

# **Grid convergence for numerical solutions of stochastic moment equations of groundwater flow**

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Submitted to

*Stochastic Environmental Research and Risk Assessment*

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**Abstract:**

22 We provide qualitative and quantitative assessment of the results of a grid  
23 convergence study in terms of (a) the rate/order of convergence and (b) the Grid  
24 Convergence Index, GCI, associated with the numerical solutions of Moment  
25 Equations (MEs) of steady-state groundwater flow. The latter are approximated at  
26 second order (in terms of the standard deviation of the natural logarithm,  $Y$ , of  
27 hydraulic conductivity). We consider (i) the analytical solutions of Riva et al. (2001)  
28 for steady-state radial flow in a randomly heterogeneous conductivity field, which  
29 we take as references; and (ii) the numerical solutions of the MEs satisfied by the  
30 (ensemble) mean and (co)variance of hydraulic head and fluxes. Based on 45  
31 numerical grids associated with differing degrees of discretization, we find a  
32 supra-linear rate of convergence for the mean and (co)variance of hydraulic head  
33 and for the variance of the transverse component of fluxes, the variance of radial  
34 fluxes being characterized by a sub-linear convergence rate. Our estimated values of  
35 GCI suggest that an accurate computation of mean and (co)variance of head and  
36 fluxes requires a space discretization comprising at least 8 grid elements per  
37 correlation length of  $Y$ , an even finer discretization being required for an accurate  
38 representation of the second-order component of mean heads.

39 **Keywords:** stochastic moment equations; groundwater flow; grid convergence  
40 index; Richardson extrapolation.

41

## 1. Introduction

42 Modeling of groundwater flow in natural aquifer systems is affected by a variety  
43 of sources of uncertainty. In this context, our incomplete knowledge of spatial  
44 distributions of hydrogeological attributes, such as hydraulic conductivity, inevitably  
45 propagates to results of numerical models. A convenient way to deal with such  
46 uncertainty is to conceptualize system attributes as random spatial fields, thus  
47 leading to a stochastic description of groundwater flow and/or transport.

48 In this context, a wide range of stochastic approaches are available including, e.g.,  
49 techniques based on numerical Monte Carlo simulations and moment differential  
50 equations (or moment equations, MEs). Our study is focused on moment  
51 differential equations of fully saturated steady-state confined groundwater flow (see,  
52 e.g., Tartakovsky and Neuman, 1997; Zhang, 2002; Li and Tchelepi, 2003, 2004; Li  
53 et al., 2003; or Winter et al., 2003 for a review on moment differential equations for  
54 groundwater flow in highly heterogeneous porous media). The latter are  
55 deterministic equations rendering the (ensemble) moments of hydraulic head  $h(\mathbf{x})$   
56 and Darcy flux  $\mathbf{q}(\mathbf{x})$  at location vector  $\mathbf{x}$ . Moment equations are obtained from the  
57 stochastic flow and mass conservation equations by integration in probability space.  
58 While the resulting system of MEs is almost never closed, closure approximations  
59 employed to make MEs workable are typically grounded on perturbation expansions  
60 (see also Section 2). Advantages of MEs-based approaches to groundwater flow as  
61 compared to numerical Monte Carlo (MC) simulations include the observation that

62 MEs provide insights on the nature of the solution which can hardly be achieved  
63 through a MC framework. Additionally, MC-based approaches rely on numerical  
64 solutions of the flow equation across a collection of many detailed realizations of  
65 hydraulic conductivity to capture the effects of heterogeneity. In some cases, this can  
66 lead to high computational costs, which can hamper the efficiency of MC-based  
67 analyses.

68 Moment differential equations of groundwater flow have been recently applied to  
69 field settings (Riva et al., 2009; Bianchi Janetti et al., 2010; Panzeri et al., 2015), to  
70 non-Gaussian fields (e.g., Hristopulos, 2006; Riva et al., 2017) and have been  
71 embedded in geostatistical inverse modeling approaches (Hernandez et al. 2003),  
72 stochastic pumping test interpretation (Neuman et al., 2004, 2007), or reactive solute  
73 transport (e.g., Hu et al., 2004). Most recent developments have allowed embedding  
74 stochastic MEs of transient groundwater flow in data assimilation/integration and  
75 parameter estimation approaches, e.g., via ensemble Kalman filter (Li and Tchelepi,  
76 2006; Panzeri et al., 2013, 2015).

77 It can be argued that grids required to accurately represent the spatial distributions  
78 of inputs to MEs can be coarser than those associated with MC simulations, MEs  
79 being grounded on smoothed, ensemble mean parameters. Nevertheless, an  
80 assessment of the degree of approximation introduced by a given numerical grid  
81 employed to solve MEs is still lacking. In this context, it is noted that the full set of  
82 MEs (i.e., the equations governing the spatial distribution of ensemble mean or

83 variance-covariance) for steady-state groundwater flow are characterized by the  
84 same mathematical format, while being associated with differing forcing terms (see  
85 also Section 2). As such, the nature of such forcing terms can play a main role in  
86 driving numerical grid convergence studies and results.

87 While a number of grid refinement analyses have been conducted on subsurface  
88 flow and transport settings (see, e.g., Slough et al., 1999; Weatherill et al., 2008;  
89 Graf and Degener, 2011), these have mainly been framed in a deterministic  
90 modeling framework. As such, they yield only limited insights about the  
91 dependencies of numerical grid size on the main geostatistical descriptors of aquifer  
92 heterogeneity. Leube et al. (2013) provided guidance about the selection of the  
93 spatial resolution of a numerical grid employed to solve groundwater flow in  
94 randomly heterogeneous reservoirs in a MC context. These authors apportion the  
95 computational complexity of numerical MC simulations according to spatial and  
96 temporal grid resolution, as well as the number of realizations to be considered in  
97 the collection employed to evaluate statistics (or quantiles) of interest. Recently,  
98 Maina et al. (2018) compared several numerical approaches to simulate  
99 breakthrough curves of solute concentrations measured during laboratory  
100 experiments performed on flow cells filled with various configurations of  
101 heterogeneous sands. Their results suggest that spatial discretization is significantly  
102 important to obtain accurate solutions in heterogeneous domains.

103 The two main objectives of our study are the assessment of the order of

104 convergence,  $p$ , and the analysis of the results of systematic grid convergence  
 105 studies for numerical solutions of steady-state groundwater flow MEs. Quantities of  
 106 interest are the (ensemble) mean of hydraulic head,  $h(\mathbf{x})$ , and flux vector,  $\mathbf{q}(\mathbf{x})$ , as  
 107 well as the corresponding spatial covariances. The qualities of the ensuing solutions  
 108 are estimated through the Grid Convergence Index (GCI), which relies on a grid  
 109 refinement error estimator grounded on the generalized Richardson extrapolation  
 110 (Richardson, 1910; Richardson and Gaunt, 1927). As a reference against which  
 111 solution accuracies of MEs are evaluated, we leverage on the analytical expressions  
 112 developed by Riva et al. (2001) for leading statistical moments of  $h(\mathbf{x})$  and  $\mathbf{q}(\mathbf{x})$   
 113 under steady-state convergent flow to a well operating in a bounded, randomly  
 114 heterogeneous reservoir.

115 This study is organized as follows. Section 2 illustrates the MEs we analyze.  
 116 Section 3 presents the details of the convergence study for the MEs. Sections 4 and 5  
 117 illustrate the set of numerical analyses and associated results, respectively. Section 6  
 118 is devoted to our main conclusions.

## 119 **2. Theoretical Background for Moment Equations of steady-state groundwater**

### 120 **flow**

121 Consider steady-state groundwater flow described by:

$$122 \left. \begin{aligned} -\nabla_{\mathbf{x}} \cdot \mathbf{q}(\mathbf{x}) + f(\mathbf{x}) &= 0 \\ \mathbf{q}(\mathbf{x}) &= -K(\mathbf{x})h(\mathbf{x}) \end{aligned} \right\} \quad (1)$$

123 subject to boundary conditions

$$124 h(\mathbf{x}) = H(\mathbf{x}) \quad \mathbf{x} \in \Gamma_D \quad (2)$$

125  $[-\mathbf{q}(\mathbf{x})] \cdot \mathbf{n}(\mathbf{x}) = Q(\mathbf{x}) \quad \mathbf{x} \in \Gamma_N \quad (3)$

126 Here,  $\mathbf{x}$  is the vector of spatial coordinates within domain  $\Omega$ ;  $\nabla_x$  is the spatial  
 127 gradient operator;  $f(\mathbf{x})$  is a (generally random) forcing term;  $K(\mathbf{x})$  is hydraulic  
 128 conductivity;  $\mathbf{n}(\mathbf{x})$  is the unit vector normal to Neumann boundary  $\Gamma_N$ ;  $Q(\mathbf{x})$  is  
 129 the (typically random) flux along  $\Gamma_N$ ;  $H(\mathbf{x})$  is a random head along Dirichlet  
 130 boundary  $\Gamma_D$ .

131 For simplicity, we consider  $f(\mathbf{x})$ ,  $H(\mathbf{x})$  and  $Q(\mathbf{x})$  as deterministic in our  
 132 analyses. Hydraulic conductivity  $K(\mathbf{x})$  is taken to be a random spatial field, its  
 133 fluctuation about the (ensemble) mean  $\langle K(\mathbf{x}) \rangle$  being expressed as  
 134  $K'(\mathbf{x}) = K(\mathbf{x}) - \langle K(\mathbf{x}) \rangle$ . We introduce  $h'(\mathbf{x}) = h(\mathbf{x}) - \langle h(\mathbf{x}) \rangle$  as the random  
 135 fluctuation of hydraulic head,  $h(\mathbf{x})$ , about (ensemble) mean,  $\langle h(\mathbf{x}) \rangle$ . One can then  
 136 recast (1)-(3) as

137  $\nabla_x \cdot [\langle K(\mathbf{x}) \rangle \nabla_x \langle h(\mathbf{x}) \rangle + \langle K(\mathbf{x}) \rangle \nabla_x h'(\mathbf{x}) + K'(\mathbf{x}) \nabla_x \langle h(\mathbf{x}) \rangle + K'(\mathbf{x}) \nabla_x h'(\mathbf{x})] + f(\mathbf{x}) = 0 \quad (4)$

138 subject to boundary conditions

139  $\langle h(\mathbf{x}) \rangle + h'(\mathbf{x}) = H(\mathbf{x}) \quad \mathbf{x} \in \Gamma_D \quad (5)$

140  $\left[ \langle K(\mathbf{x}) \rangle \nabla_x \langle h(\mathbf{x}) \rangle + \langle K(\mathbf{x}) \rangle \nabla_x h'(\mathbf{x}) \right. \\ \left. + K'(\mathbf{x}) \nabla_x \langle h(\mathbf{x}) \rangle + K'(\mathbf{x}) \nabla_x h'(\mathbf{x}) \right] \cdot \mathbf{n}(\mathbf{x}) = Q(\mathbf{x}) \quad \mathbf{x} \in \Gamma_N \quad (6)$

141 Taking ensemble averages of (4)-(6) yields exact equations satisfied by  $\langle h(\mathbf{x}) \rangle$   
 142 (see, e.g., Guadagnini and Neuman, 1999a; Zhang, 2002). Following these authors,  
 143 it is then possible to obtain exact equations satisfied by the covariance of heads  
 144 and/or the cross-covariance between conductivity and heads, as well as expressions  
 145 for the covariance tensor of flux. A strategy to solve these (deterministic) MEs relies

146 on expanding all moments appearing in them in terms of a small parameter  $\sigma_Y$ ,  
147 representing the standard deviation of the natural logarithm of hydraulic  
148 conductivity, i.e.,  $Y(\mathbf{x}) = \ln K(\mathbf{x})$ . We then obtain a set of recursive approximations  
149 of the otherwise exact MEs which we can solve up to a given order (expressed in  
150 terms of powers of  $\sigma_Y$ ). Each equation rendering a given order of approximation of  
151 a moment of interest is then local in space. In the following sections, we summarize  
152 the main formulations associated with the equations satisfied by low order  
153 approximations of ensemble mean and covariance of hydraulic heads and fluxes.  
154 Further details about the complete derivation of such equations are included, e.g., in  
155 Guadagnini and Neuman (1999a) and Zhang (2002).

## 156 **2.1 Zero-order mean head and flux**

157 The equation for the zero-order mean head  $\langle h^{(0)}(\mathbf{x}) \rangle$  is expressed as:

$$158 \quad \nabla_x \cdot [K_G(\mathbf{x}) \nabla_x \langle h^{(0)}(\mathbf{x}) \rangle] + f(\mathbf{x}) = 0 \quad (7)$$

159 subject to boundary conditions:

$$160 \quad \langle h^{(0)}(\mathbf{x}) \rangle = H(\mathbf{x}) \quad \mathbf{x} \in \Gamma_D \quad (8)$$

$$161 \quad [-\langle \mathbf{q}^{(0)}(\mathbf{x}) \rangle] \cdot \mathbf{n}(\mathbf{x}) = Q(\mathbf{x}) \quad \mathbf{x} \in \Gamma_N \quad (9)$$

162 Here and in the following, superscript ( $i$ ) identifies terms that are strictly of order  $i$   
163 (in terms of powers of  $\sigma_Y$ ),  $K_G(\mathbf{x}) = e^{\langle Y(\mathbf{x}) \rangle}$  is the geometric mean of  $K(\mathbf{x})$ , and  
164  $\langle \mathbf{q}^{(0)}(\mathbf{x}) \rangle = -K_G(\mathbf{x}) \nabla_x \langle h^{(0)}(\mathbf{x}) \rangle$  is the zero-order mean flux vector.

## 165 **2.2 Second-order cross covariance between head and conductivity**

166 Multiplying Eqs. (4-6) by  $K'(\mathbf{y})$ , taking expectation and expanding the resulting



167 equations yield the following equations for the second-order approximation of the

168 cross covariance of head and conductivity,  $u^{(2)}(\mathbf{y}, \mathbf{x}) = \langle K'(\mathbf{y})h'(\mathbf{x}) \rangle^{(2)}$ :

$$169 \quad \nabla_x \cdot \left[ K_G(\mathbf{x}) \nabla_x u^{(2)}(\mathbf{y}, \mathbf{x}) - K_G(\mathbf{y}) C_Y(\mathbf{x}, \mathbf{y}) \langle \mathbf{q}^{(0)}(\mathbf{x}) \rangle \right] = 0 \quad (10)$$

170 subject to boundary conditions:

$$171 \quad u^{(2)}(\mathbf{y}, \mathbf{x}) = 0 \quad \mathbf{x} \in \Gamma_D \quad (11)$$

$$172 \quad \left[ K_G(\mathbf{x}) \nabla_x u^{(2)}(\mathbf{y}, \mathbf{x}) - K_G(\mathbf{y}) C_Y(\mathbf{x}, \mathbf{y}) \langle \mathbf{q}^{(0)}(\mathbf{x}) \rangle \right] \cdot \mathbf{n}(\mathbf{x}) = 0 \quad \mathbf{x} \in \Gamma_N \quad (12)$$

173 Here,  $C_Y(\mathbf{x}, \mathbf{y}) = \langle Y'(\mathbf{x})Y'(\mathbf{y}) \rangle$  is the covariance of  $Y$  between locations  $\mathbf{x}$  and  $\mathbf{y}$

174 in the domain.

### 175 **2.3 Second-order head covariance**

176 Multiplying Eqs. (4-6) by head fluctuation  $h'(\mathbf{y})$ , taking expectation and

177 expanding the resulting equations yield the following equations for the second-order

178 head covariance,  $C_h^{(2)}(\mathbf{y}, \mathbf{x}) = \langle h'(\mathbf{y})h'(\mathbf{x}) \rangle^{(2)}$ :

$$179 \quad \nabla_x \cdot \left[ K_G(\mathbf{x}) \nabla_x C_h^{(2)}(\mathbf{y}, \mathbf{x}) + u^{(2)}(\mathbf{x}, \mathbf{y}) \nabla_x \langle h^{(0)}(\mathbf{x}) \rangle \right] = 0 \quad (13)$$

180 subject to boundary conditions:

$$181 \quad C_h^{(2)}(\mathbf{y}, \mathbf{x}) = 0 \quad \mathbf{x} \in \Gamma_D \quad (14)$$

$$182 \quad \left[ K_G(\mathbf{x}) \nabla_x C_h^{(2)}(\mathbf{y}, \mathbf{x}) + u^{(2)}(\mathbf{x}, \mathbf{y}) \nabla_x \langle h^{(0)}(\mathbf{x}) \rangle \right] \cdot \mathbf{n}(\mathbf{x}) = 0 \quad \mathbf{x} \in \Gamma_N \quad (15)$$

183 where  $u^{(2)}(\mathbf{x}, \mathbf{y}) = \langle K'(\mathbf{x})h'(\mathbf{y}) \rangle^{(2)}$  is given by Eqs. (10)-(12).

### 184 **2.4 Second-order mean head and flux**

185 The equation satisfied by the second-order mean head  $\langle h^{(2)}(\mathbf{x}) \rangle$  is:

$$186 \quad \nabla_x \cdot \left[ K_G(\mathbf{x}) \left[ \nabla_x \langle h^{(2)}(\mathbf{x}) \rangle + \frac{\sigma_Y^2}{2} \nabla_x \langle h^{(0)}(\mathbf{x}) \rangle \right] - \mathbf{r}^{(2)}(\mathbf{x}) \right] = 0 \quad (16)$$

187 subject to boundary conditions:

188  $\langle h^{(2)}(\mathbf{x}) \rangle = 0 \quad \mathbf{x} \in \Gamma_D \quad (17)$

189  $[-\langle \mathbf{q}^{(2)}(\mathbf{x}) \rangle] \cdot \mathbf{n}(\mathbf{x}) = 0 \quad \mathbf{x} \in \Gamma_N \quad (18)$

190 Here,  $\langle \mathbf{q}^{(2)}(\mathbf{x}) \rangle = -K_G(\mathbf{x}) \left( \nabla_x \langle h^{(2)}(\mathbf{x}) \rangle + \frac{\sigma_y^2}{2} \nabla_x \langle h^{(0)}(\mathbf{x}) \rangle \right) + \mathbf{r}^{(2)}(\mathbf{x})$  and

191  $\mathbf{r}^{(2)}(\mathbf{x}) = -\nabla_x u^{(2)}(\mathbf{x}, \mathbf{x})$  are a second-order mean flux vector and the residual flux,

192 respectively.

193 We evaluate the second-order residual flux by taking the limit for  $\mathbf{y} \rightarrow \mathbf{x}$  of the

194 negative of  $\nabla_x u^{(2)}(\mathbf{y}, \mathbf{x})$ , as:

195  $\mathbf{r}^{(2)}(\mathbf{x}) = \lim_{\mathbf{y} \rightarrow \mathbf{x}} [-\nabla_x u^{(2)}(\mathbf{y}, \mathbf{x})] \quad (19)$

196 where  $u^{(2)}(\mathbf{y}, \mathbf{x})$  is given by Eqs. (10)-(12).

197 We note that Guadagnini and Neuman (1999a, b) relied on a strategy based on a

198 Green's function approach to compute the second-order residual flux, which is

199 expressed as  $\mathbf{r}^{(2)}(\mathbf{x}) = \int_{\Omega} K_G(\mathbf{x}) K_G(\mathbf{y}) \langle Y'(\mathbf{x}) Y'(\mathbf{y}) \rangle \nabla_x \nabla_y^T \langle G^{(0)}(\mathbf{y}, \mathbf{x}) \rangle \nabla_y \langle h^{(0)}(\mathbf{y}) \rangle d\mathbf{y}$ ,

200 subscript T representing transpose, and  $\langle G^{(0)}(\mathbf{y}, \mathbf{x}) \rangle$  being the zero-order mean

201 Green's function associated with the flow problem (see Guadagnini and Neuman,

202 1999a, for details). This approach has then been employed in subsequent studies

203 (e.g., Ye et al., 2004). It is apparent that the main computation cost associated with

204 this scheme stems from the need to solve the equation satisfied by  $\langle G^{(0)}(\mathbf{y}, \mathbf{x}) \rangle$  for

205 a number of times corresponding to the number of computational nodes in domain

206  $\Omega$ , evaluating the corresponding partial derivatives, and then performing integration

207 over  $\Omega$ . Computational times associated with this approach are then exacerbated

208 when considering transient flow (see Ye et al., 2004). All of these aspects constitute

209 a limitation when considering inverse modeling for geostatistical aquifer  
 210 characterization based on Moment Equations. This is the key motivation for which  
 211 we resort here to Eqs. (10)-(12), and (19) to evaluate  $\mathbf{r}^{(2)}(\mathbf{x})$  at a much reduced  
 212 computational effort.

## 213 **2.5 Second-order tensor of flux covariance**

214 The second-order flux covariance tensor  $\mathbf{C}_q^{(2)}(\mathbf{x}, \mathbf{y}) = \langle \mathbf{q}'(\mathbf{x}) \mathbf{q}'^T(\mathbf{y}) \rangle^{(2)}$  satisfies  
 215 the following equation:

$$\begin{aligned}
 \mathbf{C}_q^{(2)}(\mathbf{x}, \mathbf{y}) = & K_G(\mathbf{x}) K_G(\mathbf{y}) [\nabla_x \nabla_y^T C_h^{(2)}(\mathbf{x}, \mathbf{y}) \\
 & + \nabla_x \langle h^{(0)}(\mathbf{x}) \rangle \nabla_y^T \langle h^{(0)}(\mathbf{y}) \rangle C_Y(\mathbf{x}, \mathbf{y}) \\
 & + \nabla_x \langle h^{(0)}(\mathbf{x}) \rangle \nabla_y^T u^{(2)}(\mathbf{x}, \mathbf{y}) \\
 & + \nabla_x u^{(2)}(\mathbf{y}, \mathbf{x}) \nabla_y^T \langle h^{(0)}(\mathbf{y}) \rangle]
 \end{aligned}
 \tag{20}$$

217 Solutions of Eqs. (7)-(15) constitute the inputs to (20).

## 218 **2.6 Numerical approach**

219 Evaluation of the statistical moments introduced above is performed in a  
 220 sequential way. We start by computing the zero-order mean head,  $\langle h^{(0)} \rangle$ , through  
 221 Eqs. (7-9). Note that all other quantities of interest depend on  $\langle h^{(0)} \rangle$ . The  
 222 zero-order mean flux,  $\langle \mathbf{q}^{(0)} \rangle$ , is obtained through Darcy's law using the derivatives  
 223 of the numerical approximation of  $\langle h^{(0)} \rangle$ . Neither  $\langle h^{(0)} \rangle$  nor  $\langle \mathbf{q}^{(0)} \rangle$  depend on  
 224 the covariance of  $Y$ .

225 The second-order cross covariance between head and conductivity,  $u^{(2)}(\mathbf{y}, \mathbf{x})$ , is  
 226 obtained by solving (10-12) and depends on the covariance of  $Y$  and on  $\langle \mathbf{q}^{(0)} \rangle$ .  
 227 Quantities such as  $\langle h^{(2)} \rangle$ ,  $\langle \mathbf{q}^{(2)} \rangle$ , and  $C_h^{(2)}$  depend strongly on  $u^{(2)}$ . The latter

228 must then be computed accurately and grid discretization should be fine enough to  
229 properly describe the contribution of the covariance function of  $Y$  to  $u^{(2)}$ . In other  
230 words, if the distance between two adjacent nodes on the computational grid is  
231 larger than the correlation length of  $Y$ , the covariance function in Eq. (10) between  
232 such nodes will tend to vanish. This would in turn lead to a poor approximation of  
233  $u^{(2)}$ , thus impacting on the quality of the results associated with all quantities that  
234 depend on  $u^{(2)}$ .

235 From a numerical point of view, Eqs. (7), (10), (13), and (16) share the same  
236 format, i.e., all of them can be cast in terms of the divergence of the gradient of a  
237 given moment multiplied by  $K_G$ , under the action of a sink/source term. Thus, their  
238 discretization leads to systems of equations where the coefficients of the unknown  
239 quantities are identical, the right-hand side (i.e., the force term) depending on the  
240 moment to be solved. In this context, one can resort to a direct solver, which allows  
241 for the transformation (factorization) of the matrix containing the coefficients of the  
242 system of equations. This transformation is performed only once and the  
243 transformed matrix enables one to solve the system of equations in a very efficient  
244 way, because only the right-hand side needs to be updated depending on the moment  
245 of interest. The MEs are here solved by linear Galerkin finite elements.

### 246 **3. Grid Convergence for Moment Equations**

247 We take the analytical solutions of moments of steady-state flow to a well of Riva  
248 et al. (2001) as the exact results,  $F_{exact}$ , against which the quality of numerical

249 solutions of the MEs illustrated in Section 2 is assessed. We focus on requirements  
 250 for grid convergence of the equations satisfied by  $\langle h^{(0)}(\mathbf{x}) \rangle$ ,  $u^{(2)}(\mathbf{y}, \mathbf{x})$ ,  $C_h^{(2)}(\mathbf{y}, \mathbf{x})$   
 251 and  $\langle h^{(2)}(\mathbf{x}) \rangle$ . It is remarked that while the equations satisfied by these quantities  
 252 are characterized by the same mathematical format, they are associated with  
 253 differing forcing terms. The latter feature can influence the rate  $p$  of grid  
 254 convergence which we examine in this study.

255 A grid convergence/refinement study is a procedure that enables us to explore the  
 256 effect of a given grid discretization level on the accuracy of the numerical solution  
 257 of a target mathematical model. We estimate the orders  $p$  of grid convergence of the  
 258 solutions of equations illustrated in Section 2 by the two procedures described in the  
 259 following.

### 260 3.1 Rate of Convergence

261 We start by defining the quantity:

$$262 \quad E(\mathcal{G}) = F(\mathcal{G}) - F_{exact} = C\mathcal{G}^p + O(p) \quad (21)$$

263 where  $\mathcal{G}$  is a metric representing grid spacing; and  $E(\mathcal{G})$  is the error between the  
 264 numerical solution  $F(\mathcal{G})$  related to grid spacing  $\mathcal{G}$  and  $F_{exact}$  (i.e., the exact  
 265 solution),  $O(p)$  representing higher order terms. One can then estimate  $C$  and  $p$  in  
 266 (21) from a linear regression on results obtained on multiple grids, according to:

$$267 \quad \ln E(\mathcal{G}) \approx \ln C + p \ln \mathcal{G} \quad (22)$$

268 We follow Vassberg and Jameson (2010) and take  $\mathcal{G} = \sqrt{1/N}$ ,  $N$  being the  
 269 number of nodes (i.e. number of unknowns) of a given computational grid. The

270 regression result typically depends on the number of grids used to perform the  
 271 analysis. As we state in Section 4, our study relies on a total of 15 families of  
 272 unstructured grids. Each family comprises a coarse, an intermediate and a fine grid,  
 273 constructed according a constant/uniform grid refinement ratio. We then obtain a  
 274 total of 3 values of  $\mathcal{G}$  for each grid family. As such, we can perform regression to  
 275 estimate  $C$  and  $p$  on the basis of 45 values of  $E(\mathcal{G})$  for target moment and location  
 276 in the domain. We do so for the set of (statistical) moments of interest (see Section  
 277 4).

### 278 3.2 Grid Convergence Index

279 We note that, in general,  $F_{exact}$  is unknown, this being a key reason underpinning  
 280 grid convergence studies. We consider three grid refinement levels for each of the 15  
 281 grid families mentioned in Section 3.1 (see also Section 4), i.e., a coarse, an  
 282 intermediate, and a fine level (hereafter termed  $\mathcal{G}_c$ ,  $\mathcal{G}_m$ , and  $\mathcal{G}_f$ , respectively) and  
 283 evaluate the corresponding (numerical) solutions  $F(\mathcal{G}_i) = F_i$  ( $i = c, m, \text{ or } f$ ). One  
 284 can then estimate  $p$  from (21) as:

$$285 \quad p \approx \ln \left( \frac{F_c - F_m}{F_m - F_f} \right) / \ln(\omega) \quad (23)$$

286 where  $\omega = \mathcal{G}_c / \mathcal{G}_m = \mathcal{G}_m / \mathcal{G}_f$  is a (constant) grid refinement ratio. High values of  $p$   
 287 correspond to high convergence rates. We can calculate 15 values of  $p$  in our  
 288 analyses, one for each grid family we construct. We can also evaluate the quality of  
 289 the convergence, based on the indicator (Stern et al., 2001):

$$290 \quad \mu = \varepsilon_{m,f} / \varepsilon_{c,m}; \quad \text{with } \varepsilon_{c,m} = F_c - F_m; \text{ and } \varepsilon_{m,f} = F_m - F_f \quad (24)$$

291 where one can distinguish among monotonic ( $0 < \mu < 1$ ) or oscillatory ( $\mu < 0$ )  
292 convergence; and divergence ( $\mu > 1$ ). It is worth noting that values of  $\mu \approx 1$   
293 indicate that  $p$  is close to zero (see (23)) which means that the numerical solution  
294 is not sensitive to the grid size.

295 We then calculate a Grid Convergence Index (GCI) for each grid family. This  
296 index rests on the theory of the generalized Richardson extrapolation and provides a  
297 measure of grid convergence as well as an error band for the grid convergence of the  
298 solution (Roache, 1994) and is defined as

$$299 \quad GCI_{k,s} = S_F \frac{|F_k - F_s|}{|F_s|(\omega^p - 1)} \times 100\% \quad (25)$$

300 Here,  $GCI_{k,s}$  is the grid convergence index corresponding to numerical solutions  
301  $F_k$  and  $F_s$ ; and  $S_F$  is a safety factor, which is typically set to 1.25 when  
302 three-grid levels are employed.

## 303 **4 Numerical analyses for radial flow configuration**

### 304 **4.1 Numerical settings**

305 Consistent with the setting of Riva et al. (2001), we perform our grid  
306 convergence study on a two-dimensional domain formed by a circle of radius  $L$   
307 (Figure 1a) and centered at the origin of a selected coordinate system. Domain  
308 discretization is implemented through an unstructured triangular mesh. Boundary  
309 conditions are of Dirichlet type and are considered as uniform and known (i.e., head  
310 is set to 0). A zero-radius well with a deterministic unit pumping rate is operating at  
311 the domain center. Hydraulic conductivity  $K(\mathbf{x})$  is considered as a (second-order

312 stationary) spatial random field characterized by a Gaussian covariance function  
 313 defined by:

$$314 \quad C_Y(\delta) = \sigma_Y^2 \exp\left[-\frac{\pi \delta^2}{4 \lambda^2}\right] \quad (26)$$

315 where  $\delta$  separation distance (lag) between two locations,  $\sigma_Y^2$  is the variance of  
 316  $Y(\mathbf{x})$  and  $\lambda$  the (isotropic) correlation scale.

317 The accuracies of the numerical simulations are analyzed by comparison against  
 318 the analytical solutions provided by Riva et al. (2001). These authors derived  
 319 analytical solutions for second-order (statistical) moments of head and flux in terms  
 320 of four-dimensional integrals. These are evaluated at given locations in the domain  
 321 by Gaussian quadrature relying on 500 Gauss points. The moments of interest, i.e.,  
 322  $\langle h^{(0)} \rangle$ ,  $\langle h^{(2)} \rangle$ ,  $\sigma_h^{2(2)}$  and the components of (second-order) flux variance tensor,  
 323 i.e.,  $\sigma_{qr}^{2(2)}$ ,  $\sigma_{q\theta}^{2(2)}$ , and  $\sigma_{qr\theta}^{2(2)} = \sigma_{q\theta r}^{2(2)}$ , are evaluated at  $N_r = 100$  (dimensionless)  
 324 values of  $\xi = r/L$  ( $r$  being distance from the well). These moments do not depend  
 325 on the angular coordinate due to symmetry. The selected 100 values of  $\xi$  are  
 326 distributed according to a geometric progression, i.e., following an arithmetic  
 327 progression of the log-transformed values of  $\xi$ , with  $\ln(0.01) \leq \xi \leq \ln(0.99)$  and  
 328 considering a constant increment of  $\frac{1}{99} \times \ln 99$ .

329 Since we rely on an unstructured mesh, we cannot take advantage of symmetry.  
 330 The numerical solutions are computed at the above indicated  $N_r$  locations and at a  
 331 set of  $N_\theta = 100$  angular coordinates (ranging according to  $0 \leq \theta \leq 99\pi/50$ , with  
 332 a regular increment of  $\pi/50$ ) for each radial distance. The ensuing  $N_r \times N_\theta$



333 reference locations are depicted in Figure 1a, the spatial arrangement of  $\xi$  values  
334 being depicted in Figure 1b for a given  $\theta$ .

335 The second-order head covariance  $C_h^{(2)}$  between locations  $(\xi, \theta)$  and  $(\xi', \theta')$  is  
336 symmetric with respect to either  $(\xi - \xi')$  (when  $\theta - \theta' = 0$ ) or  $(\theta - \theta')$  (when  
337  $\xi - \xi' = 0$ ). We consider three given  $\xi'$  values (i.e.,  $\xi' = 0.2, 0.5,$  and  $0.8$ ) and  
338 define two sets of reference locations at which we compute head covariances. The  
339 first set corresponds to three locations having the same angular coordinate and  
340 differing radial coordinates. A second set is formed by three locations with the same  
341 radial coordinate and differing  $\theta$ . In the following, we denote by  $C_h^{(2)}(\xi, \xi_1)$ ,  
342  $C_h^{(2)}(\xi, \xi_2)$  and  $C_h^{(2)}(\xi, \xi_3)$  the solutions of the first set of reference points and by  
343  $C_h^{(2)}(\theta, \xi_1)$ ,  $C_h^{(2)}(\theta, \xi_2)$  and  $C_h^{(2)}(\theta, \xi_3)$  the corresponding solutions associated  
344 with the second set of reference points.

345 The analytical solution for a given distance  $\xi$  is compared to the 100 numerical  
346 solutions obtained at the same distance to the well and corresponding to differing  
347 values of  $\theta$ . Numerical solutions are first calculated at the nodes of the triangular  
348 mesh and then projected (through linear interpolation) onto the closest reference  
349 locations where analytical solutions are evaluated.

350 Solutions for means and variances are stored in a  $N_r \times N_\theta$  matrix  $\mathbf{S}$ , whose  
351 entry  $S_{ij}$  is the numerical solution at radial coordinate  $\xi_i$  and angular coordinate  
352  $\theta_j$ . The size of the matrix associated with corresponding solutions for head  
353 covariances is  $N_r \times N_r$  or  $N_\theta \times N_\theta$  for the two sets of reference points above

354 illustrated, respectively. Entry  $S_{ij}$  of  $\mathbf{S}$  is then the numerical solution of head  
 355 covariance at radial ( $\xi_i$  and  $\xi_j$ ) or angular ( $\theta_i$  and  $\theta_j$ ) coordinates, for the first  
 356 and second set of reference points, respectively.

357 Numerical errors are estimated through the root mean square error for a given  $\xi_i$ ,  
 358 i.e.,

$$359 \quad E_r^i = \sqrt{\frac{1}{N_\theta} \sum_{j=1}^{N_\theta} (S_{ij} - S_i^a)^2} \quad (27)$$

360 and by way of the global quantity

$$361 \quad E_r = \frac{1}{N_r} \sum_{i=1}^{N_r} E_r^i \quad (28)$$

362  $S_{ij}$  and  $S_i^a$  being the numerical and the analytical solutions, respectively.

## 363 **4.2 Domain discretization and test cases**

364 We conduct our grid convergence study by relying on 15 grid families. The 15  
 365 initial triangular meshes, each associated with a given element size (expressed as  $\zeta =$   
 366  $\lambda / \Delta x$  in Table 1,  $\Delta x$  being the grid size) and termed as coarse meshes, are generated  
 367 with the public domain mesh generator Gmsh (Geuzaine and Remacle, 2009). These  
 368 initial meshes are then refined by dividing each triangle into 4 regular sub-triangles  
 369 to obtain the medium meshes (Table 1). The latter are further refined (using the same  
 370 procedure) to obtain the fine meshes. MEs are then solved on the collection of 45  
 371 different unstructured meshes listed in Table 1. Numerical simulations are hereafter  
 372 termed as  $TC_{i,j}$  (subscripts  $i = 1, 2, \dots, 15$ , and  $j = c, m, \text{ and } f$  representing the  
 373 grid family and the level of refinement, respectively). Note that the initial nodes

374 employed during the generation of the coarse mesh in the  $i^{th}$  family are then shared  
375 by the corresponding medium and fine meshes. Grid refinement also includes  
376 additional nodes, specifically employed to describe the domain boundary and  
377 generated as shown in Figure 2.

378 Numerical solutions of the various (statistical) moments of interest are computed  
379 for a combination of values of  $K_G$  and  $\sigma_Y^2$ , and for  $\kappa = L / \lambda = 1$ , and 3.

## 380 **5. Results and Discussion**

### 381 *5.1 Qualitative comparisons against analytical solutions*

382 Figure 3 juxtaposes the numerical and analytical solutions for the zero- ( $\langle h^{(0)} \rangle$ )  
383 and second- ( $\langle h^{(2)} \rangle$ ) order mean heads, as well as second-order head variance ( $\sigma_h^{2(2)}$ )  
384 for  $TC_{1,c}$  and  $TC_{15,f}$ , respectively associated with the coarsest and finest grids  
385 considered. Corresponding comparisons for the components of second-order flux  
386 variance tensors are depicted in Figure 4. Figures 5 and 6 depict the results obtained  
387 for the two sets of head covariances corresponding to the reference points indicated  
388 in Section 4.1. As expected, numerical errors for the coarse mesh are visibly  
389 significant at locations characterized by marked spatial gradients of the solution (i.e.,  
390 close to the well), the quality of the numerical results significantly increasing with  
391 the level of discretization. Values of the cross component  $\sigma_{qr\theta}^{2(2)}$  are very small and  
392 fluctuating around their analytical counterpart, which is equal to zero (Riva et al.,  
393 2001). It has to be noticed that errors are also associated with the required (linear)  
394 interpolations of the numerical solutions. This is especially critical close to the well

395 where heads tend to vary in a way which is akin to a logarithmic trend. The Dirichlet  
396 boundary contributes to stabilize the numerical solution far from the well,  
397 independent of the discretization. The seemingly periodic fluctuations appearing for  
398 the head covariance associated with  $TC_{1,c}$  (Fig. 6) are likely due to the combined  
399 effects of the interpolation and of the spatial structure of the grid.

## 400 *5.2 Grid convergence*

401 Figure 7 depicts  $\ln E_r$  (28) versus the total number of nodes associated with each  
402 of the numerical grids employed, as rendered by  $\ln(\mathcal{G}) = -0.5 \ln(N)$ . Straight  
403 (solid or dashed) lines are the results of (least square) linear regressions on  
404 numerical results. According to Eq. (21), the slopes of these regression lines  
405 correspond to estimates of the convergence orders ( $p$ ) of the numerical solutions.  
406 The values of  $p$  and of the determination coefficients ( $R^2$ ) of the regressions are  
407 listed in Table 2.

408 Results included in Figure 7b and Table 2 show that numerical solutions for  
409  $C_h^{(2)}(\xi, \xi'_1)$ ,  $C_h^{(2)}(\xi, \xi'_2)$  and  $C_h^{(2)}(\xi, \xi'_3)$  are associated with virtually the same  
410 value of  $p$ , a similar observation holding also for the second set of head covariance  
411 solutions. With reference to the latter, we note that their associated convergence  
412 orders are higher than those we find for any of the (statistical) moments considered.  
413 This result is partially attributed to the observation that numerical solutions for  
414  $C_h^{(2)}(\theta, \xi'_1)$ ,  $C_h^{(2)}(\theta, \xi'_2)$  and  $C_h^{(2)}(\theta, \xi'_3)$  are evaluated at positions apart from the  
415 pumping well (see the red plus symbols in Figure 1) and, as such, do not include the

416 zone close to the pumping location where errors are highest. While the rate of  
 417 convergence is supra-linear for the mean and (co)variance of hydraulic head and for  
 418 the variance of the transverse component of fluxes, it is sub-linear for the variance  
 419 of the radial component of fluxes.

420 Quantification of grid convergence order across the whole domain in the absence  
 421 of a reference analytical solution (as is the case in a variety of flow scenarios in  
 422 natural heterogeneous aquifers) can be assessed through Eq. (23) at nodes where the  
 423 numerical solutions are characterized by monotonic convergence conditions (i.e.,  $0$   
 424  $< \mu < 1$ ; see Eq. (24)). In our study, we start by analyzing:

$$425 \quad \alpha_i = N_i^{*mc} / N_i^* \times 100\% \quad \text{with } i = 1, 2, \dots, 15 \quad (29)$$

426 Here, subscript  $i$  denotes the grid family;  $\alpha_i$  is the percentage of grid nodes where  
 427 monotonic convergence is attained for a given statistical moment of interest;  $N_i^{*mc}$   
 428 and  $N_i^*$  are the number of nodes associated with monotonic convergence condition  
 429 and the initial number of nodes (i.e., the number of nodes in common to the coarse,  
 430 medium and fine meshes), respectively. The dependence of  $\alpha_i$  on the grid family  
 431 for the various moments considered is depicted in Figure 8a. These results indicate  
 432 that values of  $\alpha_i$  for  $\langle h^{(2)} \rangle$  are always close to 100%, while fluctuating around 90%  
 433 for  $\langle h^{(0)} \rangle$ ,  $\sigma_h^{2(2)}$  and  $C_h^{(2)\dagger}$  (the latter quantity is the head covariance solution at  
 434 the reference point corresponding to coordinates  $(\xi, \theta) \equiv (0.5, 0)$ ). Figure 8b  
 435 complements these results by depicting the values of  $\bar{p}$  computed as averages of  
 436 the corresponding values of  $p$  calculated through Eq. (23) at the fraction of nodes

437 depicted in Figure 8a. These results reveal that similar average values of  $p$ , i.e., 1.6  
 438  $\leq \bar{p} \leq 1.9$ , are obtained for  $\langle h^{(0)} \rangle$ ,  $\langle h^{(2)} \rangle$ ,  $\sigma_h^{2(2)}$  and  $C_h^{(2) \dagger}$ . These values are  
 439 consistent with those listed in Table 2.

440 A global appraisal of the grid convergence index  $GCI_{c,m}$  (as calculated  
 441 considering the coarse ( $c$ ) and medium ( $m$ ) mesh) for the whole domain can be  
 442 obtained as the average of the nodal values of (25) computed at the  $N_i^{*mc}$  grid  
 443 nodes. The dependence on the grid family of values of average  $GCI_{c,m}$  (denoted as  
 444  $\overline{GCI}_{c,m}$ ) are depicted in Figure 8c. It is noted that values of  $\overline{GCI}_{c,m}$  decrease with  
 445 increasing  $\zeta = \lambda / \Delta x$  (i.e., with decreasing grid size with respect to the correlation  
 446 scale of  $Y$ ) and converge to zero for all statistical moments. This finding implies that  
 447 numerical convergence is attained, or, in other words, that a further mesh refinement  
 448 does not lead to an improvement of the quality of the numerical results. As expected,  
 449 we note that values of  $\overline{GCI}_{c,m}$  for the second-order components of the statistical  
 450 moments analyzed generally display lower convergence rates as compared to  $\langle h^{(0)} \rangle$ .  
 451 A significantly fine grid (in terms of number of grid nodes per correlation scale) is  
 452 required to obtain accurate results for the second-order mean head, as compared to  
 453  $\langle h^{(0)} \rangle$ . Similar grid convergence behavior is observed for both  $L / \lambda = 1$  and 3 (see  
 454 the inset in Fig. 8c). On the basis of these results and Table 2, we note that grid  
 455 convergence is achieved for  $\lambda / \Delta x \geq 8$  for all statistical quantities except for the  
 456 second-order mean head  $\langle h^{(2)} \rangle$  that attains grid convergence for  $\lambda / \Delta x \geq 14$  (for  
 457 example, when considering  $\langle h^{(2)} \rangle$  one can note that  $\overline{GCI}_{c,m} < 0.5\%$  when  $\lambda / \Delta x$

458 = 16).

### 459 5.3 Dependence of numerical errors on the mean and variance of log-conductivities

460 Here, we investigate the dependence on  $\langle Y \rangle$  and  $\sigma_Y^2$  of the errors associated  
461 with the numerical solutions of the MEs. We do so by considering two settings,  
462 respectively corresponding to (i)  $\langle Y \rangle = -2.3, -0.7, 1.6, \text{ and } 2.3$  (corresponding to  
463  $K_G = 0.1, 0.5, 5 \text{ and } 10$ , in arbitrary consistent units) with  $\sigma_Y^2 = 1.0$ ; and (ii)  $\sigma_Y^2$   
464  $= 2, 4, 6 \text{ and } 8$  with  $\langle Y \rangle = 0.0$  (i.e.,  $K_G = 1.0$ ). We keep  $\kappa = L / \lambda = 1$  in both  
465 settings.

466 Figures 9 and 10 depict the dependence of  $E_r$  (28) on  $\langle Y \rangle$  and  $\mathcal{G}$  for the  
467 statistical moments considered. The error is significant for coarse meshes and low  
468 values of  $\langle Y \rangle$  for all moments of head considered. Because boundary conditions  
469 and well pumping rate are (deterministically) prescribed, low values of  $\langle Y \rangle$  give  
470 rise to marked head gradients and the linear interpolation employed tends to be  
471 ineffective. Errors associated with second-order flux variances appear to be  
472 insensitive to  $\langle Y \rangle$ . The pattern of errors associated with head covariances is similar  
473 to the one observed for the mean and variance (compare Figures 9 and 10), the  
474 errors decreasing with the distance from the well.

475 Figures 11 and 12 depict the dependence of  $E_r$  (28) on  $\sigma_Y^2$  and  $\mathcal{G}$  for the  
476 statistical moments considered, with the exception of  $\langle h^{(0)} \rangle$ , which is independent  
477 of  $\sigma_Y^2$  (see Eq. (7)). One can see that  $E_r$  generally increases with  $\sigma_Y^2$  and  $\mathcal{G}$ .  
478 The impact of  $\sigma_Y^2$  is consistent with the formats of the moment equations (see Eqs.

479 (10), (13), (16) and (20)) where  $\sigma_Y^2$  appears as a multiplicative factor, thus  
480 potentially amplifying computational errors. For example, the head gradient in Eq.  
481 (10) is multiplied by  $\sigma_Y^2$ , thus amplifying (for  $\sigma_Y^2 > 1$ ) the error due to the head  
482 gradient evaluation.

## 483 **6. Conclusions**

484 Values of grid convergence orders,  $p$ , of numerical solutions of moment  
485 equations (MEs) of steady-state groundwater flow are quantified. As test case, we  
486 consider convergent flow to a well taking place in a bounded randomly  
487 heterogeneous two-dimensional system and ground our results on comparisons  
488 between numerical solutions of MEs associated with multiple families of grids and  
489 the analytical solutions presented by Riva et al. (2001).

490 Our study leads to the following major conclusions.

- 491 1. The rate of convergence is (a) supra-linear for the mean and (co)variance of  
492 hydraulic head and for the variance of the transverse component of fluxes,  
493 and (b) sub-linear for the variance of the radial component of fluxes.  
494 Approximated values of average rate of convergence obtained by Eq. (23),  
495 relying on the use of numerical solutions of MEs associated with  
496 increasingly refined grids are consistent with their counterparts based on Eq.  
497 (22) and obtained as a linear regression on the errors between numerical and  
498 (reference) analytical solutions. Our results on grid convergence yield a  
499 pragmatic estimate of the accuracy improvement associated with the



500 evaluation of a given target statistical moment of groundwater flow with  
501 respect to grid refinement. As shown in Table 2, grid convergence rate  
502 depends on the given statistical moment, being a critical element in the  
503 evaluation of the variance of the radial component of flux while denoting the  
504 fastest achievement of a desired accuracy level for hydraulic head  
505 covariances. These findings can assist modelers to optimally refine numerical  
506 grids to achieve the highest accuracy associated with the desired prediction  
507 goal depending on the available computational resources.

508 2. The grid convergence index  $GCI_{c,m}$  (see Eq. (25)) associated with all of the  
509 statistical moments considered is shown to converge to zero with increased  
510 grid refinement. Our results suggest that employing a grid spacing  
511  $\Delta x \leq \lambda/8$  yields accurate approximations of all moments considered, an  
512 enhanced grid refinement (i.e.,  $\Delta x/\lambda \leq 1/14$ ) being required to attain grid  
513 convergence only for the second-order mean head.

514 3. Variations of log conductivity mean,  $K_G$ , and variance,  $\sigma_Y^2$ , show no  
515 appreciable impact on the percentage of nodes where uniform convergence is  
516 attained, rate of convergence, or the value of  $GCI_{c,m}$ . In addition, decreasing  
517  $K_G$  can yield increased solution errors for all computed statistical moments,  
518 with the exception of the components of second-order flux variance.  
519 Increasing  $\sigma_Y^2$  can lead to enhanced solution errors for all of the  
520 second-order statistical moments considered.

521 As noted above, our findings are associated with the particularly challenging  
522 scenario of flow driven by a pumping well, where grid refinement requirements are  
523 driven by the feedback between the geostatistical parameters of the randomly  
524 heterogeneous  $Y$  field and the degree of non-uniformity of the flow field. These  
525 results are associated with a strongly non-uniform flow condition and domain sizes  
526 (relative to the conductivity correlation length) which enable exploring the region of  
527 the domain where statistical moments of hydraulic head and fluxes are mostly  
528 affected by the action of the pumping well (see the analytical solution of Riva et al.,  
529 2001). In this context, our findings can be considered as a basis upon which one can  
530 build future studies to ascertain the effect of conditioning (e.g., on available  
531 conductivity information) on the requirements associated with numerical grids  
532 employed for the solution of groundwater flow MEs under general (non-uniform)  
533 conditions.

#### 534 **Acknowledgments**

535 This work was supported by National Nature Science Foundation of China (Grant  
536 No. J216065). Part of the work was developed while Prof. A. Guadagnini was at the  
537 University of Strasbourg with funding from Région Grand-Est and  
538 Strasbourg-Eurométropole through the ‘Chair Gutenberg’.

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## Tables

**Table 1.** Main characteristics of the 15 families of grids employed in the grid convergence study (here,  $\zeta = \lambda / \Delta x$ ,  $\lambda$  and  $\Delta x$  respectively being the correlation scale of the log-conductivity field (see Eq. (26)) and the grid size;  $N$  is the total number of nodes associated with a given grid).

Grid family	Coarse grid set		Medium grid set		Fine grid set	
	$\zeta$	$N$	$\zeta$	$N$	$\zeta$	$N$
1	4	85	8	137	16	1345
2	6	137	12	689	24	2375
3	8	297	16	1185	32	4737
4	10	449	20	1793	40	7169
5	12	645	24	2577	48	10305
6	14	849	28	3393	56	13569
7	16	1153	32	4609	64	18433
8	18	1389	36	5553	72	22209
9	20	1749	40	6993	80	27969
10	22	2085	44	8337	88	33345
11	24	2469	48	9873	96	39489
12	26	2885	52	11537	104	46145
13	28	3273	56	13089	112	52353
14	30	3881	60	15521	120	62081
15	32	4437	64	17745	128	70977

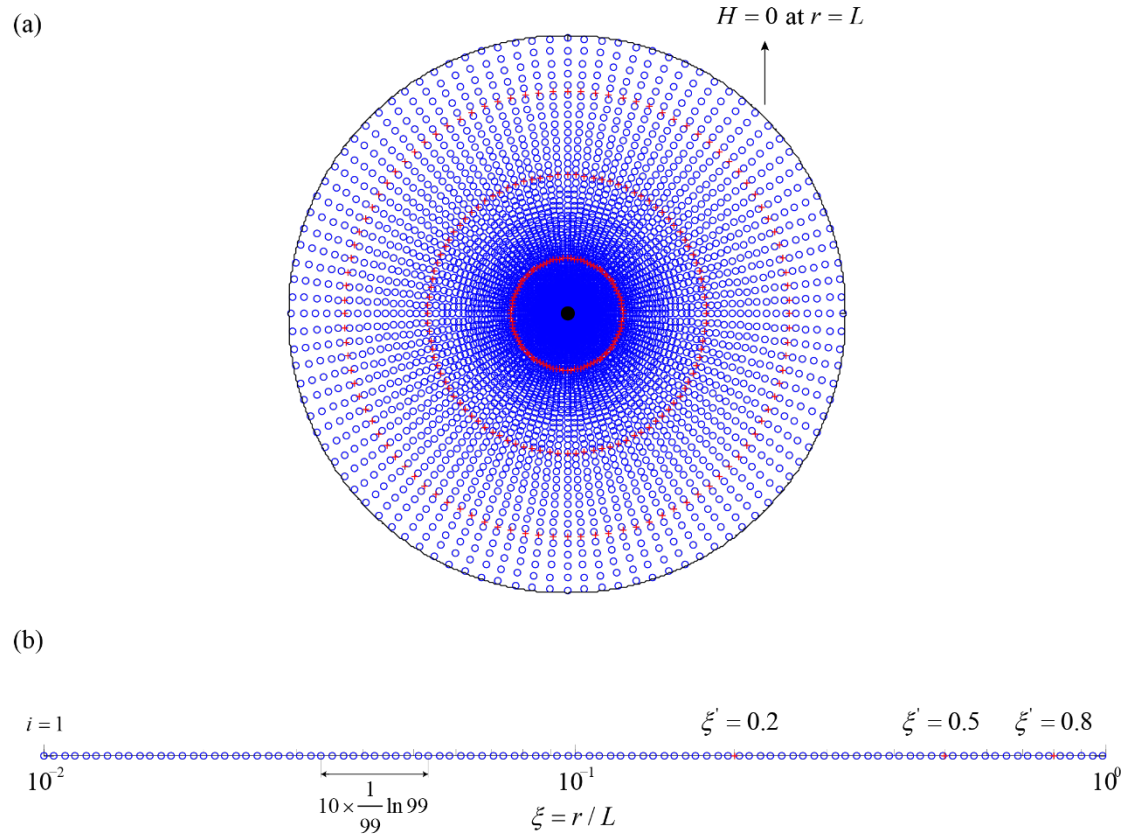


**Table 2.** Estimates of the convergence order ( $p$ ) calculated through Eq. (21) on the basis of Fig. 7. Values of the determination coefficients ( $R^2$ )

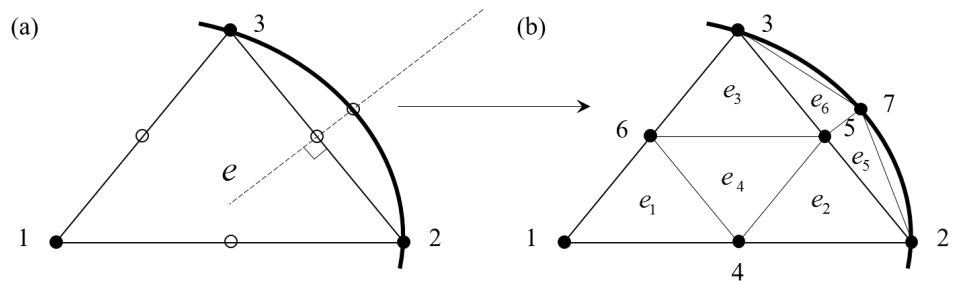
of the corresponding regressions are also listed.

Moments	$\langle h^{(0)} \rangle$	$\langle h^{(2)} \rangle$	$\sigma_h^{2(2)}$	$\sigma_{qrr}^{2(2)}$	$\sigma_{q\theta\theta}^{2(2)}$	$C_h^{(2)}(\xi, \xi_1')$	$C_h^{(2)}(\xi, \xi_2')$	$C_h^{(2)}(\xi, \xi_3')$	$C_h^{(2)}(\theta, \xi_1')$	$C_h^{(2)}(\theta, \xi_2')$	$C_h^{(2)}(\theta, \xi_3')$
$p$	1.21	1.23	1.07	0.49	1.13	1.08	1.04	1.03	2.23	2.18	2.00
$R^2$	0.93	0.93	0.85	0.89	0.91	0.82	0.81	0.81	0.96	0.98	0.98

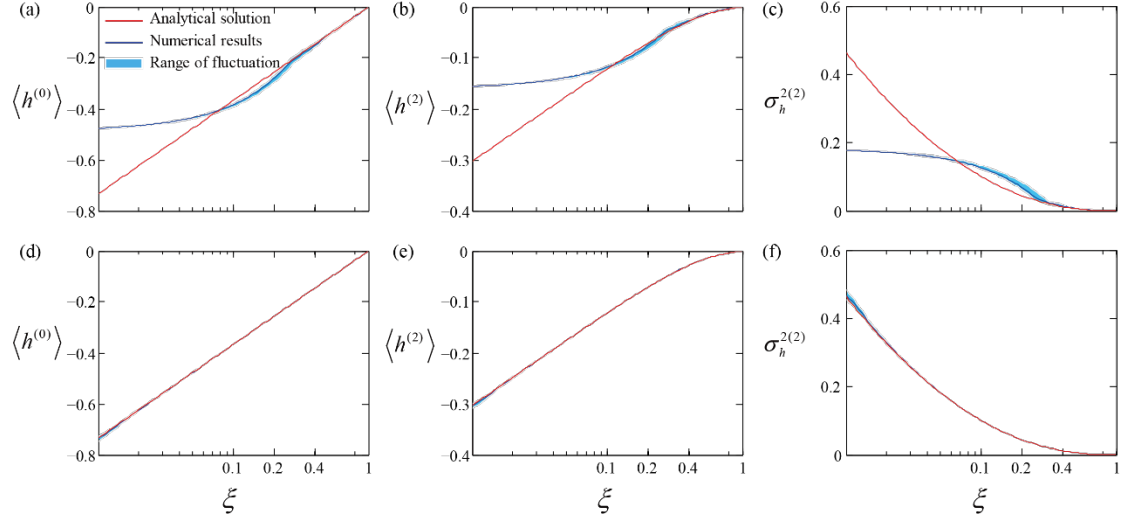
## Figures



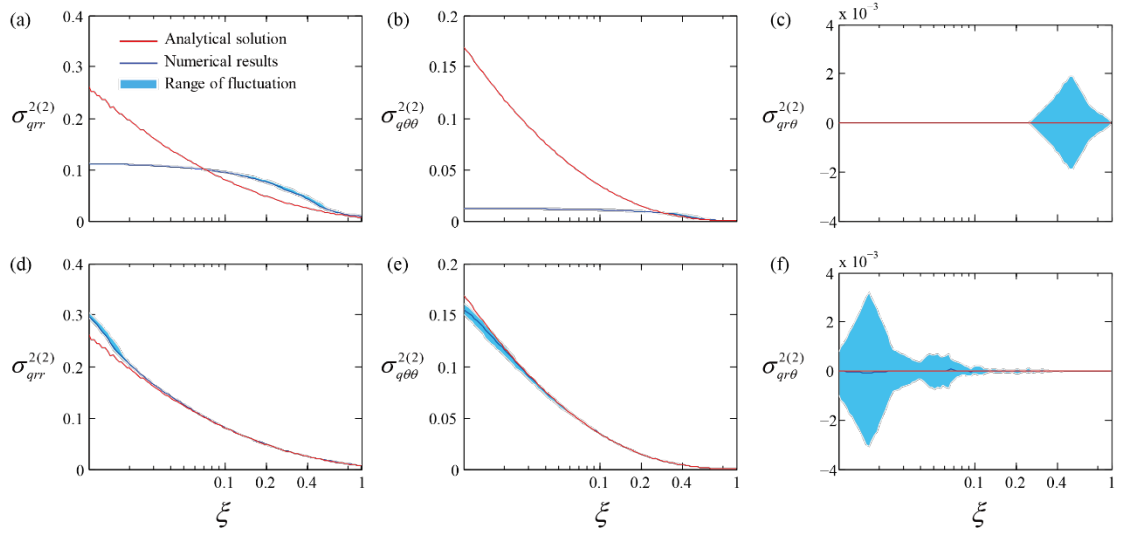
**Figure 1.** Flow domain and (a) spatial distribution of the reference points ( $\circ$ ,  $+$ ), and (b) detailed locations of the 100 reference points ( $\circ$ ) in log scale along a generic radius for the comparisons between analytical and numerical solutions of the MEs. The pumping well ( $\bullet$ ) is located at the domain center.



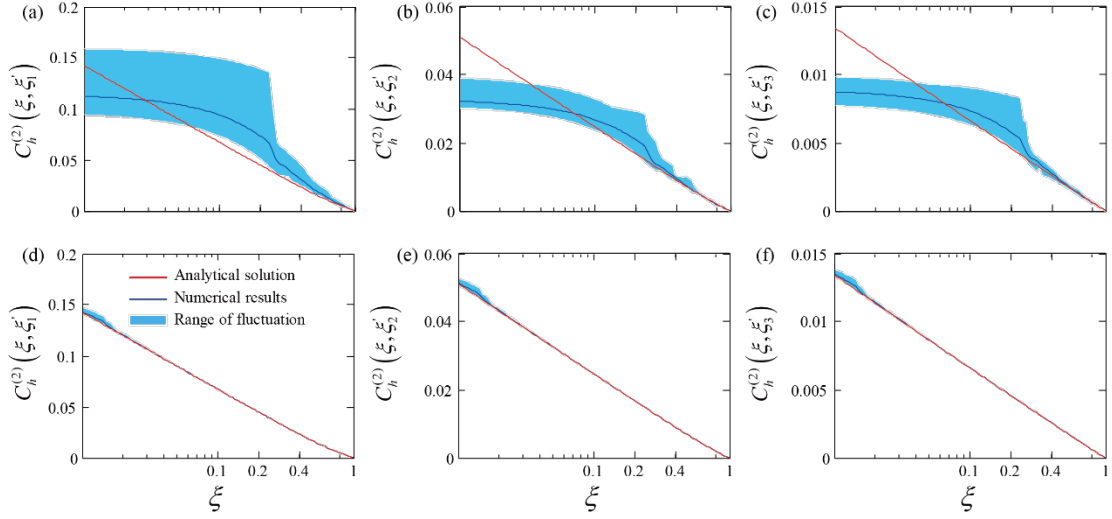
**Figure 2.** Details of the grid refinement at the domain boundary: (a) element  $e$  is divided into (b) 4 sub-elements ( $e_l; l = 1, 2, 3, 4$ ) and two additional elements are generated, i.e.,  $e_5$  and  $e_6$ ). The additional node (denoted as 7) is located on the domain boundary at equal distance from nodes 2 and 3.



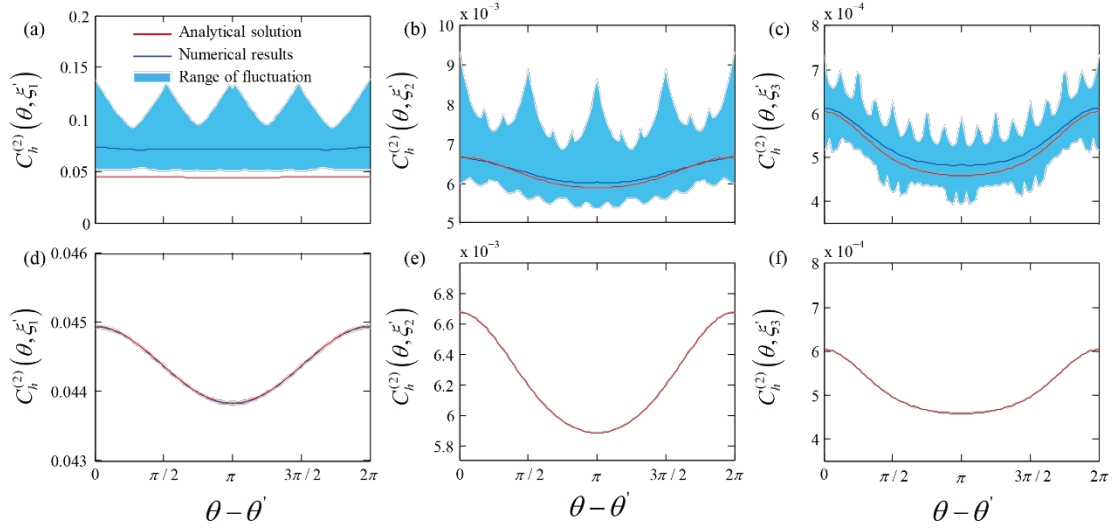
**Figure 3.** Numerical and analytical solutions for the zero- ( $\langle h^{(0)} \rangle$ ) and second- ( $\langle h^{(2)} \rangle$ ) order mean heads, together with second-order head variance ( $\sigma_h^{2(2)}$ ) for (a, b, c)  $TC_{1,c}$  and (d, e, f)  $TC_{15,f}$ . The dark blue solid curve represents the mean of the  $N_\theta$  numerical values calculated for a given radial coordinate, the light blue band describing the range of fluctuation of the solutions; the red solid curve represents the corresponding analytical solution. Results are depicted for  $L / \lambda = 1$ ,  $\sigma_Y^2 = 1$ , and  $K_G = 1$ .



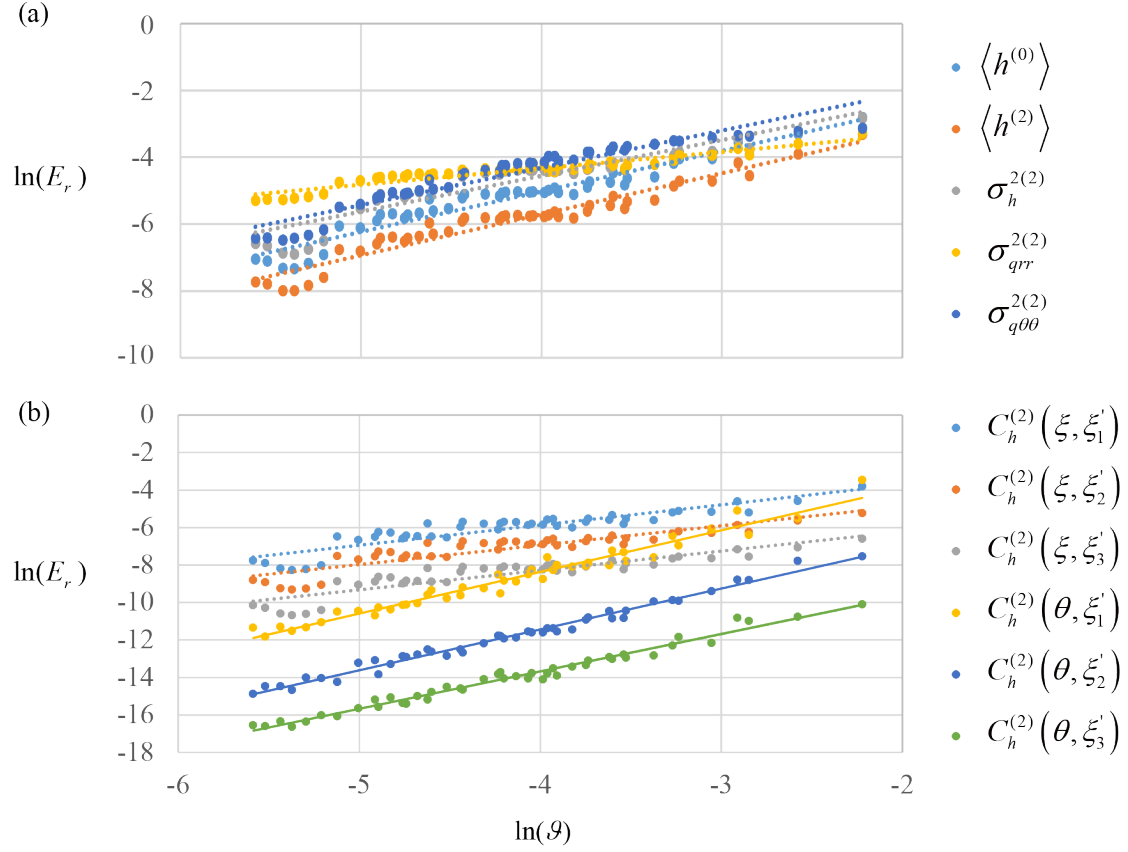
**Figure 4.** Numerical and analytical solutions of (second-order) flux variances  $\sigma_{qrr}^{2(2)}$ ,  $\sigma_{q\theta\theta}^{2(2)}$  and  $\sigma_{qr\theta}^{2(2)}$  for (a, b, c)  $TC_{1,c}$  and (d, e, f)  $TC_{15,f}$ . The dark blue solid curve represents the mean of the  $N_\theta$  numerical values calculated for a given radial coordinate, the light blue band describing the range of fluctuation of the solutions; the red solid curve represents the corresponding analytical solution. Results are depicted for  $L/\lambda = 1$ ,  $\sigma_Y^2 = 1$ , and  $K_G = 1$ .



**Figure 5.** Numerical and analytical solutions of head covariances  $C_h^{(2)}(\xi, \xi_1)$ ,  $C_h^{(2)}(\xi, \xi_2)$ , and  $C_h^{(2)}(\xi, \xi_3)$  for (a, b, c)  $TC_{1,c}$  and (d, e, f)  $TC_{15,f}$ . The dark blue solid curve represents the mean of the  $N_\theta$  numerical values calculated for a given radial coordinate, the light blue band describing the range of fluctuation of the solutions; the red solid curve represents the corresponding analytical solution. Results are depicted for  $L/\lambda = 1$ ,  $\sigma_Y^2 = 1$ , and  $K_G = 1$ .

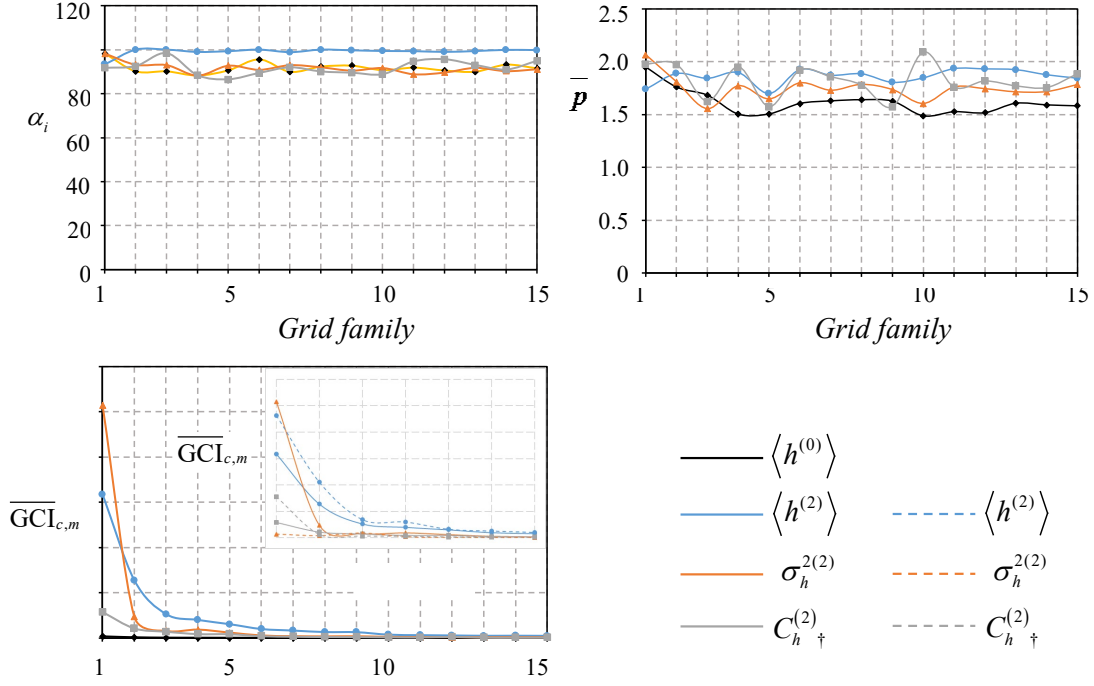


**Figure 6.** Numerical and analytical solutions of the head covariance  $C_h^{(2)}(\theta, \xi_1)$ ,  $C_h^{(2)}(\theta, \xi_2)$  and  $C_h^{(2)}(\theta, \xi_3)$  for (a, b, c)  $TC_{1,c}$  and (d, e, f)  $TC_{15,f}$ . The dark blue solid curve represents the mean of the  $N_\theta$  numerical values calculated for a given radial coordinate, the light blue band describing the range of fluctuation of the solutions; the red solid curve represents the corresponding analytical solution. Results are depicted for  $L/\lambda = 1$ ,  $\sigma_Y^2 = 1$ , and  $K_G = 1$ .

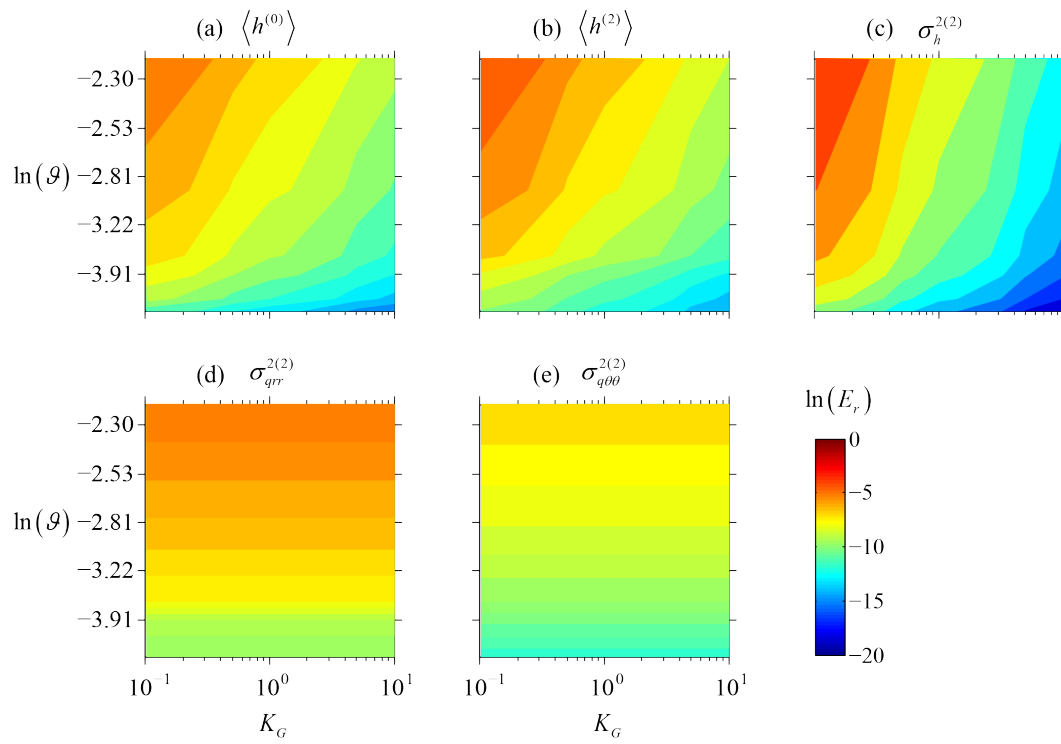


**Figure 7.** Values of  $\ln E_r$  (28) versus  $\ln(\mathcal{G}) = -0.5 \ln(N)$  for (a)  $\langle h^{(0)} \rangle$ ,  $\langle h^{(2)} \rangle$ ,  $\sigma_h^{2(2)}$ ,  $\sigma_{qrr}^{2(2)}$ , and  $\sigma_{q\theta\theta}^{2(2)}$ ; and (b)  $C_h^{(2)}(\xi, \xi'_1)$ ,  $C_h^{(2)}(\xi, \xi'_2)$  and  $C_h^{(2)}(\xi, \xi'_3)$ ,  $C_h^{(2)}(\theta, \xi'_1)$ ,  $C_h^{(2)}(\theta, \xi'_2)$  and  $C_h^{(2)}(\theta, \xi'_3)$ . Straight (solid or dashed) lines are the results of (least square) linear regressions on numerical results. Results are depicted for  $L / \lambda = 1$ ,  $\sigma_Y^2 = 1$ , and  $K_G = 1$ .

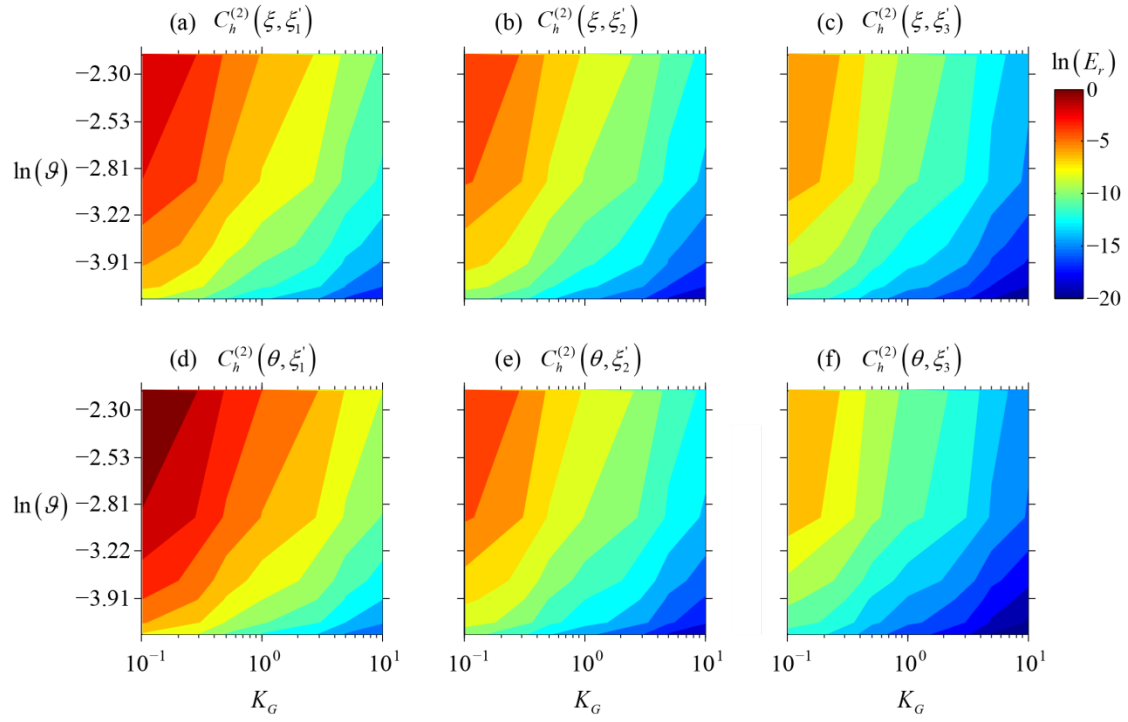




**Figure 8.** Values of (a)  $\alpha_i$  (29); (b)  $\bar{p}$  (i.e., averages of the corresponding values of  $p$  calculated via Eq. (23)) at the fraction of nodes depicted in (a); and (c) average  $GCI_{c,m}$  (25), denoted as  $\overline{GCI}_{c,m}$ , versus grid family identifier (see Table 1). Results are depicted for  $\langle h^{(2)} \rangle$ ,  $\langle h^{(0)} \rangle$ ,  $\sigma_h^{2(2)}$  and  $C_h^{(2)} \dagger$  (i.e., the head covariance for the reference point  $(\xi, \theta) \equiv (0.5, 0)$ ). Results are depicted for  $L / \lambda = 1, 3$ ,  $\sigma_Y^2 = 1$ , and  $K_G = 1$ .

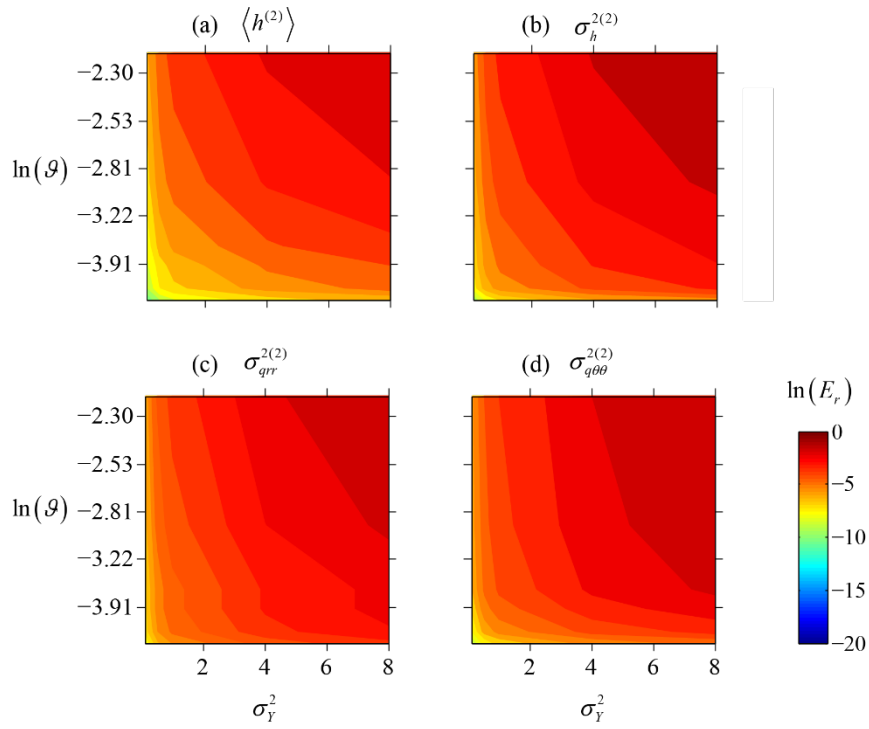


**Figure 9.** Dependence of  $E_r$  (28) on  $K_G = e^{\langle Y \rangle}$  and  $\vartheta$  for mean and variance of heads and variance of fluxes. Results are depicted for  $L / \lambda = 1$ , and  $\sigma_Y^2 = 1$ .

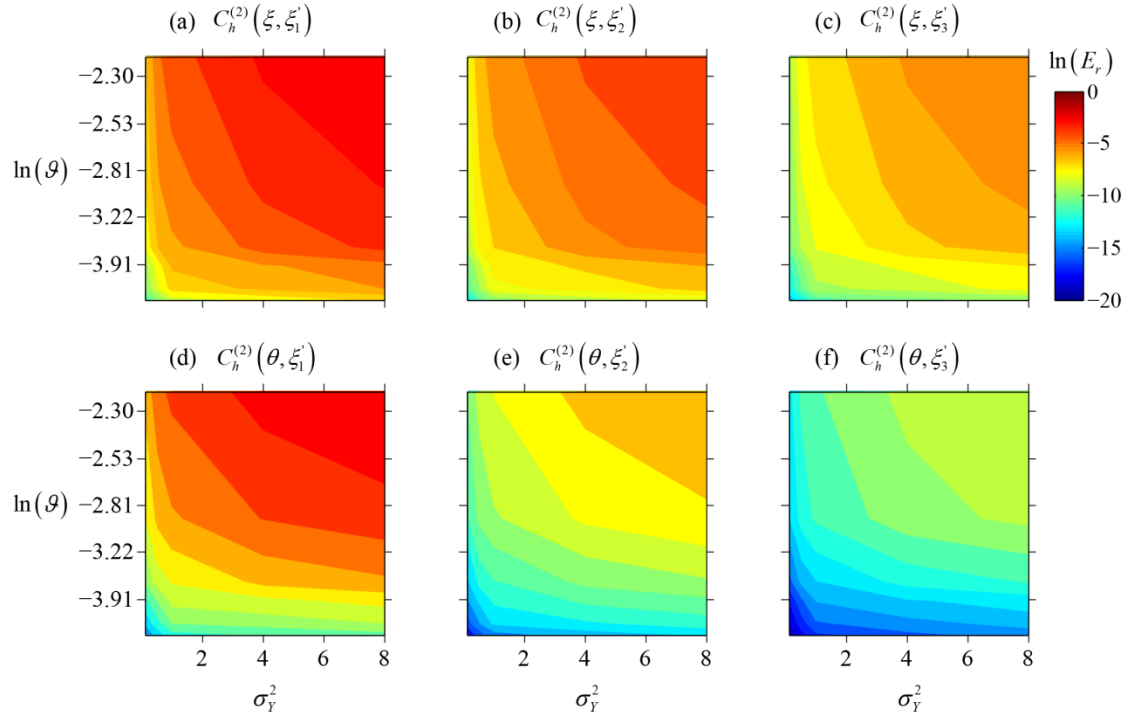


**Figure 10.** Dependence of  $E_r$  (28) on  $K_G = e^{\langle Y \rangle}$  and  $\vartheta$  for (a)  $C_h^{(2)}(\xi, \xi'_1)$ , (b)  $C_h^{(2)}(\xi, \xi'_2)$ , (c)  $C_h^{(2)}(\xi, \xi'_3)$ , (d)  $C_h^{(2)}(\theta, \xi'_1)$ , (e)  $C_h^{(2)}(\theta, \xi'_2)$ , and (f)  $C_h^{(2)}(\theta, \xi'_3)$ .

Results are depicted for  $L / \lambda = 1$ , and  $\sigma_Y^2 = 1$ .



**Figure 11.** Dependence of  $E_r$  (28) on  $\sigma_y^2$  and  $\vartheta$  for mean and variance of heads and variance of fluxes. Results are depicted for  $L / \lambda = 1$ , and  $K_G = 1$ .



**Figure 12.** Dependence of  $E_r$  (28) on  $\sigma_Y^2$  and  $\vartheta$  for (a)  $C_h^{(2)}(\xi, \xi'_1)$ , (b)  $C_h^{(2)}(\xi, \xi'_2)$ , (c)  $C_h^{(2)}(\xi, \xi'_3)$ , (d)  $C_h^{(2)}(\theta, \xi'_1)$ , (e)  $C_h^{(2)}(\theta, \xi'_2)$ , and (f)  $C_h^{(2)}(\theta, \xi'_3)$ . Results are depicted for  $L / \lambda = 1$ , and  $K_G = 1$ .