A Multilevel Multiscale Mimetic (M^3) Method for an Anisotropic Infiltration Problem

Konstantin Lipnikov, David Moulton, and Daniil Svyatskiy

Los Alamos National Laboratory, Theoretical Division,
Los Alamos, NM 87545, USA
{lipnikov,moulton,dasvyat}@lanl.gov

Abstract. Modeling of multiphase flow and transport in highly heterogeneous porous media must capture a broad range of coupled spatial and temporal scales. Recently, a hierarchical approach dubbed the Multilevel Multiscale Mimetic (M^3) method, was developed to simulate two-phase flow in porous media. The M^3 method is locally mass conserving at all levels in its hierarchy, it supports unstructured polygonal grids and full tensor permeabilities, and it can achieve large coarsening factors. In this work we consider infiltration of water into a two-dimensional layered medium. The grid is aligned with the layers but not the coordinate axes. We demonstrate that with an efficient temporal updating strategy for the coarsening parameters, fine-scale accuracy of prominent features in the flow is maintained by the M^3 method.

Keywords: multiscale, hierarchical, two-phase flow, heterogeneous porous media, infiltration.

1 Introduction

High fidelity simulations of multiphase flow and transport in porous media play a key role in driving scientific advances in a broad range of complex multiscale applications, including carbon sequestration, aquifer assessment and protection, and nuclear waste disposal. However, there are fundamental mathematical and computational hurdles that arise from the wide range of strongly coupled spatial and temporal scales. For example, the permeability of porous media is highly heterogeneous and may span several orders of magnitude, from nearly impermeable barriers to high-permeable flow channels. To address this challenge we have developed the new Multilevel Multiscale Mimetic (M^3) method [1].

The M^3 method builds recursively a problem-dependent *multilevel hierarchy of models*. Each model preserves important physical properties of the continuum model, such as *local mass conservation*. In contrast to two-level methods, such as the multiscale finite element methods [2,3,4], the multiscale mortar finite element method [5] and the Multiscale Finite Volume (MSFV) method [6], the multilevel hierarchy facilitates large total coarsening factors, of 100 or more in each coordinate direction.

Building and maintaining the hierarchy of models incurs only a moderate computational overhead especially for a small coarsening factor on each level. The M^3 method supports unstructured polygonal meshes, and is readily extended to unstructured polyhedral meshes. In addition, it can handle full permeability tensors and accommodates general coarsening strategies to capture accurately the complexity of the heterogeneous subsurface environment.

The M^3 method [1] merges two computational strategies to balance accuracy and efficiency in two-phase flow simulations. The first strategy is the algebraic coarsening developed by Y. Kuznetsov for single phase flows that reduces the degrees of freedom inside coarse-grid cells [7]. The second strategy is a *novel* approach to the conservative coarsening of velocities on the edges of a coarse-grid cell. This combination ensures that the coarse-scale system has the same sparsity structure as the fine-scale system, and with recursion leads to a multi-level algorithm. Due to its algebraic nature, the method can be adapted to other discretizations of the same algebraic form, such as the mixed finite element and finite volume methods.

In this work we demonstrate the capabilities of the M^3 method for infiltration into a stratified porous medium that is composed of sloping and non-uniform layers and strongly anisotropic inclusions. The majority of two-level methods solve localized fine-scale flow problems to capture the influence of fine-scale structures. Formulation of local problems with appropriate localized sources and boundary conditions can be problematic, particularly for anisotropic media [8]. The multiscale mortar finite element method [5] offers a more robust approach for this case, as the accuracy can be controlled via refinement of the mortar space. The M^3 method uses a different mechanism for controlling the accuracy via efficient incorporation of global information into the hierarchy of models. Numerical experiments demonstrate that the M^3 method can maintain fine-scale solution accuracy, even with large coarsening factors, while significantly reducing the overall simulation time.

The paper outline is as follows. In Section 2, we present the mathematical model of the infiltration problem. In Section 3, we describe essential features of the M^3 method. In Section 4, we illustrate the effectiveness of the method with the simulation of water infiltration into a layered anisotropic porous medium.

2 Mathematical Model of a Two-Phase Flow

We consider the flow of two immiscible phases, non-wetting (e.g., air, denoted a) and wetting (e.g., water, denoted w), in a two-dimensional domain subject to gravity (see, e.g., [9,10]). The effects of compressibility and capillary pressure are neglected. Conservation of each phase implies,

$$\phi \frac{\partial S_j}{\partial t} + \nabla \cdot \mathbf{u}_j = -q_j, \quad j = a, w, \quad (1)$$

where S_j and $\mathbf{u}_j$ are the saturation and the velocity of phase j , respectively, and the porosity, ϕ , is assumed constant. The Darcy velocity of phase j is given by,

$$\mathbf{u}_j = -\mathbb{K} \cdot \lambda_j (\nabla p_j - \rho_j \mathbf{g}), \quad (2)$$

where $\mathbb{K}$ is the absolute permeability tensor; $\lambda_j = k_{rj}/\mu_j$ is the relative mobility of phase j , with k_{rj} the relative permeability and μ_j the viscosity; ρ_j is the density and $\mathbf{g}$ is the gravitational acceleration vector.

Assuming that the two phases fill the pore volume we have the constraint $S_a + S_w = 1$. This may be combined with the sum over j of (1) to yield the bulk fluid conservation law,

$$\nabla \cdot \mathbf{u} = q_a + q_w. \quad (3)$$

Here the total or bulk fluid velocity, $\mathbf{u} = \mathbf{u}_a + \mathbf{u}_w$, may be written in the form,

$$\mathbf{u} = -\mathbb{K}(\lambda \nabla p - (\lambda_a \rho_a + \lambda_w \rho_w) \mathbf{g}), \quad (4)$$

where $\lambda = \lambda_w + \lambda_a$ is the total mobility, and neglecting capillary pressure we have set $p = p_a = p_w$ to be the reference pressure. Thus, the two-phase system that we model is comprised of an elliptic equation for the pressure, obtained by substitution of (4) into (3), and a hyperbolic equation for the water saturation, $S = S_w$, given by (1) with $j = w$. The initial and boundary conditions used to close the model are given in Section 4.

3 Multiscale IMPES Method

3.1 Time Integration and Fine-Scale Discretization

We use the IMPES (IMplicit Pressure and EXplicit Saturation) time integration method. First, the pressure equation is solved to define the velocity field. Second, the hyperbolic equation for the water saturation is integrated explicitly using the single-point upwind finite volume method [11].

To discretize the pressure we consider a polygonal partition of the domain Ω , denoted Ω_h , that is the union of the polygonal cells e_i , $i = 1, \dots, N$. We apply the Mimetic Finite Difference (MFD) method [12] to the first-order form of the pressure equation, given by (4) and (3). For each cell e_i , we define one pressure unknown, p_i , which represents the integral average of p . Similarly, for each edge ℓ_j , we define one unknown, u_j , which represents the average normal flux $\mathbf{u} \cdot \mathbf{n}$ (a scalar) through this edge. The MFD discretization of the pressure equation reads

$$\begin{bmatrix} \mathbf{M}(\mathbf{S}^n) & \mathbf{B}^T \\ \mathbf{B} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{u}^n \\ \mathbf{p}^n \end{bmatrix} = \begin{bmatrix} \mathbf{q}_g^n \\ \mathbf{q}^n \end{bmatrix}. \quad (5)$$

Here n denotes the time step, $\mathbf{M}(\mathbf{S}^n)$ is the mass matrix computed using the current saturation and $\mathbf{B}$ is the discrete divergence operator. The source $\mathbf{q}_g^n$ captures Dirichlet data and the gravitational term in (4), and $\mathbf{q}^n$ captures Neumann data and the source/sink term in (3).

3.2 Two-level Method for the Pressure Equation

We begin by describing a two-level coarsening method, a building block for the multilevel method. Let $N_0 = N$, $N_1 \leq cN_0$, with $0 < c < 1$, and

$$\Omega_H = \bigcup_{I=1}^{N_1} E_I, \quad E_I = \bigcup_{i \in \mathcal{F}(E_I)} e_i,$$

Fig. 1. Schematic of the two steps of the two-level upscaling method for a 2×2 square macro-cell. The cell-centered pressure unknowns are represented by circles, and the velocity unknowns are represented by arrows. The first step is an equivalent reduction, while the second step is approximate.

where $\mathcal{F}(E_I)$ is a set of indices of fine-grid cells forming the *macro-cell* E_I . We assume that the coarse-grid partition Ω_H is non-overlapping and conformal. Note that each *macro-edge* of a macro-cell E_I is not necessarily a straight line, as it is simply a collection of fine-grid edges.

The two-level method consists of two steps, which are illustrated in Fig. 1. For simplicity, we omit the time superscript n , and consider aggregation of four cells into a single macro-cell. First, for each macro-cell, we eliminate all internal flux unknowns, and replace all internal pressure unknowns with a single pressure [7]. By construction, this single pressure on each macro-cell is the volume-weighted average of the corresponding fine-grid pressures:

$$P_I = \frac{\sum_{i \in \mathcal{F}(E_I)} p_i |e_i|}{\sum_{i \in \mathcal{F}(E_I)} |e_i|}.$$

This first step is an *equivalent* modification of the original system (see [1] for details). The unknowns in the resulting system are shown in Fig. 1(middle).

The second step is to perform a *conservative* flux coarsening procedure that leaves one flux unknown U_J per macro-edge L_J . Mass conservation dictates that the coarse flux on a macro-edge must be a weighted sum of the corresponding fine-grid fluxes. This coarsening makes the final structure of the reduced system, shown in Fig. 1(right), identical to the original system. For each fine-grid flux u_j we introduce the coarsening parameter α_j , as follows

$$u_j = \alpha_j U_J. \quad (6)$$

This parameter is related to the first moment of the flux, and plays an important role in the M^3 algorithm. It is used to define the interpolation of the flux, and it influences the coarse-scale pressure model. Suppose that the problem (5) is solved exactly. Then we can calculate coarse-grid fluxes U_J and derive coarsening parameters α_j . Such parameters will make the upscaling procedure exact. However, these parameters are functions of time, and accurately recomputing

them at each time step would be equivalent in cost to the fine-scale IMPES formulation. In the M³ method these parameters are derived from an approximate solution of the fine-scale problem (5) and we recompute these parameters only when it is necessary to maintain accuracy (see Section 3.3).

3.3 Multilevel Hierarchy of Pressure Models

The two-level coarsening method results in coarse-grid equations that have the same structure as the fine-grid equations. Hence a multilevel algorithm follows naturally by applying this process recursively, and generates a hierarchy of discrete upscaled pressure models. To maintain the accuracy of this hierarchy without compromising the overall performance of the method, efficient update strategies are required. We have implemented the local and global update strategies described below.

Local Update Strategy. Here, the M³ method is focused on the total mobility. The total mobility changes significantly in the vicinity of a sharp water front. The M³ method updates cell-based matrices (over the whole hierarchy) that are affected by these changes. More precisely, we use the criterion proposed in [13],

$$\frac{1}{1 + \varepsilon_\lambda} \leq \frac{\lambda^n}{\lambda^{n-1}} \leq 1 + \varepsilon_\lambda,$$

where ε_λ is the user defined threshold, usually 0.1. If this condition is violated, the cell-based matrices are updated.

Global Update Strategy. In simulations of flow through porous media with long correlation lengths, or strong anisotropy, local updates of the hierarchy are not sufficient to maintain the accuracy. In these cases, the elliptic nature of the pressure equation is accentuated and global information is needed. Therefore, we recalculate flux coarsening parameters during the simulation. These updates are equi-distributed in time approximately every few hundred time steps. The impact of these updates on the accuracy of the simulation is discussed in Section 4.

To maintain the overall performance of the simulation, an efficient global approximation strategy for the α 's is needed. In [1] we proposed to leverage the strength of a robust variational multigrid method for this purpose. The saddle-point problem (5) is hybridized and reduces to a symmetric positive-definite problem for the Lagrange multipliers. We use preconditioned conjugate gradient iterations with Ruge-Stüben algebraic multigrid [14] as the preconditioner, denoted PCG(AMG), to solve approximately for the Lagrange multipliers. The convergence tolerance ε_r is usually set to $10^{-2} - 10^{-3}$, and is reached in only a few (3-10) iterations. This approach captures critical changes in global flow behavior. In our original study [1] we demonstrated its effectiveness for highly heterogeneous porous media with long correlation lengths. Here we focus on the challenging problem of infiltration into a strongly anisotropic medium.

4 Numerical Experiments

In our numerical experiments we model the infiltration of water into an unsaturated two-dimensional porous medium, shown schematically in Fig. 2(a). Initially the pore space is filled with air and a small residual water saturation. The medium is composed of four sloping layers and two elongated inclusions, and is partly motivated by the study in [15]. The interfaces of these features are not aligned with the coordinate axes. A structured orthogonal mesh is mapped onto these features so that each mesh cell has homogeneous properties. A 32×32 mesh is shown in Fig. 2(b), while the mesh used in our numerical experiments is 128×128 . Based on this mapping, we define a local coordinate system at the centroid of each mesh cell that is aligned with the associated layer or inclusion. In this local coordinate system the absolute permeability tensor is assumed to be diagonal. The diagonal permeability tensors, as well as their anisotropy ratios, are presented in Table 1. Note that since the local coordinate axes are not aligned with the Cartesian axes, the absolute permeability is a full tensor in the Cartesian system.

Fig. 2. Computational domain: (a) sloping layered structure with strongly anisotropic inclusions in Zone 5 and 6, (b) a structured mesh 32×32 is mapped onto the stratigraphy. The fine 128×128 computational mesh is constructed in a similar way.

To complete the definition of the two-phase flow model given in Section 2, we define the relative permeability curves as,

$$k_{rw}(S) = (S^*)^2, \quad k_{ra}(S) = (1 - S^*)^2, \quad S^* = \frac{S - S_{wr}}{1 - S_{wr} - S_{nwr}}, \quad (7)$$

where S^* is the normalized wetting phase saturation, and $S_{wr} = S_{nwr} = 0.1$ are the residual saturations of the wetting and non-wetting phases, respectively. In

Table 1. Absolute hydraulic permeability tensors are diagonal in the local coordinate system of each zone. Note that the anisotropy ratio is 100 within the inclusions (Zones 5 and 6) and 50 in Zone 2.

Zone	$\mathbb{K}_x(\text{m}^2)$	$\mathbb{K}_z(\text{m}^2)$	$\mathbb{K}_x/\mathbb{K}_z$
1	4×10^{-12}	4×10^{-12}	1
2	5×10^{-12}	1×10^{-13}	50
3	5×10^{-12}	5×10^{-12}	1
4	9×10^{-12}	9×10^{-12}	1
5	5×10^{-11}	5×10^{-13}	100
6	5×10^{-11}	5×10^{-13}	100

addition, the initial saturation is set to a constant, $S(t = 0) = S_{wr} = 0.1$; the porosity is constant, $\phi = 0.2$; and the phase viscosities are $\mu_w = 1.0 \times 10^{-3}$, and $\mu_a = 1.8 \times 10^{-5}$, both in units of $\text{kg} \cdot (\text{m} \cdot \text{s})^{-1}$. Boundary conditions are shown schematically in Fig.2(a) with no-flow everywhere except for the water source in the upper left and the fixed pressure in the bottom right. Fig. 2(b) shows the dimensions of the domain ($10\text{m} \times 10\text{m}$), with the infiltration and fixed pressure conditions spanning 2m each.

To study the efficiency and accuracy of the M³ method for this infiltration problem, we generate a reference solution using the standard IMPES method on a 128×128 mesh. The saturation at $T=6$ days is plotted in Fig. 3, where lighter colors represent higher water saturation. Here the rapid flow along both highly anisotropic inclusions is apparent. Also evident is the influence of gravity, which has quickly drawn the fluid down once it passed through the first inclusion. In fact, this *arm* is now reconnecting with the main flow.

Fig. 3. Reference solution: water saturation profile at $T = 6$ days computed on mesh 128×128 with the fine-scale IMPES method

Since the fine-mesh is a logically structured quadrilateral mesh, the simple aggregation strategy shown in Fig. 1 is readily applied. Thus, we coarsen by a factor of two in each direction, recursively, until the desired total coarsening factor has been reached. We set the mobility threshold, $\epsilon_\lambda = 0.1$, which controls adaptive local updates of the hierarchy. Global updates of the flux coarsening factors (i.e., the α 's) are made uniformly in time. The tolerance of the PCG(AMG) iteration for these updates is $\epsilon_r = 10^{-3}$. The time step is adapted according to the stability analysis developed by Coats [16].

We conduct two series of tests with this configuration of the M^3 method. First we consider a fixed total coarsening factor of 32 in each coordinate direction, which gives 4×4 coarse-grid for the pressure solve. We integrate to a time of $T=6$ days, and examine the affect of increasing the number of updates to the α 's, from 12, to 60, and finally 120. The saturation at $T=6$ for these three scenarios are shown in Fig4(a)-(c). Comparing the result with only 12 updates in Fig4(a), to the reference solution in Fig.3, we see that a number of features have evolved either too slowly (e.g., the flow along the upper inclusion), or too quickly (e.g., the closure of the unsaturated space under the lower inclusion). Increasing to 60 updates, Fig.4(b) begins to correct these problems, but there are still significant differences in the flow along the upper inclusion. Finally, Fig.4(c) shows that with 120 updates we recover accuracy comparable to the fine-scale solution, accurately capturing the highly anisotropic flow through both the upper and lower inclusions. To understand the cost of these multiscale simulations relative to the fine-scale IMPES simulation, it is useful to note that these update scenarios correspond to an average of 2972.7, 613.6 and 320.7 time-steps per update, respectively. Moreover, these updates are based on approximate solutions computed using only 5-10 V-cycles each. The large total coarsening factor leads to an overall speedup of more than 5 times, for all update scenarios considered here. Overall, the computational cost of the pressure solver is now negligible, compared to the cost of the transport.

Fig. 4. Multiscale solutions for different numbers of updates: (a) coarsest mesh 4×4 , 2972.7 time-steps per update, (b) coarsest mesh 4×4 , 613.6 time-steps per update, (c) coarsest mesh 4×4 , 320.7 time-steps per update

Fig. 5. Multiscale solutions for different coarsening factors: (a) coarsest mesh 16×16 , 275.5 time-steps per update, (b) coarsest mesh 8×8 , 270.7 time-steps per update, (c) coarsest mesh 4×4 , 265.8 time-steps per update

In the second set of tests we integrate to $T=6$ days with the number of updates of the α 's fixed at 150, and consider different total coarsening factors of 8, 16, and 32. The results are shown in Fig.5(a)-(c) and confirm that accuracy comparable to the fine-scale solution has been achieved in all cases. This demonstrates that with an appropriate number of updates the accuracy of multiscale solution deteriorates very slowly as the total coarsening factor increases. The M^3 method is very flexible and robust with respect to the total coarsening factor, and hence, it may be applied to very large-scale simulations where other two-level upscaling methods are insufficient.

5 Conclusion

In this research we extended the M^3 method to include gravity, and studied its effectiveness on a challenging anisotropic infiltration problem. We created a porous medium with sloping non-uniform layers and two strongly anisotropic inclusions, and we used a logically structured mapped grid to capture these features. The M^3 method performed very well, achieving accuracy comparable to the fine-scale solution, at a fraction of the computational cost. As in the original study [1], updating the flux coarsening parameters enabled the use of large coarsening factors, a factor of 32 here, while maintaining both accuracy and overall efficiency. This further highlights the importance of the global information that is provided by the updates of the flux coarsening parameters (the α 's). In the future we plan to develop an error indicator that will guide a time-adaptive update strategy for these parameters. We anticipate that this advance will further improve our ability to balance accuracy and efficiency. In addition we are interested in extending this hierarchical methodology to upscale the transport equation.

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