LOCALIZED ADJOINT METHODS: APPLICATIONS TO MULTIPHASE FLOW PROBLEMS

Ismael Herrera
Instituto de Geofisica, UNAM
Apdo. Postal 22-582
14000 México, D.F.

Richard E. Ewing
Departments of Mathematics, Chemical Engineering, and Petroleum Engineering
University of Wyoming, Laramie, Wyoming 82071

Abstract

Localized Adjoint Methods (LAM) form a broad class of numerical methods of operator-splitting type for partial differential equations, which is based in Herrera's Algebraic Theory of Boundary Value Problems. Application of LAM to flow and transport problems in porous media leads to generalized formulations of many standard approximation methods. These include Optimal Spatial Methods, with a variety of Petrov-Galerkin methods as subsets, and Characteristics Methods, with various Methods of Characteristics and Eulerian-Lagrangian Methods as subsets. After multiphase flow equations and operator-splitting techniques are presented, the LAM technique and its associated mathematical properties are discussed and its practical application to multiphase flow problems outlined.

1. INTRODUCTION

Many very difficult problems arise in the numerical simulation of multiphase or multicomponent fluid flow through porous media [1]. The mathematical models used to describe the complex flow processes are coupled systems of nonlinear partial differential equations and constraining equations. In industrial applications, these differential equations are commonly discretized via finite difference techniques in large-scale reservoir simulators. Due to the enormous size of many field-scale applications, quite large grid-spacings must be used in the simulations. The use of large grid-spacings with strongly nonlinear partial differential equations often generates spurious numerical artifacts which may destroy the usefulness of the simulation. In this paper, certain techniques are identified to help treat these problems by utilizing the basic properties of the flow more effectively.

In complex flow processes, two or more fluids can flow in an immiscible, or non-mixing, fashion at certain times or in a miscible mode, where mixing of the fluids takes place, at other times. For this reason, useful numerical techniques for multiphase or multicomponent reservoir simulators should be capable of treating both miscible and immiscible displacement phenomena.

These problems are both basically of convection/diffusion type with convection being the dominant process. Diffusion or dispersion is a small phenomenon relative to

convection, but is important for miscible flow regimes and may at times describe important capillary pressure effects in immiscible flow. Without the diffusion/dispersion terms, the model equations for each prototype would be nonlinear conservation laws which can produce shock solutions with very different flow properties. Standard upstream weighting techniques for stabilizing these hyperbolic partial differential equations can produce artificial numerical dispersion, which is of the order of the grid spacing size, and spurious effects related to the orientation of the grid.

Various authors have presented techniques to control numerical dispersion in traditional finite difference simulators for the miscible convection/diffusion models. However, they have met with limited success. On the other hand, by making use of mixed finite element techniques to study convection/diffusion models, the authors in [2–11] have been successful in greatly diminishing or essentially eliminating numerical dispersion and grid-orientation problems. We will stabilize the transport-dominated equations by utilizing methods specifically designed to treat the transport properties efficiently via special time-space test functions which follow the flow accurately. The methods are intended to treat both miscible and immiscible displacement since both give rise to nonlinear advection-dominated equations.

The numerical treatment of advection-dominated processes is quite difficult. The procedures available emanate from two main approaches: the standard temporal discretization and Eulerian-Lagrangian methods. The main distinguishing feature of the latter is the use of characteristics to carry out the discretization in time, to follow the flow. Most formulas that have been developed using a standard temporal discretization approach have been based on upstream weighting techniques, whose development is essentially ad-hoc and which can lead to serious numerical dispersion and grid-orientation problems.

In this paper, we first examine model equations for both multicomponent and multiphase flow and see that they both reduce to nonlinear advection-diffusion forms of partial differential equations. We then review some operator-splitting techniques that have been designed to treat the advective aspects of the flow. In the case of multiphase flow, we note that the operator splitting does not symmetrize the operator, and special test functions are necessary to stabilize the Petrov-Galerkin discretization procedure. We note that the Eulerian-Lagrangian techniques in operator splitting and the upstream stabilization methods are each special forms of Localized Adjoint Methods. We then present Eulerian-Lagrangian Localized Adjoint Methods (ELLAM) in some detail for one-dimensional applications, for clarity of exposition. Next, a general mathematical framework of the LAM techniques is discussed to indicate the generality of the approach. Finally, conclusions are drawn to illuminate the potential role of LAM in multiphase flow applications.

2. THE FLOW EQUATIONS

The miscible displacement of one incompressible fluid by another, completely miscible with the first, in a horizontal porous reservoir $\Omega \subset \mathbb{R}^2$ over a period $J = [T_0, T_1]$,

is given by [1,17]

$$\nabla \cdot \left(\frac{k}{\mu} \nabla p \right) \quad \nabla \cdot \mathbf{u} \quad q, \qquad \mathbf{x} \in \Omega, \quad t \in J,$$

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

where p and $\mathbf{u}$ are the pressure and Darcy velocity of the fluid mixture, ϕ and k are the porosity and the permeability of the medium, μ is the concentration-dependent viscosity of the mixture, c is the concentration of the invading fluid, q is the external rate of flow, and $\tilde{c}$ is the inlet or outlet concentration. $\mathbf{D}$ is, in general, a diffusion/dispersion tensor which has two parts, molecular diffusion and a velocity-dependent dispersion term. For simplicity in the succeeding development, the diffusion/dispersion coefficient will be assumed to be independent of velocity. Also, the viscosity μ in Equation (2.1) is assumed to be determined by some mixing rule. In addition to Equations (2.1) and (2.2), initial and no-flow boundary conditions are specified. The flow at injection and production wells is modeled in (2.1) and (2.2) via point sources and sinks.

The equations describing two-phase, immiscible, incompressible displacement in a horizontal porous medium are given by

$$\phi \frac{\partial S_w}{\partial t} - \nabla \cdot \left(k \frac{k_{rw}}{\mu_w} \nabla p_w \right) = q_w, \qquad \mathbf{x} \in \Omega, \quad t \in J, \tag{2.3}$$

$$\phi \frac{\partial S_o}{\partial t} - \nabla \cdot \left(k \frac{k_{ro}}{\mu_o} \nabla p_o \right) = q_o, \qquad \mathbf{x} \in \Omega, \quad t \in J,$$

where the subscripts w and o refer to water and oil, respectively. S_i is the saturation, p_i is the pressure, k_{ri} is the relative permeability, μ_i is the viscosity, and q_i is the external flow rates, each with respect to the ith phase.

Although formally the equations presented in (2.1) and (2.2) seem quite different from those in (2.3) and (2.4), the latter system may be rearranged in a form which very closely resembles the former system. In order to use the same basic simulator in our sample computations to treat both miscible and immiscible displacement, we briefly discuss a miscible/immiscible analogy between equations.

Adding Equations (2.3) and (2.4) and performing some simple calculations, we obtain

$$-\nabla \cdot (k \lambda(S) \nabla p) = q_w + q_o = q_t, \tag{2.5}$$

$$\mathbf{v}_t = -k \lambda(S) \nabla p\,, \tag{2.6}$$

where $k\lambda$ is the transmissibility, p is a global pressure of the fluid defined in [17], and $\mathbf{v}_t$ is the corresponding fluid velocity. Taking the difference of Equations (2.3) and (2.4), the following equation is obtained:

$$\phi \frac{\partial S}{\partial t} - \nabla \cdot (D \nabla S) + \nabla \cdot \left(\overline{\lambda}_w \mathbf{v}_t \right) \quad q_w.$$

Here the capillary diffusion term D and the fractional flow $\overline{\lambda}_w \mathbf{v}_t$ are defined in terms of relative permeabilities and capillary pressure terms as in [1,14,15,18].

With a special form of relative permeabilities and capillary pressure, the viscosity dependence in pressure equation (2.5) is the same as that specified as concentration dependence for Equation (2.1). Therefore, $\mathbf{v}_o + \mathbf{v}_w$ (i.e., $\mathbf{v}_t$), solved from Equation (2.5), will be identical to u in Equation (2.1). Moreover, Equation (2.8) has the same form as the concentration equation (2.2) if S is interpreted as a component concentration and q_w is equal to $\tilde{S}q_t$. This establishes the analogy between the two systems. They are both basically of the form of nonlinear advection-diffusion problems with dominant advection. The LAM numerical techniques presented here have been developed to treat this class of equations effectively.

3. OPERATOR-SPLITTING TECHNIQUES

In finite difference simulators the advection is stabilized via upstream weighting techniques. In a finite element setting, we use a possible combination of a modified method of characteristics and Petrov-Galerkin techniques to treat the transport separately in an operator-splitting mode. We describe this operator-splitting concept in the context of a modified method of characteristics in this section and then in terms of ELLAM techniques in the next section.

In miscible or multicomponent flow models, the convective, hyperbolic part is a linear function of the velocity. An operator-splitting technique has been developed to solve the purely hyperbolic part by time-stepping along the associated characteristics [7,9,17]. We first obtain the non-divergence form of (2.2) by using the product rule for differentiation on the $\nabla \cdot \mathbf{u}c$ term and applying (2.1) to obtain

$$\phi \frac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c \quad \nabla \cdot \mathbf{D} \nabla c = q(\tilde{c} \quad c).$$

Next, the first and second terms in Equation (3.1) are combined to form a directional derivative along what would be the characteristics for the equation if the tensor $\mathbf{D}$ were zero. The resulting equation is

$$\nabla \cdot (\mathbf{D} \nabla c) + q(\tilde{c} - c) \quad \phi \frac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c \quad \phi \frac{\partial c}{\partial \tau}.$$

The system obtained by modifying Equations (2.1)–(2.2) in this way is solved sequentially. An approximation for $\mathbf{u}$ is first obtained at time level $t = t^n$ from a solution of Equation (2.1) with the fluid viscosity μ evaluated via some mixing rule at time level t^{n-1}. Equation (2.1) can be solved as an elliptic equation for the pressure p, or via a mixed finite element method for a more accurate fluid velocity. Let $\hat{C}^n(x)$ and $\mathbf{U}^n(x)$ denote the approximations of $c(x,t)$ and $\mathbf{u}(x,t)$, respectively, at time level $t = t^n$. The directional derivative is then discretized along the "characteristic" mentioned above as

$$\phi \frac{\partial c}{\partial \tau}(x, t^n) \approx \phi \frac{C^n(c) - C^{n-1}(\overline{x}^{n-1})}{\Delta t}$$

where $\overline{x}^{n-1}$ is defined for an x as

$$\overline{x}^{n-1} = x \quad \frac{\mathbf{U}^n(x)\Delta t}{\phi} \tag{3.4}$$

This technique, first described by Russell [10] for petroleum applications, is a discretization back along the "characteristic" generated by the first order derivatives from Equation (3.2). Although the advection-dominance in the original Equation (3.2) makes it non-self-adjoint, the form with directional derivatives is self-adjoint, and discretization techniques for self-adjoint equations can be utilized. This modified method of characteristics can be combined with either finite difference or finite element Galerkin spatial discretizations.

In immiscible or multiphase flow, the convective part is nonlinear. A similar operator-splitting technique to solve this equation needs reduced time steps because the pure hyperbolic part may develop shocks. Recently, a new operator-splitting technique has been developed for immiscible flows [14–16] which retains the long time steps in the characteristic solution without introducing serious discretization errors.

The operator splitting gives the following set of equations:

$$\phi\frac{\partial \overline{S}}{\partial t} + \frac{d}{dS}\mathbf{f}^m(\overline{S})\cdot\nabla\overline{S} \equiv \phi\frac{d}{d\tau}\overline{S} \quad 0,$$

$$\phi\frac{\partial S}{\partial \tau} + \nabla\cdot(\mathbf{b}^m(S)S) - \epsilon\nabla\cdot(D(S)\nabla S) = \mathbf{q}(\mathbf{x},t), \tag{3.5}$$

$t_m \le t \le t_{m+1}$, together with proper initial and boundary conditions. As noted earlier, the saturation S is coupled to the pressure/velocity equations, which will be solved by mixed finite element methods [2,3,7–9].

The splitting of the fractional flow function into two parts: $\mathbf{f}^m(S) + \mathbf{b}(S)S$, is constructed [14] such that $\mathbf{f}^m(S)$ is linear in the shock region, $0 \le S \le S_1 < 1$, and $\mathbf{b}(S) \equiv 0$ for $S_1 \le S \le 1$. Further, Equation (3.5) produces the same unique physical solution as

$$\phi\frac{\partial S}{\partial t} + \nabla\cdot(\mathbf{f}^m(S) + \mathbf{b}(S)S) = 0 \tag{3.7}$$

with an entropy condition imposed. This means that, for a fully developed shock, the characteristic solution of Equation (3.5) always will produce a unique solution and, as in the miscible case, we may use long time steps Δt without loss of accuracy.

The solution of Equation (3.6) via variational methods leads to the following Petrov-Galerkin equations:

$$\begin{aligned} B(S_h^m,\phi_i) &\equiv (S_h^{m+1},\phi_i) - \left(\frac{\Delta t}{\phi}\mathbf{b}(\mathbf{x},t^m)S_h^{m+1},\nabla\phi_i\right) + \left(\frac{\epsilon\Delta t}{\phi}D(\mathbf{x},t^m)\nabla S_h^{m+1},\nabla\phi_i\right) \\ &= (g_h^m(\mathbf{x},t^m),\phi_i), \qquad i=1,2,\cdots,N, \quad S_h^m\in M_h, \quad \phi_i\in N_h, \end{aligned} \tag{3.8}$$

where M_h and N_h are the trial and test spaces spanned by $\{\theta_i\}$ and $\{\phi_i\}$, $i = 1,2,\cdots,N$, respectively. $B(\cdot,\cdot)$ given by Equation (3.8) is an unsymmetrical bilinear form with spatially-dependent coefficients.

In order to obtain Equation (3.8), we have used the characteristic solution from Equation (3.5) to approximate $(\partial/\partial\tau)S$ and the nonlinear coefficients [14] in Equation (3.6). The nonsymmetry in the bilinear form $B(\cdot,\cdot)$ is caused by the nonlinearity of the convective part of the equation, represented by the term $\mathbf{b}(S)S$. This term balances the diffusion forces in the shock region after a traveling front has been established.

We want to use numerical techniques which work well for the symmetric, coercive, bilinear forms to solve Equation (3.8). We consider a procedure, developed by Barrett and Morton [19], which symmetrizes the bilinear form $B(\cdot,\cdot)$ by defining a new set of test functions as follows:

$$B(S^m,\phi_i) = \left(a_{kl}\frac{\partial}{\partial x_k}S^m, \frac{\partial}{\partial x_l}\theta_i\right) \quad B^*(S^m,\theta_i), \quad 0 < a_{kl} < K. \tag{3.9}$$

One can see that the test functions defined in this way are closely related to test functions that satisfy the adjoint operator. This property will be developed in more detail below.

The test functions ϕ_i defined by Equation (3.9) have nonlocal support and would thus cause serious computational problems for large-scale problems. However, a localization procedure was developed by Demkowitz and Oden [12,13] which allows efficient computational procedures. Since the bilinear form $B(\cdot,\cdot)$ is coercive, we obtain optimal approximation properties in the norms defined by the form. For computational reasons, it may be better to use an approximate form of the optimal test function ϕ_i. An estimate for the error introduced by an approximate symmetrization of $B(\cdot,\cdot)$ is given by Barrett and Morton [19].

It seems natural to relate the size of the coarse domains to the solution of the pressure-velocity equation [14], since the velocity varies slowly and defines a natural long space scale compared to the variation of the saturation S at a front. A local error estimate, which determines if a coarse grid block must be refined, is given in reference [14]. Normally, local refinement must be performed if a fluid interface is located within the coarse grid block in order to resolve the solution there. A slightly different strategy is to make the region of local refinement big enough such that we can use the same refinements for several of the large time steps allowed by the method. The local grid refinement strategy combined with the operator splitting is defined in the literature [14–16]. The solution at each of the coarse grid vertices and the local refinement calculation may be sent to separate processors to achieve a high level of parallelism in the solution process.

The difficult problem with these techniques is the communication of the solution between the fine and coarse grids. The domain-decomposition technique described in [20] gives accurate and efficient treatment of the communication problem.

4. AN EULERIAN-LAGRANGIAN LAM FOR ADVECTION-DIFFUSION TRANSPORT EQUATIONS

Unfortunately, the modified method of characteristics techniques described above generally do not conserve mass. Also, the proper method for treating boundary conditions in a conservative and accurate manner using these techniques is not obvious. Recently, M.A. Celia, T.F. Russell, and the authors have devised Eulerian-Lagrangian localized adjoint methods (ELLAM) [21,22], a set of schemes that are defined expressly for conservation of mass properties.

The ELLAM formulation was motivated by localized methods [23,24], which are one form of the optimal test function methods discussed above [12-15,19]. We briefly describe these methods. Let

$$Lu \quad f, \quad x \in \Omega \text{ or } (x,t) \in \Omega,$$

denote a partial differential equation in space or space-time Integrating against a test function ϕ, we obtain the weak form

$$\int_\Omega Lu\phi \, d\omega \quad \int_\Omega f\phi \, d\omega .$$

If we choose test functions ϕ to satisfy the formal adjoint equation $L^*\phi = 0$, except at certain nodes or edges denoted by ℓ_i on $\partial\Omega$, and $\phi = 0$ on the boundary, then integration by parts (the divergence theorem in higher dimensions) yields

$$\sum_i \int_{\ell_i} uL^*\phi \, d\omega = \int_\Omega f\phi \, d\Omega .$$

Various different test functions can be used to focus upon different types of information. Herrera has built an extensive theory around this concept [25–29, 31]. The theory is quite general.

The formulation and usefulness of ELLAM can be seen most easily via a specific one-dimensional model problem. At first, we consider a constant-coefficient advection-diffusion equation for concreteness and simplicity of exposition and then remark about extensions to variable and nonlinear coefficients. We will see that in the context of backward Euler temporal integration, the ELLAM corresponds almost exactly (except for the more accurate treatment of boundary conditions) with the modified method of characteristics (MMOC) approach [32] presented in the previous section. ELLAM is more general and has potential for even better results than in MMOC.

Consider the one-dimensional transient advection-diffusion equation, motivated by (2.2) or (2.7),with c or S represented by a scalar function u subject to appropriate initial and boundary conditions:

$$Lc \equiv \frac{\partial u}{\partial t} + \frac{\partial}{\partial x}(Vu) - D\frac{\partial^2 u}{\partial x^2} = q\tilde{u} \equiv f(x,t)\,, \tag{4.4}$$

$$\begin{aligned} u(x,0) &= u_I(x)\,, \\ u(0,t) &= u_0(t)\,, \\ \tfrac{\partial u}{\partial x}(\ell,t) &= q_\ell(t)\,. \end{aligned}$$

First- and second-type boundary conditions are chosen for demonstration purposes only; the following development accommodates any combination of boundary conditions. The adjoint operator associated with the operator L of Equation (4.4) is

$$\frac{\partial w}{\partial t} - V\frac{\partial w}{\partial x} - D\frac{\partial^2 w}{\partial x^2}\,. \tag{4.5}$$

The LAM approach is initiated by writing the weak form of equation (4.4). Let $w(x,t)$ refer to a test function (whose precise form will be determined as part of the LAM development), so that the weak form of Equation (4.4) is

$$\int_0^\ell \int_0^\infty (Lu - f)\, w(x,t)\, dt\, dx = 0\,. \tag{4.6}$$

As discussed above, the test function w(x,t) is chosen from the solution space of the homogeneous adjoint equation (4.5).

As opposed to the simple developments for ordinary differential operators, the solution space of the partial differential equation (4.5) is infinite-dimensional. Because the objective of the numerical procedure is derivation of a finite number of algebraic equations, only a finite number of test functions should be chosen. Different choices of test functions (solutions of Equation (4.5)) lead to different classes of approximations, including families of Optimal Spatial Methods and general Characteristic Methods.

By analogy to the tensor product approach of Celia, et al. [23,24], a product solution of the form $w(x,t) = \xi(x)\tau(t)$ could be sought such that $\xi(x)$ satisfies the homogeneous spatial operator of Equation (4.5) while $\tau(t)$ satisfies the temporal part. Such a space-time split, defined on a rectangular discretization of $\Omega_{x,t}$, leads to optimal spatial algorithms involving exponential weightings in space. The result is analogous to the semi-discretizations presented in [24].

To derive a general family of Characteristic Methods (CM's), a different set of solutions to Equation (4.5) must be used. In particular, consider solutions to Equation (4.5) which satisfy the two homogeneous subequations that are grouped based on common order of derivatives, viz. $\frac{\partial w}{\partial t} + V\frac{\partial w}{\partial x} = 0$ and $D\frac{\partial^2 w}{\partial x^2} = 0$. The second constraint implies linear functions of x, while the first constraint implies w = constant along lines $x - x_0 = u(t - t_0)$. A natural choice for such a test function can be defined with respect to a rectangular array of nodes in space-time as follows,

$$w_i^{n+1}(x,t) = \begin{cases} \frac{x-x_{i-1}}{\Delta x} + V\frac{t^{n+1}-t}{\Delta x}, & (x,t) \in \Omega_1^i, \\ \frac{x_{i+1}-x}{\Delta x} \quad V\frac{t^{n+1}-t}{\Delta x}, & (x,t) \in \Omega_2^i, \\ 0, & \textit{all other } (x,t), \end{cases}$$

where subscript i denotes spatial location ($x_i \equiv i(\Delta x)$ for constant spatial step Δx), superscript n denotes time level ($t^n \equiv n(\Delta t)$ for constant time step Δt); this test function is associated with spatial location i and temporal location $n+1$. In writing Equation (4.4), constant node spacing Δx has been assumed. The regions Ω_1^i and Ω_2^i are illustrated in Figure 1, as is a typical test function. The function $w_i^{n+1}(x,t)$ has the properties that it is $C^0[\Omega_x]$ and $C^{-1}[\Omega_t]$; it is nonzero over only one time step (t^n to t^{n+1}) with discontinuities aligned along t^n and t^{n+1}; and the lines of spatial derivative discontinuities align with the characteristics that intersect the nodes x_{i-1}, x_i, and x_{i+1} at time level t^{n+1}.

Given this test function definition, the weak form of the equation can be evaluated by standard integration procedures as in [21]. Let the spatial locations at time level t^n that are on the characteristic curves that intersect points x_{i-1}, x_i, x_{i+1} at t^{n+1} be denoted as x_{i-1}^*, x_i^*, and x_{i+1}^*, respectively, as illustrated in Figure 1. These points are often referred to as the "foot of the characteristic" points. In addition, let the characteristic curves that pass through points x_{i-1}, x_i, and x_{i+1} at time t^{n+1} be identified by $x_\ell^i(t), x_c^i(t)$, and $x_r^i(t)$, respectively, as illustrated in Figure 1. The weak form of Equation (4.4) can be rewritten in an equivalent form by applying integration by parts. If $u(x,t)$ is assumed to be at least C^1-continuous in x and C^0-continuous in t (cases of less restrictive continuity are treated by the general theory of Herrera), then the integrations of Equation (4.6) can be written equivalently as a sum of elemental integrals. Integration by parts can then be applied element-by-element, where "elements" are defined as the regions Ω_1^i, Ω_2^i, etc. Evaluation of the weak form (4.3), with $w_i^{n+1}(x,t)$ used as the test function, leads to the following expression:

$$\int_0^\infty \int_0^\ell (Lu - f)\, w_i^{n+1}(x,t)\, dx\, dt = 0$$

$$\int_0^\infty \int_0^\ell \left[\frac{\partial u}{\partial t} + V\frac{\partial u}{\partial x} \quad D\frac{\partial^2 u}{\partial x^2} \quad f(x,t)\right] w_i^{n+1}(x,t)\, dx\, dt$$

$$\int_{x_{i-1}}^{x_{i+1}} u(x,t^{n+1}) w_i^{n+1}(x,t^{n+1})\, dx - \int_{x_{i-1}^*}^{x_{i+1}^*} u(x,t^n) w_i^{n+1}(x,t^n)\, dx$$

$$-D\left[\int_{t^n}^{t^{n+1}} u(x_\ell^i(t),t) \left[\!\left[\frac{\partial w_i^{n+1}}{\partial x}\right]\!\right]_{x_\ell^i(t)} + \int_{t^n}^{t^{n+1}} u(x_c^i(t),t) \left[\!\left[\frac{\partial w_i^{n+1}}{\partial x}\right]\!\right]_{x_c^i(t)}\right.$$

$$\left. + \int_{t^n}^{t^{n+1}} u(x_r^i(t),t) \left[\!\left[\frac{\partial w_i^{n+1}}{\partial x}\right]\!\right]_{x_r^i(t)}\right] + \int_{\Omega_1^i} u(x,t) L^* w_i^{n+1}\, dx\, dt$$

$$+ \int_{\Omega_2^i} u(x,t) L^* w_i^{n+1}\, dx\, dt \quad \int_{\Omega_1^i + \Omega_2^i} f(x,t) w_i^{n+1}(x,t)\, dx\, dt = 0\,,$$

where the double bracket notation denotes a spatial jump operator, $[\![\cdot]\!]_{x_k} \equiv \lim_{\epsilon \to 0} [(\cdot)_{x_k+\epsilon} - (\cdot)_{x_k-\epsilon}]$. Due to the special choice of test function given by Equation (4.7), $L^* w_i^{n+1} = 0$ in both Ω_1^i and Ω_2^i, so that the interior integrals involving $u(x,t)$ are eliminated. Furthermore, due to the constant coefficients, the spatial jump operators can be evaluated from Equation (4.4) as

$$\left[\!\!\left[\frac{\partial w_i^{n+1}}{\partial x} \right]\!\!\right]_{x_\ell^i(t)} \qquad \left[\!\!\left[\frac{\partial w_i^{n+1}}{\partial x} \right]\!\!\right]_{x_r^i(t)} \qquad \frac{1}{\Delta x} \qquad \left[\!\!\left[\frac{\partial w_i^{n+1}}{\partial x} \right]\!\!\right]_{x_c^i(t)} \qquad \frac{-2}{\Delta x}$$

Equation (4.8) can therefore be simplified as

$$\begin{aligned} &\int_{x_{i-1}}^{x_{i+1}} u(x,t^{n+1})\, w_i^{n+1}(x,t^{n+1})\, dx - \int_{x_{i-1}^*}^{x_{i+1}^*} u(x,t^n) w_i^{n+1}(x,t^n)\, dx \\ &-D\left[\left(\frac{1}{\Delta x}\right) \int_{t^n}^{t^{n+1}} u(x_\ell^i(t),t)\, dt - \left(\frac{2}{\Delta x}\right) \int_{t^n}^{t^{n+1}} u(x_c^i(t),t)\, dt \right. \\ &\left. + \left(\frac{1}{\Delta x}\right) \int_{t^n}^{t^{n+1}} u(x_r^i(t),t)\, dt \right] = \int_{\Omega_1^i+\Omega_2^i} f(x,t) w_i^{n+1}(x,t)\, dx\, dt\,. \end{aligned} \tag{4.9}$$

In addition to conservation of mass, the ELLAM give us direct information about how to accurately treat boundary conditions. When a characteristic line passing through points x_{i-1}, x_i, or x_{i+1} at time t^{n+1} crosses the boundary between times t^n and t^{n+1}, call it time t^*, the boundary information must be incorporated into the approximating equation. Based on the treatment of boundary conditions, all MMOC and ELM approximations previously proposed in the literature appear to be inherently non-mass-conservative. In variable velocity fields, failure to conserve mass may also result from inexact representations of the characteristics.

The ELLAM approach provides a systematic and consistent methodology for proper incorporation of boundary conditions. To demonstrate the incorporation of boundary conditions at the inflow boundary ($x = x_0 = 0$ for the example with $V > 0$), we consider an example for which the Courant number $Cu \equiv V(\Delta t)/(\Delta x)$ is between 1 and 2. The general case is treated in [21]. For the case of $1 \le Cu \le 2$, the characteristic curve that passes through node 1 ($x = x_1$) at time t^{n+1} intersects the boundary at $x = x_0 = 0$ at time $t_1^* \ge t^n$. Therefore, equations that involve this characteristic will be influenced by boundary conditions. Consider the ELLAM equation associated with node 1. The test function $w_1^{n+1}(x,t)$, illustrated in Figure 2, differs from the general function w_i^{n+1} of Figure 1 because part of N_1^{n+1} intersects the boundary at $x = 0$ with nonzero value. Therefore, evaluation of the general ELLAM equations are modified by boundary influence. The ELLAM equation associated with $w_i^{n+1}(x,t)$ is derived in the same way as Equations (4.8) and (4.9): elemental integration by parts is applied to each term and the condition that $L^* w_1^{n+1} = 0$ in each element is used to produce

$$\int_{x_0}^{x_2} u(x,t^{n+1})w_1^{n+1}(x,t^{n+1})\,dx \quad \left[\int_{x_0}^{x_2^*} u(x,t^n)w_1^{n+1}(x,t^n)\,dx\right.$$

$$\left.+V\int_{t^n}^{t^{n+1}} u(0,t)w_1^{n+1}(0,t)\,dt\right] - D\left[\frac{1}{(\Delta x)}\int_{t_1^*}^{t^{n+1}} u(0,t)\,dt\right.$$

$$\left.\left(\frac{2}{\Delta x)}\right)\int_{t_1^*}^{t^{n+1}} u(x_c^1(t),t)\,dt + \left(\frac{1}{\Delta x}\right)\int_{t^n}^{t^{n+1}} u(x_r^1(t),t)\,dt\right] \qquad (4.10)$$

$$+D\int_{t^n}^{t^{n+1}} \frac{\partial u}{\partial x}(0,t)w_1^{n+1}(0,t)\,dt + D\left(\frac{1}{\Delta x}\right)\int_{t^n}^{t_1^*} u(0,t)\,dt$$

$$\int_{\Omega_1^1\cup\Omega_2^1} f(x,t)w_1^{n+1}(x,t)dx\,dt$$

Examination of Equation (4.10) indicates that the spatial integration at time t^n is modified by the boundary at $x = 0$. While this equation spans a distance of $2\Delta x$ in Equation (4.7), it spans $(2 - Cu)\Delta x$ in Equation (4.10). The part that is cut off by the boundary corresponding to the distance $Cu(\Delta x)$ is picked up by the third integral on the left side of Equation (4.10), which involves the boundary value $u(0,t)$. The next three integrals in Equation (4.10) correspond to the three diffusive terms in Equation (4.8), except that the left integral is evaluated along $x = 0$ and the integrand is the boundary value $u(0,t)$. Finally, the last two integrals on the left side of Equation (4.10) are again integrals that are evaluated along the boundary $x = 0$: the second of these invloves the function $u(0,t)$, but the first involves the spatial gradient $\frac{\partial u}{\partial x}(0,t)$. Notice that this latter integral introduces an additional degree of freedom at the boundary, so that both $u(0,t)$ and $\frac{\partial u}{\partial x}(0,t)$ are present in this equation. Even when a first type boundary condition is specified at $x = 0$, the flux at the boundary may need to be determined due to the presence of this integral. Therefore, an additional equation should be written, that which corresponds to node 0, with test function $w_0^{n+1}(x,t)$ (see Figure 3). This is in constrast to standard finite element methods, wherein the boundary flux need not be explicitly determined when first type boundary conditions are prescribed. The reason that both boundary values appear in the ELLAM formulation is that the space-time LAM elements in Figure 1 are not parallel to the time axis, while standard semi-discrete finite elements correspond to rectangular space-time elements with sides parallel to the space-time coordinate axes.

Similar formulations for other Courant numbers appear in [21]. Also, outflow boundary conditions of each type and resulting matrix equations are discussed in [21] in some detail.

5. General Framework for Localized Adjoint Methods

A very promising general approach incorporating the methods described in the last section has been introduced by Herrera [25-29] and co-workers. The starting point of Herrera's approach is a rather simple and, as a matter of fact, old idea. Again, we let $\mathcal{L}$ be a differential operator that will be applied to functions defined in a region Ω and let $\mathcal{L}^*$ be its formal adjoint. Then, when u and v satisfy suitable boundary conditions, Green's formula

$$\int_\Omega v\mathcal{L}u dx = \int_\Omega u\mathcal{L}^* v dx$$

is satisfied. Equation (5.1) allows a convenient interpretation of the method of weighted residuals. Consider the problem of solving the equation

$$\mathcal{L}u = f_\Omega\,, \quad \text{in}\,\Omega\,,$$

subjected to homogeneous boundary conditions such that Green's formula (5.1) applies. In the method of weighted residuals, one usually considers a system of test functions $\{\varphi_1, \cdots, \varphi_N\}$. Then, a function u' is said to be an approximate solution of this problem when

$$\int_\Omega \varphi_\alpha \left(\mathcal{L}u' - f_\Omega\right) dx = 0, \quad \alpha = 1, \cdots, N. \tag{5.3}$$

Generally, the system of N Equations (5.3) has many solutions, but in order to obtain a system posessing a unique solution, it is customary to introduce a representation $u' = \sum A_\alpha \phi_\alpha$ of the approximate solution in terms of the system $\{\phi_1, \cdots, \phi_N\}$ of base (or trial) functions. However, this representation is an artifice that bears little relation with the *exact solution* u. Indeed, to establish a connection with the exact solution one has to resort to an approximation theory.

The following observations permit establishing the actual information, about the exact solution, contained in an approximate one. From (5.2), it is clear that the exact solution satisfies

$$\int_\Omega \varphi_\alpha \left(\mathcal{L}u - f_\Omega\right) dx = 0, \quad \alpha = 1, \cdots, N. \tag{5.4}$$

Equations (5.3) and (5.4) together imply

$$\int_\Omega \varphi_\alpha \mathcal{L}u' dx = \int_\Omega \varphi_\alpha \mathcal{L}u dx, \quad \alpha = 1, \cdots, N\,,$$

or

$$\int_\Omega u' \mathcal{L}^* \varphi_\alpha dx = \int_\Omega u\mathcal{L}^* \varphi_\alpha dx, \quad \alpha = 1, \cdots, N\,,$$

by virtue of Green's formula (5.1). Consider the Hilbert space, L^2, of square integrable functions in which the inner product of two functions, u and v, is given by $\int_\Omega uv dx$. Then, the system of Equations (5.6) allows the following interpretation:

> A function u' is an approximate solution if and only if its projection on the space spanned by the system of functions $\{\mathcal{L}^*\varphi_1,...,\mathcal{L}^*\varphi_N\}$ coincides with that of the exact solution u. As a matter of fact, this is *all the information* about the exact solution contained in an approximate one.

In this light, the representation $u' = \sum A_\alpha \phi_\alpha$ can be interpreted as a procedure for interpolating the actual information contained in the approximate solution. Thus, a judicious choice of the base functions ϕ_α, can only be made resorting to approximation theory.

The very simple and precise result just presented clarifies much of the nature of approximate solutions, and it would be desirable to apply it in a systematic manner to analyze discrete methods. For this purpose, it is necessary to have available Green's formulas similar to (5.1), but which are applicable even when the functions considered are not smooth. This is because, in most applications to numerical methods, weighting functions are localized (i.e., they have local support) and they usually do not satisfy the smoothness requirements at the boundary of their support.

Herrera [25-28], recently developed an *algebraic theory of boundary value problems*; this provides a framework for localizing the Adjoint Equation (5.6). It is natural to call the procedures obtained in this manner "Localized Adjoint Methods" since they are applied cell by cell. However, the reader should note that in previous work [25-28], this approach has been called the "Optimal Test Function Method".

Localized Adjoint Methods (LAM) consist in making systematic use of that theory to analyze the information contained in approximate solutions. Since the quality of the results obtained with a numerical method depends, in an important manner, on the weighting functions used, one of the main goals of localized adjoint methods, thus far, has consisted in motivating and developing improved test functions [21–24, 28–31].

For the specific case of L and L^* defined by Equations (4.4) and (4.5), respectively, and for the specific choices of w_i^{n+1} given by Equation (4.7), we obtained Equation (4.9). For different choices of continuity of u and w and different splittings of the adjoint equation to obtain w, we get very different methods. The generality in the LAM techniques is the choice of continuity and of test functions.

For example, for steady-state problems, leading to ordinary differential equations, four distinct algorithms were developed by Herrera et al. [28]. They were obtained by concentrating all of the information at nodes; for each one of them the sought information was: 1) the value of the function and its derivative; 2) the value of the function only; 3) the value of the derivative only; and 4) the function at some nodes and the derivative at other nodes. These algorithms were made via different choices of continuity and test functions. When the test functions exactly satisfied the adjoint equations in [28], exact values of the trial functions were obtained. In general, however, approximate test functions are developed which yield the sought information to any desired degree of accuracy.

For the extension to time-dependent problems, previous splittings grouped time and space derivatives [23,24]. For transport dominated problems, this corresponded to the addition of the first-order temporal and spatial discretization errors and inaccurate solutions. The ELLAM techniques are aimed at development of implicit time-stepping procedures which obtain a greatly improved space-time discretization error along characteristics. The continuity assumptions in space reduce the sought information along the characteristic lines, and special temporal integration schemes reduce the algorithms to MMOC-like techniques, but with more accurate treatment of boundary conditions.

The authors feel that ELLAM techniques possess great potential in multiphase flow applications. The operator-splitting techniques of [14–16] should motivate the proper choice of test functions, but better boundary condition accuracy is expected.

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