HOMOGENIZER++: A PLATFORM FOR UPSCALING MULTIPHASE FLOWS IN HETEROGENEOUS POROUS MEDIA

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Abstract. We have developed a user friendly computational tool, Homogenizer++, for the computation of effective parameters. The platform Homogenizer++ is based on Object Oriented Programming approach. It currently includes modules to compute effective permeability, effective capillary pressures and relative permeabilities, macrodiffusion in solute transport and simples code for computing solutions for flow in porous media.

Keywords: Numerical homogenization, upscaling, heterogeneous porous media, two-phase flow.

AMS classification: 65N30, 65Y15, 68U01, 68U20, 74Q99, 76T99, 76M50.

§1. Introduction

The homogenization method is used to analyse the equivalent behavior of a certain number of problems arising in flow and transport through heterogeneous porous media. We treat both single and multiphase flow in porous media. Each homogenization method leads to the definition of a global or effective model of a homogeneous medium defined by the computed effective coefficients. Homogenization methods allow the determination of these effective coefficients from knowledge of the geometrical structure of a basic cell and its heterogeneities by solving appropriate local problems. The technique is based on numerics. In the homogenization methods described and implemented in this work we use conforming, mixed finite elements and finite volume methods to compute approximate solutions of the local problems used in the calculation of the effective coefficients.

The goal of this paper is to present a short description of the methods used for computing the effective permeability, effective capillary pressures and relative permeabilities, and macrodiffusion in solute transport of heterogeneous porous media. General organization of the developed software system, called Homogenizer++, is presented in details in http://www.math.usu.edu/~ koebbe/wwwHomog/ which includes the solver and the pre/post processors with a user-friendly GUI. Examples with graphical visualization of results are presented to illustrate functionality of the program. The software is freely available for research and educational purposes. The open architecture of the program facilitates further developments and adapts to suit specific needs easily and quickly. A series of numerical examples demonstrates the effectiveness of the methodology for two-phase flow in heterogeneous reservoirs. Homogenizer++ is an extension of the platform JHomogenizer [3] to mutliphase flow in porous media.

§2. Upscaling of permeability

We consider the model problem of incompressible two-phase flow in moderately heterogeneous media. For instance in [5], using homogenization theory, the case where the phase permeabilities and the capillary pressures are identical in all parts of the medium was investigated. It was then shown, that the homogenized model has the same form as the intial model and then defining effective parameters makes sense. These methods are based on computing the average of either the energy or the flux on a Representative Elementary Volume (REV) with some boundary conditions; for instance periodic, Dirichlet, or Neumann boundary conditions (see [3]). These approximation procedures are widely used in the engineering literature.

2.1. Periodic boundary conditions

Let $\Omega \subset \mathbb{R}^d$, d=1,2, or 3, be a bounded domain with a periodic structure. More precisely, we shall scale this periodic structure by a parameter ε which represents the ratio of the cell size to the size of the whole region Ω and we assume that $0 < \varepsilon \ll 1$ in a decreasing sequence tending to zero. Let Y represent the microscopic domain of the basic cell. Assume that in such a configuration the absolute permeability tensor depends only on the microscopic variable $y = x/\varepsilon$ where x is the variable in the macroscopic scale. Namely $K^{\varepsilon}(x) = K(x/\varepsilon)$ with K a Y-periodic function in y. Assume that K is a symmetric, strictly positive definite, tensor. Then K_p^{ε} , the effective permeability, is given by

$$(K_{p}^{*})_{ij} = \frac{1}{|Y|} \int_{Y} K(y) \left[\nabla w_{i} + \overrightarrow{\mathbf{e}_{i}} \right] \cdot \left[\nabla w_{j} + \overrightarrow{\mathbf{e}_{j}} \right] dy, \qquad 1 \leq i, j \leq d,$$

$$(1)$$

with w_j , j = 1, ..., d, the solution of the so-called local or cell problem defined by:

$$\begin{cases} w_j \in H_p^1(Y) / \mathbb{R}, \\ -\nabla \cdot \left[K(y) (\nabla w_j + \overrightarrow{\mathbf{e}_j}) \right] = 0 & \text{in } Y. \end{cases}$$
 (2)

Here $\overrightarrow{\mathbf{e}_j}$ is the jth standard basis vector of \mathbb{R}^d . The computation of w_j has been performed by a conforming finite element method, then we compute an approximation of the effective permeability.

2.2. Linear boundary conditions

In this section we outline the homogenization method used for the determination of the effective permeability of heterogeneous reservoir regions without any periodic assumption on the microstructure. In the multi-dimensional case, to compute the effective permeability tensor, K_l^* , we have to solve the local problems for j = 1, ..., d

$$\begin{cases}
-\nabla \cdot [K(y)\nabla p_j] = 0 & \text{in} \quad Y, \\
p_j = y_j & \text{on} \quad \partial Y.
\end{cases}$$
(3)

where y_j is the j^{th} coordinate. Solving these local problems gives the following expression for the coefficients of the tensor K_i^* :

$$(K_l^*)_{ij} = \frac{1}{|Y|} \int_Y K(y) \nabla p_i \cdot \nabla p_j \, dy, \qquad 1 \le i, j \le d.$$
 (4)

Both conforming and mixed finite elements may be used to solve the local problems (3) and compute approximations from above and below of the effective permeability, respectively (cf. [2]). Linear boundary conditions are convenient, particularly in complicated geometries with non-rectangular coarse grid cells.

2.3. Confined boundary conditions

This technique considers each coarse grid cell separately and performs d independent flow problems with no-flow boundary conditions on four sides of the cell and constant pressure conditions on two opposing faces. Consider a domain containing fine-scale microscopic grid blocks. The effective permeability tensor, K_c^* , is given for i = 1, ..., d by:

$$(K_c^*)_{ii} = \frac{1}{|Y|} \int_Y \mathbf{K}(y) \nabla w_i \cdot \overrightarrow{\mathbf{e}_i} \, dy, \qquad 1 \le i \le d,$$
 (5)

with w_i , i = 1, ..., d, the solution of the local problem defined by:

$$\begin{cases}
-\nabla \cdot [K(y)\nabla w_i] = 0 & \text{in} \quad Y, \\
K(y)\nabla w_i \cdot \vec{v} = 0 & \text{on} \quad \mathcal{S}_i, \\
w_i = y_i & \text{on} \quad \partial Y \setminus \mathcal{S}_i,
\end{cases}$$
(6)

where \mathcal{S}_i is a union of faces of the block Y parallel to y_i axis and \vec{v} is the outward normal to $\partial \mathcal{S}_i$. Again both conforming and mixed finite elements methods may be used to solve the local problems (6). Note that this technique leads to a diagonal effective permeability tensor.

2.4. A fractured porous medium

This section is devoted to computing effective permeability for a double-porosity model describing single-phase flows in a fractured porous medium (see for instance [4]). We consider a periodic porous medium where the rescaled unit cell Y is made of two complementary parts, the matrix block Y_m and the fracture set Y_f . The effective permeability is given by:

$$(K_f^*)_{ij} = \frac{1}{|Y|} \int_{Y_f} K(y) \left[\nabla w_i + \overrightarrow{\mathbf{e}_i} \right] \cdot \left[\nabla w_j + \overrightarrow{\mathbf{e}_j} \right] dy, \qquad 1 \le i, j \le d,$$
 (7)

where w_j , j = 1, ..., d is the unique solution of the following cell problem:

$$\begin{cases} w_{j} \in H_{p}^{1}(Y) / \mathbb{R}, \\ -\nabla \cdot \left[K(y) (\nabla w_{j} + \overrightarrow{\mathbf{e}_{j}}) \right] = 0 & \text{in } Y_{f}, \\ \left[K(y) (\nabla w_{j} + \overrightarrow{\mathbf{e}_{j}}) \right] \cdot \overrightarrow{v} = 0 & \text{in } \partial Y_{f}. \end{cases}$$
(8)

As in the previous section, the effective permeability tensor is determined by solving the local problems (8) via a conforming finite elements method.

2.5. Wavelets and homogenization

In this section a brief description of an analogy between homogenization and wavelet representation will be given (cf. [8]). The analogy will be illustrated in one dimension for ease of presentation. Assume that the coefficient, k(x), for the elliptic problem

$$\frac{d}{dx}k(x)\frac{dh}{dx} = f, \qquad x \in]0,1[,$$

with appropriate boundary conditions is a piecewise constant function. Also assume that the coefficient function is defined on 2^m equally sized subintervals of the entire domain. One might imagine that some function k(x) is sampled at 2^m equally spaced points. The idea is to develop a transform method that can be used to compute the correct homogenized value for k(x).

The next step is to compute the solution of a local problem using two neighboring samples of k(x); for example, we may choose to solve for $j = 1, 2, ..., 2^{m-1}$ the local problems

$$\frac{d}{dy}k_j(y)\frac{dw_j}{dy} = -\frac{d}{dy}k_j(y),$$

with

$$k_{j}(y) = \begin{cases} k_{2j}, & 0 \le y \le 1/2, \\ k_{2j+1}, & 1/2 \le y \le 1, \\ 0, & \text{otherwise,} \end{cases}$$

and periodic boundary conditions, $w_j(0) = w_j(1) = 0$. This definition gives a total of 2^{m-1} local problems to solve. Once the problems have been solved the homogenized value for a pair can be computed using

$$k_j^{\#} = \int_0^1 k_j(y) (1 + \frac{dw_j}{dy}) dy.$$

It pays to define level estimates

$$k_{l,j}(y) = \begin{cases} k_{l,2j}, & 0 \le y \le 1/2, \\ k_{l,2j+1}, & 1/2 \le y \le 1, \\ 0, & \text{otherwise}, \end{cases}$$

and

$$k_{l-1,j} = \int_0^1 k_{l,j}(y) (1 + \frac{dw_{l,j}}{dy}) dy.$$

With these definitions it is not a difficult task to develop a fast wavelet based transform for computing a homogenized value for the entire region as defined in [8].

To do this in a computationally effective way we would need to know the solutions of the local problems. Fortunately, in one dimension the local problem defined above admits a solution of the form

$$w_{l,j}(y) = \frac{k_{l,2j+1} - k_{l,2j}}{k_{l,2j} + k_{l,2j+1}} \begin{cases} y, & 0 \le y \le 1/2, \\ 1 - y, & 1/2 \le y \le 1, \\ 0, & \text{otherwise}, \end{cases}$$

with piecewise derivative given by

$$\frac{d}{dy}w_{l,j}(y) = \frac{k_{l,2j+1} - k_{l,2j}}{k_{l,2j} + k_{l,2j+1}} \begin{cases} 1, & 0 \le y \le 1/2, \\ -1, & 1/2 \le y \le 1, \\ 0, & \text{otherwise.} \end{cases}$$
(9)

For those familiar with wavelets it is easy to see that the derivative of the solution (a piecewise constant function) is a scaled Haar wavelet. The scaling is a nonlinear combination of the two neighboring sample values or homogenized values from the previous level.

One should note that the wavelet characterization is based on the solution of the local problem that results from performing the perturbation analysis in the homogenization procedure. Thus the wavelet characterization will change as the homogenization method changes. The extension to multiple dimensions is conceptually very easy (cf. [8]).

§3. Upscaling of capillary pressures and relative permeabilities

We consider a two-phase flow in a heterogeneous porous medium $\Omega \subset \mathbb{R}^d$ of two immiscible and incompressible fluids. The porous medium is supposed to be rigid and composed of different rock types corresponding to subdomains $\Omega_1, \ldots, \Omega_n$ of Ω . Each rock type is characterized by its porosity ϕ^i , absolute permeability tensor \mathbf{K}^i , capillary pressure function $p_c^i(S)$ and two relative permeability functions $k_o^i(S)$ and $k_w^i(S)$. The viscosities and mass densities of the fluids are constant. The wetting fluid phase is denoted by index w (water) and non wetting phase by index o (oil); for simplicity we use symbol S instead of S_w .

The governing equations that describe the fluid flow in a subdomain Ω_i consist of the mass conservation law for each phase, generalized Darcy's law for fluid velocities:

$$\begin{split} \phi^i \frac{\partial S^i}{\partial t} + \operatorname{div} \vec{q}_w^{\ i} &= 0, \quad -\phi^i \frac{\partial S^i}{\partial t} + \operatorname{div} \vec{q}_o^{\ i} &= 0, \\ \vec{q}_w^{\ i} &= -\frac{1}{\mu_w} \mathbf{K}^i k_w^i (S^i) (\nabla P_w^i - \rho_w \vec{g}), \quad \vec{q}_o^{\ i} &= -\frac{1}{\mu_o} \mathbf{K}^i k_o^i (S^i) (\nabla P_o^i - \rho_o \vec{g}), \end{split}$$

and the capillary pressure law: $p_c^i(S^i) = P_o^i - P_w^i$. On the boundary between two subdomains we impose the continuity of pressures and fluxes, and on the boundary of the domain Ω different boundary conditions could be given (see for instance [7]).

In the homogenization procedure, rigorously justified in the periodic setting in [6], the fine grid blocks Ω_i are grouped in coarse grid blocks to which we apply the homogeneous properties, computed as discribed below. Let V be one such coarse grid block composed of fine grid blocks Ω_{l_i} , $i=1,2,\ldots,k\leq n$. Effective porosity of the volume V is given by arithmetic mean:

$$\phi^* = rac{1}{\mathrm{vol}(V)} \sum_{i=1}^k \mathrm{vol}(\Omega_{l_i}) \phi_{l_i}.$$

For a fixed mean value of the saturation S^* we compute the corresponding fine grid block

saturations (S^{l_i} , i = 1, 2, ..., k) by solving

$$\begin{cases} \phi^* S^* = \frac{1}{\text{vol}(V)} \sum_{i=1}^k \text{vol}(\Omega_{l_i}) \phi_{l_i} S^{l_i}, \\ p_c^{l_1}(S^{l_1}) = p_c^{l_2}(S^{l_2}) = \dots = p_c^{l_k}(S^{l_k}). \end{cases}$$
(10)

Effective capillary pressure at saturation S^* is then given by $p_c^*(S^*) = p_c^{l_1}(S^{l_1})$.

In the next step we compute effective relative permeabilities. For $\xi \in \{o, w\}$ we solve d local problems (i = 1, 2, d): find P_{ξ}^{i} such that

$$\operatorname{div}\left(\Lambda_{\xi}(x, S^*) \nabla P_{\xi}^i\right) = 0 \quad \text{in} \quad V, \tag{11}$$

$$P_{\mathcal{E}}^i = x_i \quad \text{on} \quad \partial V,$$
 (12)

where $\Lambda_{\xi}(x,S^*) = \sum_{i=1}^k \chi_{\Omega_{l_i}}(x) \mathbf{K}^{l_i} k_{\xi}^{l_i}(S^{l_i})$, and saturations S^{l_i} are given by (10). We define then the effective full permeability tensors $\Lambda_{\xi}^*(S^*)$ by

$$\Lambda_{\xi}^{*}(S^{*})\vec{e}_{i} = \frac{1}{\text{vol}(V)} \int_{V} \Lambda_{\xi}(x, S^{*}) \nabla P_{\xi}^{i} dx, \quad i = 1, 2, d, \ \xi \in \{o, w\}.$$
 (13)

Note that we have to solve 2d local problems for any chosen value of S^* . Therefore, these tensors will be computed only in a given number of saturation points. Finally, effective flow equations in a subdomain V take the form

$$\begin{split} \phi^* \frac{\partial S^*}{\partial t} + \operatorname{div} \vec{\Phi}_w^* &= 0, \\ \vec{\Phi}_w^* &= -\Lambda_w^* (S^*) (\nabla P_w^* - \rho_w \vec{g}), \end{split} \qquad \begin{aligned} -\phi^* \frac{\partial S^*}{\partial t} + \operatorname{div} \vec{\Phi}_o^* &= 0, \\ \vec{\Phi}_o^* &= -\Lambda_o^* (S^*) (\nabla P_o^* - \rho_o \vec{g}), \end{aligned}$$

with the effective capillary pressure law $p_c^*(S^*) = P_o^* - P_w^*$. On the boundary of different corse grid block we again impose the continuity of the pressures and fluxes. Finally, if necessary, the effective relative permeabilities is defined by

$$kr_{\xi}^{*}(S^{*}) = (\mathbf{K}^{*})^{-1}\Lambda_{\xi}^{*}(S^{*}),$$
 (14)

where \mathbf{K}^* is the effective absolute permeability tensor.

§4. Macrodiffusion in solute transport

A miscible displacement of an incompressible fluid with a dissolved solute in a heterogeneous confined aquifer $\Omega \subset \mathbb{R}^d$ over a time period (0,T), is given by (see, e.g., [7])

$$\phi(x)\frac{\partial c}{\partial t} + \vec{q}(x) \cdot \nabla c = \text{div}(\mathbf{D}(x)\nabla c) \quad \text{in } \Omega \times (0, T), \tag{15}$$

where $\vec{q}(x)$ is the Darcy velocity, given by the hydraulic gradient ∇H :

$$\vec{q} = -\mathbf{K}(x)\nabla H$$
, div $\vec{q} = 0$ in Ω , (16)

subject to appropriate boundary and initial conditions. Here c(x,t) is the transported solute concentration, ϕ and \mathbf{K} are the porosity and the hydraulic conductivity tensor of the heterogeneous medium, and \mathbf{D} is the diffusivity tensor at the Darcy scale. We will assume that $\phi(x) = \overline{\phi}(x/\varepsilon)$, $\mathbf{K}(x) = \overline{\mathbf{K}}(x/\varepsilon)$ and $\mathbf{D}(x) = \overline{\mathbf{D}}(x/\varepsilon)$, where $\overline{\phi}$, $\overline{\mathbf{K}}$ and $\overline{\mathbf{D}}$ are periodic functions, and ε is a small parameter.

The effective macroscale equations have the form

$$\langle \phi \rangle \frac{\partial c}{\partial t} + \vec{q}^0 \cdot \nabla c = \operatorname{div}(\mathbf{D}^h(x)\nabla c) \quad \text{in } \Omega \times (0, T),$$
 (17)

$$\vec{q}^0 = -\mathbf{K}^h \nabla H^0, \quad \operatorname{div} \vec{q}^0 = 0 \quad \text{in } \Omega. \tag{18}$$

The effective properties are computed in the following way (see [1]): First we solve the local problems defined in the periodic cell *Y*:

$$\operatorname{div}_{y}\left(\overline{\mathbf{K}}(y)(\nabla_{y}\chi_{i}^{1}+\vec{e}_{i})\right)=0 \quad \text{in} \quad Y$$
(19)

for $i = 1, 2, \dots, d$. From the vectors

$$\vec{w}^i(y) = -\overline{\mathbf{K}}(y)(\nabla \chi_i^1(y) + \vec{e}_i), \quad i = 1, 2, \dots, d,$$

we build the matrix $\mathbb{Q}(y) = [\vec{w}^1(y), \vec{w}^2(y), \dots, \vec{w}^d(y)]$ and we define the effective hydraulic conductivity

$$\mathbf{K}^{h} = -\langle \mathbb{Q} \rangle = -\frac{1}{|Y|} \int_{Y} \mathbb{Q}(y) \, dy. \tag{20}$$

For the effective macro-diffusivity $\mathbf{D}^h(x)$, we first find the *Y*-periodic solutions $y \mapsto \psi_k(y; \vec{\lambda})$ of the d convection-diffusion equations:

$$-\operatorname{div}_{y}\left(\overline{\mathbf{D}}(y)(\nabla_{y}\psi_{k}+\vec{e}_{k})\right)+\mathbb{Q}(y)\vec{\lambda}\cdot\nabla_{y}\psi_{k}=\left[\frac{\phi(y)}{\langle\phi\rangle}\langle\mathbb{Q}\rangle\vec{\lambda}-\mathbb{Q}(y)\vec{\lambda}\right]\cdot\vec{e}_{k}\quad\text{in }Y,\tag{21}$$

 $k=1,2,\ldots,d$, for every $\vec{\lambda} \in \mathbb{R}^d$, and then we compute the tensor $\mathscr{D}^h(\vec{\lambda})$ defined by

$$\mathscr{D}^{h}(\vec{\lambda})\vec{e}_{k} = \langle \overline{\mathbf{D}}(\nabla_{y}\psi_{k} + \vec{e}_{k})\rangle + \left\langle \left(\frac{\phi(y)}{\langle \phi \rangle}\langle \mathbb{Q}\rangle \vec{\lambda} - \mathbb{Q}\vec{\lambda}\right)\psi_{k}\right\rangle, \tag{22}$$

 $k=1,2,\ldots,d$. Finally we set $\mathbf{D}^h(x)=\mathcal{D}^h(\nabla H^0(x))$. The tensor $\mathcal{D}^h(\vec{\lambda})$ should be computed for any $\vec{\lambda}=\nabla H^0(x), x\in\Omega$. In practice we take an approximation procedure consisting of clustering of $\nabla H^0(x)$ vectors, and working only with a finite subset of these vectors (for more details see [1]).

Acknowledgements

This work was partially supported by the GdR MoMaS 2439 CNRS ANDRA BRGM CEA EDF, whose support is gratefully acknowledged.

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