Title: A MULTILEVEL MULTISCALE MIMETIC METHOD FOR AN ANISOTROPIC INFILTRATION PROBLEM

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Intended for: PROCEEDINGS:
SIMULATION OF MULTIPHYSICS MULTISCALE SYSTEMS
Introduction

Simulation of multiphysics and multiscale systems poses a grand challenge to computational science, with vast applications in chemical engineering, plasma physics, material science, biophysics, aerospace and automotive sectors. Most of the real-life systems involve interactions amongst a wide range of physical phenomena. In addition to that, the time and length scales of the individual processes involved often differ by orders of magnitude. Numerical simulation of these multiphysics and multiscale problems requires development of sophisticated models and methods for their integration, as well as efficient numerical algorithms and advanced computational techniques.

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Short abstract (1 page): December 6, 2008
Full paper submission: January 9, 2009
Notification of acceptance: February 2, 2009
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Early registration: March 15, 2009
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Other information
For information on conference venue, accommodation, registration, etc. please refer to the conference site or directly ask ICCS organizers.

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A Multilevel Multiscale Mimetic (M³) Method for an Anisotropic Infiltration Problem

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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 (M³) method, was developed to simulate two-phase flows in porous media. The M³ method is locally mass conserving at all levels in its hierarchy, it supports unstructured polyhedral 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 M³ method. Even for large coarsening factors, with which we achieve a speedup of xx times.

Key words: multiscale, multigrid, multilevel, hierarchical, finite volume, finite element, finite difference, two-phase flow, heterogeneous porous media

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 (M³) method [1].

The M³ 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 method [2] and the Multiscale Finite Volume (MSFV) method [3], the multilevel hierarchy facilitates large total coarsening factors, of 100 or more in each coordinate direction. Maintenance of the hierarchy
of models incurs only a moderate computational overhead due to the efficiency of recursively applying small coarsening steps, and the opportunity for spatial and temporal adaptivity. The $M^3$ method supports unstructured polyhedral meshes and accommodate general coarsening strategies to capture accurately the geometric 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 a coarse-grid cell [4]. The second 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 multilevel 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, and can handle full permeability tensors and general polygonal meshes.

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 two strongly anisotropic inclusions. The logically-structured mesh is aligned with the layers, which are not aligned with the horizontal coordinate. We note that anisotropic media are problematic for two-level MSFV style methods, because of the difficulty in finding appropriate localization conditions [5]. Yet, no special treatment is required in the $M^3$ method, which maintains an accurate hierarchy of models through the efficient temporal updates of the flux coarsening parameters. In fact, the 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, air (a) and water (w), in a two-dimensional domain subject to gravity (see, e.g., [6, 7]). The effects of compressibility and capillary pressure are neglected. Conservation of each phase implies,

\[ \phi \frac{\partial S_j}{\partial t} + \nabla \cdot u_j = -q_j, \quad j = a, w, \quad (1) \]

where $S_j$ and $u_j$ are the saturation and the velocity of phase $j$, respectively, and the porosity, $\phi$, is assumed constant. The Darcy velocity of phase $j$ is given by,

\[ u_j = -\mathbb{K} \cdot \lambda_j (\nabla p_j - \rho_j g), \quad (2) \]

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 $\mu_j$ the viscosity; $\rho_j$ is the density and $g$ 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 Eq.(1) to yield the bulk fluid conservation law,

\[ \nabla \cdot \mathbf{u} = q_a + q_w. \]

Here the total or bulk fluid velocity, \( \mathbf{u} = u_a + u_w \), may be written in the form,

\[ \mathbf{u} = -\kappa(\lambda \nabla p - (\lambda_a p_a + \lambda_w p_w) \mathbf{g}) \]

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 Eq.(4) into Eq.(3), and a hyperbolic equation for the water saturation, \( S = S_w \), given by Eq.(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 [8].

To discretize the pressure we consider a polygonal partition of the domain \( \Omega \), denoted \( \Omega_h \), that is the union of of the polygonal cells \( e_i \), \( i = 1, \ldots, N \). We apply the Mimetic Finite Difference (MFD) method [9] to the first-order form of the pressure equation, given by Eq.(4) and Eq.(3). For each cell \( e_i \), we define one pressure unknown, \( p_i \), which represents the integral average of \( p \). Similarly, for each edge \( \ell_j \) of cell \( e_i \), we define one unknown, \( u_{i,\ell_j} \), which represents the average normal flux \( \mathbf{u} \cdot \mathbf{n} \) (a scalar) through this edge. Introducing Lagrange multipliers to weakly enforce continuity of the normal flux across cell faces, we can write the MFD discretization of the pressure equation in the form,

\[
\begin{bmatrix}
M(S^n) & B^T & C^T \\
B & 0 & 0 \\
C & 0 & 0
\end{bmatrix}
\begin{bmatrix}
\mathbf{u}^n \\
p^n \\
\lambda^n
\end{bmatrix} =
\begin{bmatrix}
\mathbf{q}^n_a \\
\mathbf{q}^n_w \\
\mathbf{0}
\end{bmatrix}.
\]

Here \( n \) denotes the time step, \( M(S^n) \) is the mass matrix computed using the current saturation, \( B \) is the discrete divergence operator, \( C \) describes continuity of the normal flux across cell edges, and \( \lambda^n \) is the vector of Lagrange multipliers. The source \( \mathbf{q}^n_a \) captures nonhomogeneous Dirichlet data and the gravitational term in Eq.(4), and \( \mathbf{q}^n_w \) captures nonhomogeneous Neumann data and the source/sink term in Eq.(3).

This hybridized or local form of the discretization is desirable because the mass matrix is block-diagonal, with as many blocks as there are cells in \( \Omega_h \). Therefore, velocity and pressure unknowns can be eliminated locally, resulting in a sparse symmetric positive definite problem for the Lagrange multipliers.
Fig. 1. Schematic of the two steps of the two-level upscaling method for a $2 \times 2$ 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 is approximate.

### 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 $N_0 = N$, $cN_1 \leq N_0$, with $0 < c < 1$, and

$$
\Omega_H = \bigcup_{i=1}^{N_1} E_i, \quad E_i = \bigcup_{k \in \mathcal{F}(E_i)} e_k,
$$

where $\mathcal{F}(E_i)$ is a set of indices of fine-grid cells and $E_i$ is a macro-cell (a polygon). We assume that the coarse-grid partition $\Omega_H$ 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 $p$. By construction this single pressure on each macro-cell is the volume-weighted average of the corresponding fine-grid pressures:

$$
p_{E_i} = \frac{\sum_{k \in \mathcal{F}(E_i)} p_k |e_k|}{\sum_{k \in \mathcal{F}(E_i)} |e_k|}.
$$

Note, this first step in the elimination process is performed by equivalent modifications 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 defines one flux unknown per macro-edge. This coarsening makes the final structure of the reduced system, shown in Fig. 1(right), identical to the original system. Mass conservation dictates that the coarse flux on a macro-edge must be a weighted sum of the corresponding fine-grid fluxes. But in addition, we
need to interpolate from the coarse-grid flux, to the fine-grid fluxes. To this end we introduce the flux coarsening parameter $\alpha$. For the simple $2 \times 2$ aggregation shown in Fig. 1, an $\alpha$ for each macro-edge may be written as,

$$
\alpha = \begin{cases} 
\frac{u_1}{u_2} & u_2 \neq 0, \\
1 & \text{otherwise.}
\end{cases}
$$

(6)

where $u_1$ and $u_2$ are the corresponding fine-grid fluxes. More general flux coarsening scenarios are discussed in [1]. This parameter characterizes the first moment of the flux, and plays an important role in the M$^3$ algorithm. Specifically, it is used to define the interpolation of the flux, and it influences the coarse-scale pressure model. Indeed, there exist values of $\alpha$ that make the upscaling of pressure equation exact. However, these parameters are functions of time, and accurately recomputing them at each time step would be comparable in cost to the standard IMPES formulation. Thus, in the M$^3$ method 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 algebraic 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 M$^3$ method is focused on the total mobility. The total mobility changes significantly in the vicinity of a sharp water front. The M$^3$ method updates local matrices (in the whole hierarchy) that are affected by these changes. More precisely, we use the criterion proposed in [10],

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

where $\varepsilon_\lambda$ is the user defined threshold, usually 0.1. If this condition is not satisfied, the local 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, which includes the influence of boundary conditions, is critical. 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 \( \alpha \)'s is needed. In [1] we proposed to leverage the strength of a robust variational multigrid method for this purpose. Forming the Schur complement of Eq.(5) for the Lagrange multipliers we define the \( \alpha \)'s based on an approximate solve with a weak convergence tolerance, \( \epsilon_r \). This approximate solve is achieved efficiently with a small number of preconditioned conjugate gradient (PCG) iterations that use Ruge-Stüben algebraic multigrid (AMG) as a preconditioner [11]. Using this approach to update the \( \alpha \)'s captures critical global information about the pressure-field and flow, without introducing spurious artifacts from localizing assumptions. In our original study [1] we demonstrated the effectiveness of this approach 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. 4(a). Initially the pore space is filled with air and a small residual water saturation. The medium is composed of four layers and two elongated inclusions, and 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. 4(b), while in our numerical experiments we consider the fine mesh to be 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.

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.

<table>
<thead>
<tr>
<th>Zone</th>
<th>(K_x (m^2))</th>
<th>(K_z (m^2))</th>
<th>(K_x/K_z)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>(4 \times 10^{-12})</td>
<td>(4 \times 10^{-12})</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>(5 \times 10^{-12})</td>
<td>(1 \times 10^{-13})</td>
<td>50</td>
</tr>
<tr>
<td>3</td>
<td>(5 \times 10^{-12})</td>
<td>(5 \times 10^{-12})</td>
<td>1</td>
</tr>
<tr>
<td>4</td>
<td>(9 \times 10^{-12})</td>
<td>(9 \times 10^{-12})</td>
<td>1</td>
</tr>
<tr>
<td>5</td>
<td>(5 \times 10^{-11})</td>
<td>(5 \times 10^{-13})</td>
<td>100</td>
</tr>
<tr>
<td>6</td>
<td>(5 \times 10^{-11})</td>
<td>(5 \times 10^{-13})</td>
<td>100</td>
</tr>
</tbody>
</table>

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

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

(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 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 \(kg \cdot (m \cdot s)^{-1}\). Boundary conditions are shown schematically in Fig. 4(a) with no-flow everywhere except for the water source in the upper left and the fixed pressure in the bottom right. Fig. 4(b) shows the dimensions of the domain (10m\(\times\)10m), with the infiltration and fixed pressure conditions spanning 2m each.

To study the efficiency and accuracy of the M\(^3\) method described in Section 3.2 for this infiltration problem, we first generated a reference solution using the standard IMPES method on a 128 \(\times\) 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 \(\text{arm}\) is now reconnecting with the main flow.

To implement the M\(^3\) method, we first note that since the fine-mesh is a logically structured quadrilateral mesh, the simple aggregation strategy shown in Fig. 1 is readily applied. Thus, in this study we coarsen by a factor of two in
each direction, recursively, until the desired coarsening factor has been reached. We set the mobility threshold, \( \epsilon_A = 0.1 \), which controls adaptive local updates of the hierarchy. Global updates of the flux coarsening factors (i.e., the \( \alpha \)'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 [12].

We conduct two series of tests with this configuration of the M3 method. First we consider a fixed total coarsening factor of 32 in each coordinate direction, which gives 4 \times 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 \( \alpha \)'s, from 40, to 200, and finally 500. The saturation at \( T=6 \) for these three scenarios are shown in Fig4(a)-(c). Comparing the result with only 40 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 200 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(b) shows that with 500 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 solves, using only 2-3 V-cycles each. Thus, the M3 method is able to efficiently recover fine-scale accuracy of the solution, even with a large coarsening factor.

In the second set of tests we integrate to \( T=6 \) days with the number of updates to the \( \alpha \)'s fixed at 500, 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 the M3 method is very flexible and robust with respect to the total

![Fig. 3. Snapshots of water saturation profiles at \( T = 6 \) days. Fine-scale solution computed on mesh 128x128.](image-url)
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Fig. 4. Multiscale solutions for different numbers of updates: (a) coarsest mesh 4x4, 2972.7 time-steps per update, (b) coarsest mesh 4x4, 613.6 time-steps per update, (c) coarsest mesh 4x4, 320.7 time-steps per update.

Fig. 5. Multiscale solutions for different coarsening factors: (a) coarsest mesh 16x16, 275.5 time-steps per update, (b) coarsest mesh 8x8, 270.7 time-steps per update, (c) coarsest mesh 4x4, 265.8 time-steps per update.

cooarsening 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 \( M^3 \) 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 $\alpha$'s). Thus, 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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