Direct fluid flow simulation at pore scale with regularized hydrodynamic equations

Balashov Vladislav, Savenkov Evgeny
Keldysh Institute of Applied Mathematics of RAS, Miuskaya sq., 4 Moscow, 125047, Russia
E-mail: vladislav.balashov@gmail.com, e.savenkov@gmail.com

Abstract.
Laboratory analysis of rock samples (core material) is one of the main tools used in an analysis of oil and gas field development and methods to enhance oil recovery. A number of drawbacks are intrinsic to the laboratory techniques, among which we note the practical impossibility of carrying out parametric studies on one sample, the impossibility (and / or high cost) of taking into account reservoir conditions, and the impossibility of analyzing non-cemented rocks (sludge). With the development of computational capabilities and computed tomography methods, the “digital rock physics” technology, which consists in direct simulation of physical processes in a rock sample with resolved pore space geometry, is gaining popularity today. This technology complements the traditional laboratory studies and compensates for a number of their shortcomings. The presented work is devoted to the direct simulation of fluid flow within the scope of the digital rock physics. For simulation regularized (according to quasi-hydrodynamic technique) hydrodynamic equations are used. Both single-phase single-component flows and two-phase two-component flows, taking into account interfacial tension, are discussed. The results of simulations of fluid flows both in model domains and in domains corresponding to the pore space of real rocks are presented.

1. Introduction
Mathematical modeling is one of the main tools used in the analysis of the development and exploitation of oil and gas fields. A reservoir is a very complex physical system, which cannot be described by a single mathematical model that could be successfully applied on practice. One of the main complicating factors is the wide range of scales on which physical processes take place: from micrometers (the scale of individual pores) to kilometers (the characteristic distance between wells, the scale corresponds to the entire field). Therefore, in practice, each scale uses its own mathematical model.

In this paper we consider a model which is used at the pore scale. This scale determines the dynamics of fluid displacement at the macro level. In particular action of physical and chemical methods of enhanced oil recovery techniques (surfactants, polymers, foams, etc.) stems from this scale. Thus, detailed knowledge of dynamics at the pore scale level is an important and urgent problem, the solution of which significantly affects the method of exploiting the entire field.

Until recently, the only way to assess displacement properties at the pore scale was a laboratory experiment. At the same time, laboratory techniques are characterized by a number of drawbacks, among which we note the practical impossibility of conducting parametric studies...
on a sample, impossibility (and / or high cost) simulation of some reservoir conditions, the impossibility of analysis unconsolidated rocks (sludge). With the development of computational power and microtomography techniques “digital rock physics” technology is gaining popularity. The technology consists in direct simulation of physical processes within rock sample with direct resolution of the pore space [1, 2, 3]. This technology complements traditional full-scale experiments and compensates for a number of their shortcomings. Presented paper is devoted to direct simulation of fluid flow in relation to “digital rock physics” technology. For description of fluid flow we use quasi-hydrodynamically regularized equation of hydrodynamics. Both single-phase one-component flows and two-phase two-component flows, taking into account the interfacial tension are discussed. In latter case, to describe two-phase flows, a regularized version of the Navier–Stokes–Cahn–Hillard equations is used. Simulation results of fluid flows both in model areas and in areas corresponding to the pore space of real rocks samples are presented.

2. Geometry model

In the “digital rock physics” technology one of the most common ways for description of the geometry of pore space is its voxel model. To construct the model computer microtomography is used. Its results, which are a set of images in grayscale, are processed using segmentation algorithms: the entire area occupied by the sample is covered with a three-dimensional uniform Cartesian grid and each cell is referred to either the rock or the pore space. The result is a three-dimensional binary image of the pore space of the test sample. The cell of the introduced grid is also called a voxel (by analogy with pixel in the 2D case). In the figures 1 and 2 examples of voxel geometry of a part of solid and pore space of a sandstone sample are presented.

3. Mathematical model

This section describes the mathematical models used to modeling of both single-phase and two-phase flows. As noted in the introduction a characteristic feature of these models is their preliminary regularization according to quasi-hydrodynamic technique: it is assumed that the mass flux $j_m$ may differ from the momentum of the unit volume $\rho u$, which leads to $j_m = \rho u - \rho w$. The vector $w$ is the regularizing velocity and it is proportional to small regularizing parameter $\tau$. This leads to the appearance of additional dissipative terms in equations of the considered
model. These terms play a regularizing role when spatial approximations with central differences are used and make it possible to use a larger time step when using explicit conditionally stable methods. Used regularization is applied for different models of continuum mechanics and is actively developing at present time [4, 5, 6, 7].

3.1. Single-phase flow

To describe single phase isothermal flow of viscous compressible fluid we use following equations [8, 9]:

\[ \begin{align*}
\partial_t \rho + \text{div} \ j_m &= 0, \\
\partial_t (\rho u) + \text{div} (j_m \otimes u) + \nabla p &= \nabla \cdot \Pi,
\end{align*} \]

where \( \rho \) is the fluid density, \( u \) is the velocity, \( j_m = \rho(u - \bar{w}) \) is the mass flux, \( p = c_s^2 \rho \) is the pressure, \( c_s \) is the sound speed, \( \Pi = \Pi^{\text{NS}} + \Pi^r \) is the stress tensor, \( \Pi^{\text{NS}} = \eta \left[ (\nabla u + \nabla u^T) - (2/3)I \right] \) \( \text{div} u \) is the Navier–Stokes stress tensor, \( I \) is the identity tensor, \( \eta \) is the dynamic viscosity coefficient, \( \Pi^r = \rho u \otimes \bar{w} \) is the regularizing stress tensor, \( \bar{w} = (\tau/\rho) (\rho u \cdot \nabla u + \nabla p) \), \( \tau \) is the small parameter, which is calculated as \( \tau = 0.5h/c_s \).

3.2. Two phase flows

To describe two-phase two-component flows the regularized Navier–Stokes–Cahn–Hilliard model is used. It is a phase field model. It is which are based on the use of an order parameter \( C \). The parameter distinguishes one phase from another. Another important feature of the phase field model is a special form of free energy: it depends both on \( C \) and \( |\nabla C|^2 \). Importantly, the dependence on \( C \) is nonconvex. Free energy of such construction allows one to describe boundary between two separate phases as thin layers with finite thickness, within which the parameters of the fluid change rapidly but continuously [10, 11].

In [7] QHD-regularization technique was applied to (Navier–Stokes–Cahn–Hilliard equations). For isothermal two-component mixture the system is as follows:

\[ \begin{align*}
\partial_t \rho + \text{div} \ j_m &= 0, \\
\partial_t (\rho u) + \text{div}(j_m \otimes u) + \nabla p &= \text{div} \Pi, \\
\partial_t (\rho C) + \text{div}(j_m C) &= \text{div} (M \nabla \mu),
\end{align*} \]  

(1)

Here \( C \) is the mass concentration of mixture components: \( C = C_1, C_2 = 1 - C_1, C_i = \rho_i/\rho \), where \( \rho_i \) is a mass density of \( i \)-th component, \( i = 1, 2 \).

We set the Helmholtz free energy of the mixture as follows

\[ \Psi(\rho, C, \nabla C) = \Psi_0(\rho, C) + \frac{1}{2} \lambda_1 |\nabla C|^2, \]

\[ \Psi_0(\rho, C) = C c_{s1}^2 \ln \frac{\rho}{\bar{\rho}_1} + (1 - C) c_{s2}^2 \ln \frac{\rho}{\bar{\rho}_2} + \Psi_{\text{sep}}(C), \]

where the constant \( \lambda_1 > 0 \) is a model parameter, \( c_{s1} \) and \( \bar{\rho}_i > 0 \) are the sound speed and reference density of \( i \)-th component. There exist various ways to set the function \( \Psi_{\text{sep}}(C) \). According to [10, 11], we apply the following polynomial form

\[ \Psi_{\text{sep}}(C) = A_\psi C^2(1 - C)^2, \quad A_\psi > 0. \]  

(2)

The presence of two local minima at \( C = 0, 1 \) corresponding to “pure” components is peculiar to \( \Psi_{\text{sep}}(C) \) that is of great concern in simulation of interphase (surface) effects.
The functions $p$ and $\mu$ are introduced due to $\Psi_0(\rho, C)$:
\[
p(\rho, C) = \rho^2 \Psi'_0(\rho, C) = c_{s1}^2 \rho C + c_{s2}^2 \rho (1 - C),
\]
\[
\mu(\rho, C, \nabla C) = \Psi'_0(\rho, C) C - \frac{\lambda_1}{\rho} \text{div}(\rho \nabla C).
\]

Hereafter $(\cdot)'_\rho = \partial/\partial \rho$ and $(\cdot)'_C = \partial/\partial C$. It should be noted that the nonlinear terms with $\nabla C$ appearing in $Q$ in combination with the non-convexity in $C$ of $\Psi_0$ are responsible for the surface effects.

On the foundation of used Helmholtz free energy form using the Colleman–Noll procedure constitutive relations for stress tensor and QHD-terms can be derived \[7\]:
\[
\Pi = \Pi^{NS} - Q + \Pi^\tau, \quad Q = \lambda_1 \rho \nabla C \otimes \nabla C, \quad \mathbf{w} = (\tau/\rho) \left[ \rho (\mathbf{u} \cdot \nabla) \mathbf{u} + \nabla p + \text{div} \mathbf{Q} \right].
\]
In (1) $M = M(C) > 0$ and $\mu$ are mobility coefficient and generalized chemical potential:
\[
\mu(\rho, C) = \Psi'_0(\rho, C) C - \frac{\lambda_1}{\rho} \text{div}(\rho \nabla C).
\]

To set specific value of equilibrium contact angle $\theta$ we use following boundary condition \[12\]:
\[
\partial_n C = \frac{6 \sigma \cos \theta}{\rho \lambda_1} C (1 - C).
\]

Other boundary conditions reads
\[
\partial_n \mu = 0, \quad \mathbf{u} = \mathbf{0}.
\]

In the following simulations mixture of two liquids with same equations of state was considered. In this case $p = c_{s}^2 \rho$.

4. Numerical results

In this section some numerical results of flow simulation in pore space of core samples are presented. Voxel images are freely available and are taken from Imperial College website [13].

4.1. Single phase flows

To simulate one phase flow in pore space we set on two opposite faces of numerical domain boundary conditions corresponding to pressure drop $\Delta p = 1$ Pa. On other domain boundaries and boundary of pore space we set no-slip conditions.

Absolute permeability coefficient $k$ is obtained from Darcy law
\[
\frac{Q}{A} = -\frac{k \Delta p}{\eta L},
\]
where $Q$ stands for the volume flow rate, $L$ is the length between inlet and outlet boundaries, $A$ is the cross-section area. Values of $k$ for some core samples obtained with QHD-regularized equations, with open source software package Palabos [14] and from [15] are presented in table 1.

On the figures 3 and 4 streamlines obtained for sandstone $S_5$ and $S_8$ samples [13] are presented. Grey color indicates solid.

4.2. Two phase flows

Numerical simulation of two-phase displacement in core sample $S_9$ [13] with neutral contact angle ($\theta = 90^\circ$) was performed. Phase distributions for several intermediate time moments are presented in the figures 5(a)–5(d). Red color indicates phase with $C > 0.5$, and blue color —
Table 1. Coefficients $k$ (mDarcy) for core samples from collection [13].

| Sample | $k^{QHD}$ | $k^{Palabos}$ | $k^{[15]}$ |
|--------|-----------|---------------|------------|
| $S_1$  | 2.168     | 2.613         | 1.729      |
| $S_2$  | 4.293     | 4.928         | 3.931      |
| $S_3$  | 0.9205    | 1.264         | 0.415      |
| $S_4$  | 0.455     | 0.652         | 0.285      |
| $S_5$  | 5.915     | 6.516         | 4.810      |
| $S_6$  | 13.215    | 14.588        | 10.543     |
| $S_7$  | 9.410     | 10.387        | 7.495      |
| $S_8$  | 14.930    | 16.564        | 13.330     |
| $S_9$  | 2.539     | 2.747         | 2.066      |
| $S_{b}$| 1.542     | 1.856         | 1.287      |

Figure 3. Streamlines in $S_5$ core sample. Solid is colored with semitransparent grey.

Figure 4. Streamlines in $S_8$ core sample. Grey color indicates solid.

phase with $C \leq 0.5$. For illustration purposes only red fluid is presented. Red fluid saturation is denoted by $S$.

Also two phase displacement was performed in system of two parallel connected pore throats (so called pore doublet model). Different wettability of solid boundary was considered: (i) $\theta = 150^\circ$: wetting of the solid wall by displacing fluid is very favorable; (ii) $\theta = 30^\circ$: wetting of the solid wall by displacing fluid is unfavorable. Domain sizes are $L_x = 0.02$ m, $L_y = L_x/2$. On the figures 6 and 7 distribution of phases are presented for several consecutive time moments, where $\Delta t = 8 \cdot 10^{-8}$ s is the time step. Space step is $h = L_x/200$. Qualitative difference between two cases is obvious: if wetting of the solid wall by displacing fluid (the red one) is unfavorable then considerable part of pore space is occupied by displaced phase (the blue one); in other case the whole pore space is occupied by displacing fluid.
Figure 5. Distribution of displacing phase during displacement process for different time moments (a) $t = 10^{-6}$ s, $S = 4.3\%$; (b) $t = 50 \cdot 10^{-6}$ s, $S = 42.4\%$; (c) $t = 100 \cdot 10^{-6}$ s, $S = 73.7\%$; (d) $t = 200 \cdot 10^{-6}$ s, $S = 82\%$.

5. Conclusion

The present work is devoted to the application of regularized equations describing single-phase (Navier–Stokes equations) and two-phase flows taking into account interphase effects (Navier–Stokes–Cahn–Hillard equations) within the framework of the “digital rock physics” technology. Regularization was carried out according to the quasi-hydrodynamic technique. The simulation results are given for various flows both in artificial domains and in domains corresponding to real rock samples (sandstones).

Acknowledgments

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Figure 6. Phase distribution for several consecutive time moments for $\theta = 150^\circ$.

Figure 7. Phase distribution for several consecutive time moments for $\theta = 30^\circ$.

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