Fast Real Space Renormalization for Two-Phase Porous Media Flow

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Abstract

Upscaling of hydraulic conductivity data in space is one of the important problems in hydrological modelling.

In this article the basics of Real Space Renormalization (RSR) for upscaling hydraulic conductivity are introduced. The RSR procedure is described on a $2-D$ hydraulic conductivity grid. RSR is chosen because it can cope with correlated and anisotropic media. An up to now unanswered problem is the non-unique relationship between water fluxes and water contents or heads.

In special cases analytical solutions for two phase flow systems allow RSR to be as fast as single phase RSR. In the general case, numerical solution of the small scale flow equations are required. A new solution procedure which reduces the amount of computations is described.

1. Introduction

Upscaling of hydraulic conductivity data in space is one of the important problems in hydrological modelling. For the modelling of ground water flow and the input of climate models soil hydraulic conductivity data have to be provided which match the scale of the model. Several different techniques are proposed in the literature to solve this problem. Up to know no upscaling technique gives satisfactory results in all cases and is used widely. Current state of the art are lumped parameter models. The procedures to derive these lumped parameters vary according to the goal of the modeller and the data available, e.g. an effective conductivity which reproduces the mean flow in a grid block, will normally differ from a conductivity which reproduces the mean head.

The main question is: *how to estimate with reasonable precision the conductivity on larger scales from small scale data?* When going from the Darcy scale to the larger model grid block scale or to a scale suitable for use in weather or climate models, a closure problem arises. In addition to the spatial scaling problem, also the time step of the model changes. This article is focused only on the spatial scaling problem.

In this presentation we introduce the basics of Real Space Renormalization (RSR) [4] and apply this to a $2-D$ conductivity field. The RSR is chosen because it can cope with spatially correlated and anisotropic media.

1.1 Definition of the problem

An important issue in modelling subsurface flow is the problem of scales. Scales refer to the spatial extent or base at which porous media properties are defined. The general two-phase flow problem is highly nonlinear due to the dependency of the hydraulic conductivity on the fluid pressure. If the porous medium is heterogenous, additional nonlinearities arise in solving the flow equations due to the spatial variable parameters of the hydraulic conductivity-pressure relation.

Upscaling of hydraulic conductivity is a computational process, that transforms small scale information obtained by measurements and geostatistical methods to larger scale information suitable for numerical flow simulators. The small scale hydraulic conductivity information is usually given as sampled or interpolated point values or given as grid block values. In this article the small scale information is assumed given. The process of upscaling is necessary, because numerical flow simulators can't handle all small scale information. Quite often the output of the flow simulator is interesting only on larger scale. Because of uncertainty in the small scale data, there is a need for fast simulations. With different small scale input distributions Monte Carlo simulations can be done, which improve prediction certainty.

Given the distribution of the hydraulic conductivity $k(h)$ in space we want to calculate the flux q across the boundaries of the flow domain. With the aid of numerical techniques we can calculate this fluxes. If the flow domain is large or the information on $k(h)$ is detailed, the calculation procedure takes a lot of time. To simplify this calculation, we want to replace $k(h)$ by an effective upscaled K, take the gradient over the entire flow domain and expect the same fluxes.

The techniques for upscaling vary from simple averaging of the heterogeneous conductivities to more sophisticated inversion and probabilistic methods. During the last years *Real Space Renormalization (RSR)* has been increasingly used in upscaling conductivity from the measurement scale to the grid block scale required for numerical simulators.

RSR is a computational procedure to estimate characteristics of disordered systems. It is used in statistical physics and magneto-hydrodynamics. In the field of percolation theory it is used to describe the flow characteristics in network models of porous media. This use is binary (wet vs. dry) only, but the technique is powerful enough to derive critical scaling exponents of the networks considered, like the percolation threshold [7].

Recently RSR was also applied in the field of reservoir engineering. King e.a. [4] used it to scale up the hydraulic conductivity from the measurement scale to the flow simulator scale. Strengths and weaknesses are discussed in his publications. Also Hinrichsen e.a. [3] present RSR in the case of a fractal hydraulic conductivity distribution.

The main strength of RSR compared to effective medium approaches or other perturbation methods is that it does not rely on on the "small perturbation" expansion, basically a linear operation.

1.2 Solutions up to now

Up to now several RSR schemes exist for one-phase fluid flow [5, 3], which work quite fast and give in most cases satisfactory approximations of the actual flow. These schemes work either by replacing the finite difference grid by a modified grid, which is obtained by locally decoupling grid blocks and analytically solving the decoupled equations [4] or by removing bonds in a bond oriented network and redistributing the "lost" pore space by an averaging procedure [2].

For two-phase flow also schemes exist, but they still require a large amount of computing resources [4, 2]. As the one-phase RSR these schemes decouple the finite difference equations, but they solve the decoupled equations numerically. In general, no analytical solutions for the decoupled equations can be obtained.

1.3 Overview of the analytical and numerical approach

Both the analytical and numerical approach to RSR require small scale information on the hydraulic conductivity. Both deliver an upscaled K function. In the case of the analytic approach, K is given by an explicit function. The numerical solution only gives a table, mapping the boundary conditions to the flow. This table is an implicit description of K and can be parameterised by a function.

Two-phase flow is described with Darcy's law and and a conductivity function dependent on the fluid pressure. By directly integrating the flow equation over a grid block explicit solutions are obtained. These algebraic equations are coupled to form the RSR grid and then solved analytically. By making use of these solutions two-phase RSR is nearly as fast as one-phase RSR. In contrast to earlier two-phase RSR schemes [4, 2], in which the computing costs grow with a power function with volume, in the presented scheme computing costs grow super-linear with volume. With this method steady-state upscaled conductivity-pressure relationships are found. The method handles anisotropy of the porous medium.

Further a new, simplified numerical method is described which handles arbitrary $k(h)$ relations. It is similar to the method described by [4], but simplifies the numerical procedure by using the special boundary conditions in the RSR procedure explicitly.

2. Description of flow equations and RSR

In this article the formulation of the equations is used as in standard vadose zone hydrology. This implies two-phase flow (air and water). For the gaseous phase Richards approximation is used (high mobility of the gaseous phase). In the equations air never enters explicitly.

2.1 The basic flow equations

The basic equation which relates fluid flow through porous media to a pressure gradient is Darcy's law:

$$q = -k(h)\nabla h \tag{1}$$

with q the flow rate, $k(h)$ the hydraulic conductivity depending on the pressure h and ∇ the gradient operator. For the hydraulic conductivity different functional forms are in widespread use, e.g. van Genuchten [8], Gardner [1] and Pullan [6]. When solving (1) numerically, the exact parameterisation of the $k(h)$ relation doesn't matter. Analytical exact solutions are only possible in heterogenous media when using the form given in [6]:

$$k(h) = k_0 e^{-ah} \tag{2}$$

with k_0 the saturated hydraulic conductivity and a a spatial constant parameter.

In heterogeneous media the above equations are assumed valid on the small scale. The equations on the large scale are assumed to have the same form, just the functional form of the $k(h)$ relation will change. The gradient operator is replaced by an average gradient.

2.2 Real Space Renormalization

As an example of RSR, the (adapted) algorithm by [5] is described. The description is for a 2 by 2 block (figure 1). The main point of the renormalization procedure is that small scale blocks may be replaced by a network of resistors, using the analogy between Darcy's and Ohm's law (figure 2). Special assumptions on the boundary conditions for the small scale blocks have to be made. In our case we assume no flow boundary conditions, but periodic boundary conditions should also be possible. For the four small scale blocks the mass conservation equations are solved and the small scale $k(h)$ functions are replaced by an "upscaled" K function. The functional form of K is different from the $k(h)$ and has to be parameterized. Because a non-homogeneous $k(h)$ on the local scale implies anisotropy on a larger scale, the renormalised conductivity for the larger scale will be a second order tensor. This procedure is repeatedly applied to the conductivity field up to the required scale.

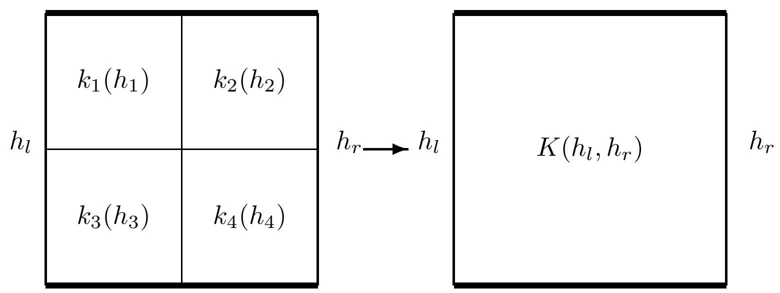

Figure 1. Basic RSR geometry

Thus the following steps have to be taken for the RSR:

- Take four small scale blocks and solve for the flow
- Use the flow and the boundary values h_1 and h_2 to find the upscaled K
- Rotate the four blocks by 90 degree and repeat the above two steps to find K in the other principal direction
- Assemble four "new" small scale blocks made of the upscaled K's
- Repeat the above steps up to the required scale

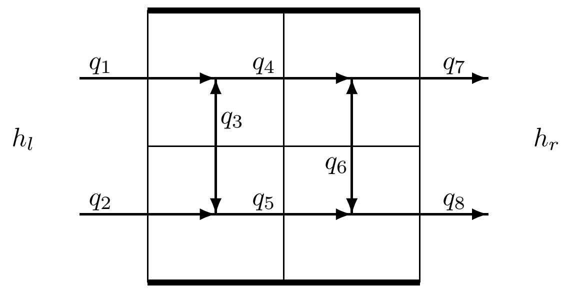

Figure 2. Flows in the small scale blocks

3. Analytical approach

In order to solve the RSR on four small scale blocks, the flow equations are discretized using a standard block-centered finite difference formulation. By combining equations (1) and (2) one obtains:

$$q = -k_0 e^{-ah} \nabla h \tag{3}$$

Integrating the above equation over the following domain and assuming q constant:

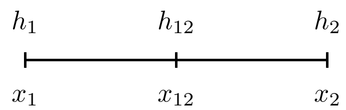

Figure 3. $1 - D$ discretized domain for analytical integration

Because of continuity of the fluxes and assuming equidistance between x_1, x_{12}, x_2 we get:

$$q = \frac{2k_{01}k_{02}}{a(x_2 - x_1)(k_{02} + k_{01})} * (e^{-ah_2} - e^{-ah_1}) \tag{4}$$

This equation is now an algebraic equation in terms of q and e^{-ah} and can be solved for these variables.

For each flow in figure 2 equation (4) is established and a system of eight algebraic equations is obtained. The system has the form:

$$\begin{aligned}
q_1 &= (\Delta x/2)^{-1}(k_{s1}/a)(H1 - HL) \\
q_2 &= (\Delta x/2)^{-1}(k_{s3}/a)(H3 - HL) \\
q_3 &= (\Delta x)^{-1}((2k_{s1}k_{s3})/(a(k_{s3} + k_{s1})))(H3 - H1) \\
q_4 &= (\Delta x)^{-1}((2k_{s1}k_{s2})/(a(k_{s1} + k_{s2})))(H2 - H1) \\
q_5 &= (\Delta x)^{-1}((2k_{s3}k_{s4})/(a(k_{s3} + k_{s4})))(H4 - H3) \\
q_6 &= (\Delta x)^{-1}((2k_{s2}k_{s4})/(a(k_{s2} + k_{s4})))(H4 - H2) \\
q_7 &= (\Delta x/2)^{-1}(k_{s2}/a)(HR - H2) \\
q_8 &= (\Delta x/2)^{-1}(k_{s4}/a)(HR - H4)
\end{aligned} \tag{5}$$

with:

$$\begin{aligned}
H1 &= e^{-ah_1} \\
H2 &= e^{-ah_2} \\
H3 &= e^{-ah_3} \\
H4 &= e^{-ah_4} \\
HL &= e^{-ah_l} \\
HR &= e^{-ah_r}
\end{aligned} \tag{6}$$

Additionally we can use the conservation of mass in the nodes:

$$\begin{aligned}
q_1 &= q_3 + q_4 \\
q_4 &= q_6 + q_7 \\
q_2 &= q_5 - q_3 \\
q_5 &= q_8 - q_6
\end{aligned} \tag{7}$$

The above set set of equations can be solved analytically. With this solution the large scale K is determined.

4. Numerical approach

When using a different functional form for $k(h)$ than above, numerical solutions to the RSR have to be found. In principle this is easy. What counts is the amount of computations. A straight forward implementation can be formulated by using a standard finite difference scheme. This leads to a matrix equation of the following form:

$$\mathbf{A}\mathbf{h} = \mathbf{b} \tag{8}$$

with $\mathbf{A}$ a four by four matrix, $\mathbf{h}$ a vector with the four small scale $h's$ and $\mathbf{b}$ another four element vector.

By numerically solving the set of FD equations on the small scale grid, one obtains upscaled $k(h)$ functions. Even if the small scale k's are isotropic, the upscaled ones will be anisotropic and non-symmetric in ∇h. Previous studies [4] used a straight forward FD implementation to solve the small scale equations. This approach still requires a numerical intensive iterative procedure to solve the equations.

By carefully analyzing the geometry and FD discretization, a simplification of the mass balance equations occurs. The given head boundary conditions and the geometry inside the four small scale blocks constrain the values the small scale h's can take. These h's are not independent, but are related to each other by:

$$h_4 - h_2 = h_3 - h_1 \tag{9}$$

Each occurrence of e.g. h_4 in the mass conservation equations can directly be replaced by:

$$h_4 = h_2 + h_3 - h_1 \tag{10}$$

The new equation (10) reduces the four above mass conservation equations (7) to only three. The new equations written in matrix form and suitable for a numerical implementation have the form:

$$\begin{bmatrix} h_1 \\ h_2 \\ h_3 \end{bmatrix} = \begin{bmatrix} \mathbf{f}\Big(h_l, h_2, h_3,\ k_1(h_1),\ k_2(h_2),\ k_3(h_3)\Big) \\ \mathbf{f}\Big(h_r, h_1, h_3,\ k_1(h_1),\ k_2(h_2),\ k_4(h_1, h_2, h_3)\Big) \\ \mathbf{f}\Big(h_l, h_1, h_2,\ k_1(h_1),\ k_3(h_3),\ k_4(h_1, h_2, h_3)\Big) \end{bmatrix} \tag{11}$$

This system can be solved in fewer steps than the straight forward FD implementation. Further reduction in the computations is possible by rewriting the iterations to implicitly include previous iteration steps.

5. Discussion

In this article the basics of RSR are described and a new analytical and numerical technique is developed. Especially the new numerical technique can help in practical upscaling problems. This is because of the flexible prameterisation of the $k(h)$ relationship. A further step in the development will be the testing of this new technique with a standard flow simulator.

Still open questions are:

- It is still open which equation or functional form to use for the upscaled $k(h)$ relation.
- Up to now I looked only at the first renormalization step. In the next renormalization step four already upscaled $k(h)$ functions are combined. Because of their different form from the original small scale description, this requires a different solution strategy.
- Still open is also the problem of time varying fluxes. Up to now the upscaling only deals with steady state fluxes.

Despite these open questions RSR holds promise for practical upscaling, especially in two-phase flow. In two phase flow there is nearly always a trend in the hydraulic conductivity because of a gradient in the fluid pressure. This also causes spatial correlation in the conductivity field. These two problems exclude simple stochastic techniques and defy up to now the solution by advanced stochastic techniques. In these cases RSR is a strong candidate for the upscaling.

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References

[1] W. R. Gardner. Some Steady-State Solutions of the Unsaturated Moisture Flow Equation with Application to Evaporation from a Water Table. *Soil Science*, 85(4):228 – 232, Apr. 1958.

[2] A. Hansen, S. Roux, A. Aharony, J. Feder, T. Jøssang, and H. H. Hardy. Real-Space Renormalization Estimates for Two-Phase Flow in Porous Media. *Transport in Porous Media*, 29(3):247 – 279, Dec. 1997.

[3] E. L. Hinrichsen, A. Aharony, J. Feder, A. Hansen, T. Jøssang, and H. H. Hardy. A Fast Algorithm for Estimating Large-Scale Permeabilities of Correlated Anisotropic Media. *Transport in Porous Media*, 12(1):55 – 72, July 1993.

[4] P. King, A. Muggeridge, and W. Price. Renormalization Calculations of Immiscible Flow. *Transport in Porous Media*, 12(3):237 – 260, Sept. 1993.

[5] P. R. King. The Use of Renormalization for Calculating Effective Permeability. *Transport in Porous Media*, 4(1):37 – 58, Feb. 1989.

[6] A. J. Pullan. The Quasilinear Approximation for Unsaturated Porous Media Flow. *Water Resources Research*, 26(6):1219 – 1234, June 1990.

[7] M. Sahimi. *Flow and Transport in Porous Media and Fractured Rock: From Classical Methods to Modern Approaches.* VCH, Weinheim, New York, Basel, Cambridge, Tokyo, 1995.

[8] M. T. van Genuchten. A Closed-form Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils. *Soil Sci. Soc. Amer. J.*, 44:892 – 898, 1980.