



**HAL**  
open science

# On the multiscale characterization of effective hydraulic conductivity in random heterogeneous media: a historical survey and some new perspectives

Iván Colecchio, Alejandro Boschan, Alejandro D Otero, Benoit Noetinger

## ► To cite this version:

Iván Colecchio, Alejandro Boschan, Alejandro D Otero, Benoit Noetinger. On the multiscale characterization of effective hydraulic conductivity in random heterogeneous media: a historical survey and some new perspectives. *Advances in Water Resources*, 2020, 140, pp.103594. 10.1016/j.advwatres.2020.103594 . hal-02871372

**HAL Id: hal-02871372**

**<https://ifp.hal.science/hal-02871372>**

Submitted on 17 Jun 2020

**HAL** is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

# On the multiscale characterization of effective hydraulic conductivity in random heterogeneous media: a historical survey and some new perspectives.

Iván Colecchio<sup>a</sup>, Alejandro Boschan<sup>a</sup>, Alejandro D. Otero<sup>a,b</sup>, Benoît Noetinger<sup>c,\*</sup>

<sup>a</sup>*Facultad de Ingeniería, Universidad de Buenos Aires, Paseo Colón 850, Buenos Aires, Argentina*

<sup>b</sup>*Centro de Simulación Computacional, CSC - CONICET, Godoy Cruz 2390, Buenos Aires, Argentina*

<sup>c</sup>*IFP Energies Nouvelles 1 & 4, avenue de Bois-Préau, 92852 Rueil-Malmaison Cedex - France*

---

## Abstract

In large scale heterogeneous aquifer simulations, determining the appropriate coarsening scale  $\lambda$  to define an effective hydraulic conductivity  $K_{eff}$  is a challenging task, that involves a trade-off between accuracy and cost. Efficiently adjusting the scale  $\lambda$  is then key, in particular for uncertainty quantification. In this paper, we obtain improved analytical results for the variance of  $K_{eff}$ , valid at any scale, in the context of energy dissipation formulation. Using this formulation, we then derive an efficient  $K_{eff}$  numerical estimator, and compare it with those of the potential-flow average and permeameter formulations in 2D, for lognormal and binary media, over a wide range of  $\lambda$  and of heterogeneity. We analyze the probability density function (pdf), mean, and variance, of these estimators, comparing them with the analytical results. In the lognormal case, the pdf's are rather similar for the three estimators, and remain lognormal at all scales. In the binary case, slow convergence to an asymptotic regime is observed close to the percolation threshold.

*Keywords:* heterogeneous aquifers; stochastic approach; volume averaging; up-scaling

---

## 1. Introduction

Describing effective properties of heterogeneous media has important applications in many fields of engineering and science. For example, the electrical or thermal effective conductivity of mixtures, or elastic properties of composites

---

\*Corresponding author

*Email address:* `benoit.noetinger@ifpen.fr` (Benoît Noetinger )

5 materials have been studied since many years ago (Maxwell, 1873, Bruggeman, 1935, Landau and Lifshitz, 1960, Auriault, 1983, Willot and Jeulin, 2009, Zhou et al., 2016). In particular, determining an effective hydraulic conductivity is of major interest in a variety of disciplines related to subsurface flow, such as groundwater flow characterization (Renard and De Marsily, 1997, Matheron, 10 1967, Dagan, 1989, Dagan et al., 2013), Carbon Capture Utilisation and Storage (CCUS) development (Akber Hassan and Jiang, 2012, Celia et al., 2015), and oil and gas reservoir engineering (King, 1989, Durlofsky, 1991, 1992, Preux, 2016, Malinouskaya et al., 2018). The scarcity of field data (Matheron, 1967, Dagan, 1989, Hristopulos, 2020) makes it necessary to perform some sort of 15 interpolation, with frequent use of a stochastic approach (Gelhar, 1993, Linde et al., 2015, Godoy et al., 2018) that treats the point conductivity values as a random process, eventually accompanied by field data conditioning. While the use of this approach permits a good management of uncertainty, it turns too costly to solve the flow at the fine scale provided by laboratory (microtomogra- 20 phy, synchrotron), or geological sources (Dagan et al., 2013), specially for large domains.

In addition, one may want to incorporate data obtained at different support scales before interpolation. To alleviate this issues, upscaling procedures allow us to perform a mapping from a fine scale onto a coarse scale, in which the 25 solution of the flow is less costly.

Fig. 1 shows the lengthscales and geometrical features of the upscaling process. The fine scale conductivity  $k(\mathbf{r})$  ( $\mathbf{r}$  is the position vector) is defined over the regional domain  $\omega \subset \mathfrak{R}^D$ , (dimension  $D=1, 2$  or  $3$ ) at a support scale  $\Delta$ . The coarsening scale  $\lambda$  determines a domain  $\vartheta$ , over which the effective hydraulic 30 conductivity  $K_{eff}$  is defined. One the one hand, for practical and conceptual purposes, we can establish an upper bound  $L$  for  $\lambda$ , determined by the largest subdomain  $\Omega$  over which it is still possible to solve the flow, eventually imposing boundary conditions at  $\partial\Omega$  if natural flow conditions are unknown. For example,  $L$  could be a characteristic aquifer scale. On the other hand, a lower 35 bound for  $\lambda$  is given by the support scale  $\Delta$ . The effective conductivity of a block or subdomain  $\vartheta$ , defined by the coarsening scale  $\lambda$ , i.e.  $K_{eff}(\lambda)$ , depends on the values of  $k(\mathbf{r})$  within  $\vartheta$ , but also on the conditions at the boundary  $\partial\vartheta$ , which may be imposed or known. Moreover,  $K_{eff}(\lambda)$  is a tensor in principle, however, for isotropic media, and certain flow conditions (Sánchez-Vila et al., 40 1995, Vereecken et al., 2007), the use of a scalar  $K_{eff}$  is appropriate. Finding a suitable coarsening scale  $\lambda$  requires dealing with a trade-off between accuracy and cost: as  $\lambda$  increases, the cost to solve the flow decreases, but some details of the heterogeneity (and of the flow) get lost, and the values of  $K_{eff}$  become less representative of the fine description. The choice of a scale  $\lambda$  that retains 45 the most salient flow features, while keeping the cost of the flow solution low, makes upscaling a challenging task.

In the following section, we revisit briefly some upscaling results, with focus on the types of media studied in most works, including the present one, i.e., lognormal and binary media, to later discuss  $K_{eff}$  distributions, and some 50 upscaling formulations.

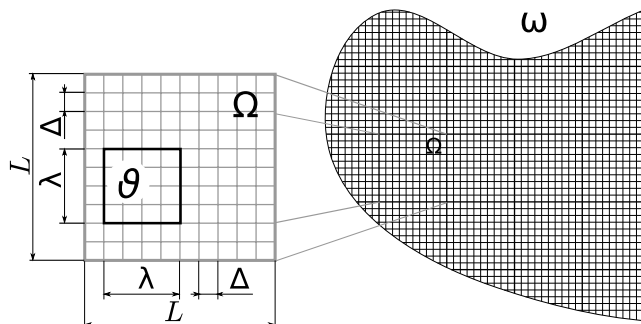


Figure 1: Lengthscales and geometry of the upscaling procedure: The fine scale conductivity  $k(\mathbf{r})$  is defined over the regional domain under investigation  $\omega$ , at a support scale  $\Delta$ . The upscaling procedure maps  $k(\mathbf{r})$  onto  $K_{eff}(\vartheta)$ , while  $\vartheta \subset \Omega$  is defined by the coarsening scale  $\lambda$ , with  $\Delta < \lambda < L$ .

### 1.1. Previous results

Analytical methods like bounds-based approaches (Hashin and Shtrikman, 1962, Renard and De Marsily, 1997, Le Loc'H, 1987, Pozdniakov and Tsang, 2004) or power averaging (Journel et al., 1986, Desbarats and Srivastava, 1991, 55 Masihi et al., 2016) provide a remarkable insight, although, as they estimate  $K_{eff}$  from the point values  $k(\mathbf{r})$  only, they disregard the influence of the flow behavior at  $\partial\Omega$ .

Depending on the detailed context, homogenization techniques (Auriault, 1983, Durlflosky, 1991, Jikov et al., 2012, Armstrong et al., 2019), volume averaging techniques (Hassanizadeh and Gray, 1979, Quintard and Whitaker, 1998, Durlflosky, 1998, Whitaker, 2013, Gray and Miller, 2005, Leung and Srinivasan, 2012, Wood and Valdés-Parada, 2013, Davit and Quintard, 2017, Aguilar-Madera et al., 2019) or stochastic perturbation theory (Landau and Lifshitz, 1960, Matheron, 1967, Dagan, 1989, King, 1989, Rubin and Gómez-Hernández, 65 1990, Indelman and Dagan, 1993a,b, Noetinger, 1994, Indelman and Abramovich, 1994, Ababou, 1994, Abramovich and Indelman, 1995, Noetinger and Gautier, 1998, Noetinger, 2000, Liao et al., 2019) were developed over many decades. All these methods provide a rigorous analytical framework supporting the existence and uniqueness of  $K_{eff}$ , for a wide variety of media types.

Analytical efforts took place mainly using perturbation theory (Gelhar, 1993, Dagan, 1989). The so called Landau-Lifschitz-Matheron (LLM) (Landau and Lifshitz, 1960, Matheron, 1967) formula reads:

$$K_{eff} \simeq \langle k^{(1-\frac{2}{D})} \rangle^{\frac{1}{(1-\frac{2}{D})}}, \quad (1)$$

In the case of a lognormal distribution of fine scale conductivity, this formula can be written under the equivalent form (King, 1989, Noetinger, 1994):

$$\langle K_{eff} \rangle = \exp \langle \log(k) \rangle e^{(\frac{1}{2}-\frac{1}{D})C_{\log k}(\mathbf{r}=0)} = K_g e^{(\frac{1}{2}-\frac{1}{D})C_{\log k}(\mathbf{r}=0)}.$$

70 The notation  $\langle \dots \rangle$  indicates ensemble arithmetic averaging over all the possible realizations of the fine scale structure.  $K_g$  denotes the geometric mean of the fine grid conductivity, and  $C_{\log k}(\mathbf{r} = 0)$  the variance of its logarithm. In this work, wherever the expressions  $\log(k)$  or  $\log(K_{eff})$  are shown, it is implied that the argument of the logarithm is divided by 1 m/day, to make it dimensionless.

In most cases, an ergodicity assumption allows to replace the ensemble average by a spatial average (Ababou, 1996, Sanchez-Vila et al., 2006), such that for finite block of size  $L$ , one estimates  $K_{eff}$  as:

$$K_{eff_{block}} \simeq \left( \frac{1}{V} \int_{block} k(\mathbf{r})^{(1-\frac{2}{D})} d^D \mathbf{r} \right)^{\frac{1}{(1-\frac{2}{D})}} \quad (2)$$

75 This formula, with dimension  $D = 1, 2, 3$  whose evaluation is straightforward, is exact in 1D for any type of media, yielding the harmonic average. In 2D, it corresponds to the geometric average that was found to be exact in 2D for lognormal media by Matheron (1967), who derived it using an elegant duality argument specific to 2 dimensions. In 3D, the formula is exact up to second  
80 order (Dagan, 1993) with respect to log-conductivity variance (using a series expansion of  $K_{eff}$  up to 4th order in powers of the log conductivity fluctuations). But in 3D, the proposed formula was shown to be inexact at third order by several authors (Indelman and Abramovich, 1994, De Wit, 1995, Stepanyants and Teodorovich, 2003).

85 Moreover, higher order results were shown to be structure dependent: this prevents the existence of a local evaluation expression like Eq. (1) in 3D. However, numerical tests carried out show that LLM formula is quite robust in 3D even for large log-conductivity variances (Dagan, 1989, Romeu and Noetinger, 1995, Renard and De Marsily, 1997). Some generalization of such approaches  
90 for anisotropic cases were revisited recently by Liao et al. (2019).

From a more geological point of view, a frequent organization of the subsurface heterogeneous formations in a number of hydrofacies, that correspond to different types of rock, or sediments, having a well defined hydraulic property, such as porosity or permeability, may be observed in natural systems (Journal  
95 et al., 1986, Beucher and Renard, 2016). Each facies possesses its own characteristic features. That promoted the study of the effective conductivity of composite media. Binary or bimodal media are the simplest cases, while still retaining the complexity of percolative systems. These types of media have been extensively studied using self-consistent effective medium approaches in  
100 the electrodynamical or elasticity contexts (Maxwell, 1873, Bruggeman, 1935, Landau and Lifshitz, 1960, Auriault, 1983, Pozdniakov and Tsang, 2004).

Analytical results, based on a mixing of characteristic conductivity values and bounds (Hashin and Shtrikman, 1962, 1963), exist for this type of media (Bernabé et al., 2004); in them, connectivity is implicitly taken into account.

105 Other authors (Pozdniakov and Tsang, 2004, Knudby and Carrera, 2005, Guin and Ritzi Jr., 2008, Bernabé et al., 2016) studied numerically the influence of the contrast between the high and low conductivity components  $k^+$  and  $k^-$ . The abrupt change in  $K_{eff}$  that takes place close to the percolation tran-

sition, when the  $k^+$  component becomes connected, poses difficulties during the upscaling procedure (Boschan and Noetinger, 2012).

Indeed, percolation theory scaling (Berkowitz and Balberg, 1993, Stauffer and Aharony, 2014, Hunt et al., 2014, Hunt and Sahimi, 2017) has been used to assess  $K_{eff}$  in this type of media, but some restrictions exist:

- This scaling is only valid for media in which the proportion of high conductivity medium is close to the percolation transition,
- Percolation transition is smeared-out by finite size effects and finite conductivity contrast values.

### 1.2. $K_{eff}$ probability distributions

Due to the fact that subsurface uncertainty is frequently dealt with by using a stochastic approach, it is appropriate to treat  $K_{eff}$  as a random variable characterized by a probability distribution more than by a deterministic value.

Although the literature mainly focuses on the firsts moments of the probability density function (pdf), such as the mean and variance (Rubin and Gómez-Hernández, 1990, Sánchez-Vila et al., 1995, Sanchez-Vila et al., 2006), the shape of the pdf provides unique insight on the underlying flow situation. For example, in media samples near percolation, a bimodal pdf may yield a mean  $K_{eff}$  value that truly has a negligible occurrence probability: this situation may easily arise when dealing with fractured media or, in general, with media possessing a high degree of heterogeneity. The pdf of  $K_{eff}$  depends on the coarsening scale  $\lambda$ , and will be noted  $P(K_{eff}, \lambda)$ .

For clarity,  $P(K_{eff}, \lambda)$  undergoes a transition from  $P(k(\mathbf{r}), \Delta)$  to  $P(K_{eff}, L)$  as  $\lambda$  goes from  $\Delta$  to  $L$ . For  $\lambda = \Delta$ , the distribution of  $k(\mathbf{r})$  is recovered, while for  $\lambda \simeq L$ ,  $P(K_{eff}, \lambda)$  will tend toward a delta-like distribution sharply peaked around a stable  $K_{eff}$  value (see Fig. 2). If it is possible to define a characteristic lengthscale (for example an integral scale  $I$ ) for the media under consideration, a crossover is expected when  $\lambda$  approaches it. More conceptually, a representative elementary volume (REV) may be determined by inspecting significant changes of the shape of  $P(K_{eff}, \lambda)$ . The fact that the statistical sampling becomes poorer as  $\lambda$  increases, can be compensated, in the framework of the stochastic theory, and assuming ergodicity, by an increase in the number of ensemble realizations.

The behavior of  $P(K_{eff}, \lambda)$  was addressed in several studies (King, 1989, Sanchez-Vila et al., 2006, Wen and Gómez-Hernández, 1996, Wu et al., 2013). In Boschan and Noetinger (2012), the convergence of  $P(K_{eff}, \lambda)$  was studied in 3D for lognormal and binary media. In the lognormal case,  $P(K_{eff}, \lambda)$  kept its lognormal nature as  $\lambda$  increased. If this result hold in 2D (this will be analyzed in the present work), it might stem from the work of Matheron (1967). In the binary case, it was shown that the convergence to a stable  $K_{eff}$  is slower when the  $k^+$  component is close to the percolation transition (Stauffer and Aharony, 2014). Finally, under the ergodic hypothesis, several studies assessed the use of filtering techniques to derive  $P(K_{eff}, \lambda)$  at all scales. (King, 1989, Noetinger

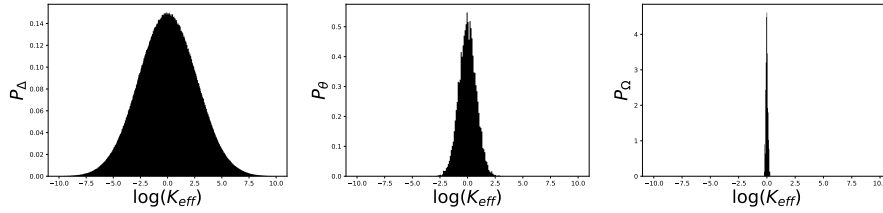


Figure 2: Probability density function  $P(K_{eff}, \lambda)$  for increasing values of the coarsening scale  $\lambda$ . Left: Fine scale distribution  $P(k(\mathbf{r}), \Delta)$ , where  $k(\mathbf{r})$  follows, as an example, a log-normal distribution. Center:  $P(K_{eff}, \lambda)$  becomes narrower as  $\lambda$  increases. Right: For  $\lambda \simeq L$ ,  $P(K_{eff}, \lambda)$  approaches a delta-like function centered on a single  $K_{eff}$  value. For dimensional reasons, the  $K_{eff}$  is normalized by a unit reference conductivity of 1 m/day.

and Gautier, 1998, Noetinger, 2000, Noetinger and Zargar, 2004, Attinger, 2003, Eberhard et al., 2004).

### 1.3. Upscaling formulations and numerical implementations

155 The fact that analytical results are limited to some academic cases, and strictly valid only up to second order in 3D, imposes the use of numerical techniques to obtain  $K_{eff}$  as well as its distribution by means of Monte Carlo simulations. Several numerical techniques were developed using different approaches and provide accurate solutions (Desbarats and Srivastava, 1991, Durlofsky, 1991, 160 Desbarats, 1992, Quintard and Whitaker, 1998, Wang et al., 2014, Zheng et al., 2017, Wang et al., 2018). The numerical implementations calculate a value  $K_{eff}$  in  $\vartheta$  from the fine conductivity field  $k(\mathbf{r})$ , and from the boundary conditions at  $\partial\vartheta$ , in what constitutes a numerical solution of the closure problem posed by the associated Laplace equation. Moreover, some of them use border regions, including information of the outer neighbourhood of  $\partial\vartheta$  (Wen et al., 2003). Two 165 aspects of the solution of the closure problem by numerical simulations stand out:

1. The task of finding the optimal scale  $\lambda$  in each flow scenario makes upscaling a multiscale problem par excellence.
- 170 2. The choice of the formulation, in particular that of the boundary conditions, strongly affects accuracy and numerical efficiency. For example, imposing boundary conditions at  $\partial\vartheta$  decouples the flow in  $\vartheta$  from its outer region, in a rather invasive procedure, in view of item 1). In that sense, solving the flow in  $\Omega$  once, and then employing this solution to estimate 175  $P(K_{eff}, \lambda)$ , i.e., seems less invasive and more efficient, but requires the ability to solve larger systems of equations.

From the existing upscaling formulations, the most widely used is the permeameter (Darcian) one, which, as a particularity, isolates the flow in  $\vartheta$ , suffering from the drawback explained above. This formulation, and its implementation, 180 will be formally introduced in Section 2.2. Another frequent formulation, (Rubin and Gómez-Hernández, 1990) and (Sánchez-Vila et al., 1995), uses the solution

of potential and the associated flow in  $\Omega$ , evaluating their averages over  $\partial\vartheta$  to obtain  $K_{eff}$ . In order to obtain a scalar  $K_{eff}$ , some assumption is required.

185 Finally, Indelman and Dagan (1993a,b), Bøe (1994) proposed that  $K_{eff}$  could be defined by assuming that the dissipated energy is conserved during the upscaling procedure. This might be the strongest conceptual definition ever formulated, however, its implementation to obtain  $K_{eff}$  is mathematically difficult.

190 Aiming to reduce the computational cost, a number of approaches that combine different formulations were proposed (Chen et al., 2003, Bauer et al., 2008, Wu et al., 2013, Karimi-Fard and Durlofsky, 2016), with the support of ergodicity considerations (Ababou et al., 1989, Ababou, 1994, 1996, Desbarats and Srivastava, 1991).

#### 1.4. Objectives

195 In this paper, we intend to explore analytically and numerically the multi-scale nature of the upscaling procedure in the context of the different formulations in 2D. On the one hand, after reviewing the existing body of literature, we update the formulae introduced in previous studies to characterize the mean and variance of  $K_{eff}$ , valid at the scale  $\Omega$  at which the boundary conditions are imposed. We derive, in the context of the energy dissipation formulation, a new  
200 expression for the variance, this time, valid at any subscale  $\vartheta \subset \Omega$ , up to second order in perturbation theory. On the other hand, using that formulation, we define and implement a new numerical estimator of  $K_{eff}$  based on a scalar energy dissipation average. This estimator can be obtained at any subscale  $\lambda$  with  
205 nearly negligible additional CPU time once the potential in  $\Omega$  is solved. Aiming to provide a comprehensive view, the pdf, the mean and the variance of this estimator are compared with those of the potential-flow average estimator, and of the permeameter Darcian one, over a wide range of coarsening scales. This study is performed over lognormal media samples with a wide range of fine grid  
210 variances, and over binary media samples spanning the percolation transition.

The paper is organized as follows: we start by presenting the overall geometry and notation, considering a steady-state Darcian flow in an heterogeneous porous medium, and perform some algebraic manipulation to express  $K_{eff}$  in terms of the viscous dissipation. We introduce then (Section 3.1) a useful variational derivation, that allows us to define  $K_{eff}$  in terms of a minimization  
215 of that dissipation. By using functional expansion techniques already developed in a previous study (Noetinger, 2013), we provide expressions for the variance of  $K_{eff}$  in  $\Omega$  up to second order in the perturbation expansion (valid for small variances), later improving it, for higher variances, by using a mean-field approximation. After some more manipulation, we get in position to show how  
220 these results are valid at any subscale (i.e., the coarsening scale  $\lambda$ ), even if the variational formulation cannot be applied at any scale smaller than  $\Omega$  (the scale in which the boundary conditions are imposed). The result depends also on the covariance of  $k(\mathbf{r})$ , and on  $\lambda$ , while it is possible to apply again the mean-field technique, now at this scale, to improve it. Section 6 introduces  
225 the numerical methodology with the implementation of the three formulations,



while Section 7, presents firstly a numerical validation, and then, the results regarding the multiscale dependence of  $K_{eff}$  under the different formulations.

## 2. Geometry, driving equations and notations

### 2.1. Geometry and local equations

We focus our attention on a block  $\Omega$  to be up scaled in  $D$  dimensions, a square in 2D or a cube in 3D. The edges of that domain are of size  $L$  in the  $D$  directions, as sketched in Fig. 1. The potential is driven by the following Laplace equation, to be solved in the domain  $\Omega$ :

$$\nabla \cdot (k(\mathbf{r})\nabla p(\mathbf{r})) = 0, \quad (3)$$

The local potential is denoted by  $p(\mathbf{r})$ . This equation is a combination of mass or charge conservation with a phenomenological equation relating the local flux to the local potential gradient, such as Joule, Darcy or Fourier's law that may arise after a proper averaging of the sub-scale transport processes (Hassanizadeh and Gray, 1979). In order to get a well defined problem, Dirichlet or Dirichlet-Neumann conditions must be specified at the frontier  $\partial\Omega$  of the domain. These conditions will be discussed in the next section. The local conductivity, denoted by  $k(\mathbf{r})$  is assumed to be scalar and to depend on position  $\mathbf{r}$ . The conductivity field can be discontinuous with respect to  $\mathbf{r}$ .

### 2.2. Classical Darcian definition of the effective conductivity

Here, we defer the discussion of the up scaling problem to references in Mathéron (1967), Durlofsky (1991), Neuman and Orr (1993), Renard and De Marsily (1997), Quintard and Whitaker (1998), Willot and Jeulin (2009), Jikov et al. (2012). The effective conductivity can be defined using the solution of the Laplace Eq. (3), to be solved with Dirichlet boundary conditions at the inlet/outlet, denoted by  $P_{in}$  and  $P_{out}$ . Neumann no-flux boundaries are imposed on the faces of the domain parallel to the average imposed flow, which will be the  $x$  direction in the rest of the paper. This definition of  $K_{eff}$  is the so-called permeameter definition that will be sometimes denoted by  $K_{perm}$ . This corresponds physically to the basic conductivity measurement that could be performed at the laboratory, both in the Darcy or electrical context. Other boundary conditions, such as periodic (Auriault, 1983, Durlofsky, 1991, Quintard and Whitaker, 1998, Noetinger, 2013) can be chosen, but that does not change drastically the analysis, so permeameter conditions will be kept throughout the paper.

By identification with the homogeneous case, effective hydraulic conductivity is given by:

$$K_{eff} = \frac{Q}{L^{D-2}(P_{in} - P_{out})}. \quad (4)$$

Here,  $Q$  denotes the total fluid flux flowing in any section of the domain perpendicular to the mean flow  $x$  direction:

$$Q = \int_{Inlet\ face} d^{D-1}\mathbf{r} k(\mathbf{r})\nabla p(\mathbf{r}) \cdot \mathbf{n}. \quad (5)$$

255 Here,  $p(\mathbf{r})$  is the unique solution of the boundary value Laplace Eq. (3) with the permeameter forcing boundary conditions.

### 3. Effective conductivity and viscous dissipation

For our purpose, it is useful to introduce an equivalent algebraic expression of  $K_{eff}$  that was introduced in the porous media context by Jacquard (1965), Matheron (1967), and revisited later by Wen and Gómez-Hernández (1996), Sánchez-Vila et al. (1995):

$$\begin{aligned} Q (P_{in} - P_{out}) &= \int_{\partial\Omega} d^{D-1} \mathbf{r} p(\mathbf{r}) k(\mathbf{r}) \nabla p(\mathbf{r}) \cdot \mathbf{n} \\ &= \int_{\Omega} d^D \mathbf{r} k(\mathbf{r}) \nabla p(\mathbf{r}) \cdot \nabla p(\mathbf{r}). \end{aligned} \quad (6)$$

In order to begin with, the first equality of Eq. (6) is obtained by expressing  $Q$  in terms of integrals over the inlet and outlet faces of the domain as in Eq. (5). In the outlet, according to the convention defining positive flow opposite to the face inward normal, the expression have the opposite sign. Then, both face pressures are moved under the integral signs obtaining similar expressions. Regarding the Neumann boundary conditions on lateral faces, imposing no pressure gradient, both integrals can be combined in only one over the whole domain boundary  $\partial\Omega$ . Using the divergence theorem combined with Laplace Eq. (3) yields the second equality. This equation has a simple physical interpretation: The RHS corresponds to the total viscous dissipated power, that must coincide with the power spent by external forcing sources set-up to create the flow.

So, the effective conductivity may be expressed as,

$$\begin{aligned} K_{eff} &= \frac{1}{(P_{in} - P_{out})^2 L^{D-2}} \int_{\Omega} d^D \mathbf{r} k(\mathbf{r}) (\nabla p(\mathbf{r}))^2 \\ &= \frac{1}{\overline{\nabla p}_{\Omega,x}^2 L^D} \int_{\Omega} d^D \mathbf{r} k(\mathbf{r}) (\nabla p(\mathbf{r}))^2, \end{aligned} \quad (7)$$

where  $\overline{\nabla p}_{\Omega,x} = -(P_{in} - P_{out})/L$  is the volume averaged gradient in the  $x$  direction (which is the mean flow direction). The average potential gradient  $\overline{\nabla p}_{\Omega}$  over the block volume  $|\Omega| = L^D$  is given by:

$$\overline{\nabla p}_{\Omega} = \frac{1}{|\Omega|} \int_{\Omega} d^D \mathbf{r} \nabla p(\mathbf{r}) = \frac{1}{|\Omega|} \int_{\partial\Omega} d^{(D-1)} \mathbf{r} p(\mathbf{r}) \mathbf{n}. \quad (8)$$

In the case of a square or cubic  $\Omega$ , the retained boundary conditions for potential  $p$  give the proposed equality in the  $x$  direction. Eq. (7) relates the effective conductivity of the whole block  $K_{eff}$  to the overall viscous dissipation and the mean forcing potential gradient norm in the imposed flow direction. It will be the starting point to define a dissipation-based effective conductivity estimator in Section 5.1.

275 *3.1. A variational characterization of  $K_{eff}$ .*

We are now in position to propose an alternative formulation that proves to be useful for estimating the sensitivity of large scale parameters to variations of local conductivity. This variational characterization of  $K_{eff}$  may be formulated as follows:

$$K_{eff} (P_{in} - P_{out})^2 L^{D-2} = Q (P_{in} - P_{out})$$

$$K_{eff} \overline{\nabla p_{\Omega,x}}^2 L^D = \text{Min}_{p(\mathbf{r})} \left\{ \Theta \{p(\mathbf{r})\} = \int_{\Omega} d^D \mathbf{r} k(\mathbf{r}) (\nabla p(\mathbf{r}))^2 \right\}. \quad (9)$$

Here, the potential fields  $p(\mathbf{r})$  among which the minimization is to be performed fulfill the boundary conditions at  $\partial\Omega$ . The justification of Eq. (9) is classical: one has to express the extremal conditions:

$$\forall \mathbf{r}, \frac{\delta \{ \Theta \{ p(\mathbf{r}) \} \}}{\delta p(\mathbf{r})} = \nabla \cdot (k(\mathbf{r}) \nabla p(\mathbf{r})) = 0.$$

The operator  $\frac{\delta \{ \Theta \{ p(\mathbf{r}) \} \}}{\delta p(\mathbf{r})}$  is a functional derivative of the functional  $\Theta \{ p(\mathbf{r}) \}$  with respect to  $p(\mathbf{r})$ . A basic presentation of functional differentiation is given in Appendix A.

280 Using thus the particular quadratic form of  $\Theta \{ p(\mathbf{r}) \}$ , these extremal conditions give rise to Laplace Eq. (3) that governs the potential. The final result may be derived using the same methods than Eq. (6).

*3.2. Functional expansion techniques for the effective conductivity*

Functional techniques combined with the variational formulation are useful to derive directly second order perturbation expansion of the effective conductivity and of its associated variance. The starting point is to evaluate the sensitivity of effective conductivity with respect to local perturbations of the local conductivity, as it was derived in Noetinger (2013) and Appendix A. The starting point is to decompose the local hydraulic conductivity as:

$$k(\mathbf{r}) = \langle k \rangle + \delta k(\mathbf{r}).$$

The brackets  $\langle \dots \rangle$  correspond to ensemble averaging over the conductivity realizations, to be not confused with volume averaging denoted by  $\overline{\dots}$ . So  $\langle \delta k(\mathbf{r}) \rangle = 0$ . One can use the formal equivalent of Taylor series formula, up to second order, also valid for functionals:

$$K_{eff} = \langle k \rangle + \int_{\Omega} d^D \mathbf{r} \frac{\delta K_{eff}}{\delta k(\mathbf{r})} \delta k(\mathbf{r}) +$$

$$+ \frac{1}{2} \int_{\Omega} d^D \mathbf{r} \int_{\Omega} d^D \mathbf{r}' \frac{\delta^2 K_{eff}}{\delta k(\mathbf{r}) \delta k(\mathbf{r}')} \delta k(\mathbf{r}) \delta k(\mathbf{r}') + \dots \quad (10)$$

The reader must note that in these equations, the functional derivative must be evaluated while the nominal value of the conductivity map is a uniform

285 value  $k(\mathbf{r}) = \langle k \rangle$  (in usual function Taylor's expansions, this corresponds to the point at which the derivative is evaluated). Averaging Eq. (10) yields a second-order expansion that coincides with LLM conjecture up to this limited order. A concise derivation using functional derivatives is given in Appendix B.

#### 4. Estimation of the variance of the effective conductivity at second order.

290 In this section, we present expressions of the variance of the effective conductivity that are obtained in the context of second order perturbation theory. The derivations are given in Appendix C. Finally, closed expressions are given for the cases when those expressions are particularized for Gaussian covariance functions.

For the variance of the effective conductivity given by

$$C_{K_{eff}}(L) = \langle K_{eff}^2 \rangle - \langle K_{eff} \rangle^2 = \langle (K_{eff} - \langle K_{eff} \rangle)^2 \rangle$$

the following expression can be obtained, Eq. (C.4):

$$C_{K_{eff}}(L) = \frac{1}{|\Omega|^2} \int_{\Omega} d^D \mathbf{r} d^D \mathbf{r}' C_k(\mathbf{r} - \mathbf{r}'). \quad (11)$$

A mean-field approximation allows to replace each occurrence of  $K_{eff}$  and  $k$  by the corresponding logarithm, Eq. (C.7), providing the following expression that can be expected to have a more extended domain of validity for practical applications:

$$C_{\log K_{eff}}(L) = \frac{1}{|\Omega|^2} \int_{\Omega} d^D \mathbf{r} d^D \mathbf{r}' C_{\log k}(\mathbf{r} - \mathbf{r}'). \quad (12)$$

The resulting formula is similar to Eq. (11), replacing the covariance function by the log conductivity covariance function. For the special case of lognormal media, this is a quite natural transformation. The same can be done with the simplified formula (C.5).

300 In the case of the Gaussian covariance with  $C_k(\mathbf{r}) = C_k(r=0) e^{-\frac{r^2}{2I_c^2}}$  where  $I_c$  is the correlation length, explicit analytical expressions can be derived for  $C_{K_{eff}}(L)$  from Eq. (11) (see Appendix C.2 Eq. (C.8))

$$C_{K_{eff}}(L) = C_k(r=0) \left( \frac{I_c}{L} \right)^{2D} \left[ \sqrt{2\pi} \frac{L}{I_c} \operatorname{erf} \left( \sqrt{2} \frac{L}{I_c} \right) + 2e^{-\frac{L^2}{2I_c^2}} - 2 \right]^D. \quad (13)$$

Likewise, using the simplified Eq. (C.5), one gets after integration (Eq. (C.9)):

$$C_{K_{eff}}(L) \simeq C_k(r=0) \left[ \sqrt{2\pi} \frac{I_c}{L} \operatorname{erf} \left( 2\sqrt{2} \frac{L}{I_c} \right) \right]^D. \quad (14)$$

305 The same calculations can be carried out for  $C_{\log K_{eff}}(L)$  applying the logarithmic transformation and give analogous results using  $C_{\log k}(r=0)$  and the same spatial dependence.

## 5. A posteriori multiscale estimators of $K_{eff}$ distributions

In this section, two estimators providing intermediate scale effective conductivity distributions are presented. Both are computed using low-cost post processing of one up scaling closure problem at the largest available scale. These distributions will be compared to reference distributions determined by computing numerically permeameter effective conductivity of every coarse block at any scale. The resulting pdf's will be compared, as well as the associated log conductivity mean and variance. For completeness, the latter will be compared with preceding analytical results.

### 5.1. Dissipation estimator

#### 5.1.1. Definition of the estimator

We consider now that the up-scaling Laplace problem was solved on a single conductivity realization on the entire block  $\Omega$ . The subscale effective conductivity  $K_{diss}(\vartheta)$  on any given cubic (or square) sub-block of size  $\lambda$  included in the overall domain  $\Omega$  can thus be defined as the relation between the dissipation and the average potential gradient at the block level by:

$$K_{diss}(\vartheta) = \frac{\int_{\vartheta} d^D \mathbf{r} k(\nabla p)^2}{\lambda^D \overline{\nabla p_{\vartheta}^2}}. \quad (15)$$

It can be observed, using Eq. (7), that if  $\vartheta = \Omega$ ,  $K_{diss}(\vartheta) = K_{eff} \times \frac{\overline{\nabla p_x^2}}{\overline{\nabla p^2}} \leq K_{eff}$ . In the case of statistically isotropic  $k(r)$ , if  $\Omega$  is sufficiently large, the average potential gradient  $\overline{\nabla p_y}$  perpendicular to the mean flow vanishes, so the effective conductivity determined by dissipation is equal to the usual definition:  $K_{diss}(\vartheta \rightarrow \Omega) \simeq K_{eff}$ .

Considering the opposite limit,  $\vartheta \rightarrow 0$ , it can be shown, using a Taylor expansion of the potential gradient under the integral sign, that  $K_{diss}(\vartheta) = k(\mathbf{r})$  if and only if  $\overline{\nabla p^2} \simeq (\nabla p)^2 \neq 0$ . This last condition corresponds to stagnation (no-flow) points. This condition is not surprising, as it can correspond to both infinite conductivity regions or to screened regions of vanishing hydraulic conductivity. In both cases, effective conductivity is not defined. Assuming that the set of these points is of vanishing measure, in most cases the original detailed conductivity map must be recovered. This criterion was already introduced and discussed by Sánchez-Vila et al. (1995) and Bauer et al. (2008). The proposed indicator fulfills two intuitive conditions for both extreme  $\vartheta$  sizes. In Appendix D it is shown that the average of the dissipation estimator is in agreement with that derived for  $K_{eff}$  for volumes  $\vartheta$  tending to  $\Omega$ , and the structure of the finite size corrections is given too. In next Section 5.1.2, it is shown up to second order that the variance of  $K_{diss}(\vartheta)$  coincides with expression (11) by replacing  $\Omega$  by  $\vartheta$  as integration domain. This implies that the evaluation of the variance  $C_{\log K_{diss}}(\lambda)$  is obtained by replacing  $L$  by the length of the considered subscale block,  $\lambda$ , in Eq. 12.

340 5.1.2. Evaluation of the variance of block dissipation conductivity  $K_{diss}$

The block equivalent conductivity  $K_{diss}(\vartheta)$  is given by Eq. (15), and its variance may be evaluated following the same steps that in Appendix C. It is defined by  $\langle K_{diss}(\vartheta)^2 \rangle - \langle K_{diss}(\vartheta) \rangle^2 = \langle (K_{diss}(\vartheta) - \langle K_{diss}(\vartheta) \rangle)^2 \rangle$ . So, one gets finally:

$$\langle K_{diss}(\vartheta)^2 \rangle - \langle K_{diss}(\vartheta) \rangle^2 = \int_{\Omega} d^D \mathbf{r} d^D \mathbf{r}' \frac{\delta K_{diss}(\vartheta)}{\delta k(\mathbf{r})} \frac{\delta K_{diss}(\vartheta)}{\delta k(\mathbf{r}')} \langle \delta k(\mathbf{r}) \delta k(\mathbf{r}') \rangle + \dots$$

Note that at present stage, the integration volume remains the whole volume  $\Omega$ , it is not restricted to  $\vartheta$  because  $K_{eff}(\vartheta)$  depends on the entire conductivity map that is defined on the support  $\Omega$  in which the Laplace equation is solved at the beginning. We have to evaluate the functional derivative  $\frac{\delta K_{diss}(\vartheta)}{\delta k(\mathbf{r})}$ . The evaluation cannot be simplified because the variational principle that characterizes  $K_{eff}$  as defined in  $\Omega$  is not relevant at any smaller scale. The derivative is given by:

$$\begin{aligned} \frac{\delta K_{diss}(\vartheta)}{\delta k(\mathbf{r})} &= \frac{(\nabla p_0(\mathbf{r}))^2}{\lambda^D \overline{\nabla p_0}^2} \mathbf{1}_{\vartheta}(\mathbf{r}) + \frac{2}{\lambda^D \overline{\nabla p_0}^2} \frac{1}{\lambda^D} \left[ \frac{1}{\overline{\nabla p_0}^2} \int_{\vartheta} d^D \mathbf{r}' k \nabla p_0(\mathbf{r}') \cdot \frac{\delta \nabla p(\mathbf{r}')}{\delta k(\mathbf{r})} - \right. \\ &\quad \left. - \frac{1}{\lambda^D} \int_{\vartheta} d^D \mathbf{r}' k \nabla p_0(\mathbf{r}')^2 \int_{\vartheta} d^D \mathbf{r}'' \nabla p_0(\mathbf{r}'') \cdot \frac{\delta \nabla p(\mathbf{r}'')}{\delta k(\mathbf{r})} \right]. \end{aligned}$$

In that equation, the first term involving the indicator function of  $\vartheta$  denoted by  $\mathbf{1}_{\vartheta}(\mathbf{r})$  is the remaining of the result that would be provided using the variational approach, as shown in Appendix C, equation C.1. The first integral arises from the derivative of  $\nabla p^2$  under the integral sign, the second corresponds to the functional derivative of  $\frac{1}{\overline{\nabla p}^2}$ . Both terms are equal to 0 if  $\vartheta = \Omega$ . At lowest order, the spatial dependence of the conductivity  $k$  must be discarded. It appears that the second line involving twice integration vanishes because  $\nabla p_0(\mathbf{r}') = \mathbf{e}_{\mathbf{x}}$  is constant up to this order, so both terms cancel each other. So we obtain the same result that would be provided by the variational approach if it was applicable for block dissipation:

$$\frac{\delta K_{diss}(\vartheta)}{\delta k(\mathbf{r})} = \frac{(\nabla p_0)(\mathbf{r})^2}{\lambda^D \overline{\nabla p}^2} \mathbf{1}_{\vartheta}(\mathbf{r}).$$

Gathering all the preceding results, we obtain the following formula for the variance of the dissipation estimator at scale  $\vartheta$ :

$$\langle (K_{diss}(\vartheta)^2 - \langle K_{diss}(\vartheta) \rangle^2) \rangle = \frac{1}{|\vartheta|^2} \int_{\vartheta} d^D \mathbf{r} d^D \mathbf{r}' C_k(\mathbf{r} - \mathbf{r}'). \quad (16)$$

Up to second order, this formula is analogous to the variance in Eq. (C.3) of the full up scaled hydraulic conductivity  $K_{eff}$ . The corresponding formulation using logarithms is similar at this order. This result allows to extend the validity of Eqs. (11) and (12) to subscale blocks  $\vartheta$ .

345 *5.2. Block average conductivity estimator*

Another  $K_{eff}$  estimator on subvolume  $\vartheta$  can be introduced, defined as

$$K_{ave}(\vartheta) = \frac{\overline{Q}_x}{\lambda^{D-1} \overline{\nabla P}_x}.$$

This expression is based on Darcy equation where  $\overline{Q}$  is the flow rate and  $\overline{\nabla P}$  the potential gradient, both volume-averaged over domain  $\vartheta$  of size  $\lambda$ . This estimator was studied by Rubin and Gómez-Hernández (1990), Sánchez-Vila et al. (1995), Renard and De Marsily (1997), Bauer et al. (2008). In particular, using a second order expansion, Rubin and Gómez-Hernández (1990) computed the average and variance of  $\log(K_{ave}(\vartheta))$  as a function of  $\vartheta$  and the input covariance function of the conductivity that correspond to the observed statistical parameters observed at scale  $L$ . They give the following expressions:

$$\begin{aligned} \langle \log K_{ave}(\vartheta) \rangle &= \log K_g + \left(\frac{1}{2} - \frac{1}{D}\right) (1 - \alpha) C_{\log k}(\mathbf{r} = 0) \\ \langle (\log K_{ave}(\vartheta) - \langle \log K_{ave}(\vartheta) \rangle)^2 \rangle &= \alpha C_{\log k}(\mathbf{r} = 0) \end{aligned}$$

The normalized variance correction factor  $\alpha$  given by

$$\alpha = \frac{1}{|\vartheta|^2} \int_{\vartheta} d^D \mathbf{r} d^D \mathbf{r}' \frac{C_{\log k}(\mathbf{r} - \mathbf{r}')}{C_{\log k}(\mathbf{r} = 0)},$$

depends only on the geometrical form of the covariance function and on the averaging volume  $\vartheta$  size  $\lambda$ . It can be observed that it shares the same form than the scale-dependant variance (11) derived before. It can be noticed that  
 350 using directly LLM formula for estimating  $K_{eff}$  for large size  $\lambda$  using these parameters, Eq. (1) under its second form is recovered as terms involving  $\alpha$  terms cancel. This highlights some internal consistency of this estimator.

In practice, once the potential is solved, the evaluation of  $K_{diss}(\vartheta)$  and  $K_{ave}(\vartheta)$  is straightforward and of negligible extra computational cost. For a  
 355 given size  $\lambda$ , one obtains a set of  $(\frac{\lambda}{\lambda})^D$ ,  $D = 2, 3$  values of  $K_{diss}(\vartheta)$  and  $K_{ave}(\vartheta)$  that can be studied using statistical tools. This will be the main topic of next sections.

## 6. Numerical methodology

### 6.1. Generation of media samples

360 We first compare the formulations over random lognormal media samples with low and high variance, and then, over binary media samples that have a high contrast of characteristic conductivities. We employed a fast Fourier transform (FFT) moving average (FFT-MA) method (Le Ravalec et al., 2000) to generate these samples. Lognormal hydraulic conductivity fields with unitary  
 365 geometric mean  $K_g$  were generated. Gaussian covariance, with an integral scale  $I = 16\Delta$  defined as the practical range of the covariance function ( $I = \sqrt{3}I_c$ ),

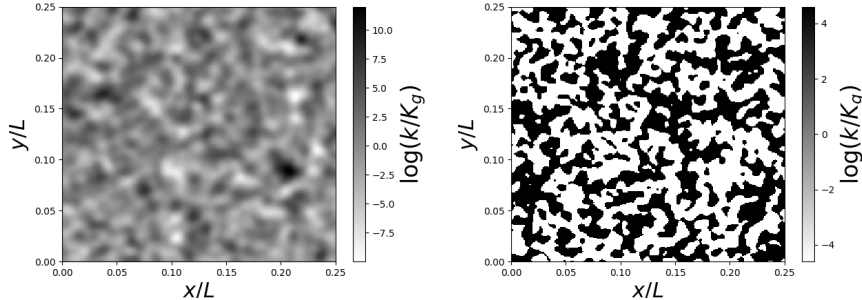


Figure 3: Maps of  $\log(k)$ . (left) Lognormal medium obtained from FFTMA. Input data:  $\sigma_{\log k}^2 = 7$ ,  $I = 16\Delta$ . (right) Binary medium. Input data:  $p = 0.5$ ,  $k^+/K_g = 100$ ,  $k^-/K_g = 0.01$ .

was used to spatially correlate the samples. Fig. 3 (left) shows, as an example, a realization of a lognormal medium obtained with this procedure. All media samples generated have  $1024 \times 1024$  cells, with a linear size of  $1024\Delta$ . In order to reduce the numerical truncation error when computing the potential field, a refining stage of degree 4 was performed (Romeu and Noetinger, 1995, Liu and Wang, 2013), resulting in a grid of  $4096 \times 4096$  computational cells of linear size  $\Delta/4$ .

Binary random media is generated as follows: We start by generating a lognormal one with an arbitrary geometric mean  $K_g$  and variance  $\sigma_{\log k}^2$ . Then, this lognormal distribution is binarized using a threshold value  $k_t$ , assigning each cell a characteristic  $k^+$  (high conductivity) or  $k^-$  (low conductivity) value (with  $k^+/k^- = 10^4$ ). The value of  $k_t$  controls the relative population  $p$  of high conductivity cells. Three values of  $p$  were studied, one at the 2D percolation threshold  $p_c = 0.5$ , one smaller ( $p = 0.4$ ) and one greater ( $p = 0.6$ ) than  $p_c$ . At  $p_c$ , 50% of the realizations percolate. We used CONNECT3D software (Pardo-Igúzquiza and Dowd, 2003) to explicitly verify the percolation condition.

The spatial correlation function of the resulting binary medium remains gaussian. In turn, the integral scale of the binary medium is determined by the integral scale of the original lognormal medium, but also by  $p$ . To be able to use the former as an input parameter, we've performed an iterative search for each of the values of  $p$  studied. Fig. 3 (right) shows, as an example, a realization of such a binary medium.

For each set of parameters, we generated 50 samples in order to obtain an acceptable statistical sampling at largest scale  $L$ .

## 6.2. Potential field calculation

For the  $K_{ave}$  and  $K_{diss}$  formulations, it is only required to solve the potential in  $\Omega$  once, and then post-processing of the obtained field is performed to obtain  $K_{eff}$  at any scale  $\lambda$ . For the  $K_{perm}$  formulation, the potential must be solved independently for all the sub-domains  $\vartheta$  under study.



To obtain the potential field we used MODFLOW-2005<sup>1</sup> software (Harbaugh, 2005) with the corresponding boundary conditions. This solver uses the finite difference method with a classical  $2D + 1$  point stencil. Particularly, the *Block-Centered Flow package (BCF6)* was used, and the linear equation system was solved with the *Preconditioned Conjugate-Gradient package (PCG)*.

### 6.3. Implementation of the permeameter scheme

We used classical permeameter boundary conditions in the computation of the potential fields. In MODFLOW, these boundary conditions are applied assigning constant potentials (Dirichlet type) to two opposite cell layers, each of them representing a domain face. A unitary potential difference ( $\Delta P$ ) between them is set. All other faces are constrained by no-flow boundary conditions (Neumann type) applied to ghost cell layers outside the domain. These boundary conditions are applied at  $\partial\vartheta$  to compute  $K_{perm}$  defined as

$$K_{perm} = \frac{Q}{\lambda \Delta P}, \quad (17)$$

The integral of the flow,  $Q$ , is calculated at the inlet or the outlet face of the block  $\vartheta$  with permeameter boundary conditions. For each medium,  $K_{perm}$  was computed for the whole set of subscales  $\lambda = 2^n$ , with integer  $n$  between 1 and 10, resulting in  $(\frac{L}{\lambda})^2 = 2^{2(10-n)}$  values at each subscale. The same procedure was followed for the other two estimators.

### 6.4. Implementation of the dissipation scheme

Based on the resulting potential field computed using MODFLOW with permeameter boundary conditions (Sections 6.2 and 6.3) on domain  $\Omega$ , and the theoretical development presented in Section 5.1, the dissipation-based block estimator computation is as follows. As the finite difference scheme adopted in MODFLOW is cell centered, after solving the potential field in  $\Omega$ , both the hydraulic conductivity  $k_{i,j}$  and potential  $P_{i,j}$  at each cell center are known. Notations are referred to cell  $(i, j)$  of  $\vartheta$ , where  $(i - 1, j)$ ,  $(i + 1, j)$ ,  $(i, j - 1)$  and  $(i, j + 1)$  are the left, right, top and bottom neighbouring cells respectively. Using an electrical analogy, the local cell dissipation can be computed as

$$\begin{aligned} \epsilon_{i,j} &= \int_{\vartheta_{i,j}} d^2\mathbf{r} k_{i,j} (\nabla p)^2 \\ &= 2k_{i,j} \left[ (P_{i+\frac{1}{2},j} - P_{i,j})^2 + (P_{i-\frac{1}{2},j} - P_{i,j})^2 + (P_{i,j+\frac{1}{2}} - P_{i,j})^2 + (P_{i,j-\frac{1}{2}} - P_{i,j})^2 \right] \end{aligned} \quad (18)$$

The factor  $2k_{i,j}$  corresponds to the conductivity of the half bond between the center and any face of  $\vartheta_{i,j}$ . The potential subscript with minus or plus halves

---

<sup>1</sup><https://water.usgs.gov/ogw/modflow/mf2005.html>

refer to cell face potentials computed invoking the equality of flux at both sides of the face. For example the potential on the left face of cell  $(i, j)$  is given by:

$$P_{i-\frac{1}{2},j} = \frac{(k_{i,j}P_{i,j} + k_{i-1,j}P_{i-1,j})}{(k_{i,j} + k_{i-1,j})}.$$

The other cell face potentials are defined analogously. Using equivalent equations to eliminate face potentials in Eq. (18), we get:

$$\epsilon_{i,j} = \frac{1}{2k_{i,j}} \left[ \left( T_{i+\frac{1}{2},j} (P_{i+1,j} - P_{i,j}) \right)^2 + \left( T_{i-\frac{1}{2},j} (P_{i-1,j} - P_{i,j}) \right)^2 + \left( T_{i,j+\frac{1}{2}} (P_{i,j+1} - P_{i,j}) \right)^2 + \left( T_{i,j-\frac{1}{2}} (P_{i,j-1} - P_{i,j}) \right)^2 \right].$$

The coefficients  $T_{.,.}$  are the usual intercell harmonic averages given by  $T_{i+\frac{1}{2},j} = \frac{2k_{i+1,j}k_{i,j}}{k_{i+1,j}+k_{i,j}}$  and  $T_{i,j+\frac{1}{2}} = \frac{2k_{i,j+1}k_{i,j}}{k_{i,j+1}+k_{i,j}}$ .

Ohm's law for dissipation can be recognized through the squares of the fluxes flowing through the faces. The cell face potentials are also used to compute the cell potential gradient as

$$\nabla P_{i,j}^T = \left[ \frac{P_{i+\frac{1}{2},j} - P_{i-\frac{1}{2},j}}{\Delta}, \frac{P_{i,j+\frac{1}{2}} - P_{i,j-\frac{1}{2}}}{\Delta} \right].$$

Thus, the averaged potential gradient of the block is

$$\overline{\nabla P} = \frac{\sum_{i,j} \nabla P_{i,j}}{n_i n_j},$$

with  $n_i, n_j$  the number of cells in each direction inside the block. In every case, the sum runs over all the fine grid-blocks included in  $\vartheta$ . Finally, the block dissipation-based estimator of Eq. (15) for block  $\vartheta$  is computed as

$$K_{diss}(\vartheta) = \frac{\sum_{i,j} \epsilon_{i,j}}{\lambda^2 \overline{\nabla P}^2}. \quad (19)$$

410 Fig. 4 presents the resulting dissipation maps for lognormal and binary media samples. A strong localization (channeling) effect may be noticed close to percolation threshold for the binary case.

### 6.5. Implementation of the block average conductivity scheme

Based on the computation of the potential field in  $\Omega$ , the second  $K_{eff}$  estimator can be defined in  $\vartheta$  as:

$$K_{ave} = \frac{\overline{Q}_x}{\lambda \overline{\nabla P}_x}. \quad (20)$$

415 This expression is based on a large-scale Darcy equation where  $\overline{Q}$  is the flow rate and  $\overline{\nabla P}$  the potential gradient, both averaged over the domain  $\vartheta$  of size  $\lambda$ . With the proper boundary conditions it is possible to recover the full hydraulic conductivity tensor (Bauer et al., 2008). In this study, we only considered the direction of the imposed potential difference  $\Delta P$ .

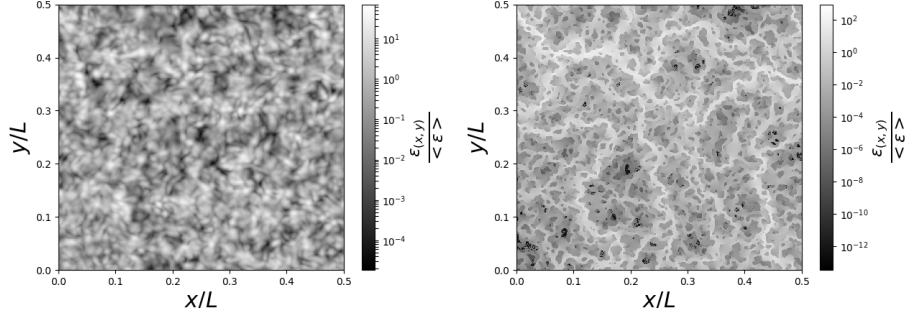


Figure 4: Local dissipation ( $\epsilon$ ) maps: (left) lognormal medium with  $\sigma_{\log k}^2 = 7$  and (right) binary medium with  $p = 0.5$ .

Table 1: Simulation parameter names, definitions and values

| Definition                             | Symbol                                | Values        |            |
|--|---------------------------------------|---------------|------------|
|  |                                       | Lognormal     | Binary     |
| Size of the full domain                | $L$                                   | 1024 $\Delta$ |            |
| Covariance function                    | $C(\mathbf{r})$                       | Gaussian      |            |
| Integral scale                         | $I$                                   | 16 $\Delta$   | 8 $\Delta$ |
| Fine grid geometric mean $K_g$ [m/day] | $K_g$                                 | 1             |            |
| Fine grid variance of $\log(K)$        | $C_{\log k}(r=0) = \sigma_{\log k}^2$ | 0.1; 7        |            |
| Characteristic conductivity [m/day]    | $k^+; k^-$                            | 100; 0.01     |            |
| Proportion of cells with $k^+$         | $p$                                   | 0.4; 0.5; 0.6 |            |

## 7. Results

420 We begin this section by comparing, as a form of validation, the outcomes of the analytical developments of Section 4, for lognormal media, with the corresponding numerical results using the well-known  $K_{perm}$  estimator. Then, for both type of media, we study the scale-dependence of the pdf of the three proposed estimators, to later focus on the first two gaussian moments i.e. mean  
425 and variance. For this latter case, a comparison with the mean-field analytical variance of  $K_{eff}$ , Eq. (13), is performed.

### 7.1. Comparison of the different analytical expressions for $C_{K_{eff}}(\lambda)$ with numerical results

430 Fig. 5 shows the variance of  $K_{eff}$  given by Eqs. (13) and (14), and their equivalent expressions within the mean-field approximation, compared with the  $K_{perm}$  estimator, as a function of the coarsening scale  $\lambda$ , that varies between fine grid scale  $\Delta$  and  $L$ . A low ( $\sigma_{\log k}^2 = 0.1$ ) and a high ( $\sigma_{\log k}^2 = 7$ ) fine grid variance are used as extreme cases.

435 The analytical results are in good agreement with the numerical simulations for  $\sigma_{\log k}^2 = 0.1$  when using the expressions based on the conductivity variance

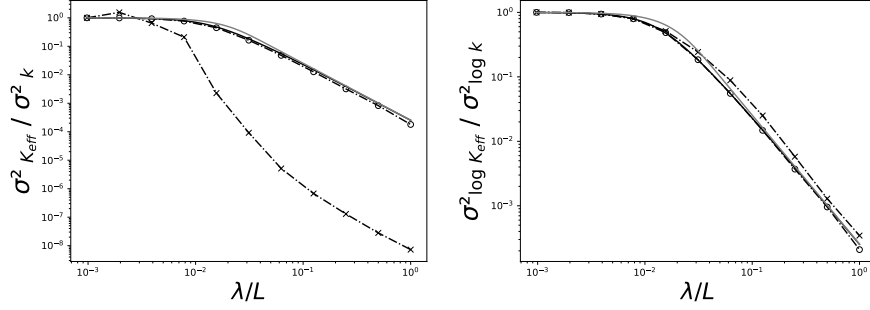


Figure 5: Analytical and numerical results for Gaussian covariance media. (Left)  $\sigma_{K_{eff}}^2$  compared against Eqs. (13) and (14). (Right)  $\sigma_{\log K_{eff}}^2$  compared against Eqs. (13) and (14) using the mean-field approximation. ( - - - ) Numerical; ( — ) Analytical; ( — ) Simplified analytical. Input variance: (o)  $\sigma_{\log k}^2 = 0.1$ , (x)  $\sigma_{\log k}^2 = 7$ .

$\sigma_{K_{eff}}^2$  (Eqs. (13) and (14)). The difference increases for the case of  $\sigma_{\log k}^2 = 7$ , specially for scales equal or greater than the integral scale, defined as the practical range of the covariance function. The estimation of the variance of the logarithm,  $\sigma_{\log K_{eff}}^2$  (Appendix C.1) provides a better agreement with the numerical results even for  $\sigma_{\log k}^2 = 7$ . In this case, the analytical equations correctly capture the tendency as the scale increases, with small discrepancy from the numerical results beyond the integral scale. In both cases, the simplified formulas (Eq. (14)) coincide to a large extent with the complete ones except at the scales close to the integral scale, where a small difference appears. In view of these observations, comparison against analytical results in the next sections will be only carried out with respect to Eq. (13) using the mean-field approximation.

## 7.2. Lognormal media

### 7.2.1. Probability density function of the different estimators

Pdf's of  $K_{diss}$ ,  $K_{ave}$  and  $K_{perm}$  are plotted in Fig. 6 (left) for  $\sigma_{\log k}^2 = 7$ . Although  $K_{diss}$  and  $K_{ave}$  present a sharper pdf, they are rather similar. The dependence of the pdf of  $K_{diss}$  with the coarsening scale  $\lambda$  is shown in Fig. 6 (right). It can be observed that the pdf remain Gaussian at all scales. As a Gaussian pdf is fully described by its mean and variance, in the following subsection, we focus our attention on these two moments..

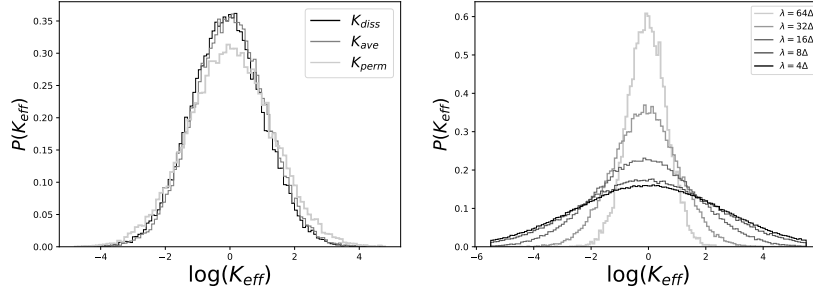


Figure 6: Pdf's of  $\log(K_{eff})$ . Input data:  $\sigma_{\log k}^2 = 7$ ,  $I=16\Delta$ . (Left) For the three estimators at  $\lambda = 32\Delta$ . (Right) Pdf of  $K_{diss}$  for  $\lambda = 4, 8, 16, 32$  and  $64\Delta$ .

455 *7.2.2. Scale dependence of the mean and variance of  $K_{eff}$*

Fig. 7 compares the values of the geometric mean of  $K_{eff}$ , indicated by  $\langle\langle \dots \rangle\rangle$  (left), and the variance  $\sigma_{\log K_{eff}}^2$  scaled by  $(\frac{\lambda}{I})^2$  (see Appendix C) (right) for the three estimators. As  $\lambda$  tends to  $\Delta$ ,  $\langle\langle K_{eff} \rangle\rangle$  approaches to the fine scale mean  $K_g$  for both variances. For  $\sigma_{\log k}^2 = 0.1$ , the three formulations yield very similar results, while for  $\sigma_{\log k}^2 = 7$  some discrepancies are observed. Moreover, for  $\lambda$  close to  $I$ , a depart from the theoretical value (of upto 12%) is observed for  $K_{diss}$ . We recall that, as developed in Section 5.1.1, if  $\vartheta = \Omega$ , the potential gradients transverse to the mean flow vanish, due to the boundary conditions applied at that scale in all cases, but, if  $\vartheta < \Omega$ , these gradients may exist and be non negligible. Also, they are stronger as the heterogeneity increases, explaining the slump in  $K_{diss}$  for  $\lambda$  close to  $I$ .

The variances of  $K_{eff}$  were evaluated analytically using the mean-field approximation of Eq. (13). In Fig. 7 (right), the variances of the three estimators show an excellent agreement with the analytical results for  $\sigma_{\log k}^2 = 0.1$ , while, for  $\sigma_{\log k}^2 = 7$ , a slight difference for  $\lambda > I$  is observed for the three estimators, probably due to discretization effects (Romeu and Noetinger, 1995).

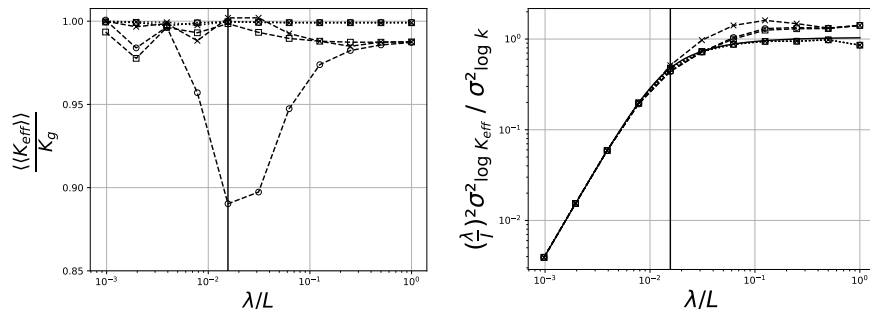


Figure 7:  $K_{eff}$  as a function of  $\lambda$ , for the three estimators, for lognormal media: (left) geometric mean and (right) rescaled variance  $\frac{\lambda^2}{L^2} C_{\log K_{eff}}$ . Input variance: ( $\cdots$ )  $\sigma_{\log k}^2 = 0.1$ , ( $--$ )  $\sigma_{\log k}^2 = 7$ . Upscaling method: ( $\times$ )  $K_{perm}$ , ( $\circ$ )  $K_{diss}$ , ( $\square$ )  $K_{ave}$ . The vertical line indicates the integral scale. ( $—$ ) Analytical variance Eq. (13) using the mean-field approximation.

### 7.3. Binary media

#### 7.3.1. Probability density functions of the $K_{eff}$ estimators

In binary media, the lower limiting case is when the upscaling scale  $\lambda$  tends to the fine grid scale  $\Delta$ , with only two possible conductivity values:  $k^+$  with probability  $p$ , and  $k^-$  with probability  $(1-p)$ . Consequently, the pdf of the effective conductivity tends to a two-peaked distribution with relative heights given by  $p$  and  $(1-p)$ , and its mean is similar to that of the original medium at the fine grid scale. On the other hand, the upper limit corresponds to the upscaling scale reaching the domain scale  $L$ . In this case, the pdf of the effective conductivity looks more like a unimodal distribution with its mean approaching  $k^+$  when  $p > p_c$ , and  $k^-$  when  $p < p_c$ . At intermediate scales, a transition between both extreme behaviors occurs. Pdf's of  $K_{diss}$ ,  $K_{ave}$  and  $K_{perm}$  are plotted in Fig. 8 in order to compare them with the expected behavior. Three situations, with  $p$  smaller, close to and greater than  $p_c = 0.5$  (for which percolation transition occurs), are shown in this figure.

In the left column of the figure, the three methods are compared for  $\lambda = 32\Delta$ . At this intermediate scale different behaviors are observed depending on the method. The pdf's of the three estimators considered here exhibit some differences: the  $K_{perm}$  estimator presents more peaked distributions with two clearly separated modes while those of global methods,  $K_{diss}$  and  $K_{ave}$ , are relatively more homogeneous, with a continuous variation between the peaks. Also, the values of conductivity corresponding to the facies that does not percolate are only retained in the case of  $K_{perm}$ , while  $K_{diss}$  and  $K_{ave}$  smooth them out. This is a direct effect of the permeability boundary conditions that are imposed for each sub domain  $\vartheta$  when computing  $K_{perm}$ . This renders percolation in  $\vartheta$  much more critical for  $K_{eff}$ . On the other hand, analyzing the behavior when small, middle and large scales are adopted for  $\lambda$ , the expected behavior is recovered.  $K_{diss}$  converges to a unimodal distribution as  $\lambda$  increases, faster as

500  $p$  departs from  $p_c$ , as it was observed in a previous study for  $K_{perm}$  (Boschan and Noetinger, 2012). In addition, as  $p$  departs from  $p_c$ , for a given  $\lambda$ , the distributions become narrower. This implies that the convergence to a representative mean is slower near percolation.

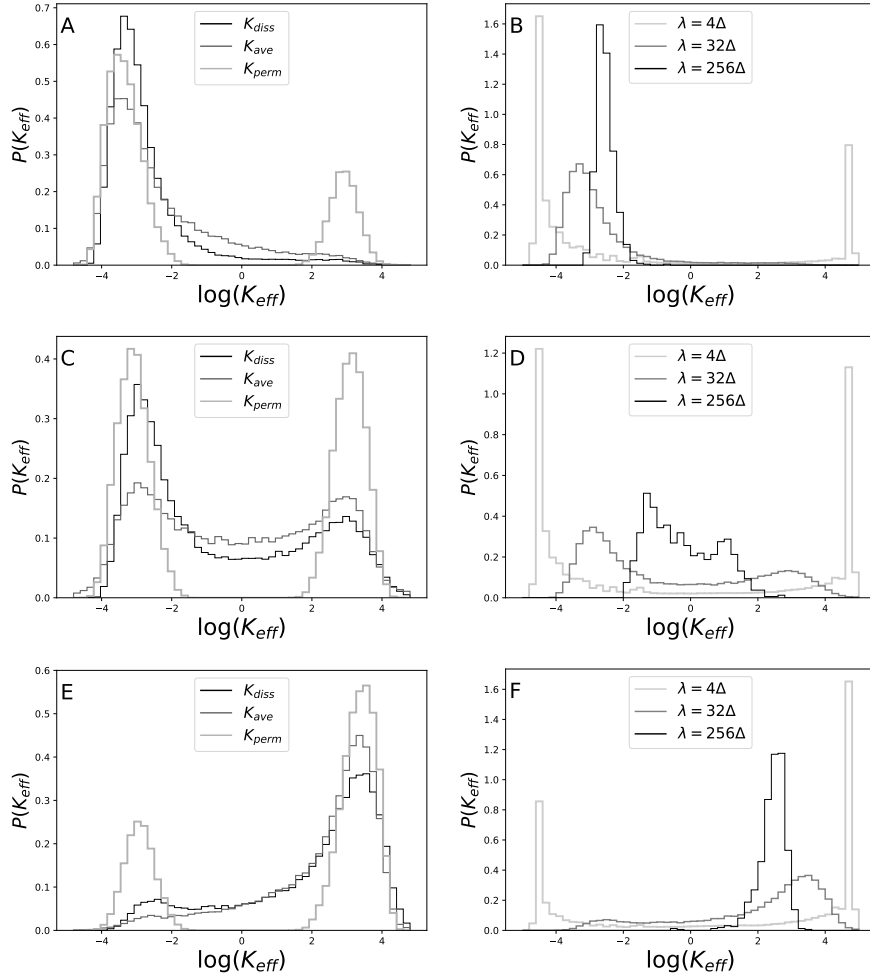


Figure 8: Pdf's of the effective conductivity  $\log(K_{eff})$  resulting from the three studied estimators. Input data: relative population  $p = 0.4$ ,  $p = 0.5$  and  $p = 0.6$  (top to bottom). (Left) Results obtained with the three methods for  $\lambda = 32\Delta$ . (Right)  $K_{diss}$  results for three block sizes  $\lambda = 4$ ,  $32$ , and  $256 \Delta$ .

### 7.3.2. Scale dependence of the mean and variance of $K_{eff}$

505 In the binary case, as it is clearly seen in Fig. 8, the pdf's of  $K_{eff}$  are far from being unimodal, and then, the mean and variance become less representative

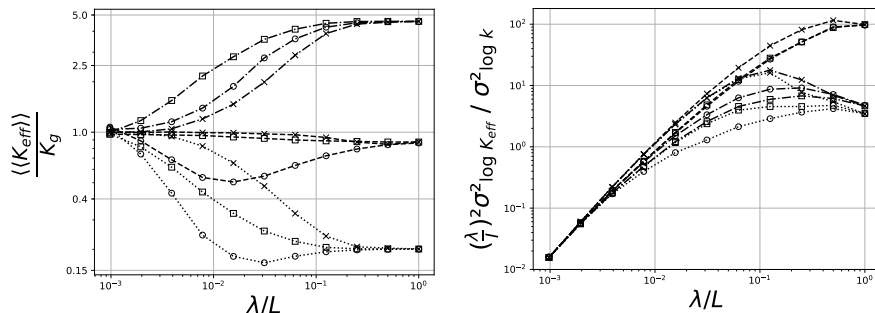


Figure 9: Dependence of the three estimators of  $K_{eff}$  with the scale in binary media: (left) geometric mean and (right) rescaled variance  $\frac{\lambda^2}{L^2} C_{\log K_{eff}}$ . Input data: ( $\cdots$ )  $p = 0.4$ , ( $-\ -$ )  $p = 0.5$ , ( $-\cdot-$ )  $p = 0.6$ . Upscaling method: ( $\times$ )  $K_{perm}$ , ( $\circ$ )  $K_{diss}$ , ( $\square$ )  $K_{ave}$ .

of the pdf, compared with the lognormal case (cf. section 7.2.1). For example, one may note that, in panel C of Fig. 8, the mean would not be particularly representative. However, previous studies analyzed the mean and variance much more frequently than the complete pdf, so we consider interesting to present them for comparison.

Fig. 9 shows the variation of geometric mean of  $K_{eff}$  (left), and of the variance  $\sigma_{\log K_{eff}}^2$  (right), for the three estimators, as a function of  $\lambda$  for  $p = 0.4$ ,  $p = 0.5$  and  $p = 0.6$ . The values of  $\langle\langle K_{eff} \rangle\rangle$  coincide as  $\lambda$  tends to the limiting  $\Delta$  or  $L$ , for all the values of  $p$ . The behavior at both limits of the range corresponds to which is expected for a representative effective conductivity. Furthermore, the behavior far from those extreme values is strongly dependent on the particular estimator. As observed in Fig. 8, the two peaks in the  $K_{perm}$  histogram remained clearly identifiable at larger  $\lambda$  values, in opposition to what happened in the cases of  $K_{diss}$  or  $K_{ave}$ . The outcome is that if  $p$  is far from  $p_c$ ,  $K_{perm}$  converges more slowly than  $K_{diss}$  or  $K_{ave}$  to the asymptotic value of  $\lambda = L$ . This is consistent with the faster homogenization shown by the global estimators in the pdf's of section 7.3.1. Comparing  $K_{diss}$  and  $K_{ave}$ , the former shows a slight bias to lower  $\langle\langle K_{eff} \rangle\rangle$  values.

The variance  $\sigma_{\log K_{eff}}^2$  computed using the three formulations also coincides as  $\lambda$  tends to  $\Delta$  or  $L$ . At intermediate scales,  $K_{perm}$  always yields the highest  $\sigma_{\log K_{eff}}^2$ , in agreement with the findings shown in section 7.3.1, where it was shown that the pdf remained bimodal for a greater  $\lambda$  than for the other two methods. Note that, in the non percolating case ( $p = 0.4$ ),  $K_{diss}$  produces lower variances than  $K_{ave}$ , while the opposite happens for the percolating case ( $p = 0.6$ ), and, at  $p_c = 0.5$ , both estimators yield similar values of  $\sigma_{\log K_{eff}}^2$ .

## 8. Summary, discussion and perspectives

After introducing an efficient  $K_{eff}$  estimator based on energy dissipation, we revisited numerically and analytically three of the most important upscaling



535 formulations, analyzing the scale dependence of the resulting  $K_{eff}$  distributions.

For 2D lognormal media,  $K_{eff}$  distributions remain lognormal at intermediate coarsening scales for all the formulations, a result that could be theoretically related to the LLM formula (Landau and Lifshitz, 1960, Matheron, 1967). The numerical results for  $\langle\langle K_{eff} \rangle\rangle$  and  $\sigma_{\log K_{eff}}^2$  are in agreement with the analytical ones. This is notable for intermediate coarsening scales, having in mind 540 that these last results are not exact. In particular, the asymptotic behavior of  $\sigma_{\log K_{eff}}^2$  for  $\lambda > I$ , varying as  $(1/\lambda)^2$ , is reminiscent to a central limit theorem.

In the binary case, for  $p$  far from  $p_c$ , the pdf of  $K_{eff}$  evolves from a bimodal to a unimodal distribution, with representative mean and variance. The mean 545 and variance of the three estimators converge to the same asymptotic  $K_{eff}$  values for  $p = 0.4$  or  $0.6$ . It can be observed that the latter obeys the scaling law with  $1/\lambda^2$  in that case. Close to percolation threshold  $p_c$ , the intermediate-scale  $K_{eff}$  distributions do not exhibit convergence to an asymptotic stable distribution. The  $\langle\langle K_{eff} \rangle\rangle$  remains close to the fine grid geometric mean  $K_g$ . 550 This may be explained by the fact that in 2D, at  $0.5 = p_c$ , the analytical result of Matheron (1967) can be applied, yielding the geometric average in that very specific case. Looking more carefully to Fig. 9, for  $p = p_c$ ,  $\sigma_{\log K_{eff}}^2$  does not follow the scaling law in  $1/\lambda^2$ . This should be related to the absence of a representative elementary volume (Berkowitz and Balberg, 1993, Hunt et al., 555 2014, Stauffer and Aharony, 2014). Quantification of such effects remains to be studied, and  $K_{eff}$  estimators that comply to finite size scaling arguments might improve the existing description.

The computation of  $K_{eff}$  through  $K_{ave}$  and  $K_{diss}$  is much more efficient than using  $K_{perm}$ , because, in this case, the potential is solved once for  $\Omega$ , 560 and then by post-treating this solution,  $K_{eff}$  can be obtained at all scales if a multiscale description is required, while providing similar results. Using  $K_{perm}$  involves solving the potential independently for each scale, due to the strong influence of the boundary conditions imposed at  $\partial\vartheta$ .

Now comparing  $K_{ave}$  and  $K_{diss}$ , we illustrate the degree of discrepancy 565 between these two estimators as a function of the coarsening scale, showing in Fig. 10 the ratio between the geometric mean of  $K_{ave}$  and that of  $K_{diss}$ . It can be observed that the greater discrepancy occurs, both for lognormal and binary media, for  $\lambda \approx I$ , where  $I$  is the practical range of the covariance function as measured in both types of media samples, giving a characteristic lengthscale for heterogeneity. Note that  $K_{diss}$  (see section 5.1) is sensible to transverse potential 570 gradients, while  $K_{ave}$  isn't, because it assumes a colinearity between potential gradient and flow. These transverse potential gradients vanish at  $\lambda = \Delta$  and at  $\lambda = L$ , while they have a maximum in-between, at a critical lengthscale, despite that media samples are statistically isotropic. The degree of discrepancy is then probably driven by the scale dependence of these transverse potential gradients.

575 Except for the lognormal case of  $\sigma_{\log k}^2 = 0.1$ ,  $K_{diss}$  is smaller than  $K_{ave}$  up to 12% in the lognormal case of  $\sigma_{\log k}^2 = 7$ , and up to 80% in the binary case. The bias of  $K_{diss}$  towards lower values was also observed in the pdf's shown in the sections 7.2.1 and 7.3.1.

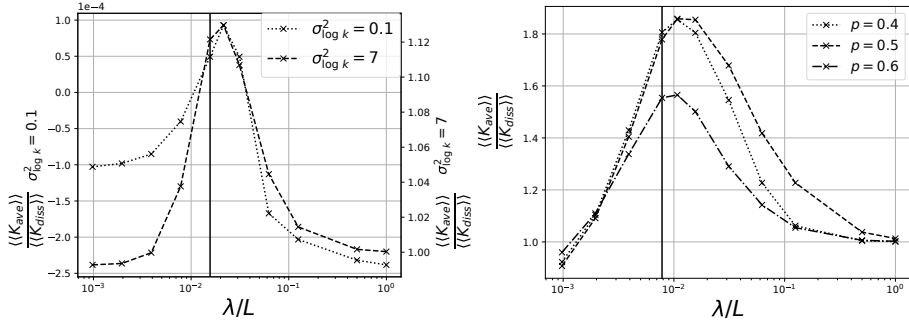


Figure 10: Discrepancy between the geometric mean of  $K_{diss}$  and that of  $K_{ave}$ . (Left) Results for lognormal media, Section 7.2.2. (Right) Results for binary media, Section 7.3.2. ( ) Integral scale.

580 The 3D generalization of this work is currently under development. In partic-  
ular, the appearance of an attractive conductivity distribution for the different  
formulations, playing in 3D an analogous role to the lognormal distribution in  
2D, is of central interest. Moreover, for binary media, it is highly interesting  
to assess the slower convergence to an homogeneous  $K_{eff}$  distribution close to  
585 the percolation transition in 3D media in the context of the different formu-  
lations. More realistic or complex distributions such as non Gaussian or power-law  
(Panzeri et al., 2016, Riva et al., 2017, Guadagnini et al., 2018) will be addressed  
in future work. A major practical issue regarding non-homogeneous materials  
is to find some self-contained estimation of the REV size allowing to determine,  
590 for a given case, if the REV size is reached. That will help to find the optimal  
meshing size, and to quantify uncertainty propagation.

## Appendix A. Functional differentiation

Functional differentiation is a generalization of calculus to functionals, i.e.,  
functions having a function as argument. Our presentation is intuitive. Let  
 $F(\{k\})$  be a functional that depends on the whole set of values of  $k$  which is  
an arbitrary function of position  $\mathbf{r} \in \Omega$ . The notation  $\{\dots\}$  recalls that  $F$  is a  
functional. Examples of functional can be the value of field  $k$  at a given location  
 $\mathbf{r}_0$ :  $F_0(\{k\}) = k(\mathbf{r}_0)$ , the weighted average  $F_{\langle \dots \rangle_f}(\{k\}) = \frac{1}{|\mathcal{V}|} \int_{\mathcal{V}} d^D \mathbf{r} f(\mathbf{r}) k(\mathbf{r})$   
in which  $f(\mathbf{r})$  is a fixed function that does not depend on  $k$ . The functional  
derivative of a functional  $F(\{k\})$  is defined by the following equation:

$$Lim_{\epsilon \rightarrow 0} \frac{F(\{k + \epsilon \delta k\}) - F(\{k\})}{\epsilon} = \int_{\mathcal{V}} d^D \mathbf{r} \frac{\delta F}{\delta k(\mathbf{r})} \delta k(\mathbf{r})$$

Here,  $\delta k$  is an arbitrary perturbation. The functional derivative has a supple-  
mentary spatial argument (that corresponds in the case of partial derivatives to

the choice of the variable with respect to which the derivative is performed). In the examples of  $F_0(\{k\})$  and  $F_{<\dots>f}(\{k\})$ , one has

$$\frac{\delta F_0}{\delta k(\mathbf{r})} = \delta((\mathbf{r} - \mathbf{r}_0))$$

$$\frac{\delta F_{<\dots>f}}{\delta k(\mathbf{r})} = \frac{f(\mathbf{r})}{|V|}$$

It gives the sensibility of the variation of  $F$  with respect to a local variation of its argument  $k$  at position  $\mathbf{r}$ . N-th order functional derivatives can be defined, as well as a Taylor formula, replacing summations by integrations.

If  $f(x)$  is a standard differentiable real function, one has the chain derivative formula:

$$\frac{\delta f(F)}{\delta k(\mathbf{r})} = \frac{df}{dx}(F) \frac{\delta F}{\delta k(\mathbf{r})}$$

If  $p(\mathbf{r})$  obeys a Laplace equation such as

$$\nabla \cdot (k(\mathbf{r}) \nabla p(\mathbf{r})) = 0,$$

Putting  $k(\mathbf{r}) = k + \delta k(\mathbf{r})$ , one obtains:

$$\nabla \cdot [(k + \delta k(\mathbf{r})) (\nabla p(\mathbf{r}) + \nabla \delta p(\mathbf{r}))] = 0,$$

Denoting by  $\delta p(\mathbf{r})$  the first order variation of potential  $p(\mathbf{r})$  with respect to  $k(\mathbf{r})$ , one obtains that  $\delta p(\mathbf{r})$  obeys the following equation, valid at first order:

$$\nabla \cdot (k \nabla \delta p(\mathbf{r})) = -\nabla \cdot [\delta k(\mathbf{r}) \nabla p(\mathbf{r})] \quad (\text{A.1})$$

As the unperturbed potential  $p(\mathbf{r})$  fulfills the boundary conditions at the domain boundary,  $\delta p(\mathbf{r}) = 0$  on Dirichlet boundaries, and same conditions for the normal flux at the Neumann boundaries. This equation has the formal solution:

$$\delta p(\mathbf{r}) = - \int_V d^D \mathbf{r}' G_k(\mathbf{r}, \mathbf{r}') \nabla \cdot [\delta k(\mathbf{r}') \nabla p_0(\mathbf{r}')]. \quad (\text{A.2})$$

Here,  $G_k(\mathbf{r}, \mathbf{r}')$  is the Green's function of the Laplace operator that obeys the following equations, to be supplemented by consistent boundary conditions:

$$\nabla \cdot (k \nabla G_k(\mathbf{r}, \mathbf{r}')) = \delta(\mathbf{r} - \mathbf{r}')$$

$$G_k(\mathbf{r}_{\mathbf{x}} = 0, 1, \mathbf{r}') = 0, \quad \partial_y G_k(\mathbf{r}_{\mathbf{y}} = 0, 1, \mathbf{r}') = 0$$

So one gets finally after one integration by parts:

$$\frac{\delta p(\mathbf{r})}{\delta k(\mathbf{r}')} = \nabla_{\mathbf{r}'} G_k(\mathbf{r}, \mathbf{r}') \cdot \nabla p_0(\mathbf{r}') \quad (\text{A.3})$$

This result may recovered directly, applying the operator  $\frac{\delta}{\delta k(\mathbf{r}' )}$  at both sides of Eq. (3), providing:

$$\nabla \cdot \left( k \nabla \frac{\delta p(\mathbf{r})}{\delta k(\mathbf{r}')} \right) = -\nabla \cdot [\delta((\mathbf{r}' - \mathbf{r}) \nabla p(\mathbf{r}))],$$

which is equivalent to Eq. (A.3). Note that the base conductivity field  $k$  may also depend on position, or be equal to  $\langle k \rangle$ , the choice depends on the application at hand.

## Appendix B. Second order estimation of the average effective conductivity

600

In order to illustrate the functional formalism, we carry out with this tool the classical second order expansion of the effective conductivity (Dagan, 1989). The Taylor expansion Eq. (10), gives directly a second order series expansion that will provide the desired expansion after averaging:

$$\langle K_{eff} \rangle = \langle k \rangle + \frac{1}{2} \int_{\Omega} d^D \mathbf{r} d^D \mathbf{r}' \frac{\delta^2 K_{eff}}{\delta k(\mathbf{r}) \delta k(\mathbf{r}')} C_k(\mathbf{r}' - \mathbf{r}). \quad (\text{B.1})$$

The main task is to evaluate explicitly the second order functional derivative that may be simplified in the following form, using Eq. (C.1) differentiated once more time:

$$\frac{\delta^2 K_{eff}}{\delta k(\mathbf{r}) \delta k(\mathbf{r}')} = \frac{1}{|\Omega|} 2 \nabla p_0(\mathbf{r}) \cdot \nabla \frac{\delta p(\mathbf{r})}{\delta k(\mathbf{r}'')}$$

In that equation,  $p_0(\mathbf{r})$  is the non-perturbed potential. The derivative  $\frac{\delta p(\mathbf{r})}{\delta k(\mathbf{r}'')}$  is given by Eq. (A.2). So, we get after substitution:

$$\frac{\delta p(\mathbf{r})}{\delta k(\mathbf{r}'')} = \frac{1}{\langle k \rangle} \nabla G(\mathbf{r}, \mathbf{r}'') \cdot \nabla p_0(\mathbf{r}''). \quad (\text{B.2})$$

In that expression,  $G(\mathbf{r}, \mathbf{r}')$  is the Green's function of Laplace operator  $\nabla^2$ , this explains the factor  $\frac{1}{\langle k \rangle}$ . Note that due to the boundary conditions that break full translational invariance of the system, this Green's function does not depend only on the argument  $(\mathbf{r} - \mathbf{r}')$ . Gathering these results in Eq. (B.1), and using the fact that  $\nabla p_0(\mathbf{r}) = e_x$ , one obtains:

$$\begin{aligned} \langle K_{eff} \rangle &= \langle k \rangle - \frac{1}{\langle k \rangle |\Omega|} \int_{\Omega} d^D \mathbf{r} d^D \mathbf{r}' \nabla p_0(\mathbf{r}) \cdot \nabla \frac{\delta p(\mathbf{r})}{\delta k(\mathbf{r}')} C_k(\mathbf{r}' - \mathbf{r}) \\ &= \langle k \rangle - \frac{1}{\langle k \rangle |\Omega|} \int_{\Omega} d^D \mathbf{r} d^D \mathbf{r}' \partial_{r_x} \partial_{r'_x} G(\mathbf{r}, \mathbf{r}') C_k(\mathbf{r}' - \mathbf{r}) \end{aligned} \quad (\text{B.3})$$

Assuming that  $|\Omega|^{1/D}$  is large compared with the integral scale  $I$ , one can replace  $G(\mathbf{r}, \mathbf{r}')$  by the free space Green's function  $G(\mathbf{r} - \mathbf{r}')$ . This is equivalent to estimate the Green's function assuming that the boundary conditions are rejected at infinity.

Using the correlation function isotropy, the integral can be simplified using a classical trace argument, yielding:

$$\langle K_{eff} \rangle = \langle k \rangle - \frac{1}{\langle k \rangle} \frac{1}{D} C_k(\mathbf{r} = 0).$$



As we are seeking a second order expansion of the variance of effective conductivity, the local quantity  $\frac{\nabla p(\mathbf{r})^2}{\overline{\nabla p_{\Omega,x}^2}}$  (resp.  $\frac{\nabla p(\mathbf{r}')^2}{\overline{\nabla p_{\Omega,x}^2}}$ ) may be replaced by 1, getting:

$$C_{K_{eff}}(L) = \frac{1}{|\Omega|^2} \int_{\Omega} d^D \mathbf{r} d^D \mathbf{r}' \langle \delta k(\mathbf{r}) \delta k(\mathbf{r}') \rangle. \quad (\text{C.3})$$

After averaging, introducing the pair correlation function  $C_k(\mathbf{r}-\mathbf{r}') = \langle \delta k(\mathbf{r}) \delta k(\mathbf{r}') \rangle$  of the hydraulic conductivity fluctuations, we get a formula already obtained by Rubin and Gómez-Hernández (1990), Sánchez-Vila et al. (1995), Wen and Gómez-Hernández (1996):

$$C_{K_{eff}}(L) = \frac{1}{|\Omega|^2} \int_{\Omega} d^D \mathbf{r} d^D \mathbf{r}' C_k(\mathbf{r}-\mathbf{r}'). \quad (\text{C.4})$$

Note that for small averaging volume size  $L$  compared to the integral scale  $I$ , this formula gives by direct inspection  $C_{K_{eff}}(L) = C_k(r=0)$ . On the other limit, assuming that the unit volume size is very large compared to the underlying integral scale, one gets the asymptotic behavior:

$$C_{K_{eff}}(L) \approx \frac{1}{|\Omega|} \int_{\Omega} d^D \mathbf{r} C_k(\mathbf{r}). \quad (\text{C.5})$$

For large  $L$ , one has the scaling :

$$\frac{L^D}{I^D} C_{K_{eff}}(L) \approx \int_{\Omega} d^D \mathbf{r} \frac{C_k(\mathbf{r})}{I^D}. \quad (\text{C.6})$$

The factor  $L^D/I^D$  corresponds to the number of independent statistical units that belong to volume  $\Omega$ . This scaling corresponds thus to a central limit theorem characterizing the emergence of a deterministic large scale effective conductivity. In other words, the system exhibits self averaging properties. Eqs. (C.4) and (C.5) are solved for the particular case of the Gaussian covariance in Appendix C.2.

#### *Appendix C.1. Improved estimation of the variance, mean-field approximation*

The preceding development is limited to small variances. In order to find an improved approximation, one can use Eq. (C.2) written on an equivalent form:

$$\langle K_{eff}^2 \rangle - \langle K_{eff} \rangle^2 = \frac{1}{|\Omega|^2} \int_{\Omega} d^D \mathbf{r} d^D \mathbf{r}' \left\langle \frac{k(\mathbf{r}) \nabla p(\mathbf{r})^2}{\overline{\nabla p_{\Omega,x}^2}} \frac{k(\mathbf{r}') \nabla p(\mathbf{r}')^2}{\overline{\nabla p_{\Omega,x}^2}} \frac{\delta k(\mathbf{r})}{k(\mathbf{r})} \frac{\delta k(\mathbf{r}')}{k(\mathbf{r}')} \right\rangle + \dots$$

Now, one can replace  $k(\mathbf{r}) \nabla p(\mathbf{r})^2$  and  $k(\mathbf{r}') \nabla p(\mathbf{r}')^2$  by their common average value  $\langle K_{eff} \rangle \overline{\nabla p_{\Omega,x}^2}$ . So one gets:

$$\frac{\langle K_{eff}^2 \rangle - \langle K_{eff} \rangle^2}{\langle K_{eff} \rangle^2} = \frac{1}{|\Omega|^2} \int_{\Omega} d^D \mathbf{r} d^D \mathbf{r}' \left\langle \frac{\delta k(\mathbf{r})}{k(\mathbf{r})} \frac{\delta k(\mathbf{r}')}{k(\mathbf{r}')} \right\rangle + \dots$$

Up to this order of approximation, the result can be identified with the variance of  $\log(K_{eff})$  and the equation can be rewritten as:

$$\begin{aligned} C_{\log K_{eff}}(L) &= \langle (\log(K_{eff}))^2 - (\log(K_{eff})) \rangle^2 \\ &= \frac{1}{|\Omega|^2} \int_{\Omega} d^D \mathbf{r} d^D \mathbf{r}' \langle \delta \log k(\mathbf{r}) \delta \log k(\mathbf{r}') \rangle + \dots \end{aligned}$$

This equation, up to this order of approximation, is equivalent to Eq. (C.4), by replacing every occurrence of a conductivity by the corresponding logarithm, so:

$$C_{\log K_{eff}}(L) = \frac{1}{|\Omega|^2} \int_{\Omega} d^D \mathbf{r} d^D \mathbf{r}' C_{\log k}(\mathbf{r} - \mathbf{r}'). \quad (\text{C.7})$$

The resulting formula is similar to Eq. (C.4), replacing the covariance function by the log conductivity covariance function. For the special case of lognormal media, this is a quite natural transformation. The same can be done with the simplified formula (C.5).

### Appendix C.2. Gaussian covariance case

In the isotropic Gaussian case, the covariance function is given by

$$C_k(\mathbf{r}) = C_k(r=0) e^{-\frac{r^2}{2I_c^2}}$$

The integral factorizes, and after changing variables  $x \rightarrow x/I_c$ , we obtain:

$$\begin{aligned} C_{K_{eff}(L)} &= C_k(r=0) \left(\frac{I_c}{L}\right)^{2D} \left[ \int_{-L/2I_c}^{L/2I_c} \int_{-L/2I_c}^{L/2I_c} dx dy e^{-\frac{(x-y)^2}{2}} \right]^D \\ &= C_k(r=0) \left(\frac{I_c}{L}\right)^{2D} \left\{ \sqrt{\frac{\pi}{2}} \int_{-L/2I_c}^{L/2I_c} dy \left[ \operatorname{erf}\left(\frac{L/I_c - 2y}{2\sqrt{2}}\right) + \operatorname{erf}\left(\frac{L/I_c + 2y}{2\sqrt{2}}\right) \right] \right\}^D \\ &= C_k(r=0) \left(\frac{I_c}{L}\right)^{2D} \left[ \sqrt{2\pi} \frac{L}{I_c} \operatorname{erf}\left(\sqrt{2} \frac{L}{I_c}\right) + 2e^{-\frac{L^2}{2I_c^2}} - 2 \right]^D \quad (\text{C.8}) \end{aligned}$$

Considering small up-scaling volume,  $L$  small compared with  $I_c$ , we obtain  $C_{K_{eff}(L)} = C_k(r=0)$  as it should. In the opposite case, considering large up-scaling volumes  $L$  provides

$$C_{K_{eff}(L)} \simeq C_k(r=0) \left( \sqrt{2\pi} \frac{I_c}{L} \right)^D$$

This is a form of a central limit theorem for effective conductivity, quantifying the variance reduction leading to convergence of the effective conductivity for large averaging volume.

Finally, using the simplified expression (C.5), one gets after integration:

$$C_{K_{eff}}(L) \simeq C_k(r=0) \left[ \sqrt{2\pi} \frac{I_c}{L} \operatorname{erf}\left(2\sqrt{2} \frac{L}{I_c}\right) \right]^D \quad (\text{C.9})$$

It shares the same asymptotic behavior for extreme  $L$  than the exact (13). The same calculations can be carried out for  $C_{\log K_{eff}}(L)$  and give the same results using  $C_{\log k}(r=0)$  and the same spatial dependence.

## Appendix D. Second order evaluation of the average of block $K_{diss}$

The block equivalent conductivity  $K_{diss}(\vartheta)$  is given by Eq. (15). Decomposing the conductivity as  $k(\mathbf{r}) = \langle k \rangle + \delta k(\mathbf{r})$ , one can carry-out a second order expansion of  $K_{diss}(\vartheta)$ :

$$K_{diss}(\vartheta) = \frac{\int_{\vartheta} d^D \mathbf{r} (\langle k \rangle + \delta k) (\nabla(p_0 + \delta p))^2}{\lambda^D \overline{(\nabla(p_0 + \delta p))^2}}.$$

This formula must be expanded up to second order in a series expansion of  $\delta k$ . Note that the technique that was presented in Appendix B cannot be followed directly because the variational formulation is efficient at the scale of the whole  $\Omega$  only, not on every subvolume  $\vartheta$ . In order to simplify notations, we introduce  $\delta p(\mathbf{r})$  as the first order variation due to a variation  $\delta k(\mathbf{r})$ . The numerator can be expanded up to second order, discarding third order terms to yield:

$$\begin{aligned} \int_{\vartheta} d^D \mathbf{r} (\langle k \rangle + \delta k) (\nabla(p_0 + \delta p))^2 &\simeq \int_{\vartheta} d^D \mathbf{r} (\langle k \rangle + \delta k) (1 + 2\nabla p_0 \cdot \nabla \delta p) + \\ &+ \int_{\vartheta} d^D \mathbf{r} \langle k \rangle (\nabla \delta p)^2. \end{aligned} \quad (\text{D.1})$$

An analogous calculation can be carried out for the denominator, recalling that  $\nabla p_0(\mathbf{r}') = \mathbf{e}_x$ :

$$\lambda^D \overline{(\nabla(p_0 + \delta p))^2} = \lambda^D \left( \overline{(\nabla p_0)^2} + 2\overline{\nabla p_0 \cdot \nabla \delta p} + \overline{(\nabla \delta p)^2} \right) = \lambda^D \left( 1 + 2\overline{\nabla p_0 \cdot \nabla \delta p} + \overline{(\nabla \delta p)^2} \right) \quad (\text{D.2})$$

Combining Eq. (D.1) and the second order expansion of Eq. (D.2), many cancellations occur, yielding still at same order of approximation:

$$\begin{aligned} K_{diss}(\vartheta) &= \bar{k} + \frac{1}{\lambda^D} \left[ 2 \int_{\vartheta} d^D \mathbf{r} \delta k (\nabla p_0 \cdot \nabla \delta p - \overline{\nabla p_0 \cdot \nabla \delta p}) + \right. \\ &\quad \left. + \langle k \rangle \int_{\vartheta} d^D \mathbf{r} ((\nabla \delta p)^2 - \overline{(\nabla \delta p)^2}) \right] \end{aligned}$$

One has in the general case  $\overline{\nabla p_0} = \nabla p_0 = \mathbf{e}_x$ . It can be observed that in the case of small averaging volume  $\vartheta$ ,  $K_{diss}(\vartheta) = k(\mathbf{r})$  as it should: all the contributions cancel each other, because in that limit a volume average is equal to the local value:  $\overline{\nabla \delta p} = \nabla \delta p$ . Further simplifications can be obtained using Green's formula on the term  $\langle k \rangle \int_{\vartheta} d^D \mathbf{r} (\nabla \delta p)^2$  combined with Eq. (A.1) that drives  $\delta p$ , yielding:

$$\begin{aligned} K_{diss}(\vartheta) &= \bar{k} + \frac{1}{\lambda^D} \int_{\vartheta} d^D \mathbf{r} \delta k \nabla p_0 \cdot \nabla \delta p - \\ &\quad - \frac{1}{\lambda^D} \left( 2 \int_{\vartheta} d^D \mathbf{r} \delta k \overline{\nabla p_0 \cdot \nabla \delta p} + \int_{\vartheta} d^D \mathbf{r} \langle k \rangle \overline{(\nabla \delta p)^2} \right) + \\ &\quad + \frac{\langle k \rangle}{\lambda^D} \int_{\partial \vartheta} d^{D-1} \mathbf{r} \delta p \nabla \delta p \cdot \mathbf{n} + \frac{1}{\lambda^D} \int_{\partial \vartheta} d^{D-1} \mathbf{r} \delta k \delta p \nabla p_0 \cdot \mathbf{n}. \end{aligned} \quad (\text{D.3})$$



We obtain after statistical averaging:

$$\begin{aligned} \langle K_{diss}(\vartheta) \rangle = \langle k \rangle &- \frac{1}{\lambda^D} \int_{\vartheta} d^D \mathbf{r} \int_{\Omega} d^D \mathbf{r}' \nabla p_0(\mathbf{r}) \cdot \nabla \frac{\delta p(\mathbf{r})}{\delta k(\mathbf{r}')} C(\mathbf{r}' - \mathbf{r}) - \\ &- \frac{1}{\lambda^D} \int_{\vartheta} d^D \mathbf{r} \left( 2 \langle \delta k \overline{\nabla p_0} \cdot \overline{\nabla \delta p} \rangle + \langle k \rangle \langle \overline{\nabla \delta p}^2 \rangle \right) + \\ &+ \frac{\langle k \rangle}{\lambda^D} \int_{\partial \vartheta} d^{D-1} \mathbf{r} \langle \delta p \nabla \delta p \cdot \mathbf{n} \rangle + \frac{1}{\lambda^D} \int_{\partial \vartheta} d^{D-1} \mathbf{r} \langle \delta k \delta p \rangle \nabla p_0 \cdot \mathbf{n}. \end{aligned}$$

Using

$$\frac{\delta p(\mathbf{r})}{\delta k(\mathbf{r}')} = \frac{1}{\langle k \rangle} \nabla \cdot [G(\mathbf{r}, \mathbf{r}') \nabla p_0(\mathbf{r}')],$$

and combining this result with Eq. (D.2), one obtains:

$$\begin{aligned} \langle K_{diss}(\vartheta) \rangle = \langle k \rangle &- \frac{1}{\langle k \rangle \lambda^D} \int_{\vartheta} d^D \mathbf{r} \int_{\Omega} d^D \mathbf{r}' \partial_{r_x} \partial_{r'_x} G(\mathbf{r}, \mathbf{r}') C_k(\mathbf{r}' - \mathbf{r}) - \\ &- \frac{1}{\lambda^D} \int_{\vartheta} d^D \mathbf{r} \left( \langle 2 \delta k \overline{\nabla p_0} \cdot \overline{\nabla \delta p} \rangle + \langle k \rangle \langle \overline{\nabla \delta p}^2 \rangle \right) + \\ &+ \frac{\langle k \rangle}{\lambda^D} \int_{\partial \vartheta} d^{D-1} \mathbf{r} \langle \delta p \nabla \delta p \cdot \mathbf{n} \rangle + \frac{1}{\lambda^D} \int_{\partial \vartheta} d^{D-1} \mathbf{r} \langle \delta k \delta p \rangle \nabla p_0 \cdot \mathbf{n}. \end{aligned} \tag{D.4}$$

640 It can be checked by direct inspection that first line of this formula compares well with Eq. (B.3). The other contributions are finite size effects that cancel if  $\vartheta = \Omega$ . They explain the observed differences in the numerical tests. If  $\vartheta$  tends to zero,  $\langle K_{diss}(\vartheta) \rangle = \langle k \rangle$ .

## Acknowledgments

645 The authors would like to acknowledge the computational time from the TUPAC cluster made available by the *CSC-CONICET* for conducting this research.

## References

- Ababou, R., 1994. Solution of stochastic groundwater flow by infinite series, and convergence of the one-dimensional expansion. *Stochastic Hydrology and Hydraulics* 8, 139–155.
- Ababou, R., 1996. Random porous media flow on large 3-D grids: numerics, performance, and application to homogenization, in: *Environmental Studies*. Springer, pp. 1–25.
- 655 Ababou, R., McLaughlin, D., Gelhar, L.W., Tompson, A.F., 1989. Numerical simulation of three-dimensional saturated flow in randomly heterogeneous porous media. *Transport in Porous Media* 4, 549–565.

- Abramovich, B., Indelman, P., 1995. Effective permittivity of log-normal isotropic random media. *Journal of Physics A: Mathematical and General* 28, 693.
- 660
- Aguilar-Madera, C.G., Herrera-Hernández, E.C., Espinosa-Paredes, G., 2019. Solute transport in heterogeneous reservoirs: Upscaling from the darcy to the reservoir scale. *Advances in Water Resources* 124, 9 – 28.
- Akber Hassan, W.A., Jiang, X., 2012. Upscaling and its application in numerical simulation of long-term CO<sub>2</sub> storage. *Greenhouse Gases: Science and Technology* 2, 408–418.
- 665
- Armstrong, S., Kuusi, T., Mourrat, J.C., 2019. Quantitative stochastic homogenization and large-scale regularity. volume 352. Springer.
- Attinger, S., 2003. Generalized coarse graining procedures for flow in porous media. *Computational Geosciences* 7, 253–273.
- 670
- Auriault, J., 1983. Effective macroscopic description for heat conduction in periodic composites. *International Journal of Heat and Mass Transfer* 26, 861–869.
- Bauer, D., Talon, L., Ehrlacher, A., 2008. Computation of the equivalent macroscopic permeability tensor of discrete networks with heterogeneous segment length. *Journal of Hydraulic Engineering* 134, 784–793.
- 675
- Berkowitz, B., Balberg, I., 1993. Percolation theory and its application to groundwater hydrology. *Water Resources Research* 29, 775–794.
- Bernabé, Y., Li, M., Tang, Y.B., Evans, B., 2016. Pore space connectivity and the transport properties of rocks. *Oil & Gas Science and Technology—Revue d’IFP Energies nouvelles* 71, 50.
- 680
- Bernabé, Y., Mok, U., Evans, B., Herrmann, F., 2004. Permeability and storativity of binary mixtures of high- and low-permeability materials. *Journal of Geophysical Research: Solid Earth* 109.
- Beucher, H., Renard, D., 2016. Truncated gaussian and derived methods. *Comptes Rendus Geoscience* 348, 510 – 519.
- 685
- Bøe, Ø., 1994. Analysis of an upscaling method based on conservation of dissipation. *Transport in Porous Media* 17, 77–86.
- Boschan, A., Noetinger, B., 2012. Scale dependence of effective hydraulic conductivity distributions in 3D heterogeneous media: a numerical study. *Transport in Porous Media* 94, 101–121.
- 690
- Bruggeman, V.D., 1935. Berechnung verschiedener physikalischer konstanten von heterogenen substanzen. i. dielektrizitätskonstanten und leitfähigkeiten der mischkörper aus isotropen substanzen. *Annalen der Physik* 416, 636–664.

- 695 Celia, M.A., Bachu, S., Nordbotten, J., Bandilla, K., 2015. Status of CO<sub>2</sub> storage in deep saline aquifers with emphasis on modeling approaches and practical simulations. *Water Resources Research* 51, 6846–6892.
- Chen, Y., Durlofsky, L.J., Gerritsen, M., Wen, X.H., 2003. A coupled local-global upscaling approach for simulating flow in highly heterogeneous formations. *Advances in Water Resources* 26, 1041–1060.  
700
- Dagan, G., 1989. *Flow and transport in porous formations*. Springer-Verlag GmbH & Co. KG.
- Dagan, G., 1993. Higher-order correction of effective permeability of heterogeneous isotropic formations of lognormal conductivity distribution. *Transport in Porous Media* 12, 279–290.  
705
- Dagan, G., Fiori, A., Jankovic, I., 2013. Upscaling of flow in heterogeneous porous formations: Critical examination and issues of principle. *Advances in Water Resources* 51, 67 – 85. 35th Year Anniversary Issue.
- Davit, Y., Quintard, M., 2017. Technical notes on volume averaging in porous media I: How to choose a spatial averaging operator for periodic and quasiperiodic structures. *Transport in Porous Media* 119, 555–584.  
710
- De Wit, A., 1995. Correlation structure dependence of the effective permeability of heterogeneous porous media. *Physics of Fluids* 7, 2553–2562.
- Desbarats, A., 1992. Spatial averaging of hydraulic conductivity in three-dimensional heterogeneous porous media. *Mathematical Geology* 24, 249–267.  
715
- Desbarats, A., Srivastava, R., 1991. Geostatistical characterization of groundwater flow parameters in a simulated aquifer. *Water Resources Research* 27, 687–698.
- Durlofsky, L., 1998. Coarse scale models of two phase flow in heterogeneous reservoirs: volume averaged equations and their relationship to existing upscaling techniques. *Computational Geosciences* 2, 73–92.  
720
- Durlofsky, L.J., 1991. Numerical calculation of equivalent grid block permeability tensors for heterogeneous porous media. *Water Resources Research* 27, 699–708.
- 725 Durlofsky, L.J., 1992. Representation of grid block permeability in coarse scale models of randomly heterogeneous porous media. *Water Resources Research* 28, 1791–1800.
- Eberhard, J., Attinger, S., Wittum, G., 2004. Coarse graining for upscaling of flow in heterogeneous porous media. *Multiscale Modeling & Simulation* 2, 269–301.  
730
- Gelhar, L.W., 1993. *Stochastic subsurface hydrology*. Prentice-Hall.

- Godoy, V.A., Zuquette, L.V., Gómez-Hernández, J.J., 2018. Stochastic analysis of three-dimensional hydraulic conductivity upscaling in a heterogeneous tropical soil. *Computers and Geotechnics* 100, 174 – 187.
- 735 Gray, W.G., Miller, C.T., 2005. Thermodynamically constrained averaging theory approach for modeling flow and transport phenomena in porous medium systems: 1. motivation and overview. *Advances in Water Resources* 28, 161 – 180.
- 740 Guadagnini, A., Riva, M., Neuman, S.P., 2018. Recent advances in scalable non-gaussian geostatistics: The generalized sub-gaussian model. *Journal of hydrology* .
- Guin, A., Ritzi Jr., R.W., 2008. Studying the effect of correlation and finite-domain size on spatial continuity of permeable sediments. *Geophysical Research Letters* 35.
- 745 Harbaugh, A.W., 2005. MODFLOW-2005, the US Geological Survey modular ground-water model: the ground-water flow process. US Department of the Interior, US Geological Survey Reston, VA.
- 750 Hashin, Z., Shtrikman, S., 1962. A variational approach to the theory of the effective magnetic permeability of multiphase materials. *Journal of Applied Physics* 33, 3125–3131.
- Hashin, Z., Shtrikman, S., 1963. A variational approach to the theory of the elastic behaviour of multiphase materials. *Journal of the Mechanics and Physics of Solids* 11, 127–140.
- 755 Hassanizadeh, M., Gray, W.G., 1979. General conservation equations for multiphase systems: 1. averaging procedure. *Advances in water resources* 2, 131–144.
- Hristopulos, D.T., 2020. *Random Fields for Spatial Data Modeling A Primer for Scientists and Engineers*. Springer.
- 760 Hunt, A., Ewing, R., Ghanbarian, B., 2014. *Percolation theory for flow in porous media*. volume 880. Springer.
- Hunt, A., Sahimi, M., 2017. Transport and reaction in porous media: Percolation scaling, critical-path analysis, and effective-medium approximation. *Reviews of Geophysics* 55.
- 765 Indelman, P., Abramovich, B., 1994. A higher-order approximation to effective conductivity in media of anisotropic random structure. *Water Resources Research* 30, 1857–1864.
- Indelman, P., Dagan, G., 1993a. Upscaling of conductivity of heterogeneous formations: General approach and application to isotropic media. *Transport in Porous Media* 12, 161–183.

- 770 Indelman, P., Dagan, G., 1993b. Upscaling of permeability of anisotropic heterogeneous formations: 2. general structure and small perturbation analysis. *Water Resources Research* 29, 925–933.
- Jacquard, P., 1965. Permeability distribution from field pressure data. *Society of Petroleum Engineers Journal* 5, 281–294.
- 775 Jikov, V.V., Kozlov, S.M., Oleinik, O.A., 2012. Homogenization of differential operators and integral functionals. Springer Science & Business Media.
- Journel, A., Deutsch, C., Desbarats, A., et al., 1986. Power averaging for block effective permeability, in: SPE California Regional Meeting, Society of Petroleum Engineers.
- 780 Karimi-Fard, M., Durlofsky, L., 2016. A general gridding, discretization, and coarsening methodology for modeling flow in porous formations with discrete geological features. *Advances in Water Resources* 96, 354 – 372.
- King, P., 1989. The use of renormalization for calculating effective permeability. *Transport in Porous Media* 4, 37–58.
- 785 Knudby, C., Carrera, J., 2005. On the relationship between indicators of geostatistical, flow and transport connectivity. *Advances in Water Resources* 28, 405–421.
- Landau, L., Lifshitz, E., 1960. *Electrodynamics of continuous media*. volume 8.
- Le Loc’H, G., 1987. Etude de la composition des perméabilités par des méthodes variationnelles. Ph.D. thesis. Thèse de doctorat dirigée par Matheron, Georges Terre, océan, espace Paris, ENMP 1987.
- 790 Le Ravalec, M., Noetinger, B., Hu, L.Y., 2000. The FFT moving average (FFT-MA) generator: An efficient numerical method for generating and conditioning gaussian simulations. *Mathematical Geology* 32, 701–723.
- 795 Leung, J.Y., Srinivasan, S., 2012. Scale-up of mass transfer and recovery performance in heterogeneous reservoirs. *Journal of Petroleum Science and Engineering* 86-87, 71 – 86.
- Liao, Q., Lei, G., Zhang, D., Patil, S., 2019. Analytical solution for upscaling hydraulic conductivity in anisotropic heterogeneous formations. *Advances in*  
800 *Water Resources* 128, 97–116.
- Linde, N., Renard, P., Mukerji, T., Caers, J., 2015. Geological realism in hydrogeological and geophysical inverse modeling: a review. *Advances in Water Resources* 86.
- 805 Liu, Z.F., Wang, X.H., 2013. Finite analytic numerical method for two-dimensional fluid flow in heterogeneous porous media. *Journal of Computational Physics* 235, 286–301.

- Malinouskaya, I., Preux, C., Guy, N., Etienne, G., 2018. Impact of geomechanical effects during sagd process in a meander belt. *Oil & Gas Sciences and Technology* 73, 17.
- 810 Masihi, M., Gago, P., King, P., 2016. Estimation of the effective permeability of heterogeneous porous media by using percolation concepts. *Transport in Porous Media* 114.
- Matheron, G., 1967. *Eléments pour une théorie des milieux poreux*. Masson.
- Maxwell, J.C., 1873. *A treatise on electricity and magnetism*. volume 1. Oxford: Clarendon Press.
- 815
- Neuman, S.P., Orr, S., 1993. Prediction of steady state flow in nonuniform geologic media by conditional moments: Exact nonlocal formalism, effective conductivities, and weak approximation. *Water Resources Research* 29, 341–364.
- 820 Noetinger, B., 1994. The effective permeability of a heterogeneous porous medium. *Transport in porous media* 15, 99–127.
- Noetinger, B., 2000. Computing the effective permeability of log-normal permeability fields using renormalization methods. *Comptes Rendus de l’Académie des Sciences-Series IIA-Earth and Planetary Science* 331, 353–357.
- 825 Noetinger, B., 2013. An explicit formula for computing the sensitivity of the effective conductivity of heterogeneous composite materials to local inclusion transport properties and geometry. *Multiscale Modeling & Simulation* 11, 907–924.
- Noetinger, B., Gautier, Y., 1998. Use of the Fourier-Laplace transform and of diagrammatical methods to interpret pumping tests in heterogeneous reservoirs. *Advances in Water Resources* 21, 581–590.
- 830
- Noetinger, B., Zargar, G., 2004. Multiscale description and upscaling of fluid flow in subsurface reservoirs. *Oil & Gas Science and Technology* 59, 119–139.
- Panzeri, M., Riva, M., Guadagnini, A., Neuman, S.P., 2016. Theory and generation of conditional, scalable sub-gaussian random fields. *Water Resources Research* 52, 1746–1761.
- 835
- Pardo-Igúzquiza, E., Dowd, P.A., 2003. CONNEC3D: a computer program for connectivity analysis of 3D random set models. *Computers & Geosciences* 29, 775 – 785.
- 840 Pozdniakov, S., Tsang, C.F., 2004. A self-consistent approach for calculating the effective hydraulic conductivity of a binary, heterogeneous medium. *Water Resources Research* 40.
- Preux, C., 2016. About the use of quality indicators to reduce information loss when performing upscaling. *Oil & Gas Science and Technology* 71, 7.

- 845 Quintard, M., Whitaker, S., 1998. Transport in chemically and mechanically heterogeneous porous media III. large-scale mechanical equilibrium and the regional form of darcy's law. *Advances in Water Resources* 21, 617–629.
- Renard, P., De Marsily, G., 1997. Calculating equivalent permeability: a review. *Advances in Water Resources* 20, 253–278.
- 850 Riva, M., Guadagnini, A., Neuman, S.P., 2017. Theoretical analysis of non-gaussian heterogeneity effects on subsurface flow and transport. *Water Resources Research* 53, 2998–3012.
- Romeu, R., Noetinger, B., 1995. Calculation of internodal transmissivities in finite difference models of flow in heterogeneous porous media. *Water Resources Research* 31, 943–959.
- 855 Rubin, Y., Gómez-Hernández, J.J., 1990. A stochastic approach to the problem of upscaling of conductivity in disordered media: Theory and unconditional numerical simulations. *Water Resources Research* 26, 691–701.
- Sánchez-Vila, X., Girardi, J.P., Carrera, J., 1995. A synthesis of approaches to upscaling of hydraulic conductivities. *Water Resources Research* 31, 867–882.
- 860 Sánchez-Vila, X., Guadagnini, A., Carrera, J., 2006. Representative hydraulic conductivities in saturated groundwater flow. *Reviews of Geophysics* 44.
- Stauffer, D., Aharony, A., 2014. *Introduction to percolation theory: revised second edition*. CRC press.
- 865 Stepanyants, Y.A., Teodorovich, E., 2003. Effective hydraulic conductivity of a randomly heterogeneous porous medium. *Water Resources research* 39.
- Vereecken, H., Kasteel, R., Vanderborght, J., Harter, T., 2007. Upscaling hydraulic properties and soil water flow processes in heterogeneous soils a review. *Vadose Zone J.* 6, 1–28.
- 870 Wang, G.W., Liu, Z.F., Wang, X.H., 2018. Finite analytic method for 2d steady fluid flows in heterogeneous porous media with unstructured grids. *International Journal for Numerical Methods in Engineering* 113, 742–766.
- Wang, Y.F., Liu, Z.F., Wang, X.H., 2014. Finite analytic numerical method for three-dimensional fluid flow in heterogeneous porous media. *Journal of Computational Physics* 278, 169–181.
- 875 Wen, X., Durlofsky, L., Edwards, M., 2003. Use of border regions for improved permeability upscaling. *Mathematical Geology* 35, 521–547.
- Wen, X.H., Gómez-Hernández, J.J., 1996. Upscaling hydraulic conductivities in heterogeneous media: An overview. *Journal of Hydrology* 183, 9–32.
- 880 Whitaker, S., 2013. *The method of volume averaging*. volume 13. Springer Science & Business Media.

- Willot, F., Jeulin, D., 2009. Elastic behavior of composites containing boolean random sets of inhomogeneities. *International Journal of Engineering Science* 47, 313–324.
- 885 Wood, B.D., Valdés-Parada, F.J., 2013. Volume averaging: Local and non local closures using a Green’s function approach. *Advances in Water Resources* 51, 139 – 167. 35th Year Anniversary Issue.
- Wu, B., Liu, Z.F., Wang, X.H., 2013. Statistical behaviors for renormalization of correlated permeability field. *Physica A: Statistical Mechanics and its*  
890 *Applications* 392, 3115 – 3121.
- Zheng, X.L., Liu, Z.F., Wang, X.H., Shi, A.F., 2017. Calculating the inter-  
nodal transmissibilities using finite analytic method and its application for  
multi-phase flow in heterogeneous porous media. *International Journal for  
Numerical and Analytical Methods in Geomechanics* 41, 79–92.
- 895 Zhou, X.Y., Gosling, P., Pearce, C., Kaczmarczyk, L., Ullah, Z., 2016. Perturbation-based stochastic multi-scale computational homogenization method for the determination of the effective properties of composite materials with random properties. *Computer Methods in Applied Mechanics and Engineering* 300, 84 – 105.