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Filtering procedures for flow in heterogeneous porous media: numerical results

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Abstract. This paper focuses on heterogeneous soil permeabilities and on the impact their resolution has on the solution of the piezometric head equation. The method of coarse graining is proposed in order to filter the piezometric head equation on arbitrary support scales: Large scale fluctuations of the permeabilities are resolved, whereas small scale fluctuations are smoothed by a spatial filtering procedure. The filtering procedure is performed in Fourier space with the aid of a low-frequency cut-off function. In the filtered equations, the impact of the small scale variability is modeled by scale dependent effective permeabilities which are determined by additional differential equations. The additional differential equations are equivalent to the piezometric head equation on cells which are solved numerically by using the software toolbox UG. The numerical results are compared with the theoretical results derived in Attinger 2001.

1 Introduction

Measurement results of soil properties which are spatially variable crucially depend on the resolution scale at which they are resolved. This paper focuses on heterogeneous soil permeabilities and on the impact their resolution has on the piezometric head equation.

In many practical problems, the analyst has data consisting of local permeability measurements across the site and several field tests. An experiment averages information over a volume determined by the support scale of the measurement procedure. The influence of the spatial average of the permeability data by using different measurement techniques has been discussed e.g. by Gelhar et al. 1977, Journel et al. 1978 or Vanmarcke 1983. A summary of permeability data from different field sites can be found e.g. in Gelhar 1993. Therefore, it is useful for the practitioner to have insight into how data collected at different scales are related to each other. In the groundwater literature, spatial filters are widely used to conceptually represent measurements of permeabilities on different scales. A detailed discussion can be found in Beckie 2001.

The derivation of large scale pressure equations has been done e.g. in the framework of stochastic theories. Mean pressure fields are determined by averaging the head equation over many realisations of different permeability fields. The fluctuating permeability fields are replaced by so-called effective permeability values. Then, approximate results for the effective permeabilities can be derived in lowest order perturbation theory of the variance of the logarithm of the permeability, see e.g. Gelhar 1993 and Dagan 1989. Higher-order perturbation theory contributions to the effective permeability were e.g. calculated by Dean et al. 1995. Moreover, effective permeability values may be determined by volume averaging methods or homogenisation techniques as well, see e.g Whitaker et al. 1999 or Papanicolaou et al. 1979. In these approaches, an effective head equation is derived. The effective permeability values are obtained from the solution of an additional differential equation (called cell problem). In the limit of small fluctuations the results reduce to the standard perturbation theory results cited above.

However, for the consistent interpretation of measurements performed at different scales, one is more interested in averaging the pressure equation on intermediate scales than on very large scales. Furthermore, the need to know how the pressure equation depends on its resolution scale becomes most apparent in constructing numerical models with coarser resolution. Upscaling methods can be used in order to incorporate subgrid-scale information into the parameter estimation of a model with coarser resolution. Numerical investigations have been performed e.g. by Hou et al. 1999, Nilson et al. 1996, Efendiev et al. 2000 or Durlofsky et al. 1992.

Filtering procedures offer a tool to derive a resolution-dependent head equation where small scale heterogeneities up to an arbitrary length scale are filtered out and large scale heterogeneities remain resolved. To that end, Attinger 2001 used a filtering procedure originally developed in the context of large eddy simulations in the theory of turbulence, for further reference see also McComb 1990. The method was also applied by Dykaar and Kitanidis 1992 for the numerical determination of the effective hydraulic conductivity. Moreover, Beckie et al. 1996 derived spatially filtered pressure equations in small perturbation assumptions. Attinger 2001 overcomes these limitations and derives spatially filtered pressure equations that are exact. In general, they are nonlocal integro-differential equations. However, for further mathematical treatment they are localised and the subscale effects are approximated by their ensemble mean. Iteration of the filtering procedure over stepwise coarser averaging volumes allowed to formulate the coarse graining procedure in terms of a differential equation which becomes a renormalisation group equation. The renormalisation group equation was solved and explicit results for the filtered pressure equation were found.

It is the aim of this article to test the quality of the theoretical approximations (localisation and mean approximation) of the filtered pressure equation by numerical simulations.

In Sect. 2, we introduce the flow model. In Sect. 3, we explain the concept of coarse graining. We recall results presented in Attinger 2001. We test the theoretical results by numerical calculations in Sect. 4. We conclude with a discussion.

2 Darcy's law in heterogeneous porous media

The steady-state pressure distribution for single-phase, incompressible flow through a heterogeneous medium is described by

$$-\nabla \cdot K_f(\boldsymbol{x})\, \nabla\phi(\boldsymbol{x}) = \varrho(\boldsymbol{x}) \tag{1}$$

where $\phi(\boldsymbol{x})$ is the pressure distribution, $K_f(\boldsymbol{x})$ a local permeability field and $\varrho(\boldsymbol{x})$ comprises source or sink terms of the pressure. It results from a combination of Darcy's law for steady-state flow

$$\boldsymbol{q}(\boldsymbol{x}) = -\, K_f(\boldsymbol{x})\, \nabla\phi(\boldsymbol{x}) \tag{2}$$

with conservation of mass $\nabla \cdot \boldsymbol{q} = \varrho$. For simplicity, we choose boundaries at infinity.

2.1 Statistical properties of the permeability field

The permeability K_f is a spatially heterogeneous field which is modelled as lognormally distributed in space

$$K_f(\boldsymbol{x}) = K\, \exp\left(f(\boldsymbol{x})\right) \tag{3}$$

where $f(\boldsymbol{x})$ is a spatially normal distributed field. We split $\log K_f$ into its mean value and the deviation from that value

$$f(\boldsymbol{x}) = \overline{f} + \tilde{f}(\boldsymbol{x})\,. \tag{4}$$

The overbar $\overline{(\ldots)}$ denotes an ensemble average over the normal distribution of $f(\boldsymbol{x})$. By construction, the ensemble average of the fluctuating part vanishes, $\overline{\tilde{f}(\boldsymbol{x})} = 0$. The correlation function is defined by

$$w\left(\boldsymbol{x}, \boldsymbol{x}'\right) \equiv \overline{\tilde{f}(\boldsymbol{x})\tilde{f}\left(\boldsymbol{x}'\right)}\,. \tag{5}$$

Assuming a stationary isotropic distribution for $f(\boldsymbol{x})$, the correlation function only depends on the distance, $w(|\boldsymbol{x}-\boldsymbol{x}'|)$. For mathematical reasons, we choose for the correlation function a Gaussian

$$w\left(|\boldsymbol{x}-\boldsymbol{x}'|\right) \equiv \sigma_f^2\, \exp\left(-\frac{|\boldsymbol{x}-\boldsymbol{x}'|^2}{2l_0^2}\right) \tag{6}$$

where σ_f^2 is the variance and l_0 an isotropic correlation length of $\log K_f$. Analogously, we split the permeability field $K_f(\boldsymbol{x})$ into its mean value and deviation from that value $K_f(\boldsymbol{x}) = \overline{K}_f + \tilde{k}_f(\boldsymbol{x})$. Using the statistical properties of $\log K_f$, the arithmetic mean follows as $\overline{K}_f = K_g\, \exp(\sigma_f^2/2)$. K_g is defined as the geometric mean, $K\exp(\overline{f})$.

3 Coarse graining: theoretical results

The pressure equation (1) and the statistical properties of the heterogeneous permeability field as introduced above are defined on the finest resolution scale. It is at least of the order of magnitude of a representative pore volume such that Darcy's law holds. Filtering changes the pressure equation as well as the statistical properties of the coarse-grained permeability fluctuations. In the limit of upscaling the pressure equation to very large scales, all permeability fluctuations are averaged out and replaced by an effective permeability tensor. These results are known from standard upscaling procedures as homogenisation theory, see Jikov et al. 1992.

The aim of coarse graining procedures, however, is to average local functions over volumes of intermediate size in order to obtain functions on coarser resolution scales. The coarse scale can be e.g. the resolution scale of a measurement or the discretisation scale of a numerical simulation. In the following, we assume that the coarse scale is characterized by a typical length λ and demonstrate the concept of the coarse graining procedure on a local pressure field $\phi(\boldsymbol{x})$.

Fluctuations of $\phi(\boldsymbol{x})$ are smoothed out over a block Ω_x with volume λ^d around the location $\boldsymbol{x}$ by the following averaging procedure

$$\phi(\boldsymbol{x})|_\lambda \equiv \frac{1}{\lambda^d} \int_{\Omega_x} d^d x'\, \phi\left(\boldsymbol{x}+\boldsymbol{x}'\right) \tag{7}$$

where $\phi(\boldsymbol{x})|_\lambda$ is the coarser pressure distribution, d the spatial dimension and $d^d x$ an infinitesimal volume element.

Now, Attinger 2001 shows by a calculation in Fourier variables that the filtered pressure field $\phi(\boldsymbol{x})|_\lambda$ approximately fulfills

$$\begin{aligned} &-\nabla \cdot \left(\overline{K}_f + \tilde{k}_f(\boldsymbol{x})|_\lambda\right)\, \nabla\phi(\boldsymbol{x})|_\lambda \\ &\quad + \nabla \cdot \delta K_f^{\mathrm{eff}}(\lambda)\, \nabla\phi(\boldsymbol{x})|_\lambda = \varrho(\boldsymbol{x})|_\lambda \end{aligned} \tag{8}$$

where $\delta K_f^{\mathrm{eff}}(\lambda)$ is derived from

$$\begin{aligned} \delta K_f^{\mathrm{eff}}(\lambda, \boldsymbol{k}) = &\int_{|\boldsymbol{k}'|>\lambda} d^d k' \int_{|\boldsymbol{k}''|>\lambda} d^d k'' \\ &\times \overline{\left(\tilde{k}_f\left(\boldsymbol{k}-\boldsymbol{k}'\right)\left(ik_i'\right) G\left(\boldsymbol{k}', -\boldsymbol{k}''\right)\left(ik_i''\right) \tilde{k}_f\left(\boldsymbol{k}''-\boldsymbol{k}\right)\right)} \end{aligned} \tag{9}$$

(equation (37) in Attinger 2001) by evaluating at $\boldsymbol{k} = 0$ which corresponds to localisation.

Here, $\delta K_f^{\mathrm{eff}}(\lambda)$ can be understood as a heterogeneity induced effective permeability value induced by small scale heterogeneities varying on typical length scales smaller than λ. It is given in the space domain by

$$\delta K_f^{\mathrm{eff}}(\lambda) = \int d^d x \int\limits_{x' \in \Omega_x} d^d x' \overline{\tilde{k}_f(\boldsymbol{x}) \partial_{x_i} G(\boldsymbol{x}, \boldsymbol{x}') \, \partial_{x'_i} \tilde{k}_f(\boldsymbol{x}')} \quad (10)$$

where Green's function $G(\boldsymbol{x}, \boldsymbol{x}')$ solves $-\nabla \cdot K_f(\boldsymbol{x}) \nabla G(\boldsymbol{x}, \boldsymbol{x}') = \delta(\boldsymbol{x} - \boldsymbol{x}')$.

One can evaluate (9) in lowest order perturbation theory or, alternatively, one can sum up higher-order contributions by a renormalisation scheme. Replacing the cut-off filter function by a Gaussian filter in real space Attinger 2001 obtains for the total effective permeability (heterogeneity induced part plus the arithmetic mean) the very compact result

$$K_f^{\mathrm{eff}}(\lambda) = \overline{K}_f \exp\left(-\frac{1}{d}\sigma_f^2 \left(1 - \left(\frac{l_0^2}{l_0^2 + \lambda^2/4}\right)^{d/2}\right)\right). \quad (11)$$

In two spatial dimensions, the partial effective permeability value reads

$$K_f^{\mathrm{eff}}(\lambda) = K_g \exp\left(\frac{1}{2}\sigma_f^2 \left(\frac{l_0^2}{l_0^2 + \lambda^2/4}\right)\right). \quad (12)$$

Here, K_g is defined as the geometric mean, $K \exp(\overline{f})$. Expression (12) models the scale dependent transition from the arithmetic mean in case of no coarse graining to the geometric mean for global upscaling. Moreover, the form is like a modified geometric mean. This is different for the result in three dimensions where we obtain

$$K_f^{\mathrm{eff}}(\lambda) = K_g \exp\left(\sigma_f^2/6\right) \exp\left(\frac{1}{3}\sigma_f^2 \left(\frac{l_0^2}{l_0^2 + \lambda^2/4}\right)^{3/2}\right) \quad (13)$$

which describes the scale dependent transition from the arithmetic mean for no coarse graining to $K_g \exp(\sigma_f^2/6)$ for global upscaling. In Fig. 1, we have plotted $K_f^{\mathrm{eff}}(\lambda)$ for $d = 2, 3$.

4 Numerical results

4.1 Numerical coarse graining

To test the result (12) from the renormalisation analysis we consider a two-dimensional example. We work on the unit square with a stationary, isotropic permeability coefficient field $K_f(\boldsymbol{x})$. The logarithm of $K_f(\boldsymbol{x})$ follows a normal distribution, i.e. $K_f(\boldsymbol{x})$ is lognormally distributed. The field is created by a Gaussian random field numerically generated as a superposition of randomly chosen cosine modes according to Kraichnan 1970 and 1976.

The heterogeneity induced effective permeability coefficient in the real space is given by (10). The ensemble average is numerically done by averaging over disjoint cells within the unit square. Therefore we choose a uniform grid τ_h of meshsize $h = 2^{-n}$. The upscaling procedure is realized by calculating the effective permeability for every cell $c_{\vec{i}} = \{\boldsymbol{x} \in [0, 1]^2 \mid i_k h \le x_k \le (i_k + 1)h, \ k = 1, 2\}$ of the grid τ_h.

For the numerical calculation of the effective permeability coefficient, we compute

$$\delta K_f^{\mathrm{eff}} = \sum_{\vec{i}} h^2 \int\limits_{c_{\vec{i}}} d^2 x \tilde{k}_f(\boldsymbol{x}) \partial_{x_i} \chi_i(\boldsymbol{x}), \quad (14)$$

where $\chi_i(\boldsymbol{x})$ fulfills the auxilliary equation

$$\nabla \cdot \left(K_f(\boldsymbol{x}) \nabla \chi_i(\boldsymbol{x})\right) = -\partial_{x_i} \tilde{k}_f(\boldsymbol{x}) \quad (15)$$

on each cell $c_{\vec{i}}$ with Dirichlet zero boundary conditions on the two sides perpendicular to the i-th coordinate direction and natural boundary conditions on the other sides. This has to be understood as an approximation to (10) where we approximate the application of the Green's function $G(\boldsymbol{x}, \boldsymbol{x}')$ (which means solving the global problem) by solving the local problem on each cell.

For obtaining the solution $\chi_i(\boldsymbol{x})$ of the partial differential equation (15) on a cell, we discretize the equation by a vertex-centered finite volume scheme. We always choose

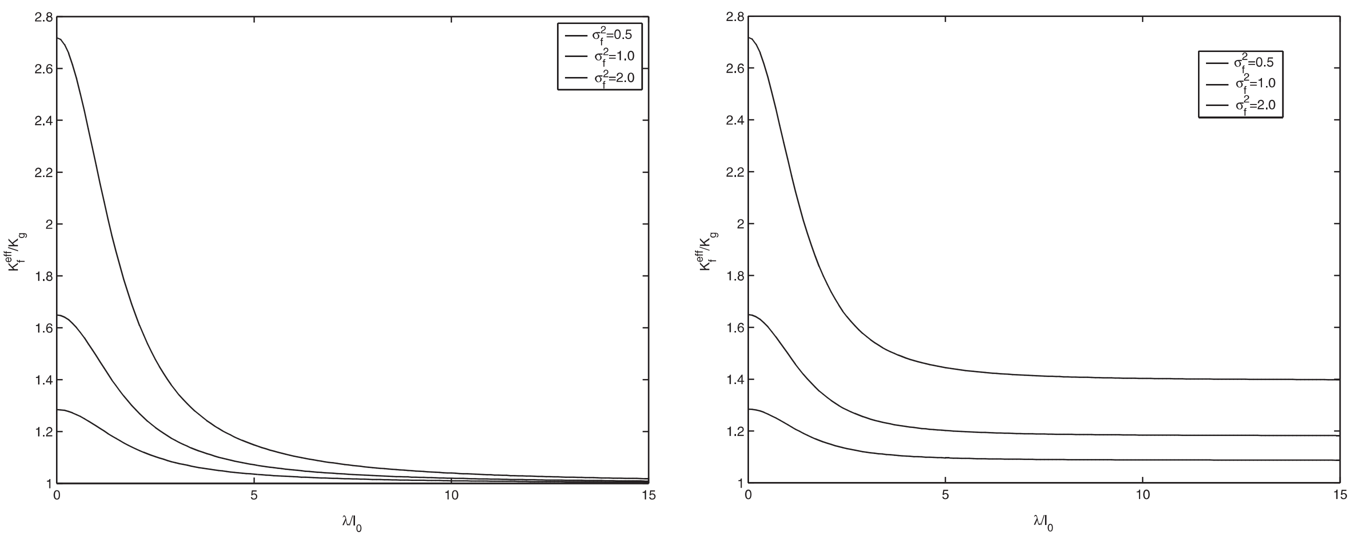

Fig. 1. K_f^{eff}/K_g for $d = 2$ (*left*) and $d = 3$ (*right*) for different σ_f^2

the discretisation mesh to be finer than the oscillations of the permeability field, i.e. $\tilde{k}_f(\boldsymbol{x})$ is constant on each element of the mesh. The resulting linear equations are solved by a geometric multigrid method, see Hackbusch (1985). The multigrid method is a very efficient tool for solving this kind of sparse system of linear equations, at least for the moderate variations of the coefficients which we consider here.

Then we calculate δK_f^{eff} according to (14). For a single cell, this is achieved by numerical integration over the elements of the discretisation mesh with a midpoint rule which gives an exact result because $\tilde{k}_f(\boldsymbol{x})$ is constant on each element. Thereafter the δK_f^{eff} values of the finite volumes are added up to obtain δK_f^{eff} for the corresponding cell. Both the discretisation and the numerical calculations have been realized with the software toolbox UG (Bastian et al. 1997).

In Figs. 2 and 3, the longitudinal component of the effective permeability tensor

$$K_f^{\text{eff}}(\lambda) = \overline{K}_f + \delta K_f^{\text{eff}}(\lambda) \tag{16}$$

is plotted in comparison with the result from the renormalisation analysis for increasing λ. This is numerically done by decreasing the number of the cells of the grid τ_h. The variance σ_f^2 of the underlying permeability field $K_f(\boldsymbol{x})$ is $\sigma_f^2 = 0.1$ (Fig. 2) and $\sigma_f^2 = 1.0$ (Fig. 3). In addition, the standard deviation of the effective permeability coefficient

$$K_f^{\pm} = K_f^{\text{eff}} \pm \Delta k_f \tag{17}$$

is plotted, where Δk_f is the deviation of the effective permeability coefficient (numerically evaluated for each cell $c_{\bar{i}}$) averaged over all cells of the grid τ_h.

The results from the renormalisation theory and the numerical simulation are in good agreement even for the higher variance. It can also be seen that the standard deviation Δk_f first increases with growing λ which is the typical length within the fluctuations are smoothed out. Especially nearby the correlation length of the permeability field, $\lambda \approx l_0$, the deviation of the effective permeability coefficient from cell to cell is highest. After having reached its maximum, Δk_f gets smaller and finally vanishes for a grid consisting of one cell.

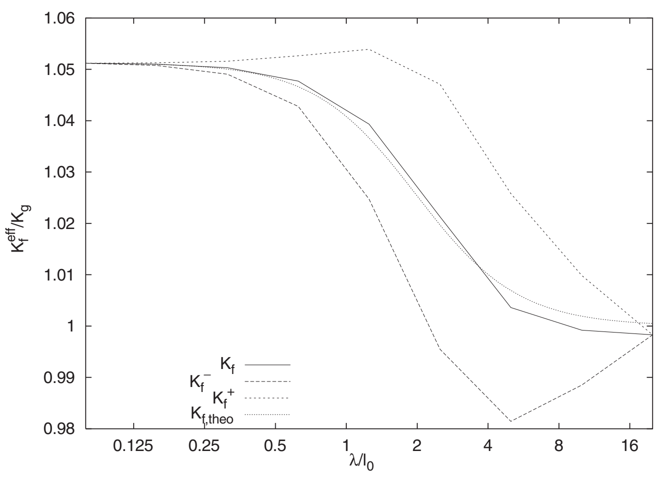

Fig. 2. The longitudinal component of K_f^{eff} and the result of the renormalisation analysis for a realisation with variance $\sigma_f^2 = 0.1$, $\overline{f} = 0$ and correlation length $l_0 = 0.05$. $K_f^{\pm}$ is given by $K_f^{\pm} = K_f^{\text{eff}} \pm \Delta k_f$ with the standard deviation Δk_f of K_f^{eff}

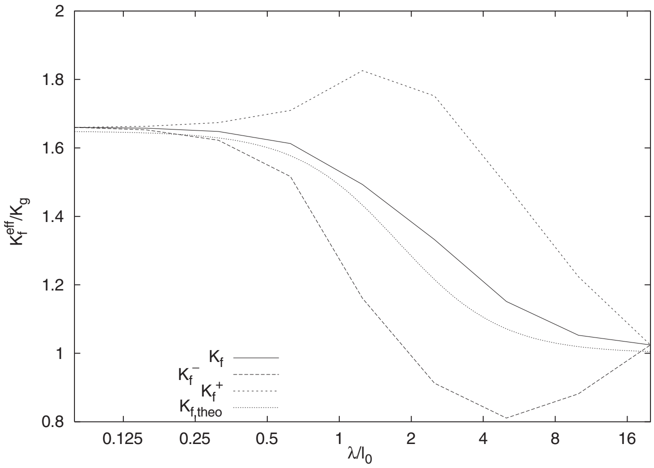

Fig. 3. The longitudinal component of K_f^{eff} and the result of the renormalisation analysis for a realisation with $\sigma_f^2 = 1.0$, $\overline{f} = 0$ and $l_0 = 0.05$

4.2 Numerical upscaling of the permeability field

For a successive upscaling of the permeability field the effective permeability field $K_f^{\text{eff}}(\lambda)$ together with the smoothed fluctuating part of the original field is considered as the new given permeability field. The fluctuating part of the permeability coefficient $\tilde{k}_f(\boldsymbol{x})$ is smoothed by arithmetic averaging over four adjacent cells within the grid.

Then the permeability field $K_f(\boldsymbol{x})|_\lambda$ on a coarser grid is given by

$$K_f(\boldsymbol{x})|_\lambda = K_f^{\text{eff}}(\lambda) + \tilde{k}_f(\boldsymbol{x})|_\lambda \,. \tag{18}$$

Figure 4 contains a set of permeability fields created in this way. The plots show the longitudinal total permeability coefficient given by equation (18) for grids with decreasing number of cells caused by the successive upscaling. The variance of the original permeability field is $\sigma_f^2 = 0.5$. Obviously, the fluctuations of the permeability field are smoothed out more and more as the coarsening of the grid proceeds.

In order to test the quality of the upscaled permeability fields of Fig. 4 we calculate the relative error in the L_2-Norm of the solution $\phi(\boldsymbol{x})$ which is given by the problem

$$-\nabla \cdot K_f(\boldsymbol{x})\, \nabla\phi(\boldsymbol{x}) = 0 \tag{19}$$

in the unit square with boundary conditions

$$\phi(\boldsymbol{x}) = \begin{cases} 1 & \text{for } x_1 = 0,\, x_2 \in [0, 1] \\ 0 & \text{for } x_1 = 1,\, x_2 \in [0, 1] \end{cases} \tag{20}$$

$$\boldsymbol{n} \cdot K_f(\boldsymbol{x}) \nabla\phi(\boldsymbol{x}) = 0 \;\text{ for } x_2 = 0 \text{ and } x_2 = 1,\, x_1 \in (0, 1)$$

($\boldsymbol{n}$ denoting the outward normal) and the solution $\phi(\boldsymbol{x})|_\lambda$ which we obtain by solving (19) with the upscaled permeability field $K_f(\boldsymbol{x})|_\lambda$. For comparison, we also solve equation (19) for upscaled permeability fields given by averaging over four adjacent cells with either the arithmetic mean or the geometric mean. Comparing the results given in Table 1 it is evident

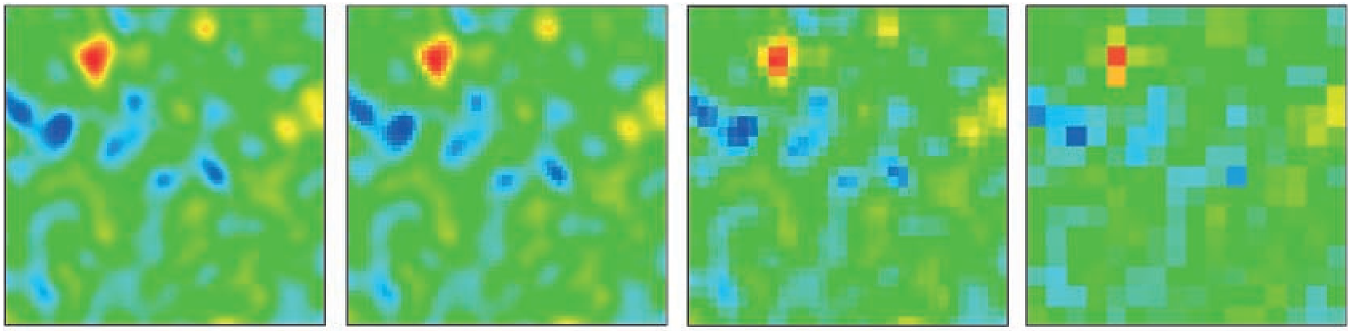

Fig. 4. Logarithmic plot of the permeability field $K_{f\,11}(\boldsymbol{x})|_\lambda/K_g$ in the unit square created by the successive upscaling for a single realisation with variance $\sigma_f^2 = 0.5$, $\overline{f} = 0$ and correlation length $l_0 = 6.4$ cells. The permeability coefficient varies from -2.37 (*blue*) to 2.94 (*red*)

Table 1. $\frac{||\phi(\boldsymbol{x})-\phi(\boldsymbol{x})|_\lambda||_{L_2}}{||\phi(\boldsymbol{x})||_{L_2}}$ for the solution $\phi(\boldsymbol{x})$ of the problem (19) and the solution $\phi(\boldsymbol{x})|_\lambda$ of (19) with a upscaled permeability field given by coarse graining or simple averaging with either arithmetic or geometric mean

Cells	64	32	16
Coarse graining	4.6×10^{-4}	2.1×10^{-3}	7.8×10^{-3}
Arithmetic averaging	5.0×10^{-4}	2.4×10^{-3}	9.0×10^{-3}
Geometric averaging	4.8×10^{-4}	2.2×10^{-3}	8.1×10^{-3}

that the coarse graining solution approximates the original solution $\phi(\boldsymbol{x})$ best, even if the difference in the relative error to the other averaging procedures is not large. We repeated this test for several other realisations with similar results.

5 Conclusions

In a former paper, Attinger 2001 derived the filtered pressure equation (8) for flow through heterogeneous porous media and presented explicit results for the heterogeneity induced part of the effective permeability value $\delta K_f^{\text{eff}}(\lambda)$ gained from renormalisation group analysis. It is the aim of this paper to test these theoretical results by numerical simulations.

The results for the mean effective permeability value from renormalisation theory and from the numerical simulation agree very well, both for smaller and higher variance of the fluctuating permeability field. In order to test the mean field approximation, we also calculated the standard deviation Δk_f. The standard deviation first increases with coarsening the numerical grid resolution. If the coarser resolution scale is of the order of the correlation length of the heterogeneous medium, $\lambda \approx l_0$, the deviation of the effective permeability coefficient from cell to cell is highest and the mean field approximation is worst. Hou et al. 1997 call that error a "resonance" error resulting from the resonance between the grid scale and typical length scale of the heterogeneous medium. The error becomes large if both scales are close. For $\lambda > l_0$, however, the error and therefore Δk_f becomes smaller. The error vanishes in the limit of total homogenisation of the medium. Hou et al. 1997 proposed an over-sampling method to overcome resonance errors. We will test that idea in our future work.

The partial differential equation for the filtered pressure distribution, (8), can easily be discretized on a coarser grid with the corresponding permeability field $K_f(\boldsymbol{x})|_\lambda$ which means much less computational work. Furthermore, suitable transfer operators for the coarse grid of a multigrid cycle can also be determined by the permeability field (18) for coarser grids. Using these transfer operators for improving the efficiency of multigrid methods and studying the connection to so-called algebraic multigrid methods will be done in future work.

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