Transp Porous Med (2008) 71:75–97
DOI 10.1007/s11242-007-9112-9

Self-similar approximants of the permeability in heterogeneous porous media from moment equation expansions

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Received: 8 May 2006 / Accepted: 7 February 2007 / Published online: 20 April 2007

Abstract We use a mathematical technique, the self-similar functional renormalization, to construct formulas for the average conductivity that apply for large heterogeneity, based on perturbative expansions in powers of a small parameter, usually the log-variance σ_Y^2 of the local conductivity. Using perturbation expansions up to third order and fourth order in σ_Y^2 obtained from the moment equation approach, we construct the general functional dependence of the scalar hydraulic conductivity in the regime where σ_Y^2 is of order 1 and larger than 1. Comparison with available numerical simulations show that the proposed method provides reasonable improvements over available expansions.

Keywords Hydraulic permeability · Heterogeneous porous media · Moment equation expansions · Renormalization · Self-similarity

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1 Introduction

Quantitative understanding of processes that govern flow and transport in porous and discontinous media is of utmost importance in many geophysical processes. For instance, the presence of fluid is one of the leading candidate to solve a variety of paradoxes in the physics of earthquakes such as the apparent weakness of mature faults (e.g., the San Andreas fault) or the heat flow paradox to cite a few (Sornette 1999). Understanding the transport properties of fluids in the fragmented crust in the presence of discontinuities occurring at many length scales is an essential component in the ultimate goal of understanding earthquakes. Understanding the properties of transport of fluids in complex porous and cracked media at many scales is also of fundamental importance from an environmental point of view as well as for a good stewardship of the storage of contaminants or pollutants or to remediate sites from contamination that arose during nuclear weapons production. It is also of critical importance at proposed nuclear waste storage sites like WIPP and Yucca Mountain, and in the simulation of oil and natural gas reservoirs.

Transport in heterogeneous porous media poses formidable challenges to model and predict with good reliability due to the multiple scales, topologies, and complex nonlinear processes. Existing models focus on end-members of a large ensemble of structures, that are chosen because they are amenable to theoretical analytical or computational attack. For instance, the moment equation approach is valid for a small variance σ_Y^2 of the log hydraulic conductivity, in contradiction with real geological settings of interest to a large variety of geophysical applications. At another extreme, the continuous-time random walk (CTRW) method takes into account extreme fluctuations and anomalous transport paths, but is only an effective phenomenological representation which may not capture the interplay between frozen and annealed disorder. Real porous media in geophysical settings are none of these limiting cartoon models. Uncertainty is usually dealt with either deterministically through upscaling or stochastically through the evaluating statistical moments. Statistical moments can be obtained through Monte Carlo simulations or development of moment differential equations, which is the method from which we start our analysis.

In the stochastic approach, parameter values determined at various points within a more-or-less distinct soil unit can be viewed as a sample from a random field defined over a continuum. This random field is characterized by a joint (multivariate) probability density function or, equivalently, its joint ensemble moments. Thus, a parameter such as (saturated, natural) log hydraulic conductivity $Y(\mathbf{x}) = \ln K_s(\mathbf{x})$ varies not only across the real space coordinates $\mathbf{x}$ within the unit, but also in probability space (this variation may be represented by another "coordinate" ξ, the configuration coordinate, which, for simplicity, we suppress). Whereas spatial moments are obtained by sampling $Y(\mathbf{x})$ in real space (across $\mathbf{x}$), ensemble moments are defined in terms of samples collected in probability space (across ξ).

In the moment equation approach, which we propose to exploit here, the stochastic differential equations are averaged first to obtain moments differential equations (MDEs) governing the statistical moments of the dependent variables. The MDEs are themselves deterministic and can be solved numerically or sometimes, analytically. The MDE approach has important advantages. First, only a small number of equations must be solved: one for the mean and one each for a small number of variances and covariances. Second, the coefficients of the MDEs are relatively smooth because they are averaged quantities. Thus the MDEs can be solved on comparatively smooth grids. Third, the MDEs are available in analytical form, even though they are usually solved numerically in applications. This holds the potential for increased physical understanding of the mechanisms of uncertainty through qualitative

analysis. Finally, in many applications MDE approaches provide a good estimate of the behavior of large variance systems despite being based on small perturbation theory.

Since the moment equation approach derives the equations of evolutions of the moments of the distribution of the scalar hydraulic conductivity by averaging the stochastic differential equations of transport in heterogeneous porous media, its fundamental limitation is the assumption that the variance σ_Y^2 of the log hydraulic conductivity is small, in contradiction with real geological settings of interest to a large variety of geophysical applications. In order to obtain reliable descriptions of the scalar hydraulic conductivity for large σ_Y^2, our goal in the present article is to adapt and extend the self-similar functional renormalization method to the moment equation approach. In essence fundamentally non-perturbative, this recently developed technique provides us with a stable and robust estimation of the scalar hydraulic conductivity at large values of the perturbation parameter σ_Y^2. The functional renormalization method associates ideas from the renormalization group theory of multiscale and critical phenomena (Sornette 2004) with methods from the theory of dynamical systems and of control theory. Using perturbation expansions up to third order and fourth order in σ_Y^2 obtained from the moment equation approach, we construct the general functional dependence of the scalar hydraulic conductivity in the regime where σ_Y^2 is of order 1 and larger than 1.

The next Sect. 2 recalls briefly how perturbation expansions are obtained from the moment equation approach. Section 3 summarizes the general formulation of the self-similar approximation theory. Section 4 gives the results of the application of the functional renormalization method to the moment equation expansions at increasing orders in σ_Y^2. Section 5 formulates the expansion in powers of $1/d$, where d is the space dimension. This procedure well-known in statistical physics is resummed by the fonctional renormalization to provide accurate formulas. Section 6 briefly discusses the results and outlines future directions of investigations.

2 Problem formulation and perturbation expansions

2.1 Basic equations

It has become common to quantify uncertainty in ground water flow models by treating hydraulic conductivity, K, and derived quantities like hydraulic head, h, as random fields. For steady-state flows in the absence of sources and sinks, the statistics of h can be obtained from the stochastic flow equation

$$\nabla \cdot [K(\mathbf{x})\, \nabla h(\mathbf{x})] \;=\; 0 \tag{1}$$

when the statistics of K are known. We further assume that the site of interest is sufficiently characterized so that available experimental data are sufficient to obtain the statistics of K, such as its (ensemble) mean, $\overline{K}$, variance, σ_K^2, and (two-point) correlation structure, $\rho_K(\mathbf{x}, \mathbf{y})$. Then one can solve directly for the moments of h by developing deterministic equations for the moments from (1). In general this involves taking the expected value of (1) and similar equations for higher-order moments, closing the system of moment equations (usually through perturbation approximations). Numerical solutions for moment equations are typically computationally more efficient than Monte Carlo simulations. In the first place, taking expected values smoothes parameters in the moment equations which in turn allows low-resolution grids for numerical solutions. Furthermore, the number of moment equations is much smaller than the number of realizations required by Monte Carlo simulations. Additionally, the moment equations lend themselves to qualitative analysis.

Here, we concentrate on flow through highly heterogeneous porous media with the variance σ_Y^2 of log hydraulic conductivity $Y = \ln K$ as the expansion parameter of the theory. We estimate the mean hydraulic head, $\overline{h}(\mathbf{x})$, and assess the errors associated with such an estimation. We represent $K(\mathbf{x}) = \overline{K}(\mathbf{x}) + K'(\mathbf{x})$ as the sum of a mean, $\overline{K}(\mathbf{x})$, and a zero-mean random deviation, $K'(\mathbf{x})$, with variance $\sigma_K^2(\mathbf{x})$. Similarly, $h(\mathbf{x}) = \overline{h}(\mathbf{x}) + h'(\mathbf{x})$ with $\overline{h'}(\mathbf{x}) \equiv 0$ and variance $\sigma_h^2(\mathbf{x})$.

The average steady-state flow equation becomes

$$\nabla \cdot \left[\overline{K}(\mathbf{x})\, \nabla \overline{h}(\mathbf{x})\right] + \nabla \cdot \overline{\mathbf{r}}(\mathbf{x}) = 0 \tag{2}$$

which consists of a deterministic mean part, $\overline{K}\nabla\overline{h}$, and a deterministic residual flux, $\overline{\mathbf{r}} = -\overline{K'\nabla h'}$. Solutions of (2) require the mean conductivity, $\overline{K}(\mathbf{x})$, and in most cases, a method for closing an expansion of $\overline{\mathbf{r}}(\mathbf{x})$. Usually $\overline{\mathbf{r}}(\mathbf{x})$ is approximated through perturbation expansions based on σ_Y^2, the variance of $Y = \ln K$, the logarithm of conductivity. This approach works well as long as σ_Y^2 is small. This restriction is a stumbling block on the road to applicability of numerous theoretical analyses to real-world problems. Our goal here is to provide a general theoretical method that exploits the limited information obtain from moment equations to derive the best guesses for the properties of the permeability in the large heterogeneity limit.

2.2 Perturbation expansions

Consider asymptotic expansions of the parameters and functions, $\overline{K} = K_g\,(1 + \sigma_Y^2/2 + \cdots)$; $\overline{h} = \overline{h}^{(0)} + \overline{h}^{(1)} + \cdots$; and $\mathbf{r} = \mathbf{r}^{(1)} + \cdots$, where $K_g = \exp(\overline{Y})$, $\overline{Y}$ being the ensemble mean of Y. The superscript (i) denotes terms that are of ith-order, i.e. contain only the ith power of σ_Y^2. The first-order (in σ_Y^2) approximation of the residual flux is given by [Tartakovsky and Neuman 1998a, b and references therein]

$$\mathbf{r}^{(1)}(\mathbf{x}) = K_g\, \sigma_Y^2 \int_\Omega \rho_Y(\mathbf{y}, \mathbf{x})\, \nabla_{\mathbf{x}} \nabla_{\mathbf{y}}^{\mathrm{T}}\, G(\mathbf{y}, \mathbf{x})\, \nabla \overline{h}^{(0)}(\mathbf{y})\, \mathrm{d}\mathbf{y}, \tag{3}$$

where $\rho_Y(\mathbf{y}, \mathbf{x})$ is the spatial two-point autocorrelation function of Y, and $G(\mathbf{y}, \mathbf{x})$ is the deterministic Green's function for Laplace equation in Ω subject to the corresponding homogeneous boundary conditions. It is a standard practice in stochastic hydrogeology to rely on the first-order approximation of $\mathbf{r}$ (Dagan 1989), but higher-order approximations are also available (Hsu et al. 1995).

Collecting the terms of the same powers of σ_Y^2 yields the zeroth-order approximation of the mean head in 2,

$$K_g\, \nabla^2 \overline{h}^{(0)}(\mathbf{x}) = 0, \tag{4}$$

and its first-order approximation,

$$K_g\, \nabla^2 \overline{h}^{(1)}(\mathbf{x}) + \nabla \cdot \left[\frac{\sigma_Y^2}{2}\, K_g\, \nabla \overline{h}^{(0)}(\mathbf{x}) - \mathbf{r}^{(1)}(\mathbf{x})\right] = 0\,. \tag{5}$$

Solving a system of these sequential approximations leads to $\overline{h}^{[1]} \equiv \overline{h}^{(0)} + \overline{h}^{(1)}$. Strictly speaking, for such expansions to be asymptotic it is necessary that $\sigma_Y^2 \ll 1$, i.e. that porous media be mildly heterogeneous. However, various numerical simulations (e.g., Guadagnini and Neuman 1999) have demonstrated that these first-order approximations remain remarkably robust even for strongly heterogeneous media with σ_Y^2 as large as 4.

2.3 Effective conductivity of porous media

For an effective conductivity to exist in the strict sense, it is necessary that $\nabla\overline{h}$ be constant. A somewhat a less restrictive assumption requires $\nabla\overline{h}$ to vary slowly in space, i.e. to have negligibly small derivatives (Dagan 1989). Then one can localize expression (3) as

$$\mathbf{r}^{(1)}(\mathbf{x}) \approx K_{\rm g}\,\sigma_Y^2\mathbf{A}^{(1)}(\mathbf{x})\,\nabla\overline{h}^{(0)}(\mathbf{x}), \quad \mathbf{A}^{(1)}(\mathbf{x}) = \int_\Omega \rho_Y(\mathbf{y},\mathbf{x})\,\nabla_{\mathbf{x}}\nabla_{\mathbf{y}}^{\rm T}\,G(\mathbf{y},\mathbf{x})\,{\rm d}\mathbf{y}. \tag{6}$$

Under these conditions, retaining the two leading terms in the asymptotic expansion of the mean Darcy flux, $\overline{\mathbf{q}} \approx \overline{\mathbf{q}}^{[1]} \equiv \overline{\mathbf{q}}^{(0)} + \mathbf{q}^{(1)}$, yields

$$-\frac{\overline{\mathbf{r}}^{[1]}(\mathbf{x})}{K_{\rm g}} = \nabla\overline{h}^{(1)}(\mathbf{x}) + \left[\mathbf{I} + \sigma_Y^2\left(\frac{1}{2}\,\mathbf{I} - \mathbf{A}^{(1)}(\mathbf{x})\right)\right]\nabla\overline{h}^{(0)}(\mathbf{x})\,. \tag{7}$$

For flow through infinite, statistically homogeneous porous media under mean uniform flow conditions, or at points away from boundaries and singularities, the mean hydraulic head gradient $\overline{\mathbf{J}} = \nabla\overline{h}^{(0)} = \text{const}$ and $\nabla\overline{h}^{(i)} = 0$ $(i \geq 1)$ (Dagan 1989; Tartakovsky and Neuman 1998a, b). This gives rise to the effective conductivity given approximately by

$$K_{\rm ef}^{[1]} \equiv K_{\rm ef}^{(0)} + K_{\rm ef}^{(1)} = K_{\rm g}\left[1 + \left(\frac{1}{2} - \frac{1}{d}\right)\sigma_Y^2\right] \tag{8}$$

where d is the space dimension.

Various attempts to generalize this asymptotic expansion to highly heterogeneous formations were attempted by conjecturing that expression (8) represents the two leading terms in the expansion of an exponent (Matheron 1967;Shvidler 1962),

$$K_{\rm ef} = K_{\rm g}\,\exp\left[\left(\frac{1}{2} - \frac{1}{d}\right)\sigma_Y^2\right]. \tag{9}$$

In recent years the question of validity of expression (9) was the focus of a thorough investigation. It was proven that expression (9) is rigorously valid under one-dimensional flow in log-normal fields where it yields the harmonic mean $K_h = K_{\rm g}\exp(-\sigma_Y^2/2)$ (Dagan 1993; Paleologos et al. 1996). It is also rigorously valid under two-dimensional flow in log-normal, statistically isotropic conductivity fields where it yields the geometric mean $K_{\rm g}$ (Matheron 1967). For three-dimensional flow in log-normal, statistically isotropic fields, the second-order (in σ_Y^2) term in (8) was found to be in agreement with the Taylor series expansion of (9) (Dagan 1993). While unsuccessfull attempts to prove (9) for three-dimensional flows in such fields have been reported (King 1989; Noetinger 1990), De Wit 1995 demonstrated that the third-order correction in (8) is not equal to the third-order term in the Taylor expansion of (9), thereby proving this conjecture to be not strictly valid for three-dimensional Gaussian isotropic media. Instead, it was demonstrated that this and higher-order terms depend on the shape of the correlation function ρ_Y.

These results suggest that it would be beneficial to view the Eq. 8 and its higher order terms as a perturbation expansion of the true scalar hydraulic conductivity in powers of the variance σ_Y^2. In this sense, the passage from (8) to (9) is a resummation procedure. It thus makes full sense to ask what could be the most general and robust resummation that can generalize (8) in order to extract the behavior of the permeability in the regime of large σ_Y^2 where the initial perturbation expansion breaks down.

It is often the case that perturbation expansions are not converging but are instead diverging series. Even if the series is convergent for small perturbation parameters σ_Y^2, one is in

general interested in the regime where σ_Y^2 is of order 1 and larger. In this case, the perturbation series is divergent and is of no direct use. The study of such summation of divergent series is the problem of great importance in theoretical physics, applied mathematics and engineering. This is because realistic problems are usually solved by means of some calculational algorithm often resulting in divergent sequence of approximations. Assigning a finite value to the limit of a divergent sequence is called renormalization or summation technique. The most widely used such technique is Padé summation (Baker 1996). However, the Padé summation method has several shortcomings. First of all, to reach a reasonable accuracy of Padé approximants, one needs to possess tens of terms of a perturbation series. In contrast, only a few terms are often available because of the complexity of the problem. Second, Padé approximants are defined for the series of integer powers. But in many cases asymptotic series arise having noninteger powers. Third, there are quite simple examples that are not Padé summable even for a sufficiently small variable. Last, Padé summation is more of a numerical technique providing answer in the form of numbers. Therefore, it is difficult, if possible, to analyze the results when the considered problem contains several parameters to be varied, since for each given set of parameters one has to repeat the whole procedure of constructing a table of Padé approximants and of selecting from them one corresponding to a visible saturation of numerical values.

We thus turn to the method of so-called self-similar approximation or functional renormalization that provide a very interesting alternative. We first summarize the idea of the technique and then apply it to calculate properties of transport in porous media in the limit of large heterogeneity.

3 General formulation of the self-similar approximation theory

General ideas and the mathematical foundation of the self-similar approximation theory have been described in detail in (Gluzman and Yukalov 1998; Yukalov and Gluzman 1997a, b; Yukalov and Gluzman 1998; Yukalov and Gluzman 1999; Gulzman and Sornette 2002; Gulzman et al. 2003; Gulzman et al. 2003; Gulzman and Yukalov 1998; Yukalov et al. 1998; Yukalov and Gluzman 1999). The approach is applicable in all cases, when either just a few terms of a series are known or when a number of such terms are available. We are always able to obtain analytical formulas that are easy to consider with respect to varying characteristic parameters. We now expose the general idea of the method of self-similar approximation. For more details on the method, see the appendix.

Consider the case, when for a sought function $f(x)$, one derives an approximate perturbative expansion

$$p_k(x) = \sum_{n=0}^{k} a_n \, x^{\alpha_n}, \tag{10}$$

in which α_n is an arbitrary real number, integer or noninteger, positive or negative. Following the method of the algebraic self-similar renormalization (Gluzman and Yukalov 1997), we define the algebraic transform

$$P_k(x, s) \equiv x^s \; p_k(x) = \sum_{n=0}^{k} a_n \, x^{s+\alpha_n}, \tag{11}$$

where s is real. Rather than constructing a trajectory in the functional space of the initial approximations, the idea behind the introduction of the transform (11) is to deform smoothly the initial functional space of the approximations $p_k(x)$ in order to obtain a faster and better controlled convergence in the space of the modified functions $P_k(x, s)$. This convergence can then be mapped back to get the relevant estimations and predictions. The exponent s depends on x in general and will be acted upon as a control function in order to accelerate convergence.

Then, by means of the equation $P_0(x, s) = a_0\, x^{s+\alpha_0} = \varphi$, we obtain the expansion function $x(\varphi, s) = \left(\frac{\varphi}{a_0}\right)^{1/(s+\alpha_0)}$. Substituting the latter into (10), we have

$$y_k(\varphi, s) \equiv P_k(x(\varphi, s), s) = \sum_{n=0}^{k} a_n \left(\frac{\varphi}{a_0}\right)^{(s+\alpha_n)/(s+\alpha_0)} . \tag{12}$$

The family $\{y_k\}$ of transforms (10) is called the approximation cascade, since its trajectory $\{y_k(\varphi, s) \mid k = 0, 1, 2 \ldots\}$ is bijective to the sequence $\{P_k(x, s) \mid k = 0, 1, 2 \ldots\}$ of approximations (11). A cascade is a dynamical system in discrete time $k = 0, 1, 2 \ldots$, whose trajectory points satisfy the semigroup property $y_{k+p}(\varphi, s) = y_k(y_p(\varphi, s), s)$. The physical meaning of the above semigroup relation can be understood as the property of functional self-similarity with respect to the varying approximation number. The self-similarity relation is a necessary condition for the fastest convergence criterion.

For the approximation cascade $\{y_k\}$, defined by transform (12), the cascade velocity is

$$v_k(\varphi, s) \equiv y_k(\varphi, s) - y_{k-1}(\varphi, s) = a_k \left(\frac{\varphi}{a_0}\right)^{(s+\alpha_k)/(s+\alpha_0)} . \tag{13}$$

This is to be substituted into the evolution integral

$$\int_{P_{k-1}}^{P_k^*} \frac{\mathrm{d}\varphi}{v_k(\varphi, s)} = \tau, \tag{14}$$

in which $P_k = P_k(x, s)$ and τ is the minimal time needed for reaching a fixed point $P_k^* = P_k^*(x, s, \tau)$. Integral (14) with velocity (13) yields

$$P_k^*(x, s, \tau) = \left[P_{k-1}^{-\nu}(x, s) - \frac{\nu\, a_k \tau}{a_0^{1+\nu}} \right]^{-1/\nu} , \tag{15}$$

where $\nu = \nu_k(s) \equiv \frac{\alpha_k - \alpha_0}{s+\alpha_0}$. Taking the algebraic transform inverse to (11), we find

$$p_k^*(x, s, \tau) \equiv x^{-s} P_k^*(x, s, \tau) = \left[p_{k-1}^{-\nu}(x) - \frac{\nu\, a_k \tau}{a_0^{1+\nu}} x^{s\nu} \right]^{-1/\nu} . \tag{16}$$

Exponential renormalization (Yukalov and Gluzman 1997a, b; Yukalov and Gluzman 1998) corresponds to the limit $s \to \infty$, at which $\lim_{s\to\infty} \nu_k(s) = 0$, $\lim_{s\to\infty} s\nu_k(s) = \alpha_k - \alpha_0$. Then (16) gives

$$\lim_{s\to\infty} p_k^*(x, s, \tau) = p_{k-1}(x) \exp\left(\frac{a_k}{a_0} \tau x^{\alpha_k - \alpha_0} \right). \tag{17}$$

Accomplishing exponential renormalization of all sums appearing in expression of type (17), we follow the bootstrap procedure (Yukalov and Gluzman 1997a, b) according to the scheme $p_k(x) \to p_k^*(x, s, \tau) \to F_k(x, \tau_1, \tau_2, \ldots, \tau_k)$, with $k \geq 1$.

Let us mention a recent innovation (Gluzman and Sornette 2002) that may improve significantly the convergence of the method, based on the determination of the control parameters from the knowledge of some moments of the function to reconstruct. Let us assume that we can obtain the first $j-1$ moments $\mu_i, i = 1, 2, \ldots, j$ of the sought function $\phi(t)$, in some interval T,

$$\mu_i = \int_0^{\mathrm{T}} t^{i-1}\phi(t)\mathrm{d}t, \tag{18}$$

so that for j=2 both zero and first moments are available etc. One can condition the control parameters $\tau_{1,}\tau_{2,\ldots}\tau_j$ as follows

$$\int_0^{\mathrm{T}} f_j^*(t, \tau_1, \tau_2, \ldots, \tau_{j-1})t^{i-1}\mathrm{d}t = \mu_i, \tag{19}$$

Based on these conditions, one can attempt to solve two different problems, the first one corresponds to an approximate reconstruction of the function $\phi(t)$ within the same interval [0,T] where moments are given or measured. The second problem consists in extrapolating to $t > T$. It is also possible to use an hybrid approach, where some controls are obtained from the agreement with the expansion, while the remaining ones are found from the conditions on moments.

4 Resummation of lower order expansions in σ_Y^2

4.1 What can be extracted from the expansion of $K_{\mathrm{ef}}^{[1]}$

Assume that the following extremely short expansion has been obtained,

$$K(\sigma_Y) \simeq 1 - a\sigma_Y^2, \quad a = \frac{1}{d} - \frac{1}{2} \quad (\sigma_Y^2 \to 0). \tag{20}$$

Consider the case $a > 0$. In order to find the behavior of $K(\sigma_Y)$ for arbitrary σ_Y^2, we continue it from the region of $\sigma_Y^2 \to 0$ self-similarly, along the most stable trajectory, with the crossover index s, determined by the condition of the minimum of the multiplier (Gluzman and Yukalov 1998; Yukalov and Gluzman 1997a, b; Yukalov and Gluzman 1999)

$$m(\sigma_Y, s) = 1 - a\sigma_Y^2\frac{1+s}{s}, \tag{21}$$

from where

$$s(\sigma_Y) = a\sigma_Y^2\left(1 - a\sigma_Y^2\right)^{-1}, \quad \sigma_Y < a^{-1/2},$$
$$s \to \infty, \quad \sigma_Y \geq a^{-1/2},$$

corresponding to the self-similar approximation

$$K^*(\sigma_Y) = \left(\frac{s(\sigma_Y)}{s(\sigma_Y)+a\sigma_Y^2}\right)^{s(\sigma_Y)} = \left(2 - a\sigma_Y^2\right)^{\frac{a\sigma_Y^2}{a\sigma_Y^2-1}}, \quad \sigma_Y < a^{-1/2}, \tag{22}$$

$$K^*(\sigma_Y) = \exp(-a\sigma_Y^2), \quad \sigma_Y \geq a^{-1/2}. \tag{23}$$

This suggests one self-similar expression (22) up to $\sigma_{Y0} = a^{-1/2}$, and another (23), exponentially "soft", above this value. Strictly speaking, formula (22) is applicable for σ_Y only

up to $(2/a)^{1/2}$, where it predicts a spurious zero of conductivity. In this particular case, the self-similar approximation plausibly reconstructs the exponential function for arbitrary σ_Y, even in the absence of any a priori assumption on the asymptotic behavior at $\sigma_Y \to \infty$.

For negative a $(d > 2)$, there is no limiting value σ_{Y0} and this yields

$$K^*(\sigma_Y) = \left(\frac{s(\sigma_Y)}{s(\sigma_Y) + a\sigma_Y^2} \right)^{s(\sigma_Y)}, \tag{24}$$

which can be used for arbitrary σ_Y. This expression appears to be more stable than the previously proposed exponential solution $\exp(-a\sigma_Y^2)$ for arbitrary σ_Y, as indicated by the analysis of the multipliers. Expression (24) also predict a smaller conductivity than the exponential function for arbitrary σ_Y suggesting that, for the most interesting case $d = 3$, the ansatz Eq. 8 should be replaced. Analysis of higher-order expansions will provide more details on the sought function.

4.2 Resummation of the second-order expansion in σ_Y^2. One-parameter formula

Available from (Dagan 1993) in the next order in σ_Y^2, we have

$$K_{\text{ef}}^{[2]} \equiv K_{\text{ef}}^{[1]} + K_{\text{ef}}^{(2)} = K_{\text{g}} \left[1 + \left(\frac{1}{2} - \frac{1}{d} \right) \sigma_Y^2 + \frac{1}{2} \left(\frac{1}{2} - \frac{1}{d} \right)^2 \sigma_Y^4 \right]. \tag{25}$$

Below, for simplicity, we apply our resummation technique to the dimensionless quantity

$$K(z) \simeq 1 + a_1 z + a_2 z^2, \quad z \equiv \sigma_Y^2, \quad a_1 = \left(\frac{1}{2} - \frac{1}{d} \right), \; a_2 = \frac{1}{2} \left(\frac{1}{2} - \frac{1}{d} \right)^2. \tag{26}$$

Application of accuracy-through-order conditions, or of the super-exponential approximants give, almost trivially, an exponential solution. Note that the Padé approximant available in this case,

$$P(z) = \frac{1 + (-a_2/a_1 \; + a_1)z}{1 - a_2/a_1 \; z}, \tag{27}$$

for $d = 3$, possesses a singularity at $z = 12$, which is wrong.

The set of approximations to $K(z)$, including the two starting terms from (26), can be written down as follows:

$$K_0 = 1,$$
$$K_1 = 1 + a_1 z,$$

and the expression for the renormalized quantity a_1^* can be readily obtained:

$$K_1^* = \left(\frac{s_1}{s_1 - a_1 z} \right)^{s_1} \Longrightarrow \left(\frac{s_1}{-a_1} \right)^{s_1} z^{-s_1} \; (z \to \infty), \tag{28}$$

where the stabilizer s_1 should be negative, if we want to reproduce in the limit of $z \to \infty$, the correct, supposedly power-law behavior of the conductivity. A different set of approximations, which does not include the constant term from (26) into the renormalization procedure, has the form:

$$\overline{K_1} = a_1 z, \tag{29}$$

$$\overline{K_2} = a_1 z + a_2 z^2, \tag{30}$$

and applying the standard procedure of (Yukalov and Gluzman 1997a, b), we obtain

$$K_2^* = 1 + a_1 z[1 - \frac{a_2 z}{a_1(1+s_2)}]^{-(1+s_2)} \Longrightarrow (-\frac{a_2}{1+s_2})^{-(1+s_2)}\, a_1^{2+s_2} z^{-s_2}\ (z \to \infty). \quad (31)$$

Demanding now that both (28) and (31) have the same power-law behavior at $z \to \infty$, we find that

$$s_2 = s_1 \equiv s.$$

Requiring now the fulfillment of the stability criteria for the two available approximations in the form of the minimal-difference condition (see Sect. 3), we obtain the condition that the *negative* stabilizer s should be determined from the *minimum* of the expression:

$$\left| \left[\left(\frac{-a_2}{1+s} \right)^{-(1+s)} a_1^{(2+s)} - \left(\frac{s}{-a_1} \right)^{s} \right] \right|. \quad (32)$$

Generally speaking, it is sufficient to ask for an extremum of this difference.

In the case of $d = 3$, the maximum is located at the point $s = -1.218$. The final formulae have the following form:

$$K_1^*(z) = \left(\frac{s}{s - a_1 z} \right)^{s}, \quad (33)$$

$$K_2^*(z) = 1 + a_1 z \left[1 - \frac{a_2 z}{a_1(1+s)} \right]^{-(1+s)}. \quad (34)$$

This last formula gives a lower bound for conductivity while the upper bound is simply $\exp(a_1 z)$ (Eq. 8) which, in this case, is the only available "factor"-approximant based on all available (three) terms from the expansion. The corresponding multiplier is

$$M_2^*(z) = \frac{a_1(1+s) + a_2 z\, s}{a_1(1+s) - a_2 z} \left(1 - \frac{a_2}{a_1(1+s)} z \right)^{-(s+1)} \quad (35)$$

and the weighted average (Yukalov and Gluzman 1999; Gluzman and Sornette 2002) is given by

$$C(z) = \frac{1 + K_2^*(z) \left| M_2^*(z) \right|^{-1}}{\exp(-a_1 z) + \left| M_2^*(z) \right|^{-1}}, \quad (36)$$

providing the one-parametric formula for 3d-conductivity. See Fig. 1 for a comparison of different formulas for the conductivity as a function of the variance $z \equiv \sigma_Y^2$ defined in Eq. 26. The solid line corresponds to the average $C(z)$, while the dotted line presents $K_2^*(z)$. The dashed line is the celebrated exponential Landau–Lifshitz–Matheron (LLM) conjecture. The dash-dotted line corresponds to the result of resummation based on first-order expansion, $K^*(\sigma_Y)$. The filled circles are the values obtained by the numerical calculations reported in Ref. Neuman and Orr 1993. One can see that the Landau–Lifshitz–Matheron (LLM) conjecture provides the best description.

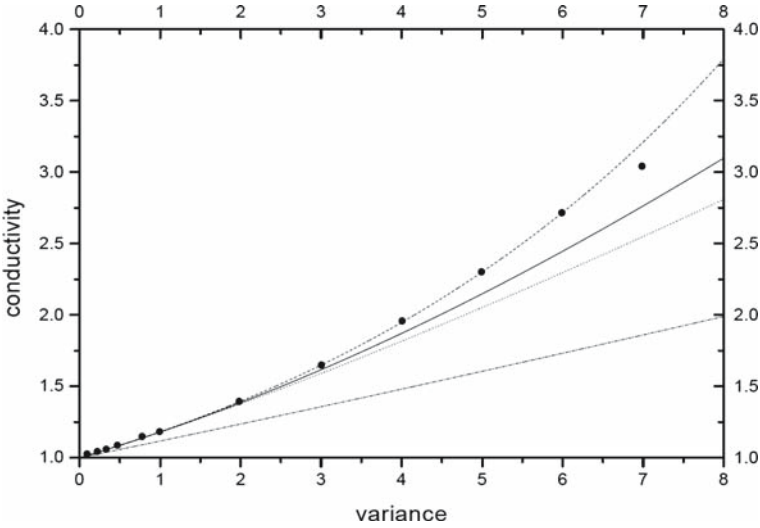

Fig. 1 Dependence of different estimators of the conductivity as a function of the variance $z \equiv \sigma_Y^2$ defined in Eq. 26. The solid line corresponds to $C(z)$, the dotted line shows $K_2^*(z)$. The dashed line is the Landau–Lifshitz–Matheron (LLM) conjecture. $K^*(\sigma_Y)$ (dash-dotted line) corresponds to the result of resummation based on the first-order expansion. The filled circles are the values obtained by the numerical calculations reported in Ref. Neumand and Orr 1993. The Landau–Lifshitz–Matheron (LLM) conjecture provides the best description

4.3 Resummation of the third-order expansion in σ_Y^2. two-parameters formula

The expansion to the next order is given by (De wit 1995),

$$K(z) \simeq 1 + a_1 z + a_2 z^2 + a_3 z^3, \quad a_3(Z) = \frac{1}{6}\left(\frac{1}{2} - \frac{1}{d}\right)^3 - Z, \tag{37}$$

where $Z = 0.0042/3$ (in the case of a Gaussian covariance), or $Z = 0.0014/3$ (in the case of an exponentially decaying covariance).

Using all terms from the expansion, we can create the following "odd" factor-approximant (Gluzman et al. 2003),

$$K_3^*(z, Z) = 1 + a_1 z \left(1 - \frac{a_2}{a_1(s_2(Z)+1)} z\right)^{-(s_2(Z)+1)}, \quad s_2(Z) = -2\frac{a_2^2 - a_3(Z)a_1}{a_2^2 - 2a_3(Z)a_1}, \tag{38}$$

while $K_2^*(z) = \exp(a_1 z)$, which recovers expression (8). The approximant $K_2^*(z)$ gives an upper bound for the conductivity coefficient, while $K_3^*(z, Z)$ given by (38) provides a lower bound. The corresponding multipliers can be readily written down,

$$M_3^*(z, Z) = \frac{a_1(1 + s_2(Z)) + a_2 z\, s_2(Z)}{a_1(1 + s_2(Z)) - a_2 z} \left(1 - \frac{a_2}{a_1(s_2(Z)+1)} z\right)^{-(s_2(Z)+1)}, \tag{39}$$

$$M_2^*(z) = \exp(a_1 z). \tag{40}$$

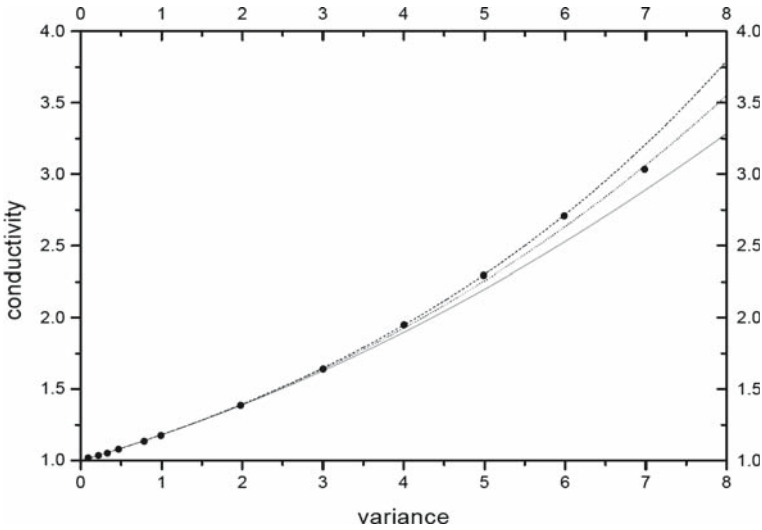

Fig. 2 Dependence of the conductivity $C(z, Z)$ as a function of the variance $z \equiv \sigma_Y^2$ defined in Eq. 26 for Gaussian and exponential covariances, shown with solid and dotted lines respectively. For comparison, the Landau–Lifshitz–Matheron (LLM) conjecture is shown in dashed lines. The filled circles are the values obtained by the numerical calculations reported in Ref. Neumand and Orr 1993. The conductivity $C(z, Z)$ for the exponential covariances is performing comparably or slightly better than the Landau–Lifshitz–Matheron (LLM) conjecture

This allows us to obtain the weighted average of the conductivity coefficient

$$C(z, Z) = \frac{1 + K_3^*(z, Z) \left| M_3^*(z, Z) \right|^{-1}}{\exp(-a_1 z) + \left| M_3^*(z, Z) \right|^{-1}}, \tag{41}$$

providing a two-parameters formula for the 3d-conductivity. The results for $C(z, Z)$ for Gaussian and exponential covariances are shown in Fig. 2, with the dotted line for the exponential case and with the solid line for the Gaussian case. These results are compared with the Landau–Lifshitz–Matheron (LLM) shown with dashed line. The filled circles are the values obtained by the numerical calculations reported in Ref. Neuman and Orr 1993. One can observe that the conductivity $C(z, Z)$ for the exponential covariances is performing comparably or slightly better than the Landau–Lifshitz–Matheron (LLM) conjecture, the difference becoming more significant for that largest available value of the variance.

Numerical data in the exponential case are available till $z = 7$ Neuman and Orr 1993 and in the Gaussian case up to $z = 6$ (Dykaar and Kitanidis 1992). Our results suggest that all formulas based on the expansion on σ_Y^2—up to the third order underestimate the conductivity and more terms are needed to improve the accuracy of the resummed expressions.

A different approach aimed at increasing the accuracy consists in getting expressions for the conductivity in the limit of $\sigma_Y^2 \to \infty$, for instance from expansions in inverse powers of σ_Y^2, It is known (see Ref. Gluzman and Yukalov 1998; Yukalov et al. 1998; Yukalov and Gluzman 1999) that when the asymptotic form of the solution is known, even only qualitatively, the formulas for the sought function can be improved very significantly. Even the knowledge of the leading power in the limit of large σ_Y^2 would be of utmost importance.

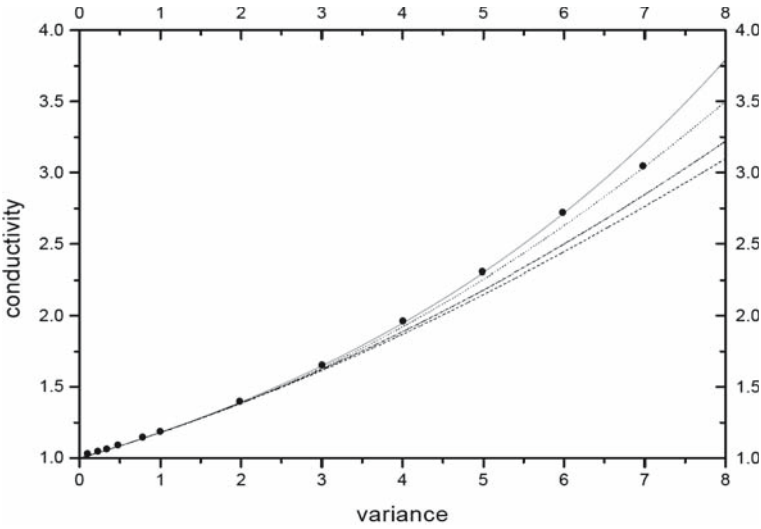

Fig. 3 As a function of the variance $z \equiv \sigma_Y^2$ defined in Eq. 26, this figure shows a comparison between the conductivity $K_2^*(m)$ (dotted line) with $C(z)$ (dashed) and with $\exp(a_1 z)$ (solid line). The Perturbative expansion $K(m)$ is shown with the dashed-dot line. The filled circles are the values obtained by the numerical calculations reported in Ref. Neumand and Orr 1993. The function $K_2^*(m)$ (dotted line) is in good agreement with these simulations

5 $1/d$-expansion and resummation

5.1 One-parametric case (d=3)

Expression (26) for $K(z)$ in the second order of perturbation theory can be re-written in the form of an expansion in the parameter $1/d$ with coefficients dependent on z,

$$K(m) \simeq b_0(z) + b_1(z)m + b_2(z)m^2, \quad m \equiv 1/d; \tag{42}$$

$$b_0(z) = 1 + \frac{z}{2} + \frac{z^2}{8}, \quad b_1(z) = -z - \frac{z^2}{2}, \quad b_2(z) = \frac{z^2}{2}. \tag{43}$$

The theory of self-similar super-exponential approximants (Yukalov and Gluzman 1997a, b; Yukalov and Gluzman 1998; Gluzman and Sornette 2002; Gluzman et al. 2003) then provides the following approximant

$$K_2^*(m) = b_0 \exp\left(\frac{b_1}{b_0}\tau_1 m \exp\left(\frac{b_2}{b_1}\tau_2 m\right)\right), \quad \tau_1 = 1, \ \tau_2 = 1 - \frac{b_1^2}{2b_0 b_2}. \tag{44}$$

$K_2^*(m)$ is located within the bounds given by $K_2^*(z)$ and $\exp(a_1 z)$ and provides a one-parametric formula for the $d = 3$-conductivity, as shown in Fig. 3. $K_2^*(m)$ (dotted line) also appears to be located within the bounds outlined by $C(z)$ (dashed) and $\exp(a_1 z)$ (solid line). The perturbative expression $K(m)$ (dashed-dot line) is shown as well for comparison. The filled circles are the values obtained by the numerical calculations reported in Ref. Neumand Orr 1993. The function $K_2^*(m)$ (dotted line) is in good agreement with these simulations.

5.2 Two-parametric case (d=3)

Expression for $K(z)$ (37) in the third order of perturbation theory can also be re-written in the form of an $1/d$-expansion with coefficients dependent on z and Z,

$$K(m, Z) \simeq b_0(z, Z) + b_1(z)m + b_2(z)m^2 + b_3(z)m^3; \tag{45}$$

$$b_0(z, Z) = 1 + \frac{z}{2} + \frac{z^2}{8} + \left(\frac{1}{48} - Z\right) z^3, \quad b_1(z) = -z - \frac{z^2}{2} - \frac{z^3}{8}, \quad b_2(z) = \frac{z^2}{2} + \frac{z^3}{4}, \tag{46}$$

$$b_2(z) = \frac{z^2}{2} + \frac{z^3}{4}, \qquad b_3(z) = -\frac{z^3}{6}. \tag{47}$$

We apply the technique of self-similar super-exponential function in its variant detailed in (Gluzman and Sornette 2002; Gluzman et al. 2003), giving the following approximants

$$K_2^*(m, Z, \tau_1, \tau_2) = b_0 \exp\left(\frac{b_1}{b_0}\tau_1 m \exp\left(\frac{b_2}{b_1}\tau_2 m\right)\right), \tag{48}$$

$$K_3^*(m, Z, \tau_1, \tau_2, \tau_3) = b_0 \exp\left(\frac{b_1}{b_0}\tau_1 m \exp\left(\frac{b_2}{b_1}\tau_2 m \exp\left(\frac{b_3}{b_2}\tau_3 m\right)\right)\right), \tag{49}$$

$$\tau_3 = \frac{1}{6}\frac{\left(-b_1^4 + 6b_0^2 b_1 b_3 - 6\tau_2 b_0 b_1^2 b_2 - 3\tau_2^2 b_0^2 b_2^2\right)}{\tau_2 b_0^2 b_1 b_3}. \tag{50}$$

In order to check whether the sequence of K_j^* converges, we study their mapping multipliers, $M_j^*(t, \tau_1, \tau_2, \ldots \tau_j)$ defined as

$$M_j^*(m, Z, \tau_1, \ldots, \tau_j) \equiv \frac{1}{b_1}\frac{\partial}{\partial t} K_j^*(m, Z, \tau_1, \ldots, \tau_j). \tag{51}$$

This definition of the multipliers allows us to compare the convergence of the expansion and of the renormalized expressions, making clear what can be expected a priori.

This provides a matrix of self-similar approximants, indexed by the order j and by the number of control parameters,

$$K_{21}^*(m, Z) = K_j^*(m, Z, \tau_1, 1), \quad K_{22}^*(m, Z) = K_j^*(m, Z, \tau_1, \tau_2), \tag{52}$$

$$\begin{aligned} &K_{31}^*(m, Z) = K_3^*(m, Z, \tau_1, 1, 1), \quad K_{32}^*(m, Z) = K_3^*(m, Z, \tau_1, \tau_2, 1), \\ &K_{33}^*(m, Z) = K_3^*(m, Z, \tau_1, \tau_2, \tau_3), \end{aligned} \tag{53}$$

Approximants $K_{22}^*(m, Z)$ and $K_{32}^*(m, Z)$ form the closest pair. Their average

$$K^*(m, Z) = \frac{K_{22}^*(m, Z)\left|M_{22}^*(m, Z)\right|^{-1} + K_{32}^*(m, Z)\left|M_{32}^*(m, Z)\right|^{-1}}{\left|M_{22}^*(m, Z)\right|^{-1} + \left|M_{32}^*(m, Z)\right|^{-1}}. \tag{54}$$

is located within the bounds given by $K_3^*(z, Z)$ (38) and $\exp(a_1 z)$ and provides a useful formula for the conductivity coefficient. The results for the exponential and Gaussian covariances are shown in Figs. 4 and 5, respectively. In the exponential case, good agreement between $K^*(m, Z)$ (dash-dot) and the Landau–Lifshitz–Matheron (LLM) conjecture (solid)

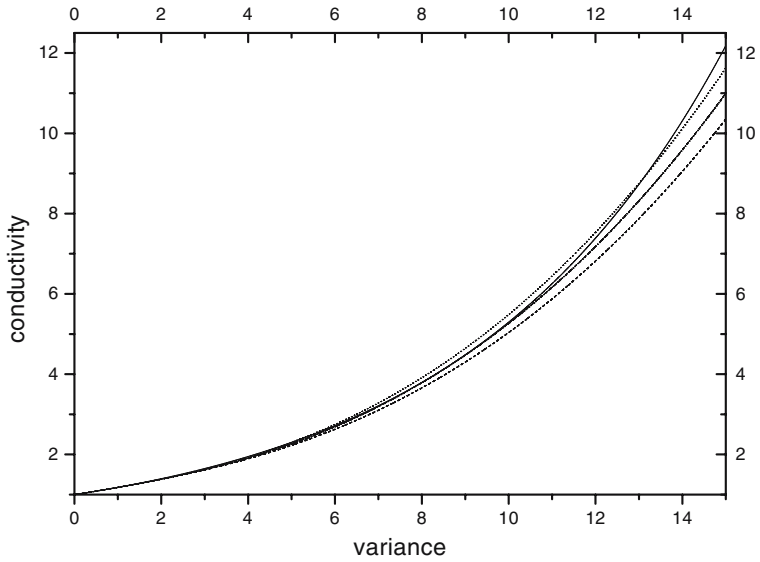

Fig. 4 Exponential covariance: $K^*(m, Z)$ (dash–dot) is compared with the Landau–Lifshitz–Matheron (LLM) conjecture (solid line). Two approximants $K^*_{22}(m, Z)$ (dashed) and $K^*_{32}(m, Z)$ (dotted) are shown as well

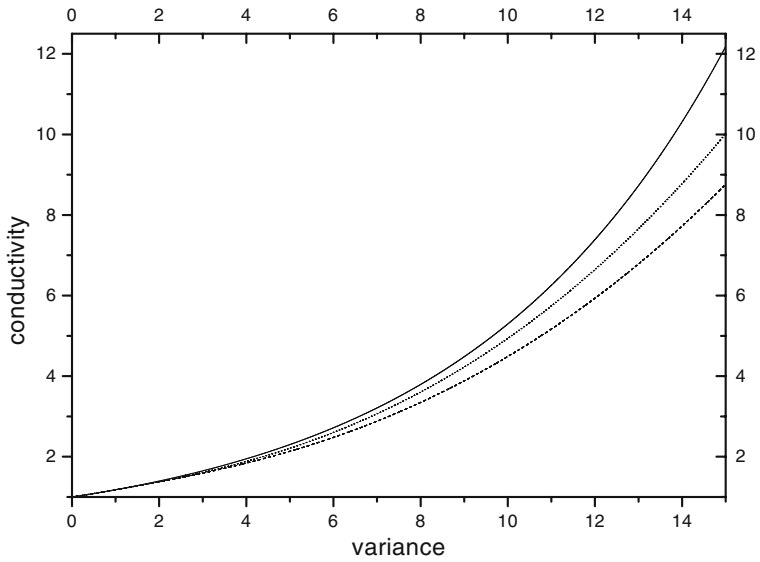

Fig. 5 Gaussian case: Approximant $K^*_{32}(m, Z)$ (dotted) compared with the Landau–Lifshitz–Matheron (LLM) conjecture (solid line). The approximant $K^*_{22}(m, Z)$ (dashed line) is shown as well

remains valid till $z \approx 11$. The average behavior appears to be located within the bounds outlined by $K^*_{22}(m, Z)$ (dashed) and $K^*_{32}(m, Z)$ (dotted) and provides a reasonable formula for the conductivity. Numerical data are available till $z = 7$ (Neuman and Orr 1993) and they agree well with our lower bound.

In the Gaussian case $K^*_{32}(m, Z)$ (dotted line) gives an approximation which is closer to the Landau–Lifshitz–Matheron (LLM) conjecture (solid) than $K^*_{22}(m, Z)$ (dashed line). In this case, numerical results are available up to $z = 6$ (Dykaar and Kitanidis 1992).

We conclude, tentatively, that all formulas based on $1/d$-expansion in the third order provide rather accurate expressions for conductivity for small and moderate variances and disagree with the LLM-conjecture for very large variances. To the best of our knowledge, the region of large variances is not accessible by other techniques, numerically or theoretically. All formulas based on the novel proposed $1/d$-expansion in the third order provide rather accurate expressions for the conductivity coefficient. We note that $1/d$-expansions may be faster converging than the original expansion in variances and should be investigated future.

6 Future directions

We have shown that it is possible to exploit the limited information obtained from moment equations to derive the best guesses for the properties of the permeability in the large heterogeneity limit. We have done this by using the self-similar functional renormalization method, which provides a more stable and robust estimation of the scalar hydraulic conductivity of the three-dimensional medium at large values of the perturbation parameter σ_Y^2.

A fundamental question on the self-similar renormalization method should be raised: Do the first terms in the expansions contain enough information about the behavior of other terms? There is not unique and universal answer to this non-trivial question. Our experience (see all the papers by Yukalov et al. and Gluzman et al.) shows that in many (most?) cases, the self-similar renormalization method does a remarkable job at providing significantly improved estimations of the true functions just from the knowledge of a few terms of the perturbative expansion. This relies evidently in some smoothness and regularity conditions in the solution which is searched for. We propose to use the self-similar renormalization method as a practical tool to obtain in most cases significantly better estimates of the observables than previously available just by using perturbation expansions. We should however mention that the proposed approach can only work if a perturbation expansion is available, which may not be the case for more complex realistic situations with complex initial and boundary conditions, source terms, and when the hydraulic conductivity is non-stationary due to conditioning on measurements. Our methodology, considered as a whole, works indeed in most of the problems in Condensed Matter, when it is possible to express them in the form of expansions; and it is possible because approximants by design possess asymptotic form well agreeing with the true physical asymptotic behavior. Our best guess therefore appears as plausible.

Future directions include the extension of the self-similar functional renormalization method to go beyond the characterization of the heterogeneity solely in terms of the variance and consider also the dependence of the transport properties with respect to the skewness (third normalized cumulant) and kurtosis (fourth normalized cumulant). In particular, most natural heterogeneous permeable media are observed to be statistically anisotropic. The application of our technique to this case is an important extension of this first preliminary work, and should follow the same lines based on the second order treatment of Abramovich and Indelman 1995.

Acknowledgements We are grateful to D.M. Tartakovsky for introducing us into the subject and for useful discussions.

Appendix: method of self-similar renormalization

The complete description of the method with the corresponding mathematical foundation can be found in Refs. Yukalov 1990, 1991, 1992; Yukalov and Yukalova 1994, 1996. In this appendix inspired from Ref. Gluzman and Yukalov 1997, we provide the ingredients which are necessary for a self-contained understanding of this paper.

Let us consider a function $f(x)$ of the variable $x \in (-\infty, \infty)$. Let this function satisfy a complicated equation that cannot be solved exactly. Assume that by means of perturbation theory we can get a sequence $\{p_k(x)\}$ of perturbative approximations $p_k(x)$, where $k = 0, 1, 2 \ldots$, enumerates the approximation order. Usually, perturbation sequences are divergent. To extract a meaningful result from a divergent sequence, one has to use so-called resummation techniques. In the method of self-similar renormalization, a divergent sequence can be made convergent by introducing additional functions ensuring convergence (see Yukalov 1990, 1991, 1992; Yukalov and Yukalova 1994, 1996). Due to their role, these functions are called governing or control functions. Let s be a set of such control functions entering into a sequence $\{F_k(x, s)\}$ obtained by a perturbation algorithm.

In addition to introducing the control functions, the main idea of the method of self-similar renormalization is to treat the passage from one approximation to another as a motion with respect to the approximation number $k = 0, 1, 2,\ldots$considered as an effective time variable. This motion is realized in the functional space of the considered function as follows. Let us define the initial approximation

$$F_0(x, s) = f \tag{55}$$

as an equation for the expansion function $x = x(f, s)$. Substitute the latter back to F_k, so that

$$y_k(f, s) \equiv F_k(x(f, s), s). \tag{56}$$

The relation inverse to (56) is

$$F_k(x, s) = y_k(F_0(x, s), s). \tag{57}$$

Let $\{y_k\}$ form a group of transformations with respect to $k = 0, 1, 2\ldots$Then, the trajectory $\{y_k(f, s)\}$ of this dynamical system, according to definitions (56) and (57), is bijective, that is in one-to-one correspondence to the approximation sequence $\{F_k(x, s)\}$. This dynamical system with discrete time k has been called (Yukalov and Yukalova 1994, 1996) the approximation cascade. The attracting fixed point of the cascade trajectory is, by construction, bijective to the limit of the approximation sequence $\{F_k(x, s)\}$, and thus corresponds to the sought function.

It is easier to deal with continuous than with discrete time. It is thus convenient to embed the approximation cascade $\{y_k\}$ into an approximation flow $\{y(t, \ldots)\}$ with continuous time $t \geq 0$. This implies that the trajectory $\{y(t, f, s)\}$ of the flow passes through all the points of the cascade trajectory at the integer times $t = k = 0, 1, 2, \ldots,$,

$$y(k, f, s) = y_k(f, s) \qquad (k = 0, 1, 2, \ldots). \tag{58}$$

The evolution equation for the flow reads

$$\frac{\partial}{\partial t} y(t, f, s) = v(y(t, f, s)), \tag{59}$$

with the right-hand side being the velocity field. The latter, in the language of renormalization-group theory, is often called the Gell–Mann–Low or β-function.

Integrating the evolution Eq. 59 from $t = k$ to $t = k^*$, we get the *evolution integral*

$$\int_{y_k}^{y_{k+1}^*} \frac{\mathrm{d}f}{v(f,s)} = k^* - k, \tag{60}$$

in which $y_k = y(k, f, s)$ and $y_{k+1}^* = y(k^*, f, s)$. Before specifying the numbers k and k^* in the limits of the evolution integral, let us note that the differential form (59) of the evolution equation, or its integral form (60), are equivalent to the functional relation

$$y(t + t', f, s) = y(t, y(t', f, s), s). \tag{61}$$

The latter in physical applications is labeled as the self-similarity relation, which explains our terminology. In general, the self-similarity can occur with respect to motion over different parameters. In our case, this is the motion over the steps of a computational procedure, the number of steps playing the role of effective time.

If there exists an attractive fixed point of the approximation-flow trajectory, then it is always possible to find a number k^* in the evolution integral (60) such that the upper limit y_k^* would correspond to an expression

$$F_k^*(x, s) \equiv y(k^*, F_0(x, s), s) \tag{62}$$

representing, with the desired accuracy, the sought function $f(x)$. If y_k^* was an exact fixed point, then (62) would give an exact answer to the problem. However, a fixed point can be reached only after infinite number of steps $k \to \infty$. For a finite number k, the limit y_k^* may represent the fixed point only approximately, and is thus named the quasi-fixed point. Our aim is to reach the latter as fast as possible, that is, during the minimal time

$$t_k^* = \min(k^* - k), \tag{63}$$

or the minimal number of steps. When there are no additional restrictions, the minimal number of steps counted by k is 1, so that

$$abs \min t_k^* = 1. \tag{64}$$

In the case where some constraints are imposed on the motion, the minimal time (63) should correspond to a conditional minimum. For instance, if a value $f_0 \equiv f(x_0)$ of the sought function $f(x)$ is given for some x_0, then we can find t_k^* by requiring that the trajectory of the approximation cascade should pass through the given point f_0.

To calculate the evolution integral (60), we need to define the velocity field. This can be done by the Euler discretization of (59) yielding the finite-difference form

$$v_k(f, s) = y_k(f, s) - y_{k-1}(f, s). \tag{65}$$

Substituting (65) into (60), and using (57), we come to the representation

$$\int_{F_k}^{F_{k+1}^*} \frac{\mathrm{d}f}{v_{k+1}(f, s)} = t_k^*, \tag{66}$$

for the evolution integral (60), where $F_k = F_k(x, s)$, $F_{k+1}^* = F_{k+1}^*(x, s)$.

Finally, we have to define the set s of control functions, whose role is to govern the convergence of the approximation sequence. This convergence can be expressed, in the language of dynamical theory, as the stability of the cascade trajectory. A useful tool for analyzing stability is the set $\{\mu_k\}$ of the local multipliers

$$\mu_k(f, s) = \frac{\partial}{\partial f} y_k(f, s). \tag{67}$$

The inequality

$$| \mu_k(f, s) | < 1 \tag{68}$$

is the condition of local stability at the step k with respect to the variation of an initial point f. The equality $| \mu_k(f, s) | = 1$ implies local neutral stability. For a convergent sequence corresponding to a contracting mapping, the condition of asymptotic stability is

$$| \mu_k(f, s) | \to 0 \qquad (k \to \infty). \tag{69}$$

The approximation cascade $\{y_k\}$ describes the motion in the functional space $\{f\}$. To return to the domain $\{x\}$, we must use the inverse transformation (57) which allows us to pass from the multiplier (67) given on the functional space $\{f\}$ to its image

$$m_k(x, s) = \mu_k(F_0(x, s), s) \tag{70}$$

being a function of x. For the image (70), the same stability condition as in (68) can be written,

$$| m_k(x, s) | < 1. \tag{71}$$

According to (69), the local multipliers decrease when approaching an attracting fixed point. This means that the variation of the initial condition f produces weaker effects on the trajectory as the attractor becomes closer. In other words, the smaller are the absolute values of the multipliers, the more stable is the trajectory. Therefore, it is reasonable to define the control functions as those minimizing the absolute values of the local multipliers, ensuring that the trajectory becomes more stable at each step k. In this way, a set s of control functions is defined by the *principle of maximal stability* written as

$$| m_k(x, s_k(x)) | = \min_s | m_k(x, s) | . \tag{72}$$

The control functions $s_k(x)$ defined by the principle (72) may be called the *stabilizing functions* or *stabilizers.*

Note that the control functions may be introduced in several ways, as discussed in the other papers by Yukalov and co-workers. However, their introduction always uses the criteria of stability conditions and the closeness of a trajectory to an attracting fixed point. In all cases, the control functions are defined so that they govern the convergence of an approximation sequence, which, from the point of view of dynamical theory, is equivalent to stabilizing the cascade trajectory.

After the stabilizers are defined, we have to substitute them into the corresponding approximations $F_k(x, s)$ getting

$$f_k(x) \equiv F_k(x, s_k(x)). \tag{73}$$

This stage can be called the *stabilizing renormalization* of a perturbative sequence.

Then, considering the motion near the renormalized quantity (73) by means of the evolution integral (66), we obtain

$$f_k^*(x) \equiv F_k^*(x, s_k(x)). \tag{74}$$

This step can be called the *dynamical renormalization*. And the whole procedure of the double renormalization (73) and (74) is named the self-similar renormalization. It is worth noting that the evolution Eq. 59 is generally nonlinear and can have several different solutions leading to different self-similar approximations (74). In such a case, to select a physically meaningful solution, we need to involve additional conditions as constraints. The constraints

can involve the properties of symmetry, the asymptotic properties at $x \to 0$ or $x \to \infty$, sum rules or other relations containing some known information on the character of the sought solution. Such additional constraints narrow down the set of possible solutions to a class with desired properties.

Since our goal is to obtain a good accuracy for the sought function from just a few availabel perturbative terms, Yukalov and co-workers have introduced tricks which amount effectively to increase the perturbation order. Here, we present the simplest algebraic method.

Suppose that there is a sequence of approximations $p_k(x)$ having polynomial structure, k showing the order of the polynomial. This order can be effectively increased by means of the multiplicative transformation

$$P_k(x, s) = x^s \; p_k(x), \;\; s \geq 0. \tag{75}$$

Then, the order of the expression (75) becomes $k + s$. The transformation inverse to (75) is

$$p_k(x) = x^{-s} \; P_k(x, s). \tag{76}$$

Following the method described above, we consider the sequence $\{P_k(x, s)\}$ and construct an approximation cascade $\{y_k\}$ whose trajectory $\{y_k(f, s)\}$ is bijective to $\{P_k(x, s)\}$. Solving the evolution integral (66), we have $P_k^*(x, s)$. From the principle of maximal stability (72) we define the stabilizers $s_k(x)$. Substituting these into $P_k^*(x, s)$ and invoking the inverse transformation (76), we obtain the self-similar approximation

$$f_k^*(x) = x^{-s_k(x)} \; P_k^*(x, s_k(x)). \tag{77}$$

The multiplicative transformation (75) is the most natural one in the case when the perturbative approximations $p_k(x)$ have the form of polynomials or series of a variable with not necessarily integer powers. The factor x^s effectively increases the approximation order, and s plays simultaneously the role of a stabilizer.

The power or effective order s is dictated by the principle of maximal stability selecting the most stable trajectory of the approximations cascade. In particular, it may happen that $s = 0$, and we do not need to proceed further, or, vice versa, we may have to go to the limit of $s \to \infty$, thus allowing for all approximation orders. In each concrete case, the effective order we need to reach depends on how good is the perturbative sequence $\{p_k(x)\}$ we start with and, how much information can be extracted from its first terms by means of the double renormalization (73) and (74). The name *algebraicself-similar renormalization* method has been used to refer to this choice wheren the control functions are introduced in the exponents of perturbative polynomials.

Concretely, the procedure works as follows.

$$p_k(x) = \sum_{n=0}^{k} a_n \; x^n, \;\; a_n \neq 0, \tag{78}$$

as a polynomial of the order k. Following (75), define

$$P_k(x, s) = \sum_{n=0}^{k} a_n \; x^{n+s}. \tag{79}$$

Similarly to (55), we have

$$P_0(x, s) = a_0 \; x^s = f, \tag{80}$$

from which the expansion function is

$$x(f,s) = \left(\frac{f}{a_0} \right)^{1/s} . \tag{81}$$

The definition (56) yields the points

$$y_k(f,s) = \sum_{n=0}^{k} a_n \left(\frac{f}{a_0} \right)^{n/s+1} \tag{82}$$

of the approximation-cascade trajectory. For the velocity field (65), we get

$$v_{k+1}(f,s) = a_{k+1} \left(\frac{f}{a_0} \right)^{\frac{k+1}{s}+1} . \tag{83}$$

From the evolution integral (66), we find

$$P_{k+1}^* = \frac{P_k}{\left(1 - \frac{(k+1)\, a_{k+1}\, t_k^*}{s\, a_0^{\frac{k+1}{s}+1}} P_k^{\frac{k+1}{s}} \right)^{\frac{s}{k+1}}} . \tag{84}$$

The multiplier (67) becomes

$$\mu_k(f,s) = \sum_{n=0}^{k} \frac{a_n}{a_0} \left(1 + \frac{n}{s} \right) \left(\frac{f}{a_0} \right)^{\frac{n}{s}} , \tag{85}$$

and its image (70) reads

$$m_k(x,s) = \sum_{n=0}^{k} \frac{a_n}{a_0} \left(1 + \frac{n}{s} \right) x^n . \tag{86}$$

The principle of maximal stability (72) defines the stabilizers $s_k(x)$, whose explicit expressions depend on the coefficients a_n. According to the transformations (75)–(77), we obtain from (84)

$$f_{k+1}^* = \frac{p_k(x)}{\left(1 - \frac{(k+1)\, a_{k+1}\, t_k^*}{s\, a_0^{\frac{k+1}{s}+1}} x^{k+1} p_k(x)^{\frac{k+1}{s}} \right)^{\frac{s}{k+1}}} , \tag{87}$$

where $s_k(x)$ defines the most stable trajectory. When there are no additional conditions, the minimal value is $t_k^* = 1$, as in (64).

As noted above, it may happen that the most stable trajectory corresponds to $s \to \infty$. It is straightforward to check that the limit of the right side in (87), as $s \to \infty$, leads to

$$f_{k+1}^*(x) = p_k(x) \exp\left(\frac{a_{k+1}}{a_0} x^{k+1} \right) . \tag{88}$$

One may notice that, renormalizing $p_k(x)$ in (88), we obtain the recurrence relation

$$f_{k+1}^*(x) = f_k^*(x) \exp\left(\frac{a_{k+1}}{a_0} x^{k+1} \right) . \tag{89}$$

It is possible also to derive several other relations permitting to repeat the self-similar renormalization several times, which is useful when working with high-order terms. Comparing

(87) with (88), we see that the self-similar renormalization can yield quite different expressions, from the fractional form to exponential one. Other extensions are described in (Gluzman et al. 2003; Gluzman et al. 2003; Tarakovsky and Neuman 1998).

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