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Upscaling: a review

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SUMMARY

Porous media have properties with heterogeneities on several length scales. It is possible to build digital models of such properties. However these can be so detailed that a computing machine of the same power as that used to build the property model is not able to solve the fluid flow equations using standard discretisation methods—storage is needed for workspace, and the discrete equations have to be solved in a reasonable time. This paper reviews averaging techniques, devised to simulate large scale features of solutions without necessarily solving all the fine scale equations. Copyright © 2002 John Wiley & Sons, Ltd.

KEY WORDS: upscaling; effective medium; homogenization; heterogeneity; renormalization

1. INTRODUCTION

This paper discusses problems of *upscaling*—the approximation of a system of partial differential equations by another, often of the same form, with known coefficients that can be solved with fewer computing resources. The material is essentially a review with some new results.

Attention is focussed on the model problem of incompressible, single phase flow. An indication of progress in the two-phase generalization of the problem is also given. We relate upscaling to the methods of homogenization, renormalization and turbulence modelling.

Other reviews can be found in References [1–5].

The summation convention regarding repeated indices is used throughout the review.

2. A MODEL PROBLEM

2.1. The flow equations

Let Ω be a finite three-dimensional region with boundary $\partial\Omega$. Let u be a flux vector with components (u, v, w), and p be the pressure field of an incompressible fluid in a porous

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medium characterized by Darcy's law. Consider a system of equations, called the 'fine problem'

$$\nabla \cdot u = 0, \quad u = -k \cdot \nabla p$$

for $x \in \Omega$, where a unit viscosity is assumed, $p = p_b$ for $x \in \partial\Omega$, p_b is a function of position on the boundary and k is a symmetric, strictly positive definite, tensor.

For simplicity of exposition suppose that Ω is a rectangular region of size $L_x.L_y.L_z$ and divide this into $N_x.N_y.N_z$ congruent boxes, called the *coarse cells* each of size $H_x.H_y.H_z$ so that $L_x = N_x.H_x$, $L_y = N_y.H_y$ and $L_z = N_z.H_z$. Also divide each of the boxes into $n_x.n_y.n_z$ congruent boxes, called the *fine cells* each of size $h_x.h_y.h_z$ so that $H_x = n_x.h_x$, $H_y = n_y.h_y$ and $H_z = n_z.h_z$. Set $M_x = N_x.n_x$, $M_y = N_y.n_y$, $M_z = N_z.n_z$. It is not assumed that these cells are, necessarily, the same as any grid cells used in simulation. In practice the cells are often used as the grid cells, but without refinement accuracy suffers [6]. In general the tensor field, k, takes a different value in each of the fine cells. The values may be the result of direct measurement, but often they result from interpolation or inversion procedures, perhaps involving a stochastic process.

It is useful to consider p_b as the restriction of a function defined throughout Ω. An assumption that $p_b = x \cdot a$, where a is a fixed, constant vector is often made, and called 'linear boundary conditions'.

Fine grid cells have lower case indices (i, j, k), where $i \in (0, \ldots, M_x - 1)$, $j \in (0, \ldots, M_y - 1)$, $k \in (0, \ldots, M_z - 1)$. The coarse grid cells have corresponding upper case indices.

2.1.1. The upscaling problem. The problem under consideration is to find, for each k, a corresponding $\tilde{k}$, without small scale heterogeneities, such that the solution of the 'coarse problem'

$$\nabla \cdot \tilde{u} = 0, \quad \tilde{u} = -\tilde{k} \cdot \nabla \tilde{p}$$

is, in some sense, near the solution of the fine scale problem, or close to a filtered solution. Filters are usually volume averages over regions such as coarse grid cells. In general we are seeking a $\tilde{k}$, calculated from one set of boundary conditions, that can also be used to obtain accurate results even when very different large scale boundary conditions are imposed.

This problem is difficult even when the fine scale solution is known. Some methods do not require fine scale solutions, although, in general, the more is known about fine scale solutions the more accurately one can tune coarse equations to fine equations. Not only are there numerical problems, there are problems of interpretation. Many methods are ad hoc and do not fit a unified framework.

2.1.2. Remarks on the origins of the fine scale data. The literature on upscaling assumes that a fine scale model has been defined. In some cases this may be the result of a careful, direct measurement procedure, but often the data will be the result of interpolation of a few measurements. This procedure makes use of the techniques of *geostatistics* [1]. Sometimes there are measurements, using methods such as seismic inversion, that provide some global, indirect, data that guides the interpolation methods. It follows that the input to upscaling methods is generally, very influenced by the choice of interpolation method. It may be possible, by exploiting the non-uniqueness in the solutions of inverse problems, to construct an interpolation that is favourable to the accuracy of a chosen upscaling method.

2.2. The standard finite volume discretization method

In this section k is a diagonal tensor and it *is* assumed that (h_x, h_y, h_z) are the grid sizes of a finite volume mesh. Denote by $\omega_{i,j,k}$ the (i,j,k)-th grid cell. Let $\partial\omega_{i+1/2,j,k}$ be the interface between cell (i,j,k) and cell $(i+1,j,k)$. The *half-cell* denoted by $\omega^-_{i+1/2,j,k}$ is the set of points in $\omega_{i,j,k}$ which are less than a distance $h_x/2$ from $\partial\omega_{i+1/2,j,k}$. Denote by $\omega^+_{i+1/2,j,k}$ the half-cell of points in $\omega_{i+1,j,k}$ which are less than a distance $h_x/2$ from $\partial\omega_{i+1/2,j,k}$. Half-cells in the j and the k directions are defined in a similar way. Also define the region $\omega_{i+1/2,j,k} = \omega^-_{i+1/2,j,k} \cup \omega^+_{i+1/2,j,k}$, composed of half-cells either side of the interface.

Introduce the basis functions

$$H_{i,j,k} = \begin{cases} 1 & x \in \omega_{i,j,k} \\ 0 & x \notin \omega_{i,j,k} \end{cases} \quad \text{and} \quad H_{i+1/2,j,k} = \begin{cases} 1 & x \in \omega_{i+1/2,j,k} \\ 0 & x \notin \omega_{i+1/2,j,k} \end{cases}$$

$H_{i,j+1/2,k}$ and $H_{i,j,k+1/2}$ have similar definitions.

Introduce piecewise constant trial functions, with parameters to be determined; for the pressure, $p = \sum_{i,j,k} H_{i,j,k}\, p_{i,j,k}$, and

$$u = \sum_{i,j,k} H_{i+1/2,j,k}\, u_{i+1/2,j,k}, \quad v = \sum_{i,j,k} H_{i,j+1/2,k}\, v_{i,j+1/2,k}, \quad w = \sum_{i,j,k} H_{i,j,k+1/2}\, w_{i,j,k+1/2}$$

for the x, y and z components of flux.

The *finite volume method*, also known as the *mixed finite element method* is obtained by substituting the trial functions for the flux into the zero divergence equation and integrating over cell (i,j,k) to obtain

$$h_y h_z (u_{i+1/2,j,k} - u_{i-1/2,j,k}) + h_x h_z (v_{i,j+1/2,k} - v_{i,j-1/2,k}) + h_x h_y (w_{i,j,k+1/2} - w_{i,j,k-1/2}) = 0$$

By rearranging the x-component of Darcy's law to read

$$\frac{u}{k_x} + \frac{\partial p}{\partial x} = 0 \tag{1}$$

and by substituting the basis functions for the flux and pressure, integrating over the region $\omega_{i+1/2,j,k}$, and setting the residual to zero, it is found that

$$0.5 h_x u_{i+1/2,j,k} \left(\frac{1}{k_{i,j,k}} + \frac{1}{k_{i+1,j,k}} \right) = -(p_{i+1,j,k} - p_{i,j,k})$$

Equations for the y and z components are derived in a similar way.

The total flux, $q_{i+1/2,j,k} = h_y h_z u_{i+1/2,j,k}$, through the face between cells i and $i+1$ is thus given by

$$q_{i+1/2,j,k} = h_y h_z u_{i+1/2,j,k} = -T_{i+1/2,j,k}(p_{i+1,j,k} - p_{i,j,k})$$

where

$$T_{i+1/2,j,k} = \frac{2 h_y h_z}{h_x (1/k_{i,j,k} + 1/k_{i+1,j,k})}$$

Similar expressions apply in the y and z directions.

It is interesting to note that the coefficients, T, called *transmissibilities* involve *harmonic* averages of permeabilities either side of cell interfaces. See Reference [7] for further discussion of this scheme and Reference [8] for more general background. A slight modification is required near the boundary, where integration is performed over only one half-cell, thus involving the boundary pressure.

For a one-dimensional system where each fine cell has, exactly, a constant permeability, this finite volume scheme gives the exact answer for the flux, and the pressures equal the volume averages over the cells.

3. UPSCALING TECHNIQUES

3.1. Overall strategy

In this section two-stage upscaling methods are reviewed.

In the first stage—the *fine grid experiment*—we solve one or more fine grid problems. These might range from a single fine scale solution over the whole of Ω or at least a substantial part of Ω to, say, three problems, one in each co-ordinate direction, on the fine grid within each of the coarse cells. This can be formalized by choosing a set of A, possibly overlapping, regions, $\Omega_\alpha(\alpha = 1, \ldots, A)$ where the union of these may or may not, cover Ω. If one or more of the Ω_α covers a substantial part of Ω one says that the experiment is *global*. Generally, more than one numerical experiment is performed, using different boundary conditions, on each subregion. When the Ω_α are small regions, of the size of a single coarse grid cell, one says that the experiment is *local*.

In the second stage—the *coarse grid calibration*—the fine grid solutions are used to determine the coarse scale properties, $\tilde{k}$. When this determination occurs locally, on a single coarse cell, or a coarse cell plus a small surrounding region, the calibration is described as *local*, otherwise the calibration is said to be *global*.

A classification into local–local, global–local, local–global and global–global methods has thus been defined. In this terminology, the first word refers to the experiment and the second to the method of calibration. Local–global methods have received little attention in the literature, but in practice there may be some merit in such an approach. This is discussed in Section 3.6.

3.2. Local–local methods

These techniques are like laboratory measurements of local properties of the porous medium, but using simulated experimental results. The simplest approach considers each coarse grid cell separately and performs three independent flow experiments with 'no-flow' or 'sealed-side' boundary conditions on four sides of the cell and constant pressure conditions on two opposing faces, say $p_b = 1$ on one face and $p_b = 0$ on the other. If the total flux is computed through one of the faces with the pressure boundary condition, it is easy to calculate an equivalent permeability on the grid cell by multiplying this flux by a simple expression: for example $\tilde{k}_x = QH_x/A\Delta P$ where Q is the total flux through the face of area $A = H_y.H_z$ and ΔP is the pressure drop. This method was first introduced into the porous medium literature by Reference [9] and promulgated in Reference [10]. Linear boundary conditions, of the form $p_b = x.a$ are convenient, particularly in complicated geometries with non-rectangular

coarse grid cells. Recently the use of flux boundary conditions has been suggested and some numerical results presented that make them worth further work [11].

3.2.1. The effective permeability tensor is symmetric. Calibration is easier if the coarse scale permeability tensor is symmetric. That such is the case was proved in the homogenization literature [12, 13] but can be shown to hold for any permeability distribution, in any shape of domain, if we impose linear boundary conditions. Our proof of symmetry, based on a similar result from p. 11 of Reference [12], uses the following preliminary result.

If p is any solution of the pressure equation in a region ω with

$$\frac{\partial}{\partial x_i}\left(k^{ij}\frac{\partial p}{\partial x_j}\right)=0$$

and ϕ is any differentiable function vanishing on the boundary $\partial\omega$ then

$$\int_\omega k^{ij}\frac{\partial p}{\partial x_j}\frac{\partial \phi}{\partial x_i}\,\mathrm{d}^3x=0 \tag{2}$$

where the three-dimensional integrals are over the x-variables.

Equation (2) can be derived by multiplying the equation for p by ϕ, applying the divergence theorem and using the property that ϕ vanishes on the boundary.

Let $p^r=x.e^r$ be the linear boundary conditions in the rth experiment where $e^0=(1,0,0)$, $e^1=(0,1,0)$, $e^2=(0,0,1)$. The pressure, p^r, satisfies the equation

$$\frac{\partial}{\partial x_i}\left(k^{ij}\frac{\partial p^r}{\partial x_j}\right)=0$$

It follows from (2) that if p^r is the rth pressure and $\phi=b_sp^s-b_sx_s$ then

$$\int_\omega k^{ij}\frac{\partial p^r}{\partial x_j}\frac{\partial p^s}{\partial x_i}b_s\,\mathrm{d}^3x=\int_\omega k^{ij}\frac{\partial p^r}{\partial x_j}b_i\,\mathrm{d}^3x \tag{3}$$

where b_s is the sth component of an arbitrary constant vector. The general solution, for an arbitrary linear boundary condition $p^r=x.a$ is then $p=p^ra_r$ and $u=u^ra_r$. Then, for a general linear boundary condition the volume averaged flux, where V is the volume of ω, is

$$\langle u^i\rangle=\frac{1}{V}\int_\omega k^{ij}\frac{\partial p^r}{\partial x_j}a_r\,\mathrm{d}^3x$$

It is thus natural to define the effective permeability of the region ω as

$$\tilde{k}^{ir}=\frac{1}{V}\int_\omega k^{ij}\frac{\partial p^r}{\partial x_j}\,\mathrm{d}^3x$$

To prove the symmetry of $\tilde{k}^{ir}$, introduce the quadratic form $\lambda=\tilde{k}^{ir}a_ib_r$ where a_i and b_r are the components of arbitrary vectors. It follows from (3) above, that

$$\lambda=\frac{1}{V}\int_\omega k^{ij}\frac{\partial p^r}{\partial x_j}a_rb_i\,\mathrm{d}^3x=\frac{1}{V}\int_\omega k^{ij}\frac{\partial p^r}{\partial x_j}\frac{\partial p^s}{\partial x_i}b_sa_r\,\mathrm{d}^3x$$

Since a and b are arbitrary vectors it follows that

$$\tilde{k}^{rs} = \frac{1}{V} \int_{\omega} k^{ij} \frac{\partial p^r}{\partial x_j} \frac{\partial p^s}{\partial x_i} \, \mathrm{d}^3 x \tag{4}$$

Symmetry of the tensor on the fine scale together with the last expression implies symmetry of the effective tensor on the coarse scale.

It follows from the expression for the effective permeability (4) that only three numerical experiments are needed. That is, the three pressure equations for p^r need to be solved. Note that the ith component of average flux in the rth numerical experiment is equal to the rth component of average flux in the ith numerical experiment.

3.2.2. An adjoint technique for a diagonal approximation to $\tilde{k}^{rs}$. As seen in the previous section, the full, effective, permeability tensor, involving six unknowns, can be determined from just three numerical experiments. Each numerical experiment involves the solution of a linear system. This is reminiscent of the situation in optimization theory, where the problem is to determine, for several right hand sides, the dot products of the solutions of a linear system with a fixed vector. It is well known that this problem is equivalent to solving a *single* system for the *adjoint* vector and taking the dot products of each of the original right hand sides with this adjoint vector. As the number of different right hand sides is increased there is an ever increasing gain in efficiency.

In an attempt to apply this idea to upscaling it was found, with a focus on the case where the effective permeability tensor is diagonal, or nearly diagonal, that the number of numerical experiments can be reduced to one.

Thus define components of an approximate diagonal tensor by $\tilde{k}^r \approx \sum_s \tilde{k}^{rs}$. Then, as proved in the next paragraph, if $\tilde{k}^{rs}$ is approximately diagonal, a single numerical experiment will suffice.

With unit basis vectors for pressure gradients (and flow directions) of the experiments, as in the previous section, the effective diagonal permeability is the sum of the average fluxes over the three directions. In numerical experiments, discretisation constructs a linear system for solution, of the form $A_{nm} p_m^i = b_n^i$ where the right hand side is a function of the basis vectors, a^i (different in each experiment) and the matrix A is independent of the experiment, where $i \in (0, 1, 2)$. Now, the discrete approximation to the volume average flux is obtained from $B_m^i p_m^r = B_m^r p_m^i$, by symmetry of the effective permeability, where B is a matrix that depends only on the fine scale permeability, and not the boundary conditions. Thus the components of the diagonal effective permeability are given by $\tilde{k}^i = c_m p_m^i$ where $c_m = \sum_r B_m^r$. By introducing an adjoint vector, v say, which satisfies the adjoint equation $A_{nm} v_m = c_n$ the three components of the effective diagonal permeability tensor can be found by solving *one* linear system (instead of three) and evaluating three scalar products $\tilde{k}^i = v_m b_m^i$. (A proof can be found in Reference [14].) This result follows from symmetry of the matrix A, itself a consequence of the symmetry of the underlying elliptic partial differential equation.

Thus, it is only necessary, when the effective permeability tensor is diagonal, to solve a *single* linear system. This, because of the dot product evaluations, is almost a factor of three faster than the usual method. As far as we are aware this upscaling method has not previously been described in the literature. The numerical results are close to those from the standard linear boundary condition method followed by the approximation $\tilde{k}^r \approx \sum_s \tilde{k}^{rs}$.

3.2.3. In one dimension, local–local methods are exact. The flow equations in one-dimension reduce to

$$\frac{\partial u}{\partial x} = 0, \quad \frac{u}{k} = -\frac{\partial p}{\partial x}$$

Integrating, with respect to x, over one coarse grid cell, the first equation shows that u is constant and the second equation gives the value

$$u = \frac{\Delta p_{I+1/2}}{\int_{I-1/2}^{I+1/2} 1/k}$$

where $\Delta p_{I+1/2} = p_I - p_{I+1}$ and the limits $I - 1/2$ and $I + 1/2$ indicate that x belongs to cell $\omega_{I+1/2}$. From the definition

$$\tilde{k} = uH_x/\Delta p_{I+1/2}$$

the effective permeability in one coarse cell is found to be the harmonic average

$$\tilde{k} = H_x \Big/ \int \frac{1}{k}$$

The total flux through all of the coarse grid cells, deduced from the coarse grid equations, is

$$\tilde{u} = \Delta p \Big/ \int_0^{L_x} 1/\tilde{k}$$

where Δp is the total pressure drop. This is the exact result because

$$\int_0^{L_x} \frac{1}{\tilde{k}} = \int_0^{1/2} \frac{1}{k} + \sum_I \int_{I-1/2}^{I+1/2} \frac{1}{k} + \int_{L_x - H_x/2}^{L_x} \frac{1}{k}$$

Noting that permeability is analogous to electrical conductivity, or inverse resistance, this result is familiar as the traditional electric circuit result that resistors in series can be replaced by a single resistor with the arithmetic averaged resistance. The exact result in one dimension is evidence, misleading as it will turn out, that upscaling might be a robust and accurate technique.

3.2.4. In three dimensions the local–local method can be very inaccurate. Now consider a three-dimensional example. For simplicity consider only two coarse grid cells with four layers. In all layers set $k_y = 0$ and $k_z = 0$. In the x-direction set k_x to either the value k or α. In the first cell the layers are ordered as (k, α, k, α). In the second coarse cell set the fine cells to (k, α, k, α) in the first case and to (α, k, α, k) in the second. The first example has layers extending through the cells, and in the other the layers in the second cell have been interchanged, so that there is discontinuity between the coarse cells.

Using the local–local method the effective k_x permeability of each coarse grid cell is $0.5(k + \alpha)$. In the first case the total effective permeability is also $0.5(k + \alpha)$ but in the second case the total effective permeability is $2k\alpha/(k + \alpha)$. In the limit as α goes to zero the error in the second case is large. This shows that care is needed in applying any local–local upscaling method. The use of such elementary arguments to show the inadequacy of upscaling methods

does not seem to be covered in the existing literature. There is no space here to give details, but it is possible, by looking at such simple, artificial examples, to see how most numerical upscaling methods will or will not work. As implied by the section on homogenization, if the length scales are well-separated then all local–local methods will give exact results.

3.2.5. The boundary condition dependence of effective permeability. Consider a case with a zero permeability barrier dividing a coarse cell into two pieces and extending just outside the boundary of the cell. If sealed-side boundary conditions, transverse to the barrier, are used then the effective permeability will be zero. If linear boundary conditions are applied, then some flux will be allowed, and a non-zero effective value will result. This clearly demonstrates that the results are dependent on the boundary conditions. A useful discussion of the choice of boundary conditions, in the context of the application of upscaling may be found in Reference [15].

3.2.6. The effect of jackets. Some authors [16] have suggested that the use of a flow region, somewhat larger than the coarse grid cell, will give improved results. One says that a *flow jacket* is in use, around the grid cell. It is possible that in most cases the results are improved, and that as the extent of the jacket is increased so does the accuracy. It is important to only use the jacket to construct the fine scale solution. Averaging is needed on the support of the coarse grid cell in focus. However, as there is no clear definition of accuracy the method is rather *ad hoc*. Furthermore, there is a danger of doing more work than in solving the fine scale problem. Nevertheless, this is an important idea which merits further study. In the context of the multiscale finite element method, Reference [17] has strongly advocated the use of a jacket which they refer to as 'oversampling'.

3.2.7. Direct upscaling for transmissibility. Another approach that has been advocated [18, 19], is to solve a local flow problem around the interface between two coarse grid cells, compute the flux through the face and assign the transmissibility as the ratio of the flux to the mean pressure drop. In one dimension this method exactly reproduces the correct flux and average pressures within a coarse cell.

In Section 3.2.4 it was noted that when there are marked discontinuities in properties at the boundaries of the local region used in the upscaling experiment, then the results can be very inaccurate. A similar effect occurs with the direct upscaling of transmissibility, where, if there is a discontinuity in, say, the x-direction permeability at the plane through the cell centre, then the x-direction transmissibility will lead to a flux through the system when it should be near to zero. Again, the application of a jacket might improve matters.

3.3. Local–local upscaling viewed as a control volume method

The local–local methods are based (apparently) on a physical rather than mathematical argument. There has been little work that tries to place upscaling in the context of numerical methods, with the exception of References [17, 20, 21]. In Reference [17] they solve a local problem, recommending the use of oversampling. Once solved, the fine scale pressure solution relating to each coarse grid cell is normalized relative to that cell so that it can be used as a basis function in a generalized finite element method. Some analysis of convergence is made which seems to indicate that a condition of separation of scales is needed to obtain accurate

results without refining the coarse grid down to the fine grid. Some interesting variants of the fine scale boundary conditions are given, where a one dimensional solution is made along an edge, to provide a boundary condition for the two dimensional solution. (These authors only work in two dimensions, but their ideas seem to generalize to three dimensions.)

In Reference [17] it is stated that the multiscale finite element is systematic and self-consistent in contrast to empirical upscaling methods. It is, of course, true that upscaling methods are presented in a physical fashion, but this does not mean that, perhaps with slight alteration, they cannot be evolved into a rigorous numerical method. Indeed, as is now shown, the local–local upscaling method is a mixed finite element version of the Galerkin approach of Reference [17]. As far as we know, this is a new result.

Suppose a local fine scale solution has been calculated. From this, normalise the pressure, to obtain, in each grid cell a fine grid function, $\hat{p}_I$, with a unit volume integral over the coarse grid cell. Consider the half-cells either side of each coarse cell face and normalize the flux vectors so that their normal components $\hat{u}_{I+1/2}$, $\hat{v}_{J+1/2}$ and $\hat{w}_{K+1/2}$, have unit surface integrals over corresponding cell faces. Note that since all subscripts involving I, J or K occur in groups of three, a 'dropped index' convention can be used, where, if an index *appears* to be missing, it is I, J or K as implied by the context. For example $J + 1/2$ stands for $(I, J + 1/2, K)$.

Now introduce trial functions $\hat{p} = \sum_I p_I \hat{p}_I$ and $\hat{u} = \sum_I u_{I+1/2} \hat{u}_{I+1/2}$, with similar expressions for v and w.

Integrating the incompressibility condition over the IJK'th cell gives us the usual discrete mass balance

$$H_y H_z (u_{I+1/2} - u_{I-1/2}) + H_x H_z (v_{J+1/2} - v_{J-1/2}) + H_x H_y (w_{K+1/2} - w_{K-1/2}) = 0$$

Writing Darcy's law in the form (1), substituting the basis functions and integrating over the two half-cells from x_I to x_{I+1}, the centre planes of coarse cells I and $I + 1$, we find

$$u_{I+1/2} \int_{\omega_{I+1/2}} \frac{\hat{u}_{I+1/2}}{k_x} \, \mathrm{d}x \, \mathrm{d}y \, \mathrm{d}z = -p_{I+1} \int \hat{p}_{I+1}(x_{I+1}, y, z) \, \mathrm{d}y \, \mathrm{d}z + p_I \int \hat{p}_I(x_I, y, z) \, \mathrm{d}y \, \mathrm{d}z$$

Now approximate the integrals on the right hand side of the last equation as unity. The usual form of the upscaled Darcy equation is then deduced, where face fluxes, rather than volume average fluxes, are used in calibration. One could, from the outset, look for piecewise constant pressure approximations, and so obtain the normal form directly. Note that if the fluxes and pressure are obtained from the exact solution, then retaining the surface integrals enables the algorithm to reconstruct the exact solution. This may be an interesting property for a numerical method to possess. Also note that if the numerical scheme is derived by direct minimisation of a Kelvin principle (in which the integral of $k^{ij} u_i u_j$ is minimized, subject to the constraint of zero divergence) yet a different numerical scheme follows.

It would be useful to pursue this line of research a little further, focusing on finite volume schemes rather than Galerkin approaches, as these are more widely used in flow problems with hyperbolic behaviour.

A challenging problem is to generalize the technique of using basis functions obtained from local numerical experiments on finer grids to the nonlinear, two-phase situation.

3.4. Global–local methods

The case where the exact solution, or at least a good approximation, is known to a problem on the whole of the fine grid is now discussed. Situations, in which solutions on substantial parts of Ω, with perhaps overlap could also be included. This is not the same as a local–local method with a flow jacket, as here there is no large region corresponding to each and every coarse grid cell. Therefore it is necessary to solve a non-trivial inverse problem. One technique is to use the integrated fine scale flux through the face of a coarse cell and use this to calibrate a local solution on the coarse grid cell of the coarse scale equations.

Applied to our test problem, with the inverted and non-inverted layers, the effective $\tilde{k}$ for cell I is easily found, using the arithmetic average of the pressures on the coarse cell faces. Then take the harmonic average of these coarse grid cell values and obtain the exact overall effective permeability of the three dimensional system. This result is encouraging, but numerical experiments [22] show this exactness not to hold when the problem is genuinely three dimensional (remember that $k_y = k_z = 0$ for tractability in the test problem). However, the global–local method provides a first guess for the optimization approach discussed in the next section.

In the two-phase case this technique, suitably generalized, is the method of *pseudo-functions* developed prominently in Reference [23].

3.5. Global–global methods

This approach minimizes a global functional measuring the difference between the fine and coarse solutions. It is possibly the most demanding, in computer resources, of the various methods and was, as far as we know, first discussed by Reference [24]. There are not many papers using this method. Reference [25] uses it in a general case; References [26, 27] provide interesting test cases and analysis. The idea is similar to history matching (data assimilation) but uses results from fine scale calculations rather than physical measurements. This was done by some contributors in the recent SPE comparison study on upscaling [28].

At first sight it seems a disadvantage to have to obtain full solutions on the fine grid. However, as stated in Reference [22], with a multigrid solver the work is proportional to the problem size, and so it is not expected, in the single phase case, that the technique requires markedly different computer times compared to a local–local method.

If the upscaled permeability from a single phase global–global method is used in a multi-phase situation, perhaps using a local–local method to average other parameters, there may be another interesting upscaling method that needs further investigation. This last suggestion is not, however, a method based on any clear principle.

3.6. Local–global methods

In a local–global method it might be possible to upscale a fine model in a few small sub-regions. In this situation the coarse scale model is under-determined. To build the complete coarse scale model it is necessary to interpolate the available data.

We remarked in Section 2.1.2 how the input to upscaling is often obtained via interpolation. It is therefore possible that an approach based on interpolating a few upscaled values, is of interest. It certainly requires less work, and if the original fine scale correlation functions are

unknown it seems rational to work on the larger scale, and easier, problem of determining the correlation function directly from the large scale measurements.

Such a method was indicated in Reference [16]. However, there is not yet any literature that evaluates this approach.

3.7. Relation of upscaling to homogenization theory

It is widely held that continuum models only work if there is separation of length scales. In the porous medium literature this point has been made in Reference [29] (who refers to the REV—the representative elementary volume). Of course, it is also believed the condition is necessary but not sufficient. There are many examples where the large scale behaviour of a system is governed by equations that are very different in form from those pertaining to the small scales.

The subject of homogenization theory takes an extreme position, whereby the limit of infinite separation is taken. In the case of diffusion equations, it can be shown that in the limit the effective medium model is exactly the same equation but with a different—one might say 'upscaled'—permeability. This is interesting and provides a rigorous formulation of the conventional intuition that the length scales must be well separated.

See Reference [30] for a delightful introduction to homogenization. An extensive collection of applications to porous media can be found in Reference [12] and more general literature can be found in Reference [13]. A wide ranging review of applications to porous media flow is in Reference [31].

There are several approaches to homogenization, amongst which is the formal approach based on an expansion in a length scale parameter ε. The permeability is assumed to be of the form $k^{ij}(x, y) = k^{ij}(x, x/\varepsilon)$ and we write

$$\nabla = \nabla_x + \frac{1}{\varepsilon}\nabla_y$$

Now expand the solution, substitute into the equations and equate the coefficients of powers of ε to zero. Some manipulation and analysis is required, involving averaging over the fast variable y and use of periodicity.

In the single phase case, the equations, after homogenization, remain essentially of the same form, although diagonal tensors become six-component symmetric tensors. The effective permeability tensor obtained by this approach is the same as Equation (4) derived using local–local upscaling with linear boundary conditions.

In the two-phase case, with different saturation functions in each of the fine grid cells, the situation is more complicated. If the heterogeneous medium consists of two types of rock, then the large scale model has the form of two superimposed continua with an exchange term. These are the dual-porosity and dual-permeability models, usually thought of as models of fractured media. Originally introduced in Reference [32] they are natural models for the large scale behaviour of multi-phase flow through heterogeneous porous media. A large growth of the literature in this area may be expected over the next few years.

3.8. Relation of upscaling to renormalized perturbation theory

Renormalized perturbation theory (RPT), in the case that the permeability distribution is a realization of a specified spatial random process, tackles the stochastic problem directly. A series

expansion about an exactly solvable problem, in powers of some parameter (not necessarily small) is derived. A particularly interesting variant of RPT expands about an exactly solvable, but initially unspecified problem. After expansion the unspecified problem is determined so that, in some sense, the rate of convergence of the expansion is optimized. The method provides interesting results for problems that are not too complicated, and have simple geometries (usually periodic or infinite). A general introduction can be found in Reference [33]. A very clear explanation is in the article [34], which relates RPT to the classical approach of Lindstedt (1883) (see Reference [35] for references and details of the Lindstedt method). For applications to turbulence (where most of the relevant techniques were developed) see References [36, 37]. RPT has been applied to the problems of heterogeneous diffusion (and hence to flow through porous media) many times over many years. For example the work of Reference [38] explicitly studies the problem of diffusion in heterogeneous media. More recently the problem has been studied by References [39, 40]. The review [41] covers both renormalized perturbation theory (in particular the 'smoothing method') and contrasts it with homogenization. The idea in homogenization theory of taking the limit of infinite separation of scales appears [41] to be due to Keller. However, the idea of computing the effective properties, of a large sample of material, made from a periodic array of identical heterogeneous components, goes back to Rayleigh and Maxwell. (See References [42–44] for further references.)

3.9. Preconditioning by adaptive grid generation of the coarse grid

It would appear that, although not sufficient, it is at least necessary for the fine grid properties within each coarse grid cell to be either constant or possess a very small length scale compared to a characteristic length scale over which averaging is performed. Given data with fine scale detail it might be possible to use adaptive gridding to build coarse grids with the desired properties.

The first to suggest methods for this was [45]. This line of investigation was deepened in Reference [46]. These approaches, where a flow equation is solved on the fine grid and the equipotentials and streamlines are used to construct an optimal coarse grid have been developed further by Reference [47]. Another, rather heuristic approach, based on solving flow problems, was introduced in Reference [48]. An alternative is to minimize the variance of some property in a cell References [49–53].

Variance minimization using the moving finite element method was proposed in Reference [49]. In References [50, 51] the combinatorial aspect of the problem was tackled using a global optimisation algorithm. This approach was made faster in Reference [53] by restricting coarse grids to consist of a strict grouping of fine grid cells.

It is the impression of this author that adaptive gridding algorithms work well on carefully chosen test problems, but on general problems in three dimensions are not yet practical. A difficulty is that *failed* attempts tend to produce adaptive grids that can make the errors larger than with a uniform grid. There are opportunities for further work in this area. By allowing unstructured grids, success might follow. In two dimensions there has been very good progress in *image segmentation*, which is a very similar problem. There are some deep results available, which look as though they generalize to three dimensions (see Reference [54] for references).

3.10. Further remarks on two-phase problems

The equations of two-phase flow introduce the phase saturation of one of the phases, a flux vector for each phase, and a pressure for each phase. A mass balance for each phase in the form of a continuity equation is needed, and also a generalized Darcy law, in which the permeability is multiplied by the 'relative permeability', a function of the saturation. The equation set is closed with a phenomenological law giving the difference in the phase pressures as a function of the saturation, known as the 'capillary pressure'. Again consider a sequence of numerical experiments, but now including investigations over a range of average saturations. By computing the volume averaged phase fluxes, calibrated upscaled relative permeability and capillary pressure functions are found.

In two special limiting cases, one where capillary pressure dominates and another where it is negligible, approximate phase saturations can be found in a simple algebraic way (although there are implementation difficulties due to non-linearity) and a single phase upscaling method can be used to compute the effective relative permeabilities. A detailed introduction to these methods can be found in Reference [6]. More recent references can be found in Reference [55]. The papers [56–58] provide a mathematical perspective with some analytical solutions, discussing when upscaling might work.

There has been progress in applying homogenization theory to the two-phase problem [59, 60]. When the relative permeability and capillary functions are independent of explicit dependence on position, then the equations can be homogenized to the same form, but using the upscaled absolute permeability, as computed in a single-phase problem. That the equations remain of the same form, is not the case more generally, as discussed earlier.

4. COMPARISONS OF UPSCALING METHODS

A classification of upscaling techniques via the type of fine grid experiment and coarse scale calibration procedure has been described. Many upscaling methods have been described in the literature, and some of these have been described in this review.

The literature does not include many systematic comparisons between different upscaling methods, or evaluations of particular techniques, on a range of different permeability distributions. Nevertheless, there are some papers which contain results that indicate some conclusion.

Of particular note is the recent SPE comparison study on upscaling [28]. Two problems were specified with given data, one of these being a 1.1 million cell model generated using a geostatistical method. The physics of the flow was two phase, but the two-phase properties were not spatially heterogeneous and there were no capillary effects. This implied that the problem was very much a test of single phase upscaling methods. The contributors to the study were allowed to choose their own methods, and this included the size of the coarse grid. It was concluded from this study that the no-flow boundary condition method, which was described in Section 3.2, was the best overall method. However, this judgment is not based on a wide selection of examples, and it is clear that much further work is needed to evaluate all upscaling methods. In the papers [22, 27] examples are given where the global–global method performs much better than the local–local, no-flow boundary condition method.

5. UPSCALING AND TURBULENCE THEORY

Upscaling methods have many similarities with large eddy simulation in the study of turbulence. (See Reference [61] for some review articles.) In turbulence studies averaging of the basic equations leads to models such as the $k-\varepsilon$ model and its generalizations. There appears to have been no attempt to derive higher order models of flow in heterogeneous porous media analogous to the Reynolds averaged Navier–Stokes approach. This is almost certainly a result of the extreme non-linearity of the two-phase flow equations, where the relative permeability and capillary functions are monotone but essentially arbitrary. The interesting analysis of Reference [62] using homogenization theory to derive turbulence models of a form similar to k–ε should encourage some research in this direction. The book [37] contains useful references on turbulence of relevance to flow through heterogeneous porous media.

As noted earlier, homogenization theory applied to two-phase flow leads to models using multiple, overlapping continua. In a sense, this is the work that is analogous to the turbulence modelling ideas.

When the displacement of fluid is unstable the problem is even closer to the turbulence problem. An early empirical approach is that reported in the exciting paper [63].

6. CONCLUDING REMARKS

When the length scales of the heterogeneity are well separated then the techniques of local–local upscaling are successful. This is justified by the theory of homogenization.

When the length scales are not well separated, the upscaling problem is much more difficult. Local–local methods can work but are unreliable; global methods meet with some success, in particular the fitting of global experiments with a global calibration, but may be too expensive in the general case. In the context of local–local methods, improvement can occur with oversampling, and the interpretation of upscaling as a generalized finite element or finite volume method is probably a fruitful line of research.

When the flow is unstable then the problem becomes like that of turbulence and there are no clear results, although some empirical models have been devised.

In some cases non-uniqueness of inverse problems may make it possible to change the input data. This occurs when the heterogeneity property model has been derived by an interpolation or modelling approach, and so it may be possible to interpolate the data in such a way that the length scales are well separated.

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