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FINITE ELEMENT METHODS FOR NONLINEAR FLOWS IN POROUS MEDIA

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A model problem is presented for fluid flow in porous media which has numerical difficulties common with many other areas of nonlinear mechanics. Special finite element techniques are described which have proved useful in alleviating many of these difficulties. A modified method of characteristics, mixed finite element methods for fluid velocities, singularity removal, and self-adaptive local grid refinement techniques are presented. Both theoretical and computational results are described, together with an indication of the present and future uses of finite element methods in large-scale reservoir simulation.

1. Introduction

Important applications of fluid flow in porous media arise in the areas of hydrology, contaminant transport, and the production of hydrocarbons. In order to understand the complex chemical, physical, and fluid flow processes occurring in these applications well enough to predict the results of various flow or production regimes, simulators are constructed involving the numerical solution of large coupled systems of nonlinear partial differential equations. Many of the computational problems involved in solving these systems of differential equations are similar to those arising in other areas of nonlinear mechanics and flow processes. This paper discusses several of the complications arising in a simple model problem describing the miscible displacement of one incompressible fluid by another in a porous medium and presents certain finite element techniques for alleviating these difficulties.

Many problems in numerical reservoir simulation involve considerably more physics and are exceedingly more difficult than the model problem considered here. The author has given an introduction to the variety of physical problems requiring simulation in [27]. We note, however, that although these more complex models involve larger coupled systems of nonlinear partial differential equations, most of these equations have forms and properties very similar to the equations described in our model problem. Except for sheer size and resulting computational complexity, the major mathematical difficulties that must be addressed are the same: (a) the resolution of sharp moving fronts in convection-dominated convection-diffusion problems, (b) the stability and accuracy of discretization of highly non-self-adjoint

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differential operators, (c) the need to have very accurate fluid velocities which dominate the flow, (d) the need to model dynamic local phenomena which govern the physics, and (e) the emphasis on development of efficient numerical procedures for the enormous problems encountered.

In general, finite difference techniques have been used in the petroleum industry for reservoir simulation applications. Several authors, beginning with work by Jim Douglas and Todd Dupont [19, 55], have considered finite element techniques for these problems. An excellent survey of finite element procedures, both theoretical and computational, developed by work of Douglas Arnold, David Brown, Bruce Darlow, Jim Douglas, Jr., Todd Dupont, Richard Kendall, Thomas Potempa, Jean Roberts, Thomas Russell, Peter Sammon, Mary Wheeler, and the author is presented in [54]. Early finite element work by Young [61] also has appeared in the petroleum engineering literature. Recent volumes [25, 26], edited by the author, were designed to give an indication of the wide variety of numerical techniques which are being applied to reservoir simulation problems in the petroleum industry.

In this paper we shall emphasize the power of finite element methods in treating many aspects of large-scale reservoir simulation problems. A model problem which illustrates many major numerical difficulties arising in reservoir simulation is presented in Section 2. The numerical stability problems associated with this transport-dominated system and the corresponding pure transport problem are discussed. A modified method of characteristics based on combining the transport and accumulation terms in the equation into a directional derivative along characteristic-like curves is then described. The modified method of characteristics is heavily dependent upon having very accurate fluid velocities. Section 3 is then devoted to the description of a mixed finite element procedure which is designed to give approximations of the fluid velocities which are just as accurate as the pressure approximations, even in the context of rapidly changing reservoir properties. Theoretical results which guided our choice of methods and corroborating computational results are discussed. Using the mixed finite element formulation a fully discrete sequential time-stepping method for the miscible displacement model problem is presented. Optimal order a priori asymptotic error estimates for this combined process are discussed together with computational results on a problem requiring the resolution and tracking of very sharp concentration fronts.

The need for adaptive local grid refinement methods to resolve certain dynamic, highly localized physical phenomena is described in Section 4. Important considerations such as a choice of versatile and efficient data structures and adaptivity techniques are discussed and a code developed by the author and coworkers at Mobil Research and Development is described. Finally, the major points of the paper are summarized in Section 5.

2. Description of model problem and modified method of characteristics

A model system of equations describing the miscible displacement of one incompressible fluid by another in a thin horizontal porous medium is given by [16, 27, 38, 46, 47, 54]

$$\nabla \cdot \boldsymbol{u} = -\nabla \cdot \frac{k}{\mu(c)} \nabla p = q, \quad x \in \Omega, \ t \in J, \tag{2.1}$$

$$\phi \frac{\partial c}{\partial t} + \nabla \cdot [\boldsymbol{u}c - D(\boldsymbol{u})\nabla c] = \tilde{c}q, \quad \boldsymbol{x} \in \Omega, \ t \in J, \tag{2.2}$$

$$\boldsymbol{u} \cdot \boldsymbol{n} = [\boldsymbol{u}c - D(\boldsymbol{u})\nabla c] \cdot \boldsymbol{n} = 0, \quad \boldsymbol{x} \in \partial\Omega, \ t \in J, \tag{2.3}$$

$$c(\boldsymbol{x}, 0) = c_0(\boldsymbol{x}), \quad \boldsymbol{x} \in \Omega, \tag{2.4}$$

for $\Omega \subset \mathbb{R}^2$ with boundary $\partial\Omega$ and $J = [0, T]$, where p and $\boldsymbol{u}$ are the pressure and velocity of the single phase fluid mixture, c is the concentration of the injected fluid, and q is the total volumetric flow rate, modeled by Dirac delta point sources and sinks describing the injection and production wells, ϕ, k, μ and $D(\boldsymbol{u})$ are assumed to be known rock and fluid properties. D is a diffusion-dispersion tensor given by [47, 54]

$$(D_{ij}(\boldsymbol{x}, \boldsymbol{u})) = \phi d_m I + \frac{d_l}{|\boldsymbol{u}|}\begin{pmatrix} u_1^2 & u_1u_2 \\ u_1u_2 & u_2^2 \end{pmatrix} + \frac{d_t}{|\boldsymbol{u}|}\begin{pmatrix} u_2^2 & -u_1u_2 \\ -u_1u_2 & u_1^2 \end{pmatrix}, \tag{2.5}$$

where $\boldsymbol{u} = (u_1, u_2)$, $|\boldsymbol{u}|$ is the Euclidean norm of $\boldsymbol{u}$, d_m is the molecular diffusion coefficient, and d_l and d_t are the magnitudes of longitudinal and transverse dispersion. An excellent discussion of the importance of incorporating the effects of dispersion in our simulation work appeared in [54]. In general, d_m is assumed to be quite small with d_l and d_t somewhat larger. Often the assumption is made that $d_l \simeq 10d_t$. Since the magnitudes of the last two terms in (2.5) are approximately $d_l|\boldsymbol{u}|$ and $d_t|\boldsymbol{u}|$, we see more dispersive mixing where the velocities are higher, around the wells, and less out in the reservoir. Equation (2.2) is an example of a transport-dominated convection-diffusion equation. Since diffusion is small, the solution c exhibits very sharp fronts or concentration gradients which move in time across the reservoir and finger into production wells. The frontal width is very narrow in general, but must be resolved accurately via the numerical method since it describes the physics of the mixing zone and governs the speed of the frontal movement, and thus the production history of the hydrocarbons.

Most finite difference simulators ignore the dispersion tensor (2.5), partially because the mixed derivatives it causes in (2.2) would normally require a nine-point difference formulation for areal problems and twenty-seven point formulas in three space dimensions. Thus if (2.5) is incorporated, the bandwidth of the matrices obtained from finite differences would be the same as that required for finite element methods. This would greatly reduce the normal computational complexity advantage held by finite differences over finite elements. Due to grid-orientation problems, to be discussed later, many finite difference codes are already being shifted to the expanded finite difference stars for accuracy purposes.

Of course if the dispersion tensor in (2.2) is ignored as in most simulators in use today, (2.2) becomes a first-order hyperbolic problem instead of a transport-dominated convection-diffusion equation. Standard highly accurate finite difference schemes for hyperbolic partial differential equations are known to be unstable and various upstream weighting or 'artificial diffusion' techniques have been utilized to stabilize the variant of (2.2). The upstream weighting techniques (described in [27]) used in the petroleum industry introduce artificial diffusion in the direction of the grid axes and of a size proportional to the grid spacings. Thus, although this stabilizing effect would be small if very fine grid block spacings were used, the enormous size of petroleum simulation problems necessitates the use of large grid blocks and hence large, directionally-dependent artificially induced numerical diffusion which has nothing

to do with the physics of the flow. Two major problems in numerical reservoir simulation today are due essentially to the use of standard upstream weighting techniques. First, the upstream methods, by introducing a large artificial numerical diffusion or dispersion, smear sharp fluid interfaces producing erroneous predictions of the degree of mixing and incorrect frontal velocities. Second, the numerical diffusion is generated along grid lines and, coupled with the standard use of five-point difference formulas which have difficulty describing radial flow in areal problems, produce results which are radically different if the orientation of the grid is rotated forty-five degrees. This 'grid-orientation problem' and several attempts to alleviate it are described in more detail in [27].

If one ignores $D(\boldsymbol{u})$ in (2.2) and must stabilize the result, or if $D(\boldsymbol{u})$ is not sufficiently large to stabilize (2.2) as it is, one should add a stabilizing artificial diffusion in the form of a rotationally invariant tensor which will not cause grid-orientation effects. Since D, as given in (2.5), is already in the form of a rotationally invariant tensor, this would amount to increasing d_l and d_t until stabilization is achieved. Thus we see that rotationally invariant stabilization will require a tensor formulation in (2.2) which will require the use of finite difference stars and matrices of the same size as those used for finite element methods. Clearly, if more diffusion or dispersion is required to stabilize (2.2), sharp fluid interfaces will be diffused and smeared artificially, reducing accuracy and physical realism. Thus we have tried to develop techniques for stabilizing (2.2) without adding artificial diffusion or dispersion and which maintain rotational invariance of the operators in (2.2).

In [51, 52], Russell described a technique based on a method of characteristics approach for treating the first-order hyperbolic part of (2.2). This technique [17, 23, 51, 52], based on a form of (2.2) which is analogous to a convection-diffusion equation, was implemented by Russell [52] and now forms the basis for our time-stepping scheme.

In order to introduce a nondivergence form of (2.2) that is used in our numerical schemes, we first expand the convection $(\nabla \cdot \boldsymbol{u}c)$ term in (2.2) with the product rule and use (2.1) to obtain

$$\phi \frac{\partial c}{\partial t} + \boldsymbol{u} \cdot \nabla c - \nabla \cdot [D(\boldsymbol{u}) \nabla c] = (\bar{c} - c)\bar{q}, \quad \boldsymbol{x} \in \Omega, \ t \in J, \tag{2.6}$$

where $\bar{q} = \max\{q, 0\}$ is nonzero at injection wells only. To avoid technical boundary difficulties associated with our modified method of characteristics for (2.6), we assume that Ω is a rectangle and that the problem (2.1), (2.6), (2.3) and (2.4) is Ω-periodic. This is physically reasonable since the no-flow condition (2.3) can be treated as a reflection boundary condition and because boundary effects in reservoir simulation are of considerably less interest than interior flow patterns.

The modified method of characteristics is a time-stepping procedure that can be combined with any spatial discretization. First introduced into the present application areas in [51, 52], it has been used predominantly with finite element spatial discretizations.

The basic idea is to consider the hyperbolic part of (2.6), namely, $\phi \, \partial c/\partial t + \boldsymbol{u} \cdot \nabla c$, as a directional derivative. Accordingly, let $\boldsymbol{s}$ denote the unit vector in the direction of (u_1, u_2, ϕ) in $\Omega \times J$, and set

$$\psi(\boldsymbol{x}) = (u_1(\boldsymbol{x})^2 + u_2(\boldsymbol{x})^2 + \phi^2)^{1/2}. \tag{2.7}$$

Then (2.6) can be rewritten in the form

$$\psi \frac{\partial c}{\partial s} - \nabla \cdot (D \nabla c) + \bar{q} c = \bar{q} \bar{c} . \tag{2.8}$$

Note that the spatial operator in (2.8) is now self-adjoint, symmetric matrices will result from spatial discretization, and the associated numerical methods will be better behaved. Since iterative solution techniques are used to solve the nonlinear equations resulting from finite element discretization of (2.8), and since symmetry is very important in any of the useful conjugate-gradient iterative solvers, this change to symmetric matrices is very important.

We must next discretize the directional derivative $\partial c/\partial s$ in an accurate fashion. Partition J into $0 = t^0 < t^1 < t^2 < \cdots < t^N = T$ with $\Delta t_c^n = t^n - t^{n-1}$. For simplicity of exposition we will henceforth assume uniform time steps. For functions f on $\Omega \times J$, we denote $f(x, t^n)$ by $f^n(x)$. We shall assume that u^n is a known function. We shall then discuss the coupling of (2.1) and (2.6) in more detail. Approximate $\partial c/\partial s$ by a backward difference quotient in the s-direction [23, 34, 51, 52],

$$\frac{\partial c^n}{\partial s}(x) = \frac{c^n(x) - c^{n-1}\left(x - \dfrac{u(x)}{\phi(x)} \Delta t_c\right)}{\Delta t_c (1 + u_1^2(x) + u_2^2(x) + \phi^2(x))^{1/2}} . \tag{2.9}$$

If we let $\bar{x} = x - [u(x)/\phi(x)]\Delta t_c$ and $\bar{f}(x) = f(\bar{x})$, then, differencing back along the characteristic yields

$$\psi^n \frac{\partial c^n}{\partial s} \simeq \psi \frac{c^n(x) - c^{n-1}(\bar{x})}{\Delta t_c \left(1 + \dfrac{u^n}{\phi}\right)^{1/2}} = \phi \frac{c^n(x) - c^{n-1}(\bar{x})}{\Delta t_c} . \tag{2.10}$$

Extensions of some of these ideas to higher-order time-stepping procedures and nonlinear problems appear in [34, 53].

As discussed in [54], the critical aspect of the modified method of characteristics is the accurate approximation of the directional derivative $\partial c/\partial s$. Many methods based upon characteristics fix a grid at time t^{n-1} and try to determine where these points would move under the action of the characteristics. These 'moving point' or 'front tracking' methods must then discretize (2.6) and solve for the unknowns c^n on a mesh of irregular or unpredictable nature. If too large a time step in chosen, serious difficulties can arise from the spatial and temporal behavior of the characteristics. Front-tracking in two space dimensions is difficult while in three dimensions, it is considerably more difficult. Similar arguments can be made about some of the moving finite element methods [42, 43].

In this method, a fixed grid is considered at the advanced time level n, and information is sought back along the characteristic from which the grid point came. Therefore the solution mesh is controlled by the method and not by the flow. Although all numerical work on this method has previously used a fixed grid, making extensions to two and three space dimensions very straightforward, the grid could be adjusted to changing flow patterns in an uncomplicated way to take advantage of a priori estimates of the flow.

We note that in general $\bar{x}$, found by following the tangent to the characteristic from a grid point back to time level $n-1$, will not coincide with grid point at time level $n-1$. If finite difference spatial techniques are used, this will necessitate interpolation from grid points at time level $n-1$ to obtain $c^{n-1}(\bar{x})$. Using finite element techniques, a functional approximation of c^{n-1} is known and must simply be evaluated at $\bar{x}$, once $\bar{x}$ is found. At this point this interpolation or function evaluation can cause mass balance errors, especially if the characteristic reaches out of neighboring grid blocks during the time step. Some of the recovery techniques of Morton [44] may help to eliminate small mass balance errors and overshoot and undershoot associated with the basic finite element approximation of sharp fronts.

In the next section we will define our discrete approximations for both p and $\boldsymbol{u}$. We will then define a sequential time-stepping method which decouples the equations and makes the assumption of a known approximation for $\boldsymbol{u}^{n-1}$, which was made in this section, natural.

3. Mixed finite element methods for pressure and velocity

Since both the modified method of characteristics and the diffusion-dispersion term in (2.6) are governed by the fluid velocity, accurate simulation requires an accurate approximation of the velocity $\boldsymbol{u}$. Using the Dirac delta functions for well models, we see that $\boldsymbol{u}$ is not even square integrable at the wells and thus standard approximations for $\boldsymbol{u}$ do not converge at the wells. A technique for removing the leading singularity in $\boldsymbol{u}$ and accurately approximating the result is presented. Also, since the lithology in the reservoir can change abruptly, causing rapid changes in the flow capabilities of the rock, the coefficient k in (2.1) can be discontinuous. In this case, in order for the flow to remain relatively smooth, the pressure changes extremely rapidly. Thus standard procedures of solving (2.1) as an elliptic partial differential equation for pressure, differentiating or differencing the result to approximate the pressure gradient, and then multiplying by the discontinuous k/μ can produce very poor approximations to the velocity $\boldsymbol{u}$. In this section a mixed finite element method for approximating $\boldsymbol{u}$ and p simultaneously, via a coupled system of first-order partial differential equations, will be discussed. This formulation allows the removal of singular terms in the equations and accurately treats the problem of rapidly changing flow properties in the reservoir. We shall define a coupled weak form of (2.1) as well as special finite element spaces for the method.

The coupled system of first-order equations used to define our methods arise from Darcy's Law and conservation of mass,

$$\boldsymbol{u} = -\frac{k}{\mu}\nabla p, \quad \boldsymbol{x} \in \Omega, \tag{3.1}$$

$$\nabla \cdot \boldsymbol{u} = q, \qquad \boldsymbol{x} \in \Omega, \tag{3.2}$$

subject to the boundary condition

$$\boldsymbol{u} \cdot \boldsymbol{n} = 0, \quad \boldsymbol{x} \in \partial\Omega. \tag{3.3}$$

Clearly (3.1)–(3.3) will determine p only to within an additive constant. Thus a normalizing

constraint such as $\int_\Omega p(x)\,dx = 0$ or $p(x_s) = 0$ for some $x_s \in \Omega$ is required in the computation to prevent a singular system.

We next define certain function spaces and notation. Let $L^2(\Omega)$ be the set of all functions on Ω whose square is finite integrable. Let $H^1 = H^1(\Omega)$ consist of those functions in $L^2(\Omega)$ whose first-order partial derivatives are also in L^2. Let $H(\mathrm{div}; \Omega)$ be the set of vector functions $v \in [L^2(\Omega)]^2$ such that $\nabla \cdot v \in L^2(\Omega)$ and let

$$V = H(\mathrm{div}; \Omega) \cap \{v \cdot n = 0 \text{ on } \partial\Omega\}. \tag{3.4}$$

Let $W = L^2(\Omega)$. Since p is determined only up to an additive constant, where approximate, one should think of W as the quotient space $L^2(\Omega)/\{\text{constant functions}\}$.

Let $(v, w) = \int_\Omega vw\,dx$, $\langle v, w\rangle = \int_{\partial\Omega} wv\,ds$, and $\|v\|^2 = (v, v)$ be the standard L^2 inner-products and norm on Ω and $\partial\Omega$. We obtain the weak solution form of (3.1)–(3.3) by dividing each side of (3.1) by k/μ, multiplying by a test function $v \in V$, and integrating the result to obtain

$$\left(\frac{\mu}{k} u, v\right) = (p, \nabla v), \quad v \in V. \tag{3.5}$$

The right-hand side of (3.5) was obtained by further integration by parts and use of (3.4). Next, multiplying (3.2) by $w \in W$ and integrating the result, we complete our weak formulation, obtaining

$$(\nabla \cdot u, w) = (q, w), \quad w \in W. \tag{3.6}$$

For a sequence of mesh parameters $h > 0$, we choose finite-dimensional subspaces V_h and W_h with $V_h \subset V$ and $W_h \subset W$ and seek a solution pair $(U_h; P_h) \in V_h \times W_h$ satisfying

$$\left(\frac{\mu}{k} U_h, v_h\right) - (P_h, \mathrm{div}\, v_h) = 0, \quad v_h \in V_h, \tag{3.7}$$

$$(\mathrm{div}\, U_h, w_h) = (q, w_h), \qquad w_h \in W_h. \tag{3.8}$$

We can now complete the description of our mixed finite element methods with a discussion of particular choices of V_h and W_h.

For a region S, let $C^j(S)$ be the set of all functions which are j times continuously differentiable on S with $C^{-1}(S)$ being the set of discontinuous functions. Let $P_m(S)$ be the set of polynomials of degree not greater than m on S. For a partition δ of an interval S given by $\delta = \{x_0, x_1, \ldots, x_{N_x}\}$, $x_i > x_{i-1}$, we define

$$M_j^m(\delta) = \{\psi \in C^j(S): \psi|_{(x_{i-1}, x_i)} \in P_m,\ i = 1, 2, \ldots, N_x\}.$$

Assume that δ_x is a partition of (a, b) and δ_y is a partition of (c, d) and let

$$h = \max_{i=1,2,\ldots,N_x, j=1,2,\ldots,N_y} \{(x_i - x_{i-1}), (y_j - y_{j-1})\}.$$

We next define two different sets of Raviart–Thomas [48] subspaces on $(a, b)\times(c, d)$. The first-order or 'lowest-order' spaces are denoted by

$$\begin{aligned} W_h &= M^0_{-1}(\delta_x)\otimes M^0_{-1}(\delta_y), \\ \hat{V}_h &= M^1_0(\delta_x)\otimes M^0_{-1}(\delta_y)\times M^0_{-1}(\delta_x)\otimes M^1_0(\delta_y), \\ V_h &= \{v\in \hat{V}_h : v\cdot n = 0 \text{ on } \partial\Omega\}. \end{aligned} \tag{I}$$

Thus the first-order space for pressures is composed of discontinuous constant functions on each grid block. The associated space for the x-component of the velocity is C^0-linears in x tensored with discontinuous constants in y. The space for the y-component of the velocity is similar, with the roles of x and y interchanged. Since cell-centered finite difference methods can be considered as utilizing piecewise constant pressures and velocity approximation at cell boundaries, there is a close relationship between the first-order mixed method and cell-centered finite difference methods as noted in [54].

The second-order Raviart–Thomas spaces in this paper can be described on $(a, b)\times(c, d)$ by

$$\begin{aligned} W_h &= M^1_{-1}(\delta_x)\otimes M^1_{-1}(\delta_y), \\ \hat{V}_h &= M^2_0(\delta_x)\otimes M^1_{-1}(\delta_y)\times M^1_{-1}(\delta_x)\otimes M^2_0(\delta_y), \\ V_h &= \{v\in \hat{V}_h : v\cdot n = 0 \text{ on } \partial\Omega\}. \end{aligned} \tag{II}$$

Thus the second-order space for pressures is composed of discontinuous linears in x tensored with discontinuous linears in y, while the x-component of V_h is composed of C^0-quadratics in x tensored with discontinuous linears in y. Again the space for the y-component of velocities is obtained by interchanging x and y in the above description. We recall again that $W_h \subset W$, $\hat{V}_h \subset V$ and $V_h \subset V$ for each of the two sets of Raviart–Thomas subspaces.

In order to treat the point sources and sinks which model wells in our codes, we remove the singularities at the wells for the velocities and then solve for the remaining portions via the mixed finite element techniques described above. As suggested by Douglas Arnold and presented in [12, 20, 21, 32, 33, 36, 40], we decompose u into its regular and singular parts (u_r and u_s, respectively):

$$u = u_r + u_s, \tag{3.9}$$

$$u_s = \sum_{j=1}^{N_w} Q_j(t)\nabla N_j, \tag{3.10}$$

$$N_j = \frac{1}{2\pi}\log|x - x_j|, \quad j = 1, 2, \ldots, N_w, \tag{3.11}$$

where N_w is the number of wells, $Q_j(t)$ are the flow rates at the wells located at x_j, and u_r, the regular part of u, satisfies the relations

$$\nabla\cdot u_r = 0, \qquad x\in\Omega, \tag{3.12}$$

$$u_r\cdot n = -u_s\cdot n, \quad x\in\partial\Omega. \tag{3.13}$$

Let $\boldsymbol{U}_r$ be the finite element approximation to $\boldsymbol{u}_r$ from V_h; let

$$\boldsymbol{U} = \boldsymbol{U}_r + \boldsymbol{u}_s \tag{3.14}$$

be our numerical approximation of $\boldsymbol{u}$, and let $P_h \in W_h$ be our approximation to p. We then see that $\boldsymbol{U}_r \in V_h$ satisfies

$$\left(\frac{\mu}{k}\boldsymbol{U}_r, \boldsymbol{v}_h\right) - (P_h, \operatorname{div} \boldsymbol{v}_h) = -\left(\frac{\mu}{k}\boldsymbol{u}_s, \boldsymbol{u}_h\right), \qquad \boldsymbol{v}_h \in V_h, \tag{3.15}$$

$$(\operatorname{div} \boldsymbol{U}_r, w_h) = 0, \qquad w_h \in W_h, \tag{3.16}$$

$$\langle (\boldsymbol{U}_r + \boldsymbol{u}_s)\cdot \boldsymbol{n}, \boldsymbol{v}_h \cdot \boldsymbol{n}\rangle = 0, \qquad \boldsymbol{v}_h \in V_h. \tag{3.17}$$

We note that (3.17) requires that the net flow across $\partial\Omega$ of each boundary element be zero.

Extensions of the techniques to compressible fluids and thus mixed methods for parabolic partial differential equations have been considered [22, 32, 50]. Douglas and co-workers continue to study more efficient methods for solving the resulting linear equations.

For problems with smooth coefficients and smooth forcing functions, standard approximation theory results show that, by using higher-order basis functions, correspondingly higher-order convergence rates can be obtained. For the fluid flow in porous media applications, the source and sink terms q are not smoothly distributed, but are sums of Dirac delta functions. As shown by Ewing and Wheeler [34], the resulting smoothness of $\boldsymbol{u}$ is reduced; $\boldsymbol{u}$ is not contained in the space L^2 and thus using the methods described by (3.7) and (3.8), the velocity approximations $\boldsymbol{U}_h$ *would not converge at the wells.* This result was obtained theoretically by Ewing and Wheeler [39] and Douglas et al. [20, 21] and computationally in [33]. By removing the leading term of the singularities (the logarithm terms), the remaining parts of the velocities are now in $H^{2-\varepsilon}$ for any $\varepsilon > 0$. Thus the approximations to these parts will now converge at the wells since we have regained sufficient regularity for convergence.

Douglas, Ewing and Wheeler [20, 21] have obtained the following theoretical results.

THEOREM 3.1. With q defined as a sum of Dirac delta functions, if the leading terms in the singularities are removed and the remaining parts of $\boldsymbol{u}$ *are approximated by either the first- or second-order mixed method, we obtain*

$$\|\boldsymbol{U} - \boldsymbol{u}\| \leq C_1 h \ln h^{-1}, \tag{3.18}$$

and

$$\|P - p\| \leq C_2 h \ln h^{-1}, \tag{3.19}$$

where C_1 *and* C_2 *are constants depending upon the smoothness of* $\boldsymbol{u}$ *and* p.

If no wells are present in the model and all sources and sinks are smoothly distributed, Douglas, Ewing and Wheeler [20, 21] obtained the following stronger results.

THEOREM 3.2. For smoothly distributed sources and sinks, for the first- and second-order spaces, respectively, we obtain

$$\|U - u\| \leq C_3 h \quad \text{and} \quad \|P - p\| \leq C_4 h\,, \tag{3.20}$$

and

$$\|U - u\| \leq C_5 h^2 \quad \text{and} \quad \|P - p\| \leq C_6 h^2\,, \tag{3.21}$$

where C_3, C_4, C_5 and C_6 are constants depending upon the smoothness of u and p.

Special choices of basis functions for the Raviart–Thomas spaces based upon Gauss-point nodal functions and related quadrature rules have significantly aided in the computational efficiency of these methods. For detailed descriptions of these bases and computational results, see [12, 33, 40, 59]. The observed convergence rates matched those predicted in Theorems 3.1 and 3.2 above. Also superconvergence results were obtained at specific locations which can be utilized in quadrature and reduced quadrature considerations in the coupled systems described in Section 2.

The algebraic system arising from our mixed method system can be written as

$$\begin{pmatrix} A_1 & 0 & B_1 \\ 0 & A_2 & B_2 \\ B_1^t & B_2^t & 0 \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \beta \end{pmatrix} = \begin{pmatrix} R_1 \\ R_2 \\ R_3 \end{pmatrix}, \tag{3.22}$$

where the vectors α_1 and α_2 contain the coefficients of the x- and y-components of the velocity and β contains the coefficients of the pressure p. Eliminating α_1 and α_2 from (27) yields the system for β given by

$$(B_1^t A_1^{-1} B_1 + B_2^t A_2^{-1} B_2)\beta = B_1^t A_1^{-1} R_1 + B_2^t A_2^{-1} R_2 - R_3\,. \tag{3.23}$$

The matrix found on the left-hand side of (3.23) is not positive definite and care must be exercised in its solution. Similarly with the explicit A_1^{-1} and A_2^{-1} appearing, it is inefficient to even form this matrix, much less invert it directly. This motivates our use of preconditioned conjugate-gradient techniques for obtaining β from (3.23). For efficient ideas for preconditioning and solving (3.22) see [9, 33, 60].

Now that we have described the mixed finite element process for approximating u and p from (2.1) we can define the sequential time-stepping procedure for the system (2.3)–(2.5), (2.8) and (3.15)–(3.17). In practice, the velocity may change less rapidly in time than the concentration, even if characteristics are taken into account. Thus, it is appropriate to use a longer time step for (3.15)–(3.17) than for (2.8). Partition J into pressure time steps $0 = t_0 < t_1 < \cdots < t_n = T$, with $\Delta t_p^m = t_m - t_{m-1}$. Each pressure step is also a concentration step. Thus for each m there exists an n such that $t_m = t^n$. In general $\Delta t_p > \Delta t_c$. For pressure time steps we write $f_m(x) = f(x, t_m)$, hence distinguishing subscripts for pressure time steps and superscripts for concentration time steps.

If concentration step t^n relates to pressure steps by $t_{m-1} < t^n \leq t_m$, we need a velocity approximation for (2.8) based upon U_{m-1} and earlier values. If $m \geq 2$, we take the linear extrapolation of U_{m-1} and U_{m-2} defined by [35, 37, 51]

$$EU^n = \left(1 + \frac{t^n - t_{m-1}}{t_{m-1} - t_{m-2}}\right) U_{m-1} - \frac{t^n - t_{m-1}}{t_{m-1} - t_{m-2}}\, U_{m-2}\,. \tag{3.24}$$

If $n = 1$, set

$$EU^n = U_0 . \tag{3.25}$$

For $h > 0$, let M_h denote the family of subspaces of $H^1(\Omega)$ consisting of C^0 piecewise bilinear functions on a concentration grid. This will define our test and trial spaces for the concentration approximation.

The fully discrete time-stepping procedure for our miscible displacement problem can now be considered as a map $C_h : \{t^0, t^1, \ldots, t^N\} \to M_h$ and a map $(U_h, P_h) : \{t_0, t_1, \ldots, t_n\} \to V_h \times W_h$ defined by

$$C^0 = \hat{C}^0 , \quad x \in \Omega , \tag{3.26}$$

$$\left(\phi \frac{C^n - \bar{C}^{n-1}}{\Delta t}, \chi\right) + (D(EU^n)\nabla C^n, \nabla\chi) = (\bar{q}^n(\bar{c}^n - C^n), \chi) , \quad \chi \in M_h, \ n \geq 1 , \tag{3.27}$$

$$\left(\frac{\mu(C_m)}{k} U_m, v\right) - (P_m, \operatorname{div} v) = 0 , \quad v \in V_h, \ m \geq 0 , \tag{3.28}$$

$$(\operatorname{div} U_m, w) = (q_m, w), \qquad w \in W_h, \ m \geq 0 , \tag{3.29}$$

where

$$\bar{C}^{n-1}(x) = C^{n-1}(\bar{x}) = C^{n-1}\left(x - \frac{EU^n(x)}{\phi(x)} \Delta t\right) . \tag{3.30}$$

We first solve for C^0, then $(U_0 P_0)$, then $C^1, C^2, \ldots, C^{n_1}$ such that $t^{n_1} = t_1$, then (U_1, P_1), and so on.

Theoretical convergence estimates for this coupled system using both the modified method of characteristics and mixed methods will appear in [37]. We recall that Δt_c and Δt_p are time steps for the concentration and pressure equations; let h_c and h_p denote corresponding average spatial grid sizes. Briefly, an a priori error estimate of the following form is valid [37].

THEOREM 3.3. Under appropriate smoothness assumptions on the coefficients and functions and smoothly distributed sources and sinks, and if the discretization parameters satisfy, for $l \geq 1$, and $k \geq 0$,

$$\Delta t_c = o(h_p) , \qquad h_c^{l+1} = O(h_p) , \qquad (\Delta t_p)^{3/2} = O(h_p) , \qquad (\Delta t_p)^2 = O(h_p) ,$$

then we have

$$\max_{0 \leq n \leq N} \|c^n - C^n\| \leq K[h_c^{l+1} + h_p^{k+1} + \Delta t_c + (\Delta t_p^1)^{3/2} + (\Delta t_p)^2] . \tag{3.31}$$

The size of the Δt_c term depends principally upon $\|\partial^2 c/\partial\tau^2\|$ where τ approximates the characteristic direction s (Section 2). The size of the Δt_p terms depends principally on $\|\partial u/\partial t\|$ and $\|\partial^2 u/\partial t^2\|$. The spatial terms depend principally upon the spatial smoothness assumptions [37].

Computational results and further discussion appeared in [36]. Chavent et al. [10, 11] have used mixed methods in an immiscible displacement process where the fluids do not mix but flow as separate competing phases. Similar applications for accurately approximating separate phase velocities in compositional simulation describing multiphase flow with mass transfer between phases appear in [30, 31]. Mixed finite element techniques have also been applied successfully to compressible and time-dependent flows by Ewing and Koebbe [32].

In order to illustrate the accuracy and usefulness of finite element techniques in reservoir-simulation problems, we next present some computational results obtained by Tom Russell, Mary Wheeler and the author [36] using mixed finite element methods and the modified method of characteristics in the miscible displacement setting. The numerical results stem from the simulation of a quarter of a five-spot flooding pattern. The computational domain was a square with an injection well in one corner, a production well in the opposite corner, and no-flow boundary conditions. The concentration grids were nonuniform with finer subdivision near the wells. For more details of specific grids, see [52]. The pressure grids were uniform but of different size than the concentration grids. Time steps in the range of 0.01 to 0.04 pore volumes were found to be appropriate for these computations. These are larger by an order of magnitude than time steps required for comparable methods not utilizing the method of characteristics. This is an important feature of these methods.

There was slight overshoot and undershoot around the moving front, but they were everywhere less than 3.5%, even on coarse (20×20) concentration grids. The overshoot and undershoot occurred only in the neighborhood of the moving front and did not persist as the front moved on. Thus, they were not instabilities in the method, but merely indications that the grids chosen were too coarse to accurately resolve the very sharp fronts caused by high mobility ratios and dispersion coefficient ratios. As the grid was refined, the overshoot and undershoot were reduced correspondingly.

The recovery curves and concentration profiles indicated that, even with high mobility ratios and dispersion ratios, there was little grid-orientation problem. Concentration profiles are shown at 0.3 and 1 pore volumes injected in Figs. 1 and 2, respectively. The 20×20 concentration grids had diagonal grid orientation (see [27]) while the 28×28 concentration grid had parallel orientation. As noted in Figs. 1 and 2, the profiles are very similar before and after breakthrough to the production well indicating little grid-orientation effect.

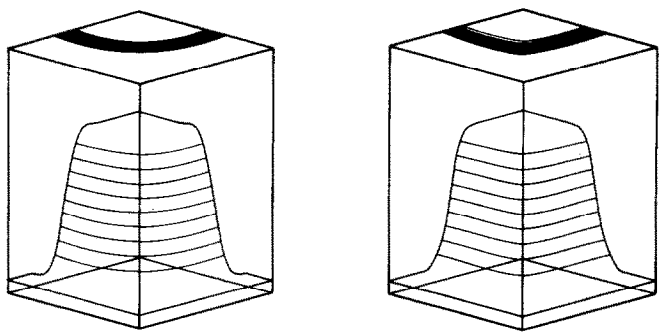

Fig. 1. Concentration profile, 0.3 PV injected. $M = 10$, $\phi d_m = 0$, $\phi d_l = 10$, $\phi d_t = 1$. (a) Diagonal orientation, 20×20 concentration, 15×15 pressure. (b) Parallel orientation, 28×28 Concentration, 20×20 pressure.

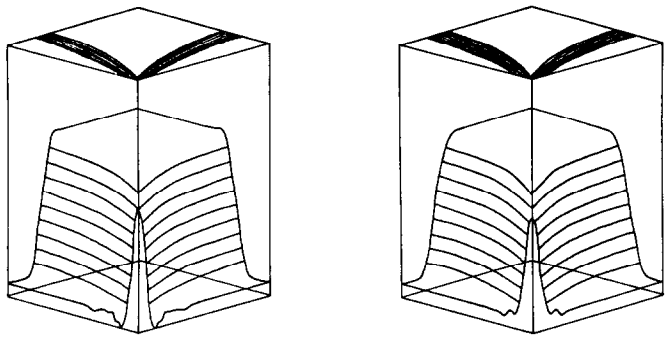

Fig. 2. Concentration profile, 1 PV injected. $M = 10$, $\phi d_m = 0$, $\phi d_l = 10$, $\phi d_t = 1$. (a) Diagonal orientation, 20×20 concentration, 15×15 pressure. (b) Parallel orientation, 28×28 concentration, 20×20 pressure.

In order to illustrate that our model will propagate fingers due to grid-size permeability variations, a problem with mobility ratio one hundred, $\phi d_m = 0$, $\phi d_l = 10$ and $\phi d_t = 1$ was simulated by Thom Potempa and Mary Wheeler, using a random number generator to choose a permeability variation between 0.002 and 1016 millidarcies. The results of the fingering produced in this way are illustrated in Fig. 3. Note that due to the ratio of the dispersion coefficients, the width of the front in the direction transverse to flow is very narrow while the contours are highly dispersed in the direction parallel to flow.

4. Adaptive local grid refinement

The objective of reservoir simulation is to understand the complex chemical, physical and fluid flow processes occurring in a petroleum reservoir sufficiently well to be able to optimize the recovery of hydrocarbon. Many of the chemical and physical phenomena which govern enhanced recovery processes have extremely important local character. Therefore the models used to simulate these processes must be capable of resolving these critical local features. Field scale hydrocarbon simulations normally involve reservoirs of such great size that uniform gridding on the length scale of the local phenomena would involve systems of discrete equations of such enormous size as to make solution on even the largest computers prohibitive. Therefore local grid refinement capabilities are becoming more important in reservoir simulation as the enhanced recovery procedures being used become more complex with more localized phenomena (see [27]).

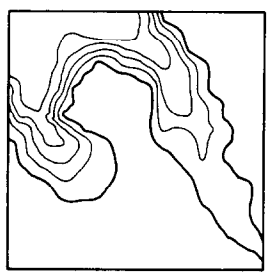

Fig. 3. Fingering for variable permeability.

In most enhanced recovery processes, fluids are injected into some wells in a reservoir while petroleum is produced through other wells. As one fluid displaces the others the localized phenomena occur along the moving interface between the fluids. If the complex fluid interactions in the region of this moving interface are not accurately resolved, the physics is lost and inaccurate frontal velocities and fluid behaviors are often predicted. Since this is the region that must be resolved accurately via local grid refinement we are naturally led to the need of dynamic grid-refinement capabilities. Since large-scale reservoir simulation involves hours or even days of computer usage, monitoring the simulation process and changing the grid refinement manually as the displacement proceeds would be impossible. Therefore self-adaptive local grid refinement is essential for accurate simulation of many of the dynamic recovery processes.

As we have described earlier, the pressure and velocity have near-singular behavior in the vicinities of wells with Dirac delta functions serving as good models. If special well models are not used, extremely high fluid pressure and velocity gradients near the well bore require that a fine gridding be placed in the neighborhood of each well to accurately resolve these variables. It has been shown [57] that local refinement around these singularities greatly increases the accuracy throughout the reservoir, if the discretization scheme properly treats the local refinement.

In an involved production strategy, new wells are drilled and old wells are often shut in to produce optimal sweep by the injected fluid and increase the hydrocarbon recovery. Thus the need to dynamically turn wells on or off necessitates the ability to add or remove local refinements around the wells without regenerating the entire grid. The ability to dynamically change the number of elements without greatly disrupting the solution process is highly desirable. A data structure and solution process with these capabilities will be discussed. Many of the local or moving grid refinement methods currently in use do not have these features. Techniques which rely upon mapping from a regular grid system (e.g., see papers in [56]) have great difficulty in smoothly adding or removing elements since this greatly disrupts the matrix solution process. The same argument applies to the moving finite element methods [42, 43]. The multigrid techniques however are designed to efficiently treat the use of several grids and have had preliminary success in local grid refinement.

A fairly sophisticated data structure is required to support an adaptive local grid-refinement capability. There are several excellent data structures available in the literature, each with its own advantages and disadvantages when reservoir simulation applications are considered. Due to the enormous size of reservoir problems, data storage requirements are already large, even for supercomputers, and the storage burdens of a data structure must be carefully balanced against natural efficiency requirements.

A data structure and corresponding code have been developed by Uhler, Jones and the author [14, 15, 28, 29] at Mobil Research and Development Corporation which has attempted to utilize the best aspects of the data structures of Rheinboldt and Mesztenyi [49] and Bank and Sherman [6, 7]. The structure of Rheinboldt and Mesztenyi is very efficient if data storage is severely limited. It is a general labeled tree structure and is designed for storage of minimal data and pointers at the expense of possibly a considerable amount of traveling the tree to obtain necessary data to build and solve the associated matrix problems [41, 49]. We have added some pointer storage to facilitate access to this needed information efficiently.

The data structure presented by Bank and Sherman [6, 7] is an excellent one if storage

restrictions are not a problem. By storing all essential information locally, extremely efficient construction and solution of the finite element matrices are possible. In large-scale reservoir-simulation problems where storage restrictions are severe, this structure is too storage intensive and time spent in data management severely deteriorates its efficiency. The Uhler–Jones–Ewing structure [14, 15, 28, 29] has both storage requirements and solution efficiency intermediate between the Rheinboldt–Mesztenyi structure and that of Bank and Sherman. The code also supports local enrichment and removal of refinement without regenerating a new grid, a capability missing in the other structures. This feature is extremely important for time-dependent problems where the grid may need to be changed only slightly from one time step to the next. A more detailed description of the data structure mentioned here and comparisons with other structures appear in [15, 28, 29].

Application of any of the data structures and algorithms mentioned above to finite difference discretization requires special treatment but is important since essentially all field-scale reservoir simulators now in use utilize finite difference techniques. Special solution stars must be determined in the neighborhood of local refinement [57]. We are currently trying to use the finite element formulations to determine suitable finite difference stars for these applications. Similarly, desire to incorporate the grid-refinement ideas in finite difference simulators in two and three space dimensions motivates the use of rectangular grid structures. In a finite element setting, this requires care to maintain continuity across element boundaries and conservation of mass in the presence of local grid refinement. Finite difference techniques have been applied successfully in [8]. They have a patch-type of local refinement so the difficulties of special finite difference stars are restricted only to the boundaries of the patches and the communication between the different grids. They have also addressed the problem of conservation of mass between grids.

Many different adaptive methods have recently been proposed for the solution of partial differential equations (see [1–5, 8, 13–15, 18, 24, 42, 43, 58]). For a 'state-of-the-art' survey of adaptive refinement for finite elements, see [4]. Adaptive multigrid methods include [5] while adaptive finite element methods have been presented in [2, 3, 5, 13, 42, 43, 58]. For large-scale reservoir-simulation problems, any dynamic refinement decisions must be made in a self-adaptive fashion. Also, the efficiency of the decision process is critical since these decisions must be made repeatedly, at each time step throughout the simulation.

The adaptivity of a method is driven by some estimate of the errors present in different spatial locations which need to be reduced. Traditional error estimates for finite element methods are a priori bounds, predicting the asymptotic rate of convergence as the mesh size tends to zero. Unfortunately, this tells us little about the true error for a fixed grid size in a difficult problem. Recently, locally-computable a posteriori error estimators have been developed, primarily by Babuška and Rheinboldt [1, 3], Bank [4] and Weiser [58]. Under suitable assumptions, these error estimators converge to the norm of the actual error as the mesh size tends to zero. The most recently developed estimators are asymptotically upper bounds for the norm of the true error and can be computed locally, element by element (see [58]). These a posteriori error estimators are extremely important for problems involving elliptic partial differential equations in determining the reliability of estimates for a fixed grid and a fixed error tolerance in a given norm. The error estimators are used to successively refine locally until the errors in some specified norm are, in some sense, equilibrated. These techniques have proven to be very effective for elliptic problems. However, the estimators

drive the local refinement at only one or two levels per iteration. Thus obtaining an 'optimal' grid normally takes several iterations. Although the local error estimation is a relatively small part of the solution of an elliptic problem, this is *not* the case for time-dependent problems.

For the parabolic or transport-dominated problems arising in reservoir simulation, there is much information which can be used from preceding time steps to help drive the adaptivity process. In parabolic problems, where the solution changes smoothly in time, the 'optimal' grid used at the previous time step should be a very good approximation to the desired grid at the advanced time step. Thus beginning with a new course grid at each time step and using the elliptic techniques of error estimators to drive the local refinement would be wasteful. The estimators would also need to have the capability of initiating removal of unnecessary grid as well as placement of needed grid.

The placement or removal of refinement in the Mobil code SAFES [14, 15] is triggered through a problem-independent grid analysis based on local cell indicators. The analysis is local in that only neighboring cells are considered in the decision process. An attempt is made to equalize the indicators on a local level rather than on a global level as in [1]. The local indicators used in the computations for [14, 15] were L^2-norms of the gradients of the solution. For other tolerance criteria, other norms can be used for the local indicators. These techniques are similar to those used in [13].

For hyperbolic or transport-dominated parabolic partial differential equations, sharp fronts move along characteristic or near-characteristic directions. Therefore the computed velocity determines both the local speed and direction of the regions where local refinement will be needed at the next time steps. This information should be utilized in the adaptive method to move local refinement with the front. Using these techniques, the refinement is not 'optimal' as with the methods described earlier or the moving finite element method to be discussed later. However, these methods are considerably cheaper to perform and some waste in using more grid than absolutely necessary is compensated for by the overall efficiency. In applying these techniques, we have found that moving the grid at each time step is inefficient. A considerably more effective technique is to use a larger, refined area within which the front will remain for several time steps and move the patch less frequently, after several steps. This concept is similar to the patch-refinement techniques of [8]. Efficiency is crucial in large-scale reservoir simulation.

More detailed discussions of the adaptive criteria used in the code developed at Mobil and termed SAFES (Self-Adaptive Finite Element Simulator) appear in [15, 28, 29] together with calculations on typical simple reservoir-simulation problems. This code is presently capable of treating only linear parabolic or elliptic partial differential equations and major extensions are necessary before many reservoir applications are accessible.

5. Conclusions

In this section we shall summarize several of the main points of this paper.

(1) Fluid flow in porous media shares many computational problems with other areas of nonlinear mechanics: (a) stabilization of large-scale transport or transport-dominated processes, (b) accurate resolution of sharp moving fronts, (c) accurate treatment of geometry or other singularities.

(2) The modified method of characteristics can efficiently stabilize convection-diffusion processes in several space dimensions without the addition of artificial diffusion which can smear sharp fronts and cause grid-orientation problems.

(3) Mixed finite element methods produce very accurate approximations to fluid velocities, even in the presence of rapidly changing flow properties and singularities. Singularities for velocities at the wells must be treated in a special manner to obtain convergence there.

(4) Analysis and a priori asymptotic error estimates have been instrumental in the choice of numerical techniques used in reservoir simulation.

(5) Dynamic local physical phenomena which may govern the entire flow process must be resolved with efficient, self-adaptive local grid-refinement capabilities.

(6) Finite element techniques have the versatility and power to yield very effective techniques in large-scale reservoir-simulation applications.

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