Multiscale Methods for Multiphase Flow in Porous Media

Jan M. Nordbotten

Department of Mathematics, University of Bergen jan.nordbotten@math.uib.no
Department of Civil and Environmental Engineering, Princeton University

Summary. We aim in this paper to give a unified presentation to some important approaches in multi-phase flow in porous media within the framework of multiscale methods. Thereafter, we will present a modern outlook indicating future research directions in this field.

1 Introduction

Understanding flow in porous media is crucial in applications as diverse as petroleum and geothermal energy recovery, ground water management, waste disposal (including CO_2) in geological formations, and the production of porous materials. Simultaneously, the mathematical and numerical challenges associated with accurate modeling of the strongly non-linear governing equations are profound. Difficulties are characterized by parameters which are anisotropic and discontinuous on all scales of observation, while the solutions are nearly discontinuous and globally coupled even for idealized homogeneous problems.

The equations for porous media flow have an elliptic-hyperbolic structure, where the pressure is governed by an equation which is nearly elliptic, while the fluid saturation is governed by an equation which is nearly hyperbolic. In applications, the principle of mass conservation (which is embedded in both equations), is considered essential. Thus efficient numerical solution techniques are needed which appropriately handle discontinuous coefficients, while honoring mass conservation strictly (see e.g. [3]).

Standard methods are often unsuitable under these circumstances. In terms of spatial discretization, either control volume methods or mixed (or discontinuous) finite element methods are needed to enforce mass conservation in a strong sense [8]. The non-linearities and time dependencies lead to implicit discretizations (in particular for the pressure step). Finally, many of the challenges encountered by multi-grid preconditioners in continuum fluid dynamics (see [6]) are present or even enhanced in porous media (see e.g. [29]). Therefore, domain decomposition preconditioners have become popular.

In industrial petroleum recovery applications, it is common that the parameter field (e.g. permeability), is given at a far higher resolution than what can be resolved with the available computational resources. This has led to a large focus on upscaling methods, and lately this effort has focused on multiscale methods. Frequently, these methods show strong resemblance not only to upscaling, but also to domain decomposition (see e.g. [25]).

We define by "multiscale" in this paper methods which deal with problems defined at a resolution finer than what can be computationally resolved. In reality, this defines two scales, that of the problem and that of the computational resolution, and all the methods herein might well be labeled "twoscale".

We will continue this paper by outlining a framework for classifying various multiscale methods. Thereafter, we will discuss several methods from literature, and identify their proper definition as a multiscale method. Our focus will not be on discussing abstract frameworks, but practical implementations. In particular, we will discuss how permeability upscaling, relative permeability upscaling, and vertical equilibrium formulations all can be seen as multiscale methods. We then give an introduction to state of the art multiscale simulation. Finally, we summarize by giving examples indicating prospects for future developments.

2 A Framework for Discussing Multiscale Methods

There are several frameworks to discuss multiscale methods in. Some useful approaches are Volume Averaging [30], Systematic Upscaling [7] and Variational Multiscale [16]. We will herein use the terminology of the Heterogeneous Multiscale Method (HMM) [12]. Similarities between these frameworks have been discussed elsewhere [11].

Following the presentation of HMM [12], we recall that for a problem

$$f(u,d) = 0, \tag{1}$$

where u is the unknown and d is data, we can postulate the exitence of a "coarse" variable u_D, which satisfies

$$F(u_D,D) = 0. \tag{2}$$

We will assume the functional form of $F(u_D,D)$ to be known, however the coarse data D must be estimated from the fine scale model. The coarse and fine scale models are associated through a compression (also referred to as interpolation) operator $u_D = \mathcal{Q}u$, and some reconstruction (or extrapolation) operator $\mathcal{R}u_D$. Note that while we require $\mathcal{Q}\mathcal{R} = \mathcal{I}$, the reverse does not in general hold.

Of particular interest to the remaing discussion is the finite element formulation of HMM (HMFEM), which consideres minimization problems on the form: Denote by u an element which minimizes

$$\min_{v \in V} A(v) - B(v) \tag{3}$$

for non-linear and linear forms A and B, respectively.

Consider the minimization problem given in Equation (3), and assume it has a unique solution. By introducing a compression operator $\mathcal{Q} : V \rightarrow V_D$, where V_D is some coarse scale solution domain, we have the minimization problem equivalent to (3):

$$\min_{v_D \in V_D} \min_{v:\mathcal{Q}v=v_D} A(v) - B(v). \tag{4}$$

We restrict the choice of compression operators under consideration such that also (4) has a unique solution. We note that an 'exact' reconstruction operator with respect to the minimization problem can be defined from (4): $\mathcal{R}_e u_D$ solves

$$\min_{v:\mathcal{Q}v=u_D} A(v) - B(v). \tag{5}$$

We now have the exact coarse scale HMFEM minimization problem

$$\min_{v_D \in V_D} A(\mathcal{R}_e v_D) - B(\mathcal{R}_e v_D). \tag{6}$$

For practical purposes, calulating $\mathcal{R}_e$ is excessively expensive, and an approximation is introduced; $\tilde{\mathcal{R}} \approx \mathcal{R}_e$. It is usually advocated (see e.g. [12]) that since u_D is a macro-scale function, it should vary smoothly, thus it is sufficient to evaluate the integrals appearing in the variational formulation at quadrature points. This allows for great flexibility in localization strategies for approximating $\tilde{\mathcal{R}}$.

3 A Model Problem for Multiphase Flow

The model equation for multiphase flow in porous media is the standard extension of Darcy's law to two phases $\alpha = \{0,1\}$ (see e.g. [5, 8, 19, 22]):

$$\mathbf{u}_\alpha = -K\lambda_\alpha(\nabla p - \rho_\alpha \mathbf{g}). \tag{7}$$

Here $\mathbf{u}_\alpha$ is the volumetric flux with units [L/T] , K is the intrinsic permeability of the medium [L^2], $\lambda_\alpha = \lambda_\alpha(s_\alpha)$ is the phase mobility as a function of the phase saturation s_α [TLM^{-1}], p is pressure [$ML^{-1}T^{-2}$], $\rho_\alpha = \rho_\alpha(p)$ is phase density [ML^3], and finally $\mathbf{g}$ is the gravitational vector [LT^{-2}], positive downwards. We have neglected the difference between phase pressures, which is a common assumption at reservoir scales [19].

The equations for flow satisfy conservation of mass for each phase

$$\phi \partial_t(\rho_\alpha s_\alpha) = \nabla \cdot (\rho_\alpha \mathbf{u}_\alpha) = b_\alpha, \tag{8}$$

where ϕ denotes the void fraction (porosity) [L^0], which is kept constant is time, but is allowed to vary in space, while b_α represents source and sink terms [$ML^{-3}T^{-1}$].

We close the system by requiring that no more than two phases are present,

$$s_0 + s_1 = 1, \tag{9}$$

and assigning constitutive relationships:

$$K = K(\mathbf{x}), \qquad \phi = \phi(x), \qquad \lambda_\alpha = \lambda_\alpha(s_\alpha). \tag{10}$$

Note that we will frequently use the shorthand $s = s_0$ and $s = 1 - s_1$ in the derivations. In this work we will neglect compressibility.

The key difficulties in (7) and (8) lie firstly in the pronounced heterogeneity in the permeability, which may be discontinuous and contain long-range correlations. Further, the solution may contain shocks due to the non-linear relative permebility functions.

A total pressure - fractional flow formulation is often used for (7)–(10) as this formulation allows for the application of a splitting to exploit the (relatively) weak time dependence of pressure [8]. We obtain a total pressure equation by eliminating $\partial_t s$ from (8):

$$\nabla \cdot \mathbf{u}_T = b_T \tag{11}$$

$$\mathbf{u}_T = -K\lambda_T(\nabla p - \rho_T \mathbf{g}). \tag{12}$$

Equations (11) and (12) are written in two parts to retain the physical fluxes explicitly. This is important to get the mass conservation equation discretized correctly. The flux, source, mobility and density are defined as:

$$b_T = \sum_\alpha b_\alpha \rho_\alpha^{-1}, \qquad \mathbf{u}_T = \sum_\alpha u_\alpha, \qquad \lambda_T = \sum_\alpha \lambda_\alpha, \qquad \rho_T = \lambda_T^{-1} \sum_\alpha \lambda_\alpha \rho_\alpha. \tag{13}$$

The individual phase fluxes can be recovered from $\mathbf{u}_T$;

$$\mathbf{u}_\alpha = \lambda_\alpha \lambda_T^{-1} \mathbf{u}_T + \lambda_\alpha \lambda_\beta \lambda_T^{-1} K(\rho_\alpha - \rho_\beta)\mathbf{g}, \tag{14}$$

where $\beta = 1 - \alpha$. Equations (11)–(14) together with either of (8) form an equivalent system of equations to (7)–(10).

4 Some Upscaling Methods

In this section, we will investigate upscaling methods aimed at the two main difficulties outlined in our model multiphase flow equations: The heterogeity of the permeability data and the heterogeneity of the saturation solution.

4.1 Permeability Upscaling

Upscaling of permeability by itself is essentially a single phase problem. As such, it is analogous to many other problems in the physical sciences, including most famously heat conduction. Many strategies are applicable to this problem, particularly in the case where scale separation exists. We will herein consider a form of numerical homogenization popular in the porous media community. We recognize that permeability upscaling has previously been discussed within the framework of HMM [2, 12], however the approach taken here is different.

Typically, in porous media, every coarse grid block is assigned a permeability, based on fine scale flow properties. Depending on the level of complexity of the coarse scale numerical solver, this permeability is either isotropic, anisotropic aligned with the grid, or generally anisotropic.

The coarse block permeability is calculated by solving some fine scale problem. The appropriate boundary conditions for this problem can be a cause of debate, but for the sake of the argument, we follow [5] and use a linear potential (we need not consider gravity when upscaling absolute permeability). The coarse permeability is then calculated by postulating the existence of a coarse scale Darcy law for the grid block

$$\langle \mathbf{u} \rangle = -\frac{K_D}{\mu} \langle \nabla p \rangle. \tag{15}$$

Here $< \mathbf{u} >$ is the mean of the calculated velocity, and $< \nabla p >$ is (by Green's theorem) a function of the boundary conditions. By varying the boundary conditions, one can infer the coarse scale permeability K_D.

We will avoid a lengthier discussion of upscaling methods for absolute permeability, and consider how the approach taken above can be seen as within the framework of the HMM.

Consider the following choice of discrete coarse scale variables: a potential vector $\mathbf{p}_D$ and coarse permeability vector (or tensor) $\mathbf{K}_D$. We assume that the coarse scale equations are some appropriate discretization of the elliptic equation on the coarse scale grid, e.g. $F(\mathbf{p}_D, \mathbf{K}_D) = 0$. We define the compression for coarse cell Ω_i as

$$p_{D,i} = \mathcal{Q}p = \frac{1}{L} \int_{\Omega_i} p \mathrm{d}s,$$

where L is the arc length of the integral.

The constrained variational form of (5) for the fine scale HMM problem can then be written [24]: Find p' s.t. $p_D = \mathcal{Q}p'$ and

$$(K\nabla p', \nabla q') = 0 \quad \forall\, q' \text{ s.t. } 0 = \mathcal{Q}q'. \tag{16}$$

The data K_D is then obtained from (15), subject to the additional constraint that the anisotropy directions are known (e.g. aligned with the flow or the grid).

We see now that the classical permeability upscaling approach can be seen as a localization of the global fine scale problem in the HMM. Indeed, if we use a piecewise linear potential to impose $p_D = \mathcal{Q}p'$, and solve (16) separately on each subdomain, we obtain exactly the numerical upscaling approach described earlier.

We emphasize that the intuitive, or one might say engineering, approach to upscaling permeability can thus be shown to be related to a multiscale modeling framework. However, this relationship comes at a considerable cost: We have assumed the existence of an equivalent homogeneous coarse scale permeability K_D; defined a highly specialized compression operator; and subsequently made a very crude approximation to what is the known "true" fine scale problem. Indeed, we would encourage interpreting this section not in support of classical permeability upscaling, but rather as a critique pointing out the expected weaknesses.

The observations regarding potential problems with permeability upscaling are not new, and they have previously motivated what is known as transmissibility upscaling for finite volume methods (see e.g. [10, 20]). With this approach, the coarse scale is assumed to satisfy a discrete conservation law of the form

$$\mathbf{f}_D = -B\mathbf{p}_D; \qquad -C\mathbf{f}_D = \mathbf{b}_D. \tag{17}$$

Here, $\mathbf{f}_D$ and $\mathbf{b}_D$ are the coarse fluxes and sources, while B and C are sparse matrices representing conductivity and mass conservation, respectively. The mass conservation matrix C is known, and an upscaling approach is used to determine the coefficients of B.

We note that from a general perspective, permeability upscaling and transmissivity upscaling are closely related, and the previous remarks about the relationship to a HMM framework apply also to transmissibility upscaling. The case of transmissivity upscaling is discussed in more detail in [13]. Our main point of including the transmissivity upscaling, is to show how the macroscale model may be either discrete *a posteriori*, as in the case of permeability upscaling, or *a priori* as in the case of transmissivity upscaling. Note that the advantage of an *a priori* discrete model in this case is that no explicit assumptions are made on a macroscale permeability K_D

4.2 Saturation Upscaling

The second challenge of porous media upscaling is the saturation equation. We will here outline the industry standard perspective.

As with the permeability, we assume the existence of a macroscale extension of Darcy's law. This macroscale extension can as in the previous section be either continuous or discrete; for the sake of the argument we will make assumption that it is continuous, e.g.:

$$\langle \mathbf{u}_\alpha \rangle = -k_{D,\alpha}(s_{D,\alpha})\frac{K_D}{\mu_\alpha}\langle \nabla p_\alpha \rangle. \tag{18}$$

Here s_D is the macroscale saturation, while k_D is the macroscale relative permeability. The compression operator for the macroscale saturation must for mass conservation reasons be defined simply as the cell average saturation.

Applying a similar approach to the permeability upscaling case, one obtains the following rather interesting observations: Firstly, the results are highly sensitive to how one treats the coarse scale potential gradient term [27]. Secondly, the results are (as expected), influenced by imposed boundary conditions. Finally, and more importantly, we note that in analog to permeability upscaling where we saw induced anisotropy at the coarse scale (even without anisotropy at the fine scale), for saturation upscaling we see a strong history dependence on the coarse scale, even when none is present at the fine scale.

From a HMM perspective, we first observe that for the hyperbolic part, these simple approaches are variants of a Godunov method. This allows us to make a more natural interpretation of the hysteresis point: While saturation has a unique compression operator, the problem unfortunately has a strong dependence on the degrees of freedom in the reconstruction operator. Indeed, the problem is that the upscaling method described above aims at being more accurate than a naive first order Godunov method, but the price then becomes selective accuracy, depending on the quality of the reconstruction.

4.3 Vertically Integrated Models

For some porous media applications, such as saltwater intrusion [5] and storage of CO_2 in saline aquifers, vertically integrated models may be applicable [14, 28]. The features allowing a successful application of such a formulation are the dominance of horizontal length scales over vertical length scales, combined by gravity segregation in the systems.

The key concept behind vertically averaged models is to consider equations for an interface between the two fluids resulting from gravity segregation. By integrating over the vertical direction, we obtain governing equations for the interface, which are essentially 2D conservation equations combined by flux functions involving integrals over the vertical direction;

$$F = \int f \, \mathrm{d}z. \tag{19}$$

These integrals contain subscale information through the explicit dependence on the vertical solution structure. To apply this formulation, effective approximations must be introduced regarding the vertical structure of the pressure field in addition to that of segregated fluids. Common choices are vertical equilibrium (the Dupuit approximation), although more complex choices are possible [26].

Let us consider this approach again within the framework of a multiscale methodology. The scale assumption is that the vertical scales are short, and the associated time scale of equilibration are short. To honor mass conservation, the compression operator taking saturation to interface thickness is vertical integration. A compression operator for the pressure can be taken as the pressure at the bottom of the domain (as in the above references). Following the assumption of short equilibration time in the vertical direction, and reconstruction of initial conditions for a fine scale solver will lead to a vertically segregated, fluid-static system. We will therefore simply assume that the reconstruction operator is the fluid-static distribution. The combined operator $\mathcal{RQ}$ will be exact for problems where the fine scale indeed is vertically segregated.

It is interesting to note how the Dupuit approximation in the vertically integrated model appears immediately with the multiscale framework. Also worth noting is how HMM provides an abstract framework for discussing this approximation beyond the ususal asymptotic arguments.

We conclude this section by reiterating the purpose of these examples. Through relating well established concepts to a common framework, we hope to achieve two aims: Firstly, to provide a unified way of considering physical based (as opposed to strictly numerical) upscaling methods. Secondly, to build support for HMM (or a similar multiscale design) as a general framework to guide upscaling methods.

5 Multiscale Numerical Methods

In this section, we will expand upon the ideas from the previous section, and discuss newer methods gaining interest in porous media. In particular we will discuss a class of numerical methods, which term themselves also multiscale methods, which aim at creating approximate solutions on a coarse scale, retaining a physically plausible fine scale structure. The methods discussed here primarily address the pressure equation, which due to ellipticity is the harder equation, while the saturation equation is resolved on a fine scale [1, 4, 17, 23]. While these methods have much in common with domain decomposition [9, 25], they differ in the focus on fast approximations to the fine scale problem which are physically plausible, rather than the solution to the fine scale problem itself. We will focus in particular on the so-called variational multiscale methods, the general ideas are similar between the formulations.

5.1 The Variational Multiscale Method

The Variational MultiScale (VMS) Method is a general approach to solving partial differential equations [15, 16]. While more specialized in approach than the HMM, we see in VMS a sharper focus on the nature and structure of the fine scale problems. When applied in a similar manner, it can be shown that VMS can be considered a special case of HMM [24].

We therefore consider: Find $u \in U$ such that

$$a(u,v) = b(v) \quad \forall\, v \in V. \tag{20}$$

We take a and b to be bilinear and linear operators, respectively. Although in general the spaces U and V may be different, we will here use $U = V$.

Hughes et. al discuss finite element approximations in terms of the following argument: Let V' be defined such that $V_H \oplus V' = V$, noting that in general V_H and V' need not be orthogonal. Then the following coupled problems are equivalent to (20): Find $u_H \in V_H$ and $v' \in V'$ such that

$$a(u_H, v_H) + a(u', v_H) = b(v_H) \quad \forall\, v_H \in V_H \tag{21}$$

and

$$a(u_H, v') + a(u', v') = b(v') \quad \forall\, v' \in V', \tag{22}$$

The term $a(u', v_H)$ can be quanitified by representing u' in terms of a Green's function for the original problem constrained to the space V' [15]. Thus, we can write the solution of (22) formally as

$$u' = -G'(b - \mathcal{L}u_H), \tag{23}$$

where $b - \mathcal{L}u_H$ is the residual error of the approximate solution u_H to the underlying PDE:

$$\mathcal{L}u - b = 0, \tag{24}$$

and G' is an integral Green's transform, where the kernel is simply the Green's function in V'. By combining (22) and (23), we obtain the finite dimensional variational problem: Find $u_H \in V_H$ such that

$$a(u_H + G'(u_H), v_H) = b(v_H) + a(G'(b), v_H) \quad \forall\, v_H \in V_H. \tag{25}$$

This equation is refered to as a paradigm for multiscale simulation [16].

5.2 A VMS Approach for the Implicit Time-Discretized Pressure Equation

We consider the following coupled partial differential equations, which serve as a prototype for the pressure equation in porous media flow.

$$\nabla \cdot \mathbf{u} = b \quad \text{in } \Omega, \tag{26}$$

$$\mathbf{u} + d(\nabla p - \mathbf{c}) = 0 \quad \text{in } \Omega, \tag{27}$$

$$\mathbf{u} \cdot \nu = 0 \quad \text{on } \partial\Omega. \tag{28}$$

We consider for simplicity only zero Neumann (no-flow) boundaries. These boundary conditions are prevailing in applications. On variational form, the mixed problem can be stated as: Find $p \in W$ and $\mathbf{u} \in \mathbf{V}$ such that

$$(\nabla \cdot \mathbf{u}, w) = (b, w) \quad \forall\, w \in W, \tag{29}$$

$$(d^{-1}\mathbf{u}, \mathbf{v}) - (p, \nabla \cdot \mathbf{v}) = (\mathbf{c}, \mathbf{v}) \quad \forall\, \mathbf{v} \in \mathbf{V}. \tag{30}$$

The permeability is a symmetric and positive definite matrix, justifying the inverse used in (30). The mixed space $\mathbf{V}$ must honor the boundary condition.

Given (29) and (30), we are prepared to introduce our VMS method. Thus, let W and $\mathbf{V}$ be direct sum decompositions $W = W_H \oplus W'$ and $\mathbf{V} = \mathbf{V}_H \oplus \mathbf{V}'$. Our coarse scale variational problem is thus: Find $p_H \in W_H$ and $\mathbf{u}_H \in \mathbf{V}_H$ such that

$$\begin{aligned}&(\nabla \cdot (\mathbf{u}_H + G'_{\mathbf{u}}(\nabla \cdot \mathbf{u}_H, \nabla p_H + d^{-1}\mathbf{u}_H)), w_H)\\ &\quad = (b + \nabla \cdot G'_{\mathbf{u}}(b, \mathbf{c}), w_H) \quad \forall\, w_H \in W_H\end{aligned} \tag{31}$$

and

$$\begin{aligned}&(d^{-1}(\mathbf{u}_H + G'_{\mathbf{u}}(\nabla \cdot \mathbf{u}_H, \nabla p_H + d^{-1}\mathbf{u}_H), \mathbf{v}_H)\\ &\quad - (p_H + G'_p(\nabla \cdot \mathbf{u}_H, \nabla p_H + d^{-1}\mathbf{u}_H), \nabla \cdot \mathbf{v}_H)\\ &\qquad = (\mathbf{c} + d^{-1}G'_{\mathbf{u}}(b, \mathbf{c}), \mathbf{v}_H) - (G'_p(b, \mathbf{c}), \nabla \cdot \mathbf{v}_H) \quad \forall\, \mathbf{v} \in \mathbf{V}.\end{aligned} \tag{32}$$

The integral operators $G'_p \in W'$ and $G'_{\mathbf{u}} \in \mathbf{V}'$, which we will refer to as Green's transforms, are the formal solutions to the following (linear) equations:

$$(\nabla \cdot G'_{\mathbf{u}}(g,\mathbf{f}), w') = (g, w') \quad \forall\, w' \in W', \tag{33}$$

$$(d^{-1} G'_{\mathbf{u}}(g,\mathbf{f}), \mathbf{v}') - (G'_p(g,\mathbf{f}), \nabla \cdot \mathbf{v}') = (\mathbf{f}, \mathbf{v}') \quad \forall\, \mathbf{v}' \in \mathbf{V}'. \tag{34}$$

We note that in (31) and (32), we need the Green's transforms evaluated for all members of the spaces W_H and $\mathbf{V}_H$. Since (33) and (34) are linear, it suffices to evaluate (or approximate, as the case will be) G'_p and $G'_{\mathbf{u}}$ for a set of basis functions for W_H and $\mathbf{V}_H$, in addition to the right hand side components b and $\mathbf{c}$.

To proceed further, it is necessary to make an appropriate choice of spaces W_H, $\mathbf{V}_H$, W' and $\mathbf{V}'$. This will not be elaborated here, alternative choices can be found in e.g. [4, 18, 21, 23].

6 Conclusions

In this paper we have made an initial attempt at bringing together diverse approaches to upscaling for multiphase porous media flow problems under the umbrella of multiscale methods. The goal has not been to complete a comprehensive survey, but rather to illustrate how key ideas can be related.

We have considered upscaling, both static and dynamic; vertically integrated formulations; and modern multiscale simulation. While there is still work to be done before these approaches can be presented seamlessly, we hope that the current exposition will allow the reader to appreciate the subtle similarities.

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