Dynamically adaptive upwind finite volume methods for contaminant transport

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Abstract

In order to accurately model chemically reactive transport, one needs to incorporate some type of grid adaptivity into the numerical simulator. In this paper we give an example of a two-component contaminant transport model, which exhibits some interesting physical phenomena and motivates our desire for grid adaptivity. A dynamically adaptive method is then developed in the context of a Godunov-mixed method for a scalar equation. Theoretical and numerical results for this approach are presented.

1 Introduction

The accurate modeling of chemically reactive transport in a porous medium is crucial to monitoring and remediating contaminant sites. Over the past several years, mathematical and numerical models which describe transport, geochemical and biogeochemical reactions between chemical species in the subsurface have been developed, see, for example, Yeh and Salvage [1] and Wheeler *et al* [2].

These problems are difficult to model computationally for several reasons. First, the combination of highly advective flow and chemical reactions can give rise to very sharp concentration fronts, which must be modeled with minimal numerical diffusion and oscillation. Second, the chemical reactions themselves can be in equilibrium or non-equilibrium, which gives rise to non-linear couplings and problems with highly varying time-scales. Finally,

these contaminant species are flowing through highly heterogeneous porous media, and the flow field must accurately account for these heterogeneities.

At the Center for Subsurface Modeling, we have developed a parallel contaminant transport simulator, PARSSIM, which models single phase flow and transport of multiple contaminant species. In this simulator, advection and diffusion are modeled using either a characteristic-mixed method, described in Arbogast and Wheeler [3], or a Godunov-mixed method, described in Dawson [4]. In the latter approach, a higher-order Godunov method is used to simulate advection, and diffusion is incorporated using a mixed finite element method. Chemical reactions are handled through a split step, and solved as a system of nonlinear algebraic and/or ordinary differential equations. Here, an interior point method is used to handle inequality contraints which can arise in geochemical modeling. For a complete description of the methodology, see Wheeler *et al* [2].

PARSSIM does not, at the present time, have any adaptive capability. Not surprisingly, we have found in some of our recent simulations that such a capability is not only desirable but necessary. Therefore, we are presently in the process of studying adaptive methods in more detail and incorporating them into our simulators.

The outline of this paper is as follows. In the next section, we describe a simple two-component contaminant transport problem and give numerical results which motivate our need for dynamic adaptivity. In Section 3, we will describe our dynamically adaptive method in some detail, and state a theoretical result on the overall accuracy of this method.

2 An example of two-component transport

In this section, we consider a simple case of two-component sorptive transport. The model concerns the flow of a metal cation and a pH front through one-dimensional porous medium. Competition for adsorption sites between the two species occurs, giving rise to some potentially interesting physical behavior.

Consider the one-dimensional flow of fluid containing a sorbing species such as a metal cation (e.g. Sr^{++}, Ca^{++}, Na^{+}, etc.) through a porous medium containing a sorbent onto which proton and metal cation adsorption occurs. The adsorption reactions may be written as

$$M^{+n} + S \Leftrightarrow SM^{+n}$$
$$H^{+} + S \Leftrightarrow SH^{+}$$

where M^{+n} represents a cation of charge +n, S represents an adsorption site, and H^+ represents the proton. The equilibrium expressions for these reactions are written

$$K_M = \frac{Z_M}{C_M Z_S}, \tag{1}$$

$$K_H = \frac{Z_H}{C_H Z_S}, \tag{2}$$

where Z_S is the concentration of unoccupied sites on the substrate, C_i is the fluid phase concentraton of species i, Z_i is its sorbed concentration, and K_i is the corresponding equilibrium constant. Because the total number of sites on the substrate, Z_O is constant, we have the following conservation equation:

$$Z_M + Z_H + Z_S = Z_O. \tag{3}$$

Substitution of the equilibrium expressions (1)-(2) into this equation allows elimination of the concentration of unoccupied sites:

$$Z_S = \frac{Z_O}{1 + K_M C_M + K_H C_H}$$

and substitution for Z_S in (1) and (2) leads to the familiar Langmuir adsorption isotherms:

$$Z_M = \frac{K_M C_M Z_O}{1 + K_M C_M + K_H C_H}, \tag{4}$$

$$Z_H = \frac{K_H C_H Z_O}{1 + K_M C_M + K_H C_H}. \tag{5}$$

Assuming chemical equilibrium between the flowing phase and the sorbent at every point within a one-dimensional porous medium, the mass balance for the metal cation may be written:

$$(C_M + Z_M)_t + (C_M)_x - \frac{1}{N_{Pe}}(C_M)_{xx} = 0, \tag{6}$$

where t is dimensionless time, x is dimensionless distance and N_{Pe} is the Peclet number. The concentration units are in moles per unit pore volume.

For an aqueous phase the dissociation of water always occurs and can be written

$$H_2O - H^+ \Leftrightarrow OH^-.$$

At chemical equilibrium this reaction imposes a relationship between the proton and hydroxyl concentrations:

$$C_{OH^-} = \frac{K_W}{C_H}.$$

Considering the simplest possible aqueous system, where there are no other species involving protons or hydroxyls, we have that the total proton concentration, or "acidity" satisfies

$$C_A = C_H - C_{OH^-} = C_H - \frac{K_W}{C_H}. \tag{7}$$

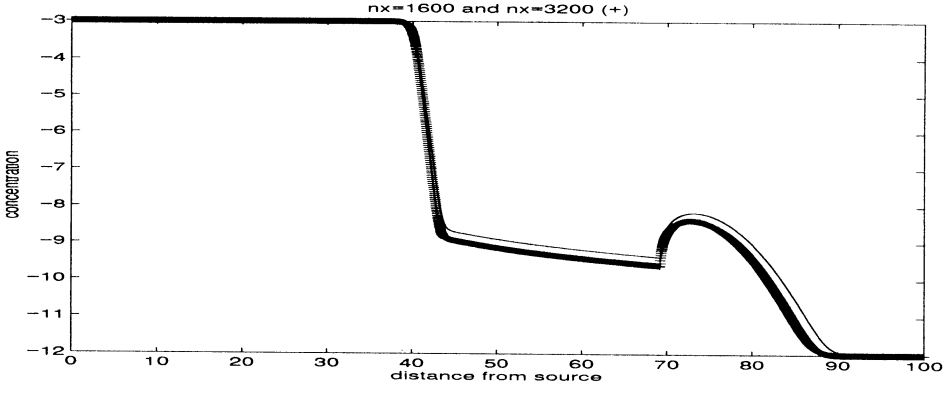
The mass balance for transport of protons becomes

$$(C_A + Z_H)_t + (C_A)_x - \frac{1}{N_{Pe}}(C_A)_{xx} = 0. \tag{8}$$

Combining (6)-(8) with appropriate boundary and initial conditions give our two-component model.

As an application of the above model, we consider the following parameters: $K_H = 10^4$, $K_M = 10^3$, $K_W = 10^{-14}$ and $Z_O = 2 * 10^{-3}$. We solve the problem over a domain $0 < x < 100$, with initial conditions $C_H = 10^-$ and $C_M = 10^{-12}$, and boundary conditions at $x = 0$, $C_H = 10^{-12}$ an $C_M = 10^{-3}$. We also choose $N_{Pe} = 10$. The model is discretized using a extension of the numerical approach described in the next section, with r adaptivity. In Figure 1 below, the numerical approximations to the con centration C_M for two different grid spacings ($\Delta x = 1/16$ and $\Delta x = 1/3$ are given at time $t = 80$. As the figure indicates, a "bump" or "fast wave forms ahead of the main front, carrying a small but significant concentr tion. Understanding the nature of this fast wave phenomena, in particula whether it is a physical occurrence or merely a numerical artifact, is th subject of ongoing research. The origin of the bump occurs at the preci location of the C_H front, suggesting that it is caused by the phenomen of competitive adsorption. We have observed that the resolution of the fa wave requires extremely fine grid in the region of the C_H front. As th Peclet number increases, even finer grid is required, to the point where t number of grid points needed to observe numerical convergence, even in one-dimensional setting, becomes prohibitive. Attempting these simulatio in multi-dimensions would be nearly impossible without some sort of gr adaptivity.

Figure 1: Concentration of cation at $t = 80$ for two different grid spacings



3 An adaptive Godunov-mixed method

n this section, we describe an adaptive upwind mixed finite element method. Ve consider the transport equation for a single component:

$$(c + z(c))_t + uc_x - Dc_{xx} = 0, \quad 0 < x < L. \tag{9}$$

Ve assume $u > 0$ and combine (9) with initial condition $c(x, 0) = c^0(x)$ and oundary conditions:

$$(uc - Dc_x)(0, t) = ug(t), \tag{10}$$

$$Dc_x(L, t) = 0, \tag{11}$$

here $g(t)$ is specified. The adsorption isotherm z is assumed to be mono- one increasing in c. Let $T(c) = c + z(c)$, and assume $\eta(T) = c$ is the inverse ap of T, which exists since z is monotone. Then (9) can be written as ollows:

$$T_t + u\eta(T)_x + q_x = 0, \tag{12}$$

$$q = -Dc_x. \tag{13}$$

Discretize the interval $[0, L]$ into grid blocks $B_j = [x_{j-1/2}, x_{j+1/2}]$, $j = , \ldots, J$, with midpoints x_j, and choose a sequence of time steps $\Delta t^n > 0$. et Δx_j denote the length of B_j. Denote by $f_j^n = f(x_j, t^n)$, where $t^n = \sum_{j=1}^{n} \Delta t^j$.

We approximate T and q using the lowest order Raviart-Thomas space, hich in one dimension consists of the set $W_h = \{w : w \text{ is a constant on } B_j\}$

and $V_h = \{v : v$ is continuous and piecewise linear$\}$. Define $V_{h,0} = V_h \cap \{v : v(L) = 0\}$. Thus, if $w \in W_h$, $w = \sum_{j=1}^{J} w_j \chi_j(x)$, where $\chi_j = 1$ on B_j and zero elsewhere. Moreover, if $v \in V_h$, $v = \sum_{j=0}^{J} v_{j+1/2} \xi_{j+1/2}(x)$ where $\xi_{j+1/2}$ is a continuous, piecewise linear with $\xi_{j+1/2}(x_{k+1/2}) = 1$ if $k = j$ and zero otherwise.

When dynamically adapting the mesh, we choose a discretization into grid blocks $\{B_j^n\}$, where the superscript n indicates that the discretization may vary with time step. Associated with this discretization, we have finite element spaces W_h^n and V_h^n. Our method can be described as follows. Find $T_h^n \in W_h^n$, $F_h^n \in V_h^n$, $Q_h^n \in V_{h,0}^n$ and $C_h^n \in W_h^n$ satisfying

$$\left(\frac{T_h^n - \bar{T}_h^{n-1}}{\Delta t^n}, w^n \right) + ((F_h^n + Q_h^n)_x, w^n) = 0, \quad w^n \in W_h^n,$$

$$(D^{-1} Q_h^n, v^n) = (C^n, v_x^n) + \lambda^n v^n(0), \quad v^n \in V_{h,0}^n.$$

Here $(\cdot, \cdot)$ is the L^2 inner product on $[0, L]$. Note that $T_h^n \approx T^n$, $F_h^n \approx u\eta(T^n)$ $Q_h^n \approx q^n$, and $C_h^n \approx c^n$ with $C_h^n = \eta(T_h^n)$. The term λ^n approximates c^n at $x = 0$. From (10),

$$\lambda^n = g^n - \frac{Q_h^n(0)}{u}. \tag{14}$$

The term $\bar{T}_h^{n-1}$ is computed as follows. On the grid $\{B_j^{n-1}\}$, we compute a discontinuous, piecewise linear function $\bar{T}_h^{n-1}$ satisfying

$$\bar{T}_h^{n-1}(x) = (T_h)_j^{n-1} + \delta_x (T_h)_j^{n-1}, \quad x \in B_j^{n-1}, \tag{15}$$

where the slope $\delta_x (T_h)_j^{n-1}$ is computed using a "slope-limiting" procedure see Dawson [4]. Note that once T_h^{n-1} is known, (14) is a simple, cheap post processing step. The reason this step is needed is to maintain the accuracy of the method, as noted below.

In order to compute F_h^n, we use a higher-order upwind approximation First, let $\tilde{T}_h^n$ denote the L^2 projection of $\bar{T}_h^{n-1}$ into W_h^n, that is

$$(\tilde{T}_h^n, w^n) = (\bar{T}_h^{n-1}, w^n), \quad w^n \in W_h^n.$$

We note that by Taylor's series,

$$T(x_{j+1/2}^n, t^{n-1/2}) \approx T(x_j^n, t^{n-1}) + \frac{\Delta x_j^n}{2} T_x + \frac{\Delta t^n}{2} T_t,$$

where the latter two terms are computed at (x_j^n, t^{n-1}). The superscript n on x_j is meant to indicate that this is the midpoint of block B_j^n. Using the the differential equation, we find

$$\begin{aligned} T(x_{j+1/2}^n, t^{n-1/2}) &\approx T(x_j^n, t^{n-1}) + \frac{\Delta x_j^n}{2} T_x - \frac{\Delta t}{2}(u\eta_x + q_x) \\ &= T(x_j^n, t^{n-1}) + \frac{\Delta x_j^n}{2} T_x - \frac{\Delta t}{2}(u\eta'(T(x_j^n, t^{n-1})T_x + q_x). \end{aligned}$$

Using the slope-limiting procedure to approximate T_x and dropping the q_x term we find

$$\begin{aligned} T(x_{j+1/2}^n, t^{n-1/2}) &\approx (\tilde{T}_h)_j^n + (\frac{\Delta x_j^n}{2} - \frac{\Delta t}{2} u\eta'((\tilde{T}_h)_j^n))\delta_x(\tilde{T}_h)_j^n \\ &\equiv \tilde{T}_{j+1/2}^n. \end{aligned}$$

Thus

$$(F_h^n)(x_{j+1/2}^n) = u\eta(\tilde{T}_{j+1/2}^n).$$

The boundary conditions at $x = 0$ and $x = L$ are enforced by setting

$$F_h^n(0) = u\lambda^n, \quad Q_h^n(L) = 0.$$

Note that by (14), $F_h^n(0) + Q_h^n(0) = ug^n$.

In the simple case where $z = 0$ and $u = 0$, we have the following method. Find $C_h^n \in W_h^n$ and $Q_h^n \in V_{h,0}^n$ satisfying

$$\left(\frac{C_h^n - \bar{C}_h^{n-1}}{\Delta t^n}, w^n\right) + ((Q_h^n)_x, w^n) = 0, \quad w^n \in W_h^n, \tag{16}$$

$$(D^{-1}Q_h^n, v^n) = (C^n, v_x^n), \quad v^n \in V_{h,0}^n. \tag{17}$$

In this case we have the following error estimate:

Theorem 1 *Assume c is a smooth function. Let $\Delta x = \max_{j,n} \Delta x_j^n$ and assume $\Delta x/\Delta t^n \leq K_1$ for each n, where K_1 is a constant independent of Δx and Δt^n. Then the method (16)-(17) satisfies*

$$\max_n ||C^n - c^n|| \leq K\Delta x,$$

where K is a constant independent of Δx.

Table 1: Convergence study for dynamic mesh

Maximum Δx	L^2 error at t=1.0
.018228	9.218508e-04
.009228	4.2799185e-04
.004628	2.421769e-04

Thus, the method (16)-(17) has the same global accuracy as the static method where W_h and V_h do not vary with time. The additional linear term in $\bar{C}$ makes this result possible. We expect that this estimate carries through when $u \neq 0$ and for smooth $z(c)$. This research is ongoing.

In order to verify the accuracy of the method, we considered a test problem

$$c_t + c_x - c_{xx} = f,$$

where f and the initial and boundary data were chosen so that $c(x,t) = xe^{xt}$. For each run, an initial uniform mesh was chosen. Then at each time step, the nodes in the mesh were perturbed randomly with a maximum change in location of 10% per time step. A comparison of L^2 errors at $t = 1.0$ for decreasing maximum mesh spacing is given in Table 1. These errors indicate a convergence rate of close to one, as expected from the theorem above.

References

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