \Gamma_D$, ***otherwise,*** $\tilde{b}_n = 0$
$\langle G^{(0,0)} \rangle_{mp}$	$\tilde{b}_n = \delta_{np}$
$\langle \beta' G^{(0,1)} \rangle_{mp}$	$\tilde{b}_n = -g\alpha_G \sigma_\beta^2 \sum_e \sum_{m=1}^{N} \langle G_{mp}^{(0,0)} \rangle^{(e)} \boldsymbol{e}_2^T \boldsymbol{B}_{nm}^{(e)}$
$\langle Y' G^{(1,0)} \rangle_{mp}^{(e'')}$	$\tilde{b}_n = -\sum_e C_Y(e,e'') \sum_{m=1}^{N} \langle A_{nm}^{(e)} + g\alpha_G \boldsymbol{e}_2^T \boldsymbol{B}_{nm}^{(e)} \rangle \; G_{mp}^{(0,0)(e)}$
$\langle \beta' Y' G^{(1,1)} \rangle_{mp}^{(e'')}$	$\tilde{b}_n = -\sum_e C_Y(e,e'') \sum_{m=1}^{N} \left[\langle \beta' G^{(0,1)}(y,x) \rangle_{mp}^{(e)} \left(A_{mn}^{(e)} + g\alpha_G \boldsymbol{e}_2^T \boldsymbol{B}_{nm}^{(e)} \right) + g\alpha_G \sigma_\beta^2 \langle G_{mp}^{(0,0)} \rangle^{(e)} \boldsymbol{e}_2^T \boldsymbol{B}_{nm}^{(e)} \right]$
$\langle G_{mp}^{(0,2)} \rangle$	$\tilde{b}_n = -g\alpha_G \sum_e \sum_{m=1}^{N} \left(\langle \beta' G^{(0,1)} \rangle_{mp} + \frac{1}{2}\sigma_\beta^2 \langle G_{mp}^{(0,0)} \rangle^{(e)} \right) \boldsymbol{e}_2^T \boldsymbol{B}_{nm}^{(e)}$
$\langle G_{mp}^{(2,0)} \rangle$	$\tilde{b}_n = -\sum_e \sum_{m=1}^{N} \left(\frac{1}{N_{E_1}} \sum_{e_1 \in E_1} \langle Y'(e_1) G^{(1,0)} \rangle_{mp}^{(e)} + \frac{1}{2}\sigma_Y^2(e) \langle G_{mp}^{(0,0)} \rangle^{(e)} \right) \left(A_{mn}^{(e)} + g\alpha_G \boldsymbol{e}_2^T \boldsymbol{B}_{nm}^{(e)} \right)$
$\langle Y' G^{(1,2)} \rangle_{mp}^{(e'')}$	$\tilde{b}_n = -g\alpha_G \sum_e C_Y(e,e'') \sum_{m=1}^{N} \left(\langle G_{mp}^{(0,2)(e)} \rangle + \langle \beta' G^{(0,1)} \rangle^{(e)} + \frac{1}{2}\sigma_\beta^2 \langle G_{mp}^{(0,0)(e)} \rangle \right) \boldsymbol{e}_2^T \boldsymbol{B}_{nm}^{(e)}$
$\langle \beta' G^{(2,1)} \rangle_{mp}$	$\tilde{b}_n = -\sum_e \sum_{m=1}^{N} \left(\frac{1}{N_{E_1}} \sum_{e_1 \in E_1} \langle \beta' Y'(e') G^{(1,1)} \rangle_{mp}^{(e)} + \frac{1}{2}\sigma_Y^2(e) \langle \beta' G^{(0,1)} \rangle_{mp}^{(e)} \right) A_{mn}^{(e)}$ $- g\alpha_G \sum_e \sum_{m=1}^{N} \left(\sigma_\beta^2 \langle G_{mp}^{(2,0)(e)} \rangle + \frac{1}{2}\sigma_Y^2(e) \langle \beta' G^{(0,1)} \rangle_{mp}^{(e)} + \frac{1}{2}\sigma_\beta^2 \sigma_Y^2(e) \langle G_{mp}^{(0,0)(e)} \rangle \right) \boldsymbol{e}_2^T \boldsymbol{B}_{nm}^{(e)}$ $- g\alpha_G \sum_e \sum_{m=1}^{N} \frac{1}{N_{E_1}} \sum_{e_1 \in E_1} \left(\langle \beta' Y'(e') G^{(1,1)} \rangle_{mp}^{(e)} + \sigma_\beta^2 \langle Y'(e') G^{(1,0)} \rangle_{mp}^{(e)} \right) \boldsymbol{e}_2^T \boldsymbol{B}_{nm}^{(e)}$
$\langle G_{mp}^{(2,2)} \rangle$	$\tilde{b}_n = -\sum_e \sum_{m=1}^{N} \frac{1}{N_{E_1}} \sum_{e_1 \in E_1} \langle Y'(e_1) G^{(1,2)} \rangle_{mp}^{(e)} A_{mn}^{(e)} - \frac{1}{2} \sum_e \sigma_Y^2(e) \sum_{m=1}^{N} \langle G_{mp}^{(0,2)(e)} \rangle A_{mn}^{(e)}$ $- g\alpha_G \sum_e \sum_{m=1}^{N} \left(\langle \beta' G^{(2,1)} \rangle_{mp}^{(e)} + \frac{1}{2}\sigma_\beta^2 \langle G_{mp}^{(2,0)(e)} \rangle \right) \boldsymbol{e}_2^T \boldsymbol{B}_{nm}^{(e)}$ $- g\alpha_G \sum_e \sum_{m=1}^{N} \frac{1}{N_{E_1}} \sum_{e_1 \in E_1} \left(\langle Y'(e') G^{(1,2)} \rangle_{mp}^{(e)} + \langle \beta' Y'(e') G^{(1,1)} \rangle_{mp}^{(e)} + \frac{1}{2}\sigma_\beta^2 \langle G_{mp}^{(2,0)(e)} \rangle \right) \boldsymbol{e}_2^T \boldsymbol{B}_{nm}^{(e)}$ $-\frac{1}{2} g\alpha_G \sum_e \sigma_Y^2(e) \sum_{m=1}^{N} \left(\langle G_{mp}^{(0,2)(e)} \rangle + \langle \beta' G^{(0,1)} \rangle_{mp}^{(e)} + \frac{1}{2}\sigma_\beta^2 \langle G_{mp}^{(0,0)(e)} \rangle \right) \boldsymbol{e}_2^T \boldsymbol{B}_{nm}^{(e)}$

*All required G-related terms satisfy an equation of form $\sum_{m=1}^{NN} \tilde{A}_{nm} X_{mp} = \tilde{b}_n \quad n, p = \overline{1, NN}$, where $\tilde{A}_{nm}$ is defined in (D-9).

$$
\begin{aligned}
&C_{Y\Phi}^{(2,2)}(\boldsymbol{x},\boldsymbol{y}) \\
&= -\sum_{e''} C_Y(e,e'') \sum_{j,k,p=1}^{N} \left(G_{jk}^{(0,2)(e'',e')} \left\langle \Phi_p^{(0,0)(e'')} \right\rangle + G_{jk}^{(0,0)(e'',e')} \left\langle \Phi_p^{(0,2)(e'')} \right\rangle \right) \left(A_{pj}^{(e'')} + g\alpha_{\mathrm{G}} \boldsymbol{e}_2^T \boldsymbol{B}_{pj}^{(e'')} \right) \xi_k^{(e')}(\boldsymbol{y}) \\
&-\frac{1}{2} g\alpha_{\mathrm{G}} \sigma_\beta^2 \sum_{e''} C_Y(e,e'') \sum_{j,k,p=1}^{N} G_{jk}^{(0,0)(e'',e')} \left\langle \Phi_p^{(0,0)(e'')} \right\rangle \boldsymbol{e}_2^T \boldsymbol{B}_{pj}^{(e'')} \xi_k^{(e')}(\boldsymbol{y}) \\
&-g\alpha_{\mathrm{G}} \sigma_\beta^2 \sum_{e''} \sum_{j,k,p=1}^{N} \left[C_Y(e,e'') \left\langle \beta' G^{(0,1)(e'',e')} \right\rangle_{jk} + \left\langle \beta' Y'(e) G^{(0,1)(e'',e')} \right\rangle_{jk} \right] \left\langle \Phi_p^{(0,0)(e'')} \right\rangle \boldsymbol{e}_2^T \boldsymbol{B}_{pj}^{(e'')} \xi_k^{(e')}(\boldsymbol{y}) \\
&+g \sum_{e''} \sum_{j,k,p=1}^{N} \left\langle Y'(e) G^{(1,0)(e'',e')} \right\rangle_{jk} R_{\alpha\Phi,p}^{(0,2)(e'')} \boldsymbol{e}_2^T \boldsymbol{B}_{pj}^{(e'')} \xi_k^{(e')}(\boldsymbol{y}) \\
&-\sum_{e_D} \left\langle Y'(\boldsymbol{x}) H'(\boldsymbol{z}) \nabla_z^T G(\boldsymbol{x},\boldsymbol{y}) K_s(\boldsymbol{z}) \right\rangle^{(2,2)(e,e',e_D)} \boldsymbol{n}(e_D)\, d_e
\end{aligned}
\tag{D-16}
$$

Here the last summation is over all elements on the Dirichlet boundary (e_{D}), d_{e} is the length of the element segment on Γ_{D}, $\boldsymbol{n}(e_D)$ is the normal to this boundary segment, and $\left\langle Y'(\boldsymbol{x}) H'(\boldsymbol{z}) \nabla_z^T G(\boldsymbol{x},\boldsymbol{y}) K_s(\boldsymbol{z}) \right\rangle^{(2,2)}$ is given in Appendix A.

The term $\xi_k^{(e')}(\boldsymbol{y})$ in (D-15) and (D-16) allows us to evaluate $\langle Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle^{(2,0)}$ and $\langle Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle^{(2,2)}$ for $\boldsymbol{x}$ in an element and $\boldsymbol{y}$ at a local node, i.e., the cross-covariance between Y in an element and Φ at a node. This is preferred because Φ is defined at nodal points. However, because (D-15) and (D-16) are formulated for $\boldsymbol{y}$ in any element e' in the domain, the question remains are these results consistent if we evaluate them from different elements that share the same node point? The answer is positive. Take (D-15) as an example. Suppose we calculate $\langle Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle^{(2,0)}$ for Y' in any element e and Φ' at node 2 of element e_1, as shown in the

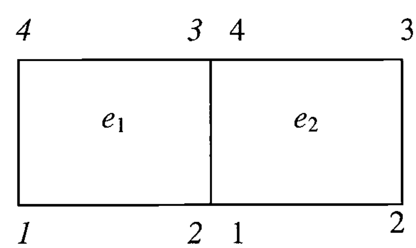


figure on the right. Replace e' by e_1 in (D-15) and note that only $G_{jk}^{(0,0)(e'',e_1)}$ and $\xi_k^{(e_1)}$ are related to element e_1. The product of these two, according to the definition of ξ_k, is

$$G^{(0,0)(e'',e_1)}\xi^{(e_1)} = \left(G_{12}^{(0,0)(e'',e_1)}, G_{22}^{(0,0)(e'',e_1)}, G_{32}^{(0,0)(e'',e_1)}, G_{42}^{(0,0)(e'',e_1)}\right)^T \tag{D-17}$$

where $G^{(0,0)(e'',e_1)}$ is 4x4 matrix defining G at all nodes in e'' with respect to all nodes in e_1, and $\xi^{(e_1)}$ the vector of the weighting functions evaluated at node 2 in e_1. Similarly, if we evaluate $\langle Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle^{(2,0)}$ for Y' in the same element e and Φ' at node 1 of element e_2, which is the same node as node 2 of element e_1, then we have

$$G^{(0,0)(e'',e_2)}\xi^{(e_1)} = \left(G_{11}^{(0,0)(e'',e_2)}, G_{21}^{(0,0)(e'',e_2)}, G_{31}^{(0,0)(e'',e_2)}, G_{41}^{(0,0)(e'',e_2)}\right)^T \tag{D-18}$$

which is the same as (D-17), because for any j, $G_{j2}^{(0,0)(e'',e_1)} = G_{j1}^{(0,0)(e'',e_2)}$.

The solutions for $\langle K_s'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle^{(2,0)}$ and $\langle K_s'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle^{(2,2)}$ can be obtained simply upon multiplying (D-15) and (D-16) by $K_G(\boldsymbol{e})$. Taking the derivatives of $\langle K_s'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle^{(2,0)}$ and $\langle K_s'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle^{(2,2)}$ with respect to $\boldsymbol{y}$ gives the solutions for $\boldsymbol{R}^{(2,0)}(\boldsymbol{x},\boldsymbol{y})=\langle K_s'(\boldsymbol{x})\nabla\Phi'(\boldsymbol{y})\rangle^{(2,0)}$ and $\boldsymbol{R}^{(2,0)}(\boldsymbol{x},\boldsymbol{y})=\langle K_s'(\boldsymbol{x})\nabla\Phi'(\boldsymbol{y})\rangle^{(2,2)}$.

D.3.2 $\langle\alpha'\Phi'(\mathrm{y})\rangle$ and $\langle\alpha'^2\Phi'(\mathrm{y})\rangle$

From (D-11) and (D-12), for any $\boldsymbol{x}\in e$, $\boldsymbol{y}\in e'$, interpolating terms when necessary, as shown (D-12)-(D-14), yields

$$\begin{aligned} R_{\alpha\Phi}^{(0,2)}(\boldsymbol{x}) = &-g\alpha_G\sigma_\beta^2\sum_{e'}\sum_{j,k,p=1}^{N} G_{jk}^{(0,0)(e',e)}\left\langle\Phi_p^{(0,0)(e')}\right\rangle \boldsymbol{e}_2^T\boldsymbol{B}_{pj}^{(e')}\xi_k^{(e)}(\boldsymbol{x}) \\ &-\sum_{e_D}\left\langle\alpha' H'(\boldsymbol{y})\nabla_y^T G(\boldsymbol{y},\boldsymbol{x})K_s(\boldsymbol{y})\right\rangle^{(0,2)(e,e_D)}\boldsymbol{n}(e_D)\, d_e \end{aligned} \tag{D-19}$$

and

$$
\begin{aligned}
&R_{\alpha\Phi}^{(2,2)}(\boldsymbol{x}) = \\
&-\alpha_G \sum_{e'} \sum_{j,k,p=1}^{N} \left(\sum_{e_1 \in E_1} \frac{1}{N_{E_1}} \left\langle \beta' Y'(e_1) G^{(1,1)} \right\rangle_{jk}^{(e',e)} \right) \left\langle \Phi_p^{(0,0)(e')} \right\rangle \left(A_{pj}^{(e')} + g\alpha_G \boldsymbol{e}_2^T \boldsymbol{B}_{pj}^{(e')} \right) \xi_k^{(e)}(\boldsymbol{x}) \\
&-\alpha_G \sum_{e'} \sum_{j,k=1}^{N} \left\langle \beta' G^{(0,1)} \right\rangle_{jk}^{(e',e)} \left(r_1^{(2,0)(e')} C_{1n} + r_2^{(2,0)(e')} C_{2n} \right) \xi_k^{(e)}(\boldsymbol{x}) \\
&-g\alpha_G^2 \sigma_\beta^2 \sum_{e'} \sum_{j,k,p=1}^{N} \left(\frac{1}{2} \sigma_Y^{2(e')} \left\langle G_{jk}^{(0,0)(e',e)} \right\rangle + \sum_{e_1 \in E_1} \frac{1}{N_{E_1}} \left\langle Y'(e_1) G^{(1,0)} \right\rangle_{jk}^{(e',e)} + \left\langle G_{jk}^{(2,0)(e',e)} \right\rangle \right) \left\langle \Phi_p^{(0,0)(e')} \right\rangle \boldsymbol{e}_2^T \boldsymbol{B}_{pj}^{(e')} \xi_k^{(e)}(\boldsymbol{x}) \\
&-g\alpha_G^2 \sigma_\beta^2 \sum_{e'} \sum_{j,k,p=1}^{N} \left\langle G_{jk}^{(0,0)(e',e)} \right\rangle \left\langle \Phi_p^{(2,0)(e')} \right\rangle \boldsymbol{e}_2^T \boldsymbol{B}_{pj}^{(e')} \xi_k^{(e)}(\boldsymbol{x}) \\
&-g\alpha_G^2 \sum_{e'} \sum_{j,k=1}^{N} \left\langle \beta' G^{(0,1)} \right\rangle_{jk}^{(e',e)} R_{K\Phi}^{(2,0)(e')} C_{2n} \xi_k^{(e)}(\boldsymbol{x}) \\
&-\sum_{e_D} \left\langle \alpha' H'(\boldsymbol{y}) \nabla_y^T G(\boldsymbol{y},\boldsymbol{x}) K_s(\boldsymbol{y}) \right\rangle^{(2,2)(e,e_D)} \boldsymbol{n}(e_D)\, d_e
\end{aligned}
\tag{D-20}
$$

For $\left\langle \alpha'^2 \Phi'(\boldsymbol{x}) \right\rangle$, from (D-14) and (D-15), for any $\boldsymbol{x} \in e$, we have

$$
\left\langle \alpha'^2 \Phi'(\boldsymbol{x}) \right\rangle^{(2,2)} = -\alpha_G \sigma_\beta^2 \sum_{e'} \sum_{j,k,p=1}^{N} \left\langle G_{jk}^{(0,0)(e',e)} \right\rangle \left\langle \Phi_p^{(0,0)(e')} \right\rangle \left(A_{pj}^{(e')} + g\alpha_G \boldsymbol{e}_2^T \boldsymbol{B}_{pj}^{(e')} \right) \xi_k^{(e)}(\boldsymbol{x}) \tag{D-21}
$$

and

$$
\begin{aligned}
&\left\langle \alpha'^2 \Phi'(\boldsymbol{x}) \right\rangle^{(2,2)} \\
&= -\alpha_G^2 \sigma_\beta^2 \sum_{e'} \sum_{j,k,p=1}^{N} \left(\left\langle G_{jk}^{(2,0)(e',e)} \right\rangle + \sum_{e_1 \in E_1} \frac{1}{N_{E_1}} \left\langle Y'(e_1) G^{(1,0)} \right\rangle_{jk}^{(e',e)} \right) \left\langle \Phi_p^{(0,0)(e')} \right\rangle \left(A_{pj}^{(e')} + g\alpha_G \boldsymbol{e}_2^T \boldsymbol{B}_{pj}^{(e')} \right) \xi_k^{(e)}(\boldsymbol{x}) \\
&\quad -\alpha_G^2 \sigma_\beta^2 \sum_{e'} \sum_{j,k,p=1}^{N} \left\langle G_{jk}^{(0,0)(e',e)} \right\rangle \left\langle \Phi_p^{(2,0)(e')} \right\rangle \left(A_{pj}^{(e')} + g\alpha_G \boldsymbol{e}_2^T \boldsymbol{B}_{pj}^{(e')} \right) \xi_k^{(e)}(\boldsymbol{x}) \\
&\quad -\alpha_G^2 \sigma_\beta^2 \sum_{e'} \sum_{j,k,p=1}^{N} \left\langle G_{jk}^{(0,0)(e',e)} \right\rangle \nabla_y^T \xi_k^{(e')}(\boldsymbol{y}) \xi_k^{(e)}(\boldsymbol{x}) \left(r^{(2,0)}(e) - g\alpha_G \boldsymbol{e}_2 R_{\alpha\Phi}^{(2,0)}(e) \right)
\end{aligned}
\tag{D-22}
$$

D.3.3 $\langle\alpha' \mathbf{K}_s'(\mathrm{x})\Phi'(\mathrm{y})\rangle$

For any $x \in e$, and $y \in e'$, from (D-17) we have

$$
\begin{aligned}
&C^{(2,2)}_{\alpha K \Phi}(\boldsymbol{x},\boldsymbol{y}) \\
&= -\alpha_G \sum_{e''} C_Y(e,e'') K_G^{(e)} \sum_{j,k,p=1}^{N} \left\langle \beta' G^{(2,0)} \right\rangle_{jk}^{(e'',e')} \left\langle \Phi_p^{(0,0)(e'')} \right\rangle \left(A_{pj}^{(e'')} + g\alpha_G \boldsymbol{e}_2^T \boldsymbol{B}_{pj}^{(e'')} \right) \xi_k^{(e')}(\boldsymbol{y}) \\
&\quad - g\alpha_G^2 \sigma_\beta^2 \sum_{e'} \sum_{j,k,p=1}^{N} \left\langle G_{jk}^{(0,0)(e',e)} \right\rangle \left\langle \Phi_p^{(2,0)(e')} \right\rangle \left(A_{pj}^{(e')} + g\alpha_G \boldsymbol{e}_2^T \boldsymbol{B}_{pj}^{(e')} \right) \xi_k^{(e')}(\boldsymbol{y}) \\
&\quad - \alpha_G^2 \sigma_\beta^2 \sum_{e'} \sum_{j,k,p=1}^{N} \left(\sum_{e_1 \in E_1} \frac{1}{N_{E_1}} \left\langle Y'(e) G^{(1,0)} \right\rangle_{jk}^{(e'',e')} \right) \left\langle \Phi_p^{(0,0)(e')} \right\rangle \boldsymbol{e}_2^T \boldsymbol{B}_{pj}^{(e'')} \xi_k^{(e')}(\boldsymbol{y}) \\
&\quad - K_G^{(e)} \sum_{e_D} \left\langle \alpha' Y'(\boldsymbol{x}) H'(z) \nabla_z^T G(z,\boldsymbol{y}) K_s(z) \right\rangle^{(2,2)(e,e',e_D)} \boldsymbol{n}(e_D) d_e
\end{aligned}
\tag{D-23}
$$

D.3.4 $\langle\alpha'^2 \mathbf{Y}'(\mathrm{x})\Phi'(\mathrm{y})\rangle$

For any $x \in e$, and $y \in e'$, from (D-19) we have

$$
\left\langle \alpha'^2 Y'(\boldsymbol{x}) \Phi'(\boldsymbol{y}) \right\rangle^{(2,2)} = -\alpha_G^2 \sigma_\beta^2 \sum_{e''} C_Y(e,e'') \sum_{j,k,p=1}^{N} \left\langle G_{\mathrm{jk}}^{(0,0)(e'',e')} \right\rangle \left\langle \Phi_p^{(0,0)(e'')} \right\rangle \left(A_{pj}^{(e'')} + g\alpha_G \boldsymbol{e}_2^T \boldsymbol{B}_{pj}^{(e'')} \right) \xi_k^{(e')}(\boldsymbol{y})
\tag{D-24}
$$

D.3.5 $\langle\alpha' \Phi'(\mathrm{x})\Phi'(\mathrm{y})\rangle$ and $\langle\alpha'^2 \Phi'(\mathrm{x})\Phi'(\mathrm{y})\rangle$

From (D-22), we note that the implicit equation for $\langle \alpha' \Phi'(x) \Phi'(y) \rangle^{(0,2)}$ has the same structure as that of mean $\mathbf{\Phi}$, thus, for any fixed $\boldsymbol{x}$ at global node p, the finite element equation has a form of

$$
\sum_{m=1}^{NN} \tilde{A}_{nm} \left\langle \alpha' \Phi'(\boldsymbol{x}) \Phi'(\boldsymbol{y}) \right\rangle_{pm}^{(0,2)} = \tilde{b}_n \qquad n, p = \overline{1, NN}
\tag{D-25}
$$

$$\tilde{A}_{nm} = \begin{cases} A_{nm} + g\alpha_G e_2^T \boldsymbol{B}_{mn} & \text{if } n \notin \Gamma_D \\ 1 & \text{if } n \in \Gamma_D \text{ and } n = m \\ 0 & \text{if } n \in \Gamma_D \text{ and } n \neq m \end{cases} \tag{D-26}$$

$$\tilde{b}_n = \begin{cases} \left\langle \alpha'\Phi'(\boldsymbol{x})H'(\boldsymbol{y})\right\rangle_{pn}^{(0,2)} & \text{if } n \in \Gamma_D \\ 0 & \text{if } n \notin \Gamma_D \end{cases} \tag{D-27}$$

Here $\langle \alpha'\Phi'(\boldsymbol{x})H'(\boldsymbol{y})\rangle_{pn}^{(0,2)}$ is cross-covariance of $\langle \alpha'\Phi'(\boldsymbol{x})H'(\boldsymbol{y})\rangle^{(0,2)}$ associated with Φ' at global node p and $\boldsymbol{y}$ at global node n. Equation (D-25) needs to be solved for each global node p. Note that (D-26) is different from (D-9). For $\langle \alpha'\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle^{(2,2)}$, we have

$$\tilde{b}_n = \begin{cases} \left\langle \alpha'\Phi'(x)H'(y)\right\rangle_{pn}^{(2,2)} & \text{if } n \in \Gamma_D \\ -\sum_e \sum_{m=1}^{N} \left(\frac{1}{N_{E_1}} \sum_{e_1 \in E_1} \left\langle \alpha' K_s'(e_1)\Phi'(x)\Phi'(y)\right\rangle_{pm}^{(2,2)} + C_{\alpha K\Phi,p}^{(2,2)(e)} \left\langle \Phi_m^{(0,0)(e)} \right\rangle \right) A_{mn}^{\prime(e)} & \text{if } n \notin \Gamma_D \\ -R_{\alpha\Phi,p}^{(0,2)} \sum_e \left(r_1^{(2,0)(e)} C_{1n} + r_2^{(2,0)(e)} C_{2n} \right) - g \sum_e K_G'(e) \sum_{m=1}^{N} \boldsymbol{B}_{mn}^{(e)} \left\langle \Phi_m^{(2,0)(e)} \right\rangle \left\langle \alpha'^2 \Phi'(x)\Phi'(y)\right\rangle_{pm}^{(2,2)} \boldsymbol{e}_2^T \boldsymbol{B}_{mn}^{\prime(e)} & \\ -g \sum_e \sum_{m=1}^{N} \left(K_G'(e) \left\langle \alpha'\Phi'(x)\right\rangle_p^{(2,2)} + \left\langle \alpha'^2 K_s'(e_1)\Phi'(x)\right\rangle_{pm}^{(2,2)} + \alpha_G C_{\alpha K\Phi,p}^{(2,2)(e)} \left\langle \Phi_m^{(0,0)(e)} \right\rangle \right) \boldsymbol{e}_2^T \boldsymbol{B}_{mn}^{\prime(e)} & \\ +g\alpha_G R_{\alpha\Phi,p}^{(0,2)} \sum_e R_{K\Phi}^{(2,0)(e)} C_{2n} & \end{cases}$$

(D-28)

where

$$\begin{aligned} A_{nm}' &= \sum_e A_{nm}^{\prime(e)} = \int_\Omega \nabla_y \xi_n(\boldsymbol{y}) \cdot \nabla_y \xi_m(\boldsymbol{y}) d\Omega \\ \boldsymbol{B}_{nm}' &= \sum_e \boldsymbol{B}_{nm}^{\prime(e)} = \int_\Omega \xi_n(\boldsymbol{y}) \nabla_y \xi_m(\boldsymbol{y}) d\Omega \end{aligned} \tag{D-29}$$

Similarly, for $\langle \alpha'^2\Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle^{(0,2)}$ we have

$$\tilde{b}_n = \begin{cases} \left\langle \alpha'^2 \Phi'(\boldsymbol{x}) H'(\boldsymbol{y}) \right\rangle_{pn}^{(0,2)} & \text{if } n \in \Gamma_D \\ 0 & \text{if } n \notin \Gamma_D \end{cases} \tag{D-30}$$

and for $\left\langle \alpha'^2 \Phi'(\boldsymbol{x}) \Phi'(\boldsymbol{y}) \right\rangle^{(2,2)}$

$$\tilde{b}_n = \begin{cases} \left\langle \alpha'^2 \Phi'(x) H'(y) \right\rangle_{pn}^{(2,2)} & \text{if } n \in \Gamma_D \\ -\sum_e \sum_{m=1}^{N} \frac{1}{N_{E_1}} \sum_{e_1 \in E_1} \left\langle \alpha'^2 K_s'(e_1) \Phi'(x) \Phi'(y) \right\rangle_{pm}^{(2,2)} A_{mn}'^{(e)} & \text{if } n \notin \Gamma_D \\ -\sum_e \sum_{m=1}^{N} \left\langle \alpha'^2 K_s'(e_1) \Phi'(x) \Phi'(y) \right\rangle_{pm}^{(2,2)} \left\langle \Phi_m^{(0,0)(e)} \right\rangle \left(A_{mn}'^{(e)} + g\alpha_G \boldsymbol{e}_2^T \boldsymbol{B}_{mn}'^{(e)} \right) & \end{cases} \tag{D-31}$$

D.3.6 ⟨ Y′(x)Y′(y)Φ′(z)⟩

From (D-33), for any $\boldsymbol{x} \in e$, $\boldsymbol{y} \in e'$, and $z \in e''$, we have

$$\begin{aligned} &\left\langle Y'(\boldsymbol{x}) Y'(\boldsymbol{y}) \Phi'(z) \right\rangle^{(2,2)} \\ &= -gC_Y(e,e') \sum_{e''} \sum_{j,k,p=1}^{N} \left(\alpha_G \left\langle \beta' G^{(0,1)} \right\rangle_{jk}^{(e'',e')} \left\langle \Phi_p^{(0,0)(e'')} \right\rangle - G_{jk}^{(0,0)(e'',e')} R_{\alpha\Phi,p}^{(0,2)(e'')} \right) \boldsymbol{e}_2^T \boldsymbol{B}_{pj}^{(e'')} \xi_k^{(e')}(z) \\ &\quad - \sum_{e_D} \left\langle Y'(e) Y'(e') H'(\tau) \nabla_\tau^T \mathrm{G}(\tau, z) K_s(\tau) \right\rangle^{(2,2)} n(e_D) d_e \end{aligned} \tag{D-32}$$

D.3.7 ⟨Y′(x)Φ′(y)Φ′(z)⟩

From (D-36) and (D-37), equations for $\langle Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Phi'(z)\rangle^{(2,0)}$ and $\langle Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Phi'(z)\rangle^{(2,2)}$ have the form of (D-25) and exactly the same $\tilde{A}$ as defined in (D-26), the vector $\tilde{b}$ for $\langle Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Phi'(z)\rangle^{(2,0)}$ and $\langle Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Phi'(z)\rangle^{(2,2)}$ are

$$\tilde{b}_n \begin{cases} \left\langle Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})H'(z)\right\rangle_{pn}^{(2,0)} & \text{if } n\in\Gamma_D \\ -\sum_{e''}\sum_{m=1}^{N}\left(\frac{1}{N_{E_1}}\sum_{e_1\in E_1}\left\langle Y'(e)K_s'(e_1)\Phi'(\boldsymbol{y})\Phi'(z)\right\rangle_{pm}^{(2,0)(e'')}+\left\langle Y'(e)K_s'(e'')\Phi'(\boldsymbol{y})\right\rangle_{p}^{(2,0)}\left\langle\Phi_m^{(0,0)(e)}\right\rangle\right)A_{mn}^{\prime(e'')} & \\ -g\alpha_G\sum_{e''}\sum_{m=1}^{N}\left(\left\langle Y'(e)K_s'(e'')\Phi'(\boldsymbol{y})\Phi'(z)\right\rangle_{pm}^{(2,0)(e'')}+\left\langle Y'(e)K_s'(e'')\Phi'(\boldsymbol{y})\right\rangle_{p}^{(2,0)}\left\langle\Phi_m^{(0,0)(e)}\right\rangle\right)\boldsymbol{e}_2^T\boldsymbol{B}_{mn}^{\prime(e'')} & \\ & \text{if } n\notin\Gamma_D \end{cases} \tag{D-33}$$

and

$$\tilde{b}_n \begin{cases} \left\langle Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})H'(z)\right\rangle_{pn}^{(2,2)} & \text{if } n\in\Gamma_D \\ -\sum_{e''}\sum_{m=1}^{N}\left(\frac{1}{N_{E_1}}\sum_{e_1\in E_1}\left\langle Y'(e)K_s'(e_1)\Phi'(\boldsymbol{y})\Phi'(z)\right\rangle_{pm}^{(2,2)(e'')}+\left\langle Y'(e)K_s'(e'')\Phi'(\boldsymbol{y})\right\rangle_{p}^{(2,2)}\left\langle\Phi_m^{(0,0)(e'')}\right\rangle\right)A_{mn}^{\prime(e'')} & \text{if } n\notin\Gamma_D \\ -g\sum_{e''}\sum_{m=1}^{N}\left(\alpha_G\left\langle Y'(e)K_s'(e'')\Phi'(\boldsymbol{y})\Phi'(z)\right\rangle_{pm}^{(2,2)(e'')}+K_G(e'')\left\langle\alpha'Y'(e)\Phi'(\boldsymbol{y})\Phi'(z)\right\rangle_{pm}^{(2,0)}\right)\boldsymbol{e}_2^T\boldsymbol{B}_{mn}^{\prime(e'')} & \\ -g\alpha_G\sum_{e''}\sum_{m=1}^{N}\left\langle Y'(e)K_s'(e'')\Phi'(\boldsymbol{y})\right\rangle_{p}^{(2,2)}\left\langle\Phi_m^{(0,0)(e'')}\right\rangle\boldsymbol{e}_2^T\boldsymbol{B}_{mn}^{\prime(e'')} & \end{cases} \tag{D-34}$$

respectively. Equations (D-34) and (D-35) have to be solved for Y' at each element and $\Phi'(\boldsymbol{y})$ at all nodes.

D.3.8 $\langle \alpha' \, Y'(x) \, Y'(y)\Phi'(z)\rangle$

For any fixed $\boldsymbol{x}\in e$, $\boldsymbol{y}\in e'$, interpolating $G^{(0,0)}$ and $\langle \Phi^{(0,0)}\rangle$ as weighted combination of their values at node points, as shown in (D-12)-(D-13), gives the

$$\begin{aligned} &\left\langle \alpha' Y'(\boldsymbol{x})Y'(\boldsymbol{y})\Phi'(z)\right\rangle^{(2,2)} \\ &= -g\alpha_G^2\sigma_\beta^2 C_Y(e,e')\sum_{e''}\sum_{j,k,p=1}^{N}\left\langle G_{jk}^{(0,0)(e'',e')}\right\rangle\left\langle\Phi_p^{(0,0)(e'')}\right\rangle\boldsymbol{e}_2^T\boldsymbol{B}_{pj}^{(e'')}\xi_k^{(e')}(z) \\ &\quad -\sum_{e_D}\left\langle\alpha' Y'(e)Y'(e')H'(\tau)\nabla_\tau^T G(\tau,z)K_s(\tau)\right\rangle^{(2,2)} n(e_D)d_e \end{aligned} \tag{D-35}$$

D.3.9 $\langle\alpha'Y'(x)\Phi'(y)\Phi'(z)\rangle$

From (D-44), for any fixed $\boldsymbol{x}\in e$, $\boldsymbol{y}$ at global node p, the equation for $\langle\alpha'Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Phi'(\boldsymbol{z})\rangle^{(2,2)}$ has the form of (D-25) and the same $\tilde{A}$ defined in (D-26), the vector $\tilde{b}$ for $\langle Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Phi'(\boldsymbol{z})\rangle^{(2,2)}$ is

$$\tilde{b}_n \begin{cases} \left\langle \alpha' Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})H'(\boldsymbol{z})\right\rangle_{pn}^{(2,2)} & \text{if } n\in\Gamma_{\mathrm{D}} \\ -\sum_{e''}\sum_{m=1}^{N}\frac{1}{N_{E_1}}\sum_{e_1\in E_1}\left\langle \alpha' Y'(e)K_s'(e_1)\Phi'(\boldsymbol{y})\Phi'(\boldsymbol{z})\right\rangle_{pm}^{(2,2)(e'')}\left(A_{mn}^{\prime(e'')}+g\alpha_G\boldsymbol{e}_2^T\boldsymbol{B}_{mn}^{\prime(e'')}\right) & \text{if } n\notin\Gamma_{\mathrm{D}} \\ -\sum_{e''}\sum_{m=1}^{N}\left\langle \alpha' Y'(e)K_s'(e'')\Phi'(\boldsymbol{y})\right\rangle_{pm}^{(2,2)(e'')}\left\langle \Phi_m^{(0,0)(e'')}\right\rangle A_{mn}^{\prime(e'')} & \\ -g\sum_{e''}\sum_{m=1}^{N}\frac{1}{N_{E_1}}\sum_{e_1\in E_1}\left(\left\langle \alpha'^2 Y'(e)K_s'(e_1)\Phi'(\boldsymbol{y})\Phi'(\boldsymbol{z})\right\rangle_{pm}^{(2,2)(e'')}\right)\boldsymbol{e}_2^T B_{mn}^{\prime(e'')} & \\ -g\sum_{e''}K_G(e'')\sum_{m=1}^{N}\left\langle \alpha'^2 Y'(e)\Phi'(\boldsymbol{y})\right\rangle_{pm}^{(2,2)(e'')}\left\langle \Phi_m^{(0,0)(e'')}\right\rangle \boldsymbol{e}_2^T\boldsymbol{B}_{mn}^{\prime(e'')} & \\ -g\alpha_G\sum_{e''}\sum_{m=1}^{N}\left\langle \alpha' Y'(e)K_s'(e'')\Phi'(\boldsymbol{y})\right\rangle_{p}^{(2,2)}\left\langle \Phi_m^{(0,0)(e'')}\right\rangle \boldsymbol{e}_2^T\boldsymbol{B}_{mn}^{\prime(e'')} & \end{cases} \tag{D-36}$$

D.3.10 $\langle Y'(x)Y'(y)\Phi'(x)\Phi'(z)\rangle$

From (D-48) and (D-49), equations for $\langle Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Phi'(\boldsymbol{z})\rangle^{(2,0)}$ and $\langle Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Phi'(\boldsymbol{z})\rangle^{(2,2)}$ have the form of (D-25) and exactly the same $\tilde{A}$ as defined in (D-26), the vector $\tilde{b}$ for $\langle Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Phi'(\boldsymbol{z})\rangle^{(2,0)}$ and $\langle Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Phi'(\boldsymbol{z})\rangle^{(2,2)}$ are

$$\tilde{b}_n = \begin{cases} \left\langle Y'(\boldsymbol{x})Y'(\boldsymbol{y})\Phi'(\boldsymbol{x})H'(\boldsymbol{z})\right\rangle_{pn}^{(2,0)} & \text{if } n\in\Gamma_{\mathrm{D}} \\ 0 & \text{if } n\notin\Gamma_{\mathrm{D}} \end{cases} \tag{D-37}$$

$$\tilde{b}_n \begin{cases} \left\langle Y'(\boldsymbol{x})Y'(\boldsymbol{y})\Phi'(\boldsymbol{x})H'(\boldsymbol{z})\right\rangle_{pn}^{(2,2)} & \text{if } n\in\Gamma_{\mathrm{D}} \\ -\sum_{e''}K_G(e'')\sum_{m=1}^{N}\left\langle \alpha' Y'(e)Y'(e')\Phi'(\boldsymbol{x})\right\rangle_{p}^{(2,2)}\left\langle \Phi_m^{(0,0)(e)}\right\rangle \boldsymbol{e}_2^T\boldsymbol{B}_{mn}^{\prime(e'')} & \text{if } n\notin\Gamma_{\mathrm{D}} \end{cases} \tag{D-38}$$

D.3.11 $\langle \alpha'^2 Y'(x)\Phi'(y)\Phi'(z)\rangle$

From (D-56), the vector $\tilde{b}$ for $\langle \alpha'^2 Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})\Phi'(\boldsymbol{z})\rangle^{(2,2)}$ is

$$\tilde{b}_n \begin{cases} \left\langle \alpha'^2 Y'(\boldsymbol{x})\Phi'(\boldsymbol{y})H'(\boldsymbol{z})\right\rangle_{pn}^{(2,2)} & \text{if } n \in \Gamma_D \\ 0 & \text{if } n \notin \Gamma_D \end{cases}$$

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