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Local modeling of instability onset for global finger evolution

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ABSTRACT

Simulation of density-driven instabilities requires flexible methods to deal with the different spatial and temporal scales involved. Downscaling approaches based on standard adaptive grid refinement aim at resolving the fine-scale details only in the region of interest, but they may become computationally expensive in presence of very corrugated unstable fronts because the problem to be solved approaches the size of the fully refined system. The Downscaling Multiscale Finite-Volume (DMsFV) method overcomes this issue by splitting the problems into a set of localized subproblems that interact only through a global problem. However, in presence of convective instabilities (e.g. density-driven fingers) the diffusion scale has to be resolved only at early times to capture the evolution of infinitesimal random perturbations, whereas at later times fingers have developed and merged, allowing the use of a coarser numerical description. Based on this observation, we present an adaptive algorithm which splits the simulation into three stages: an onset stage in which a set of localized problems is solved independently to capture the initial growth of the instabilities; a transition stage in which the DMsFV method is used to couple local and global scales; and a global stage in which only a fully coarsened description of the problem is employed. The dissolution–diffusion–convection problem (which is typically studied in the context of CO_2 sequestration) is chosen as an example to evaluate the accuracy of the adaptive algorithm. For this problem, the use of a coarse grid that does not resolve the fine-scale details at earlier times leads to a dramatic underestimation of mass influx and penetration depth. On the contrary, the solutions obtained with the adaptive algorithm are in good agreement with the reference solution (obtained with a fully refined discretization) and are able to capture total mass influx and penetration depth with excellent accuracy. This demonstrates the need and the effectiveness of modeling local details during the instability onset to capture large-scale features of the concentration patterns at later times.

1. Introduction

Density-driven instabilities can occur in a variety of subsurface-flow processes, e.g. sea-water intrusion in coastal aquifers [15], geological storage of CO_2 [12,13,18], or in the presence of geothermal gradients [4,5]. As a consequence of the convective instability, rapidly moving fingers form, which can drastically reduce the travel time. Although, they have been extensively studied in the last decades, e.g. [3,6,7,31,32,37], accurate simulations in field-scale aquifer or reservoir modeling remain a challenge due to the disparity of scales involved.

To correctly capture the onset of instability and the finger-growth rate, it is important to resolve the fastest growing wavelength, which is the smallest mode that is not damped by diffusion and emerges from any initial infinitesimal random perturbation. This requires a very fine numerical discretization (with grid size below a centimeter, e.g. [30]) at least at early simulation times. In contrast, field-scale models consider subsurface flow processes that take place over several kilometers and normally employ cell-sizes in the order of several meters, which is dictated by geological heterogeneities and by the constraints set by the computational costs.

This discrepancy between a computationally realistic and a physically sound discretization has fostered the development of several adaptive grid-refinement algorithms (e.g. [30]) that refine the computational grid around the unstable front to capture the small scale behavior. In these methods, however, the size of the larger problem that has to be solved, may approach the size of the fully refined problem if the instability front is large and complex. To avoid this issue, we have proposed a downscaling algorithm [21] that is based on the Multiscale Finite-Volume (MsFV) method [10,16,17,25,26,28,29]. The problem is downscaled by solving local problems, that are coupled through a global problem defined on the original grid; therefore, the largest problem to be solved is

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independent of the fraction of the domain that has to be refined. This framework, which employs clearly separated local and global problems, is particularly well suited to model instabilities.

In case of density instability, after an initial period dominated by diffusion, a critical time is reached at which convection starts to dominate. At early time, convection patterns are small compared to the size of the original discretization: their evolution is local and does not require global information. At later time, the convective patterns have grown such that they can be described by the original discretization and local details can be neglected. These observations naturally lead to define three stages that characterize finger evolution with respect to the original discretization: an onset or local stage; a transition stage; and a global stage.

In this paper, we propose to solve only local decoupled problems during the onset stage, whereas the Downscaling MsFV (DMsFV) algorithm [21] is used for the transition stage, and the problem is solved on the original grid in the global stage. In this approach global and local problems can be solved adaptively.

The paper is organized as follows. The equations governing density-driven flow and transport are given in Section 2. In Section 3 we discuss the different scales involved, whereas Section 4 describes the three numerical schemes employed in the three different time stages. In Section 5 the performance of the adaptive algorithm is investigated with the help of the dissolution-diffusion-convection problem [8,30,31] for different durations of the onset stage and the results for an ensemble of realizations are analyzed. Finally, conclusions are drawn in Section 6.

2. Governing equations

We consider the flow of a single phase which consists of a solvent fluid and a solute. If we assume that the fluid is incompressible and employ the Boussinesq approximation (e.g. [15]), the fluid conservation equation takes the form

$$\nabla \cdot \boldsymbol{v} = 0, \tag{1}$$

where

$$\boldsymbol{v} = -\frac{k}{\mu}[\nabla p - \rho(c)\boldsymbol{g}] \tag{2}$$

is the Darcy velocity.

In Eq. (2), k (m^2) is the absolute permeability (which is assumed isotropic); p (Pa) the pressure; $\boldsymbol{g}$ (m/s^2) the gravity acceleration; ρ (kg/m^3) the density of the fluid, which depends on the normalized concentration $0 \leqslant c \leqslant 1$ (–); and μ (kg/m/s) the viscosity (concentration effects on viscosity are neglected for simplicity). The conservation equation for the solute mass can then be written as

$$\frac{\partial}{\partial t}(\phi c) + \nabla \cdot [c\boldsymbol{v} - \phi D_m \nabla c] = 0, \tag{3}$$

where ϕ (–) is the porosity; and D_m (m^2/s) the molecular diffusion in the bulk solvent (we neglect mechanical dispersion). The equations above form a system of non-linear differential equations that are coupled by the density dependence on the solute concentration and by the velocity. To be solved, the equations need to be complemented with a constitutive relationship for $\rho(c)$ [15,19]. As we are mainly concerned with moderate density contrasts, we assume a simple linear relationship of the form

$$\rho(c) = (1-c)\rho_{\min} + c\rho_{\max}, \tag{4}$$

where $\rho_{\min}$ and $\rho_{\max}$ are the density at $c = 0$ and $c = 1$, respectively (see, e.g. [1,14]).

By defining the dimensionless quantities

$$\boldsymbol{v}^* = \frac{\boldsymbol{v}}{k\Delta\rho g/\mu}, \quad t^* = \frac{t}{L^2/\phi D_m}, \quad x^* = \frac{x}{L}, \tag{5}$$

where L is the characteristic length and $\Delta\rho = \rho_{\max} - \rho_{\min}$, we can write the system of non-dimensional equations as

$$\nabla \cdot \boldsymbol{v}^* = 0, \tag{6}$$

$$\frac{\partial c}{\partial t^*} + \mathrm{Ra}\,\boldsymbol{v}^* \cdot \nabla c - \nabla^2 c = 0, \tag{7}$$

where

$$\mathrm{Ra} = \frac{k\Delta\rho g L}{\phi\mu D_m} \tag{8}$$

is the dimensionless Rayleigh number, which describes the relative importance of convective to diffusive processes.

3. Characteristic length scales and adaptive algorithm

In the following, we will consider the dissolution-diffusion–convection (DDC) problem which has been extensively investigated in the past decade in the context of long-term geological storage of carbon dioxide in deep saline aquifer when instability arises due to the presence of a layer of supercritical CO_2 located above a brine layer: the CO_2 dissolves into the brine increasing its density and creating a denser layer of CO_2-saturated brine [8,30,31]. This problem, which is a variant of classical density instability problems related to Rayleigh–Bérnard convection [15], such as the Elder problem [3,9,36], is chosen as an example, but the method proposed is general. For instance, a similar process can take place in presence of mineral dissolution that can sensibly increase the density of the solution. Also, similar instabilities are triggered in presence of temperature gradients as in the case of a porous medium cooled from above (or heated from below); in this case the role played by diffusion is replaced by conduction and the density is modified by the thermal expansion of the fluid.

3.1. Physical length scales

The DDC problem is illustrated in Fig. 1. We consider a porous medium of height H and width W, which is initially saturated by a solvent. At time $t = 0$, a solute starts to dissolve at the top boundary and diffuses into the solution, forming a diffusive boundary layer, Fig. 1(a). Since the solution has higher density than the solvent, the system is gravitationally unstable and small perturbations grow by affecting the velocity field, Fig. 2. Linear stability analysis applies at early times because concentration fluctuations are small; it can be shown that the fastest growing perturbation is characterized by the critical wavelength

$$\lambda_c = 96.23\frac{\mu\phi D_m}{\Delta\rho g k}, \tag{9}$$

which is solely a function of the fluid and aquifer properties, e.g. [37]. This is the smallest perturbation that is not damped by diffusion and emerges from any infinitesimal random perturbation.

At early times, linear instability generates small, local convective cells that are characterized by a width λ_c. When perturbations become larger, the nonlinear regimes starts and fingers grow and merge into larger convective cells, Fig. 1(b). At later times, a fully developed nonlinear fingering regime leads to the formation of complex concentration patterns, Fig. 1(c). From this brief description it is clear that the size of the fingers (or of the convective cells, which are intimately related) is a function of time, $\ell_F(t)$, and is equal to the critical wavelength, λ_c, only in the initially linear regime.