Simulating Density-Dependent Flows Using the Lattice Boltzmann Method

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ABSTRACT
Seawater intrusion is a continuing concern in south Florida and in many other coastal areas. Although there is extensive research on this topic, more tools are required to fully understand and predict the location and behavior of the freshwater/seawater boundary. The lattice Boltzmann method is a radically different numerical tool because it is not based on discretization of a series of differential equations. It has been used to simulate fluid flow in various disciplines. Recent advances in lattice Boltzmann modeling permit simulation of large-scale density-dependent ground water flow and heat/solute transport. These simulations can be accomplished while retaining the advantages of 'regular' lattice Boltzmann methods, such as solute/heat transport at high Reynolds numbers (characteristic of flow inside a conduit). We show how this method can be applied to density-dependent flows, including a Henry-like problem.

INTRODUCTION
Seawater intrusion is a classic density-dependent problem in hydrogeology. It must be fully understood in order to be able to predict and prevent groundwater deterioration in coastal areas. Various software programs have been developed and are being used to model coupled fluid flow and solute transport for density-dependent applications: SUTRA, SEAWAT, and HST3D are popular examples. All of the current programs are either finite difference or finite element methods. Density-dependent flow problems are exceptionally challenging for conventional numerical methods due to inherent non-linearity; definitive solutions are often elusive and a completely different modeling approach may be advantageous. The lattice Boltzmann method (LBM) represents such a numerical tool because it is not based on discretization of a series of differential equations. Instead, its foundation lies in the kinetic theory of gasses as proposed by Boltzmann. A key advantage of lattice Boltzmann method is that it has the ability to solve the Navier-Stokes equations in larger conduits and pores. Hence it allows for eddy diffusion brought on by inertial components of flow at higher Reynolds numbers, which may occur in some coastal aquifers. Simulation of these phenomena is not possible with traditional Darcy's law-based groundwater models. Some geologists and engineers have been able to successfully apply LBM to fluid flow and contaminant transport problems (Ginzburg and d'Humieres, 2003; Anwar et al., 2008). There are only a handful of scientists attempting to apply LBM to density-dependent flows in general (e.g., Shan, 1997; Dixit and Babu, 2006); even fewer have considered seawater intrusion (Servan Camas, 2007).

LATTICE BOLTZMANN METHOD BASICS
Most numerical modeling tools are based on discretization of differential equations. LBMs are based on discretization of the movement and interaction of hypothetical particles using a particle distribution function, f (Sukop and Thorne, 2006). The moments of the particle distribution function provide the macroscopic fluid properties, e.g., density and velocity. In LBMs, time, space, and velocity directions are all discretized. On each point in space, called a lattice node, a discrete set of f_a corresponding to a choice of velocity directions $\mathbf{e}_a$ are stored. Directions in two dimensions are (0,0), (±1,0), (0, ±1), (±1, ±1), and the lattice based on these nine directions is referred to as the D2Q9 grid (Figure 1).

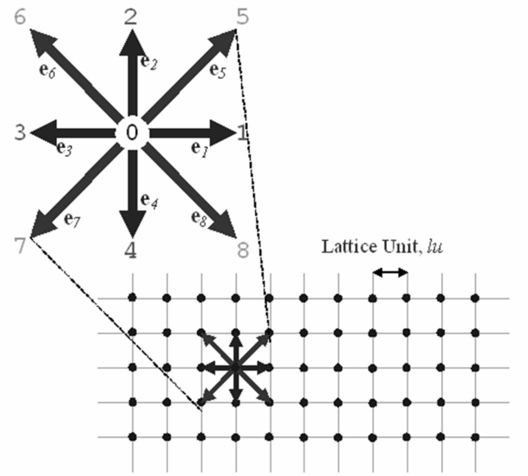

Figure 1. D2Q9 grid (Sukop and Thorne, 2006), $\mathbf{e}_{1\text{-}8}$ are unit velocity vectors

At each time step, the f_a are updated according to a *collision* step $f_a^*(\mathbf{x},t) = f_a(\mathbf{x},t) - \frac{1}{\tau}\left(f_a^{eq}(\mathbf{x},t) - f_a(\mathbf{x},t)\right)$ and a *streaming* step $f_a(\mathbf{x}+\mathbf{e}_a, t+1) = f_a^*(\mathbf{x},t)$ (Sukop and Thorne, 2006). The assumptions of unit time step $\Delta t = 1$ time step (*ts*) and unit node spacing $\Delta x = \Delta y = 1$ lattice unit (*lu*) have been incorporated. The key to the collision step is the equilibrium distribution function f^{eq}, which is defined per direction as $f_a^{eq} = w_a \rho\left(1 + 3\mathbf{e}_a \cdot \mathbf{u}^{eq} + \frac{9}{2}\left(\mathbf{e}_a \cdot \mathbf{u}^{eq}\right)^2 + \frac{3}{2}\mathbf{u}^{eq} \cdot \mathbf{u}^{eq}\right)$ where $w_0 = \frac{4}{9}$, $w_1 = w_2 = w_3 = w_4 = \frac{1}{9}$, $w_5 = w_6 = w_7 = w_8 = \frac{1}{36}$, $\rho = \sum_a f_a$ and $\mathbf{u}^{eq} = \frac{1}{\rho}\sum_a f_a \mathbf{e}_a$.

The superscript on $\mathbf{u}^{eq}$ is to distinguish it from the actual macroscopic velocity that is computed after the collision step. Additional details of LBMs including incorporation of buoyant forces can be found in Sukop and Thorne (2006).

BUOYANCY

We present two density-dependent flow problem examples here. The first example is an initial value problem with half of the domain filled with saltwater.

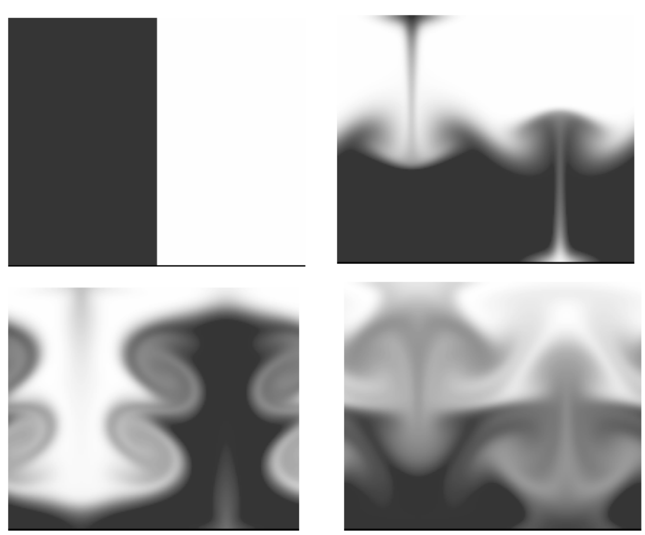

Figure 2. Initial time at upper left to approaching equilibrium at bottom right.

The second example involves fluid flow through a narrow opening between two plates at different temperatures. We have compared our results with the analytic equation:

$$v = \frac{\Delta T g \beta \rho B^2}{12\mu}\left[\left(\frac{y}{B}\right)^3 - \left(\frac{y}{B}\right)\right]$$

where: v = velocity, ΔT = temperature difference between plates, g = gravity, β = coefficient of volume expansion, ρ = fluid density, B = half width of opening, y = position in opening. Figure 3 is the result of the comparison.

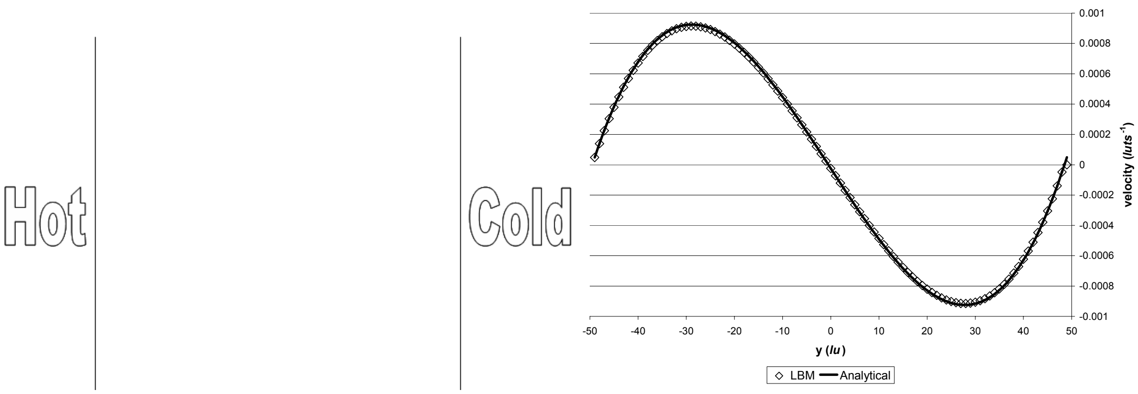

Figure 3. Left: Simulation domain, Right: Solid line analytical, dashed line LBM solution. This grid resolution results in two percent error.

HENRY-LIKE PROBLEM

The next step is to model the classic Henry problem. The Henry problem consists of a rectangular domain representing a confined aquifer with a freshwater inflow boundary condition on the right and a saltwater inflow boundary along the left. The top and bottom boundaries are closed (Henry, 1964). We were able to simulate a problem similar to the Henry problem. However we have yet to simulate the classic Henry problem with LBM using the physical parameters.

CONCLUSION

We used LBM to simulate three density-dependent flow problems. One available analytical solution was closely matched by LBM. Further work is needed to translate the physical Henry problem parameters into LBM inputs.

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