HIGH PERFORMANCE COMPUTING IN PETROLEUM APPLICATIONS

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Abstract. The purpose of mathematical reservoir simulation models in petroleum applications is to try to optimize the recovery of hydrocarbon from permeable underground reservoirs. To accomplish this, one must be able to predict the performance of the reservoir under various production schemes. There are two essential issues, modeling and software architecture design, while developing a comprehensive oil reservoir modeling platform that should be an integration of subsurface models, facility network models and economic models. Effective subsurface models must be constructed to describe the complex geomechanical, physical, and multiphase fluid flow processes that accompany the various recovery mechanisms. Upscaling needs to be utilized to provide effective rock properties for coarse-grid models used for field-scale simulations. However, localized flow regimes at sub-coarse grid scales must often be resolved using local grid refinement techniques. Finite volume element methods for accurate resolution of localized geometrics can be coupled with cell-centered finite difference methods used in many existing simulators. Aspects of coupling different grids, different discretization schemes, and different physical equations via mortar techniques will be presented. Reservoir simulation is an integration of various technologies through the construction of a reservoir model as well as optimization of production strategies. A comprehensive oil reservoir modeling platform should be an integration of different software applications or components and its software architecture should be scaleable, extendable and should have the capability to create and modify a workflow. Beyond the traditional three-tier software architecture, data, application, and user-interface, separation of control and business logic through those three tiers is proposed to achieve those goals. The aspect of the software architecture design will be discussed.

Key Words. Eulerian-Lagrangian localized adjoint method, mixed finite element method, petroleum reservoir simulation, separation of control and business logic, three-tier software architecture

1. Introduction

With rapid advances in information technology and computing power, large-scale oil reservoir simulations become the routine work in upstream asset development. The objective of oil reservoir simulation is to understand the complex chemical, physical, and fluid flow processes occurring in an underground porous medium sufficiently well so as to be able to optimize oil production strategy that is usually constrained by the volatile oil prices. To do this, one must be able to predict

the performance of the reservoir under various recovery scenarios. Consequently, a comprehensive oil reservoir modeling platform that is an integration of subsurface, facility network technologies and economics needs to be developed. There are two essential issues in development of this platform. An integrated model of reservoir, facility network and economic models must be efficiently constructed to yield information about complex subsurface phenomena and surface facility network accompanying different recovery scenarios. The software architecture design of the platform should be extendable to plug-in new software components and be flexible to create and to modify workflows that address various simulation scenarios. Among various important physical, mathematical and software development issues, we focus on the complex subsurface modeling processes and an improved software architecture design in this paper.

There are four major stages to the subsurface modeling process. First, a physical model of the flow processes is developed incorporating as much geology, chemistry, and physics as is deemed necessary to describe the essential phenomena. This requires the interaction of geologists, geophysicists, chemical and petroleum engineers, etc. Second, a mathematical formulation of the physical model is obtained, usually involving coupled systems of nonlinear, time-dependent partial differential equations. The analyses of these systems of differential equations are often quite complex mathematically. Third, once the properties of the mathematical model, such as existence, uniqueness, and regularity of the solution, are sufficiently well understood, a discretized numerical model of the mathematical equations is produced. A numerical model is determined that has the required properties of accuracy and stability and which produces solutions representing the basic physical features as well as possible without introducing spurious phenomena associated with the specific numerical scheme. Finally, a computer code capable of efficiently performing the necessary computations for the numerical model is developed. The total modeling process encompasses aspects of each of these four intermediate steps. This involves the multidisciplinary interaction of a wide variety of scientists. It is rare to find all of this expertise in one group or at one location. Thus the effective simulation of these problems should entail collaboration of scientists, often across disciplines and institutions, to address the enormous complexity of these models. Finally, the modeling process is not complete with one pass through these four steps. An optimized subsurface model should be developed by minimizing the difference between simulation results and field and lab observations by iterations through those four stages.

A comprehensive oil reservoir modeling platform should provide such a collaborative environment to support the multi-disciplinary collaborations. The aspects involved in the architecture design are three folds, an integrated central data repository that extracts, transforms and archives large amounts of incongruous data from domain specific data sources such as well log data, seismic data, well testing data, production data, rock and fluid properties, etc. and the flexibility to efficiently create, to manage and to modify a workflow that addresses various recovery scenarios. Beyond the traditional three tier software architecture, data, application and user-interface, separation of control and business logic through those three tiers is proposed to effectively and efficiently address those issues.

In this paper, we will discuss and survey some of the advanced numerical technologies that can be applied to improve the subsurface modeling as well as advanced software architecture design that allows effective integration of subsurface technologies. Some simulation results will be presented to illustrate those concepts.

2. Reservoir Characterization

The processes of both single- and multiphase flow involve convection, or physical transport, of the fluids through a heterogeneous porous medium. The equations used to simulate this flow at a macroscopic level are variations of Darcy's law. Darcy's law has been derived via a volume averaging of the Navier-Stokes equations, which govern flow through the porous medium at a microscopic or pore-volume level. Reservoirs themselves have scales of heterogeneity ranging from pore-level to field scale. In the standard averaging process for Darcy's law, many important physical phenomena which may eventually govern the macroscopic flow are lost. We discuss certain techniques that are beginning to address these scaling problems.

Since the velocity variations are influenced at all relevant length scales by the heterogeneous properties of the reservoir, much work must be done in volume averaging or homogenizing or flow-based upscaling of terms like porosity and permeability. Statistical methods that can be calibrated with existing field observations have shown promise in this area [4, 18].

Many of the multiphase flow processes are characterized by the chemical and physical interaction of the fluids. Therefore, diffusive or dispersive mixing of fluids is sometime critical to the flow processes and should be understood and modeled accurately. Molecular diffusion is typically quite small. However, hydrodynamic dispersion, or the mechanical mixing caused by velocity variations and flow through heterogeneous rock, can be extremely important and should be incorporated in some way in our models.

The effects of dispersion in various flow processes have been discussed extensively in the literature. Russell and Wheeler [53] and Young [59] have given excellent surveys of the influence of dispersion and attempts to incorporate it in present reservoir simulators. Various terms which affect the length of the dispersive mixing zone include viscosity and velocity variations and reservoir heterogeneity. The dispersion tensor has strong velocity dependence [26, 53]. Initial work on correlation of dispersion coefficients presented with statistical simulations was presented in [36].

3. Model Equations for Porous Media Flow

3.1. Model Equantions. The basic one is the model of multi-phase and multi-component fluids flow in compressible porous media. The simplified version such as black oil model can be derived from the multi-phase and multi-component model by honoring some specific assumptions. The mathematical formulation is based on the Darcy's law and mass balance equations as follows (see, e.g., [7]):

$$(1) \qquad \mathbf{u}_\alpha = -\frac{\mathbf{K}k_r\alpha}{\mu_\alpha}(\nabla p_\alpha - \gamma_\alpha \mathbf{g}), \qquad \text{in } \Omega,$$

where ρ_α is the fluid density, $\mathbf{K}$ is the absolute permeability tensor and $k_{r\alpha}$ is relative permeability that is generally a function of phase saturations, μ_α is the dynamic fluid viscosity that depends on pressure and temperature, p_α is the phase pressure of multi-phase fluid, and $\mathbf{g}$ is the acceleration vector due to gravity. The subscript α in the equation is referred to various phases, oil, water and gas.

Darcy's law provides a relation between the volumetric flux in the mass conservation equation and the pressure in the fluid. This relation is valid for viscous dominated flows which occur at relatively low velocities.

Physically, fluid mass should be conserved in terms of component that may present in phases. It is common in petroleum reservoir simulation to assume that mass exchange between hydrocarbon phases and water is negligible. Consequently, the mass balance equation of hydrocarbon component can be derived accordingly:

(2) $\dfrac{\partial(\phi m^i)}{\partial t} + \nabla \cdot (\rho_o \mathbf{u_o} c_o^i) + \nabla \cdot (\rho_g \mathbf{u_g} c_g^i) = F^i, \quad i = 1, \dots, N_c, \quad \text{in } \Omega, \quad t > 0.$

(3) $\dfrac{\partial(\phi m^w)}{\partial t} + \nabla \cdot (\rho_w \mathbf{u_w}) = F^w, \qquad i = 1, \dots, N_c, \qquad \text{in } \Omega, \quad t > 0.$

Here m^i or m^w represents the total number of moles of hydrocarbon component i or water component, c_o^i and c_g^i are the mole fraction of hydrocarbon component i in oil and gas phase, respectively, ρ_o, ρ_g and ρ_w are the molar density of oil, gas and water phase, ϕ is the porosity of rocks, and N_c is the total number of hydrocarbon components. $F^i (i = 1, \dots, N_c, w)$ represents sink/source terms that should be a function of different variables in regarding to various well constraints. Under the assumption that pore volume of porous media is fully filled with fluids, the following volumetric constraint holds [1, 13, 54]:

(4) $$S_T = S_w + S_o + S_g = 1.$$

where S_w, S_o and S_g are the water, oil and gas saturations.

Assumption of thermodynamic phase equilibrium for a given pressure-volume-temperature state at every moment is imposed to calculate the phase distribution. Phase equilibrium is characterized by equalization of chemical potentials of each component in different phases. Equation (1),(2), and (3) form a coupled system of nonlinear partial differential equations that is coupled with phase equilibrium constraints and volumetric constraint (4).

In order to solve such a system, an efficient linearization technique needs to be applied to solve this system numerically. One of the important issues in linearization process is the choice of solution unknowns that will result in various compositional formulations [1, 3, 14, 17, 50, 54]. By the Gibbs phase rule one conclude that the system is uniquely determined by $N_c + 2$ extensive variables, which are called primary variables. Other variables are the functions of the primary variables.

In addition to Equations (1) – (3), initial and boundary conditions are specified. The flow at injection and production wells is modeled in Equations (2) and (3) via point or line sources and sinks.

The equations presented above describe multi-phase and multi-component fluid flow in porous media. However, in order to use these equations effectively, parameters that describe the rock and fluid properties for the particular reservoir application must be input into the model. The relative permeabilities, which are nonlinear functions of water and gas saturations, can be estimated via laboratory experiments using reservoir cores and resident fluids. However, the permeability $\mathbf{K}$ and the porosity ϕ are effective values that must be obtained from local properties via scaling techniques. In addition, the inaccessibility of the reservoir to measurement of even the local properties increases the difficulties [29, 34, 58].

3.2. Linearization Techniques. Once the primary varibles are chosen, an effective linearization technique should be proposed to decouple Equaitons (1) – (3). There are various linearization strategies being discussed [1, 14, 50, 54]. In this paper, we propose a sequential solution procedure for the linearization with the choice of primary variables $p, m^i, (i = 1, \dots, N_c)$ and S_w. Here p is oil phase pressure, m^i is the total number of moles of i hydrocarbon component and S_w is water saturation.

Notice that the constraint (4) is a function of the primary variables. If one differentiates the constraint equation (4) with time t and replaces $\partial S_w / \partial t$ and

$\partial m^i / \partial t$ with Equations (2) and (3) incorporated with Darcy's law (1), one obtains the following pressure equations [1, 50, 54]:

$$(5) \quad \beta_T \frac{\partial p}{\partial t} - \mathbf{K} \left[\sum_{i=1}^{N_c} \frac{\partial S_T}{\partial m^i} \nabla \cdot (\rho_o \lambda_o c_o^i + \rho_g \lambda_g c_g^i) \nabla + \frac{\partial S_T}{\partial S_w} \nabla \cdot (\lambda_w \nabla) \right] p = r_p,$$

where β_T is the total compressibility, $\lambda_\alpha = k_{r\alpha}/\mu_\alpha, \alpha = oil, gas, water$ and the right-hand-side r_p is volumetric discrepancy error [1, 54]. Equaiton (5) is a parabolic PDE with respect to the pressure p and can be solved by finite difference, finite element and finite volume methods. After numerical solution p^h is obtained, one computes the numerical phase velocities using Equation (1). Then $m^i(i = 1, \ldots, N_c)$ and S_w can be obtained using Equations (2) and (3). In this paper, we will discuss the numerical solution methods for solving those equations.

4. Mixed Methods for Accurate Velocity Approximations

In reality, the subsurface geology is strongly heterogeneous, the absolute permeability $\mathbf{K}$ can be very rough. In this case the exact solution of pressure of Equation (4) is not neccessarily smooth and so the numerical solution p^h might not be accurate. As a result, the numerical Darcy's velocities u_o^h, u_g^h and u_w^h obtained from Equation (1) by numerically differentiating p^h and multiplying p^h by a rough coefficient $\mathbf{K}$ are even less accurate. This in turn affects the accuracy of thenumerical approximations to other primary variables through the substitution of phase velocities into Equations (2) and (3). While pressure p may be rough, the total velocity $\mathbf{u} = \mathbf{u}_o + \mathbf{u}_g + \mathbf{u}_w$ is usualy smooth. Consequently, we adopt an mixed finite element method to solve the following system of first-order PDEs for pressure p and total velocity $\mathbf{u}$ [50, 54]:

$$(6) \quad \frac{dp}{dt} + \nabla \cdot \mathbf{u} = R_p, \mathbf{u} + \lambda_T \mathbf{K} \nabla p = R_u.$$

Here $\lambda_T = \lambda_o + \lambda_g + \lambda_w$ and the total derivative d/dt is defined:

$$(7) \quad \frac{d}{dt} = \beta_T \frac{\partial}{\partial t} + \sum_{i=1}^{N_c} \nabla \frac{\partial S_T}{\partial m^i} (\rho_o \lambda_o c_o^i + \rho_g \lambda_g c_g^i) \nabla + \nabla \frac{\partial S_T}{\partial S_w} (\lambda_w \nabla),$$

After total velocity $\mathbf{u}$ is obtained from equation (6), the phase velocities can be computed by:

$$(8) \quad \mathbf{u}_\alpha = f_\alpha \mathbf{u}_\alpha + f_\alpha \mathbf{K} \sum_{j \neq \alpha} \lambda_j [\nabla (p_{cjo} - p_{c\alpha o}) - (\gamma_j - \gamma_\alpha) g \nabla z],$$

where the fractional flow functions f_α is defined as $f_\alpha = \lambda_\alpha / \lambda_T$.

In this section, we describe mixed finite element methods for the accurate approximation of the total velocity $\mathbf{u}$. Among the disadvantages of the conforming discretizations are the lack of local mass conservation of the numerical model and some difficulties in computing the phase velocities needed in the transport and saturation equations. The straightforward numerical differentiation is far from being justifiable in problems formulated in a highly heterogeneous medium with complex geometry. On the other hand, the mixed finite element method [10] offers an attractive alternative. In fact, this method conserves mass cell by cell and produces a direct approximation of the two variables of interest—pressure and velocity. Below we explain briefly the mixed finite element method for the pressure equation.

To describe the mixed method we introduce two Hilbert spaces. Let

$$W = L^2(\Omega), \qquad \boldsymbol{V} = \left\{ \boldsymbol{\varphi} \in L^2(\Omega)^3, \ \nabla \cdot \boldsymbol{\varphi} \in L^2(\Omega) \right\}.$$

The inner product in $L^2(\Omega)$ is denoted by $(\cdot, \cdot)$. For the sake of simplicity, $(\cdot, \cdot)$ is also used as the inner product in the product space $L^2(\Omega)^3$.

The pressure equation is written in the following mixed weak form: for $W = L^2(\Omega)$ and $\boldsymbol{V} = H(\text{div}, \Omega)$, find $(p, \mathbf{u}) \in W \times \boldsymbol{V}$ such that [10]

$$
\begin{aligned}
(A\mathbf{u}, \boldsymbol{\varphi}) - (p, \nabla \cdot \boldsymbol{\varphi}) &= (R_u, \boldsymbol{\varphi}), &&\forall \, \boldsymbol{\varphi} \in \boldsymbol{V}, \ t > 0, \\
(p_t, \psi) + (\nabla \cdot \mathbf{u}, \psi) &= (R_p, \psi), &&\forall \, \psi \in W, \ t > 0, \\
p(0) \in L^2(\Omega) &\text{ is the given initial pressure.}
\end{aligned}
$$
(9)

Here $p_t = dp/dt$, $A = (\mathbf{K}\lambda_T)^{-1}$. We note that A is always symmetric and positive definite which leads to a well defined problem.

We triangulate the domain Ω in tetrahedras with characteristic diameter h. Next we introduce the finite element spaces $W_h \subset W$ and $\boldsymbol{V}_h \subset \boldsymbol{V}$ of piecewise polynomials with respect to the triangulation and time discretization $t_n = n\Delta t$, $n = 0, 1, \ldots$. The mixed finite element approximation $(P^n, \boldsymbol{V}^n) \in W_h \times \boldsymbol{V}_h$ of $(p(t_n), \mathbf{u}(t_n)) \in W \times \boldsymbol{V}$ is the solution of the following problem:

$$
\begin{aligned}
(A^n\mathbf{u}^n, \boldsymbol{\varphi}_h) - (\nabla \cdot \boldsymbol{\varphi}_h, P^n) &= (R_{uv}^n, \boldsymbol{\varphi}_h), &&\forall \, \boldsymbol{\varphi}_h \in \mathbf{V_h}, \\
\frac{1}{\Delta t}(\beta^n(P^n - P^{n-1}), \psi_h) + (\nabla \cdot \mathbf{u}^n, \psi_h) &= (R_p^n, \psi_h), &&\forall \, \psi_h \in W_h, \\
P^0 \in W_h &\text{ is expressed through given initial data.}
\end{aligned}
$$
(10)

This is an implicit Euler approximation of a nonlinear problem which can be solved by Picard or Newton iterations.

5. Eulerian-Lagrangian Techniques

Sustituting the phase velocities $\mathbf{u}_o$, $\mathbf{u}_g$ and $\mathbf{u}_w$ obtained from Equation (8) into Equations (2) and (3) and assuming that water phase and rocks are incompressible, we rewrite Equations (2) and (3) as follows:

$$\phi \frac{\partial m^i}{\partial t} + \nabla \cdot (\mathbf{u}^i m^i) - \nabla \cdot (D^i \nabla m^i) = R^i,$$
(11)

and

$$\phi \frac{\partial S_w}{\partial t} + \nabla \cdot (\mathbf{u} f_w(S_w)) - \nabla \cdot (D^w \nabla S_w) = R^w.$$
(12)

Here the right-hand-side are given as follows:

$$\text{(13)} \quad R^w = \nabla \cdot \left(\sum_{i=1}^{N_c} D^i \nabla m^i \right) + q^w, \quad \text{and} \quad R^i = \nabla \cdot \left(\sum_{j=1; j \neq i}^{N_c} D^j \nabla m^j \right) + q^i,$$

the barycentric velocity is defined as follows:

$$\text{(14)} \qquad \mathbf{u}^i = \left[\left(\frac{m_o^i}{m^i} \right) \left(\frac{f_o}{v_o} \right) + \left(\frac{m_g^i}{m^i} \right) \left(\frac{f_g}{v_g} \right) \right] \mathbf{u}.$$

In Equation (11), 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 [23, 35, 51]. The analogue of Equation (11) can be written as follows:

$$(15) \qquad \phi\frac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c - \nabla \cdot \mathbf{D}\nabla c = q \ .$$

Here c stands for m^i, $\mathbf{u}$ for $\mathbf{u}^i$ and q for R^i. Next, the first and second terms in Equation (15) 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

$$(16) \qquad \nabla \cdot (\mathbf{D}\nabla c) + q = \phi\frac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c \equiv \phi\frac{\partial c}{\partial \tau} \ .$$

The system obtained by modifying Equations (1) and (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 Equations (1) and (2) with the fluid viscosity μ evaluated via some mixing rule at time level t^{n-1}. Equations (1) and (2) can be solved as a mixed finite element method for a more accurate fluid velocity as in the last section. Let $C^n(x)$ 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

$$(17) \qquad \phi\frac{\partial c}{\partial \tau}(x,t^n) \approx \phi\frac{C^n(c) - C^{n-1}(\bar{x}^{n-1})}{\Delta t} \ ,$$

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

$$(18) \qquad \bar{x}^{n-1} = x - \frac{\mathbf{U}^n(x)\Delta t}{\phi}.$$

This technique is a discretization back along the "characteristic" generated by the first-order derivatives from Equation (16). Although the advection-dominance in the original Equation (16) 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 spatial discretizations.

In multiphase and multi-component flow, it is common to assume that there is no mass exchange between water and hydrocarbon components. The advection-diffusion equaiton for water concentration is highly nonlinear and the equation is given as follows:

In Equation (12), the convective part is nonlinear. A similar operator-splitting technique with a focus on splitting the fractional flow function to solve the water concentration Equation (19) needs reduced time steps because the pure hyperbolic part may develop shocks. An operator-splitting technique has been developed for multiphase flows [20, 21, 24, 25] which retains the long time steps in the characteristic solution without introducing serious discretization errors.

Let S stand for S_w. The operator splitting gives the following set of equations:

$$(19) \qquad \phi\frac{\partial \bar{S}}{\partial t} + \frac{d}{dS}\mathbf{f}^m(\bar{S}) \cdot \nabla \bar{S} \equiv \phi\frac{d}{d\tau}\bar{S} = 0 \ ,$$

$$(20) \qquad \phi\frac{\partial S}{\partial \tau} + \nabla \cdot (\mathbf{b}^m(S)S) - \epsilon\nabla \cdot (D(S)\nabla S) = \mathbf{q}(\mathbf{x},t) \ ,$$

$t_m \leq t \leq t_{m+1}$, 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 described in the last section.

The splitting of the fractional flow function into two parts: $\mathbf{f}^m(S) + \mathbf{b}(S)S$, is constructed [25] such that $\mathbf{f}^m(S)$ is linear in the shock region, $0 \leq S \leq S_1 < 1$,

and $\mathbf{b}(S) \equiv 0$ for $S_1 \leq S \leq 1$. Further, Equation (19) produces the same unique physical solution as

$$(21) \qquad \frac{\partial S}{\partial t} + \nabla \cdot (\mathbf{f}^m(S) + \mathbf{b}(S)S) = 0$$

with an entropy condition imposed. This means that, for a fully developed shock, the characteristic solution of Equation (19) always will produce a unique solution and, as in the single-phase case, we may use long time steps Δt without loss of accuracy.

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, I. Herrera, and the author have devised Eulerian-Lagrangian localized adjoint methods (ELLAM) [12, 47], a set of schemes that are defined expressly for conservation of mass properties.

The ELLAM formulation was motivated by localized adjoint methods [11, 46], which are one form of the optimal test function methods discussed above [5, 21, 25].

We next extend the ELLAM techniques to the nonlinear multiphase flow equations (see e.g., [19, 20, 21, 22, 28]). We consider the divergence form of the multiphase flow equation given by Equation (12) with ϕ assumed constant in time and ignoring the gravity term for simplicity:

$$(22) \qquad LS \equiv \phi \frac{\partial S}{\partial t} + \nabla \cdot (f_w \mathbf{u}) - \nabla \cdot D\nabla S = q_w, \quad x \in \Omega, \ t \in J,$$

$$(23) \qquad (f_w \mathbf{u} - D\nabla S) \cdot \nu = h, \quad x \in \partial\Omega, \ t \in J,$$

where ν is the outward unit normal to the boundary $\partial\Omega$. Let $\Sigma = \Omega \times J$ denote the space-time domain. Then we obtain a weak formulation of Equation (22) by integrating against a test function $w = w(x,t)$. This yields a weak form, $\int_\Sigma (LS)w\,dxdt = \int_\Sigma q_w\,dxdt$. We obtain the specific equation

$$(24) \qquad \begin{aligned} &\int_\Omega \int_J \phi(Sw)_t dtdx + \int_J \int_\Omega \nabla \cdot (f_w \mathbf{u} - D\nabla S)wdtdx + \int_\Sigma D\nabla S \cdot \nabla w\,dxdt \\ &- \int_\Sigma (\phi S w_t + f_w \mathbf{u} \cdot \nabla w)dxdt = \int_\Sigma q_w w\,dxdt. \end{aligned}$$

Then, as in [52], we begin to study the time dependence of the potentially useful test functions by looking at a semidiscrete scheme on the time interval $J^{n+1} = [t^n, t^{n+1}]$ or over the space time region $\sum^{n+1} = \Omega \times J^{n+1}$. By applying the divergence theorem to (24), we obtain

$$(25) \qquad \begin{aligned} &\int_\Omega \phi S(x, t^{n+1})w(x, t^{n+1})dx \ + \int_{\Sigma^{n+1}} D\nabla S \cdot \nabla w\,dxdt \\ &+ \int_{J^{n+1}} \int_{\partial\Omega} (f_w \mathbf{u} - D\nabla S) \cdot \nu \ wd\sigma dt \\ &- \int_{\Sigma^{n+1}} (\phi S w_t + \lambda_w \mathbf{u} \cdot \nabla w)dxdt \\ &= \int_\Omega \phi S(x, t^n)w(x, t^n)dx + \int_{\Sigma^{n+1}} q_w w\,dxdt. \end{aligned}$$

In order to consider the ELLAM formulation from [12] directly, we should look for solutions of the adjoint to treat the term of the form

$$(26) \qquad \int_{\Sigma^{n+1}} SL^* w \, dxdt = 0 \,.$$

Since L is not a linear operator, we must perform some linearizations before we apply the analogue of Equation (26) to treat the fourth term in Equation (25).

Motivated by [24], we define

$$(27) \qquad \bar{f}(S)S \equiv \begin{cases} \dfrac{df_w}{ds}(S^1)S, & 0 \le S \le S^1, \\[2mm] \dfrac{(1-r)}{(1-S^1)}S + c, & S^1 \le S \le 1, \end{cases}$$

where S^1 is the top saturation of an established front. This is the piecewise linearization of f_w using the top saturation of the established front and its value $f_w(S^1)$. Then, we define $b(s)$ by the difference of f_w and $\bar{f}S$. Thus,

$$(28) \qquad f_w = \bar{f}(S)S + b(S)S.$$

For $0 \le S \le S^1, b(S)S$ is an antidiffusive term causing the fronts to tend to sharpen. For $S^1 \le S \le 1, b(S)S$ is a diffusive term. Using these definitions, the fourth term in Equation (25) can be written as

$$(29) \qquad \begin{aligned} &\int_{\Sigma^{n+1}} S\left(\phi w_t + \left\{\bar{f}(S) + b(S)\right\} \mathbf{u} \cdot \nabla w\right) dxdt \\ &= \int_{\Sigma^{n+1}} S\left(\phi w_t + \bar{f}\mathbf{u} \cdot \nabla w\right) dxdt + \int_{\Sigma^{n+1}} Sb\mathbf{u} \cdot \nabla w \, dxdt. \end{aligned}$$

We cannot, in general, determine a test function w that satisfies $\phi w_t + \bar{f}\mathbf{u}\cdot\nabla w = 0$, even locally within each small space-time element. However, we will make a choice of test functions that will make this term small. Analysis of the size of this term will be presented elsewhere.

By choosing a test function $w(x,t)$ that is constant in time along the characteristics that define the moving Lagrangian frame of reference, we can make the first term in Equation (29) small. If the test function were a standard chapeau basis function in the x-direction, it would also make second term in Equation (25) small. This would be an effective test function if the second term on the right side of Equation (29) were zero or were small. However, in many multiphase flow problems, the $b(S)\mathbf{u}$ term is not small and the use of characteristics has not symmetrized the form which is analagous to the form in Equation (25). As above, the use of an upwinded form of the test function for constant x will efficiently treat the b term from Equation (29) together with the D term from Equation (25).

We thus arrive at a choice of $w(x,t)$ which is constant along the characteristics determined by the directional derivative along τ with $\bar{f}$ defined in Equation (27). Using these test functions, our approximation scheme can be defined in the interior of the region on prisms as in [52]. Also see [52] for treatments at the boundaries of domain.

Recently ELLAM techniques have been extended to a wide variety of applications [57, 50, 22, 38, 39, 40, 41, 42, 43, 55, 56]. Optimal order error estimates have been developed for advection [39], advection-diffusion [42, 56], advection-reaction [22, 38, 39, 40, 41, 42], and advection-diffusion-reaction [40, 55] systems.

6. Software Architecture

Software Architecture is critical in high performance computation in petroleum applications and it is even more critical in building an integrated petroleum application platforms. Software architecture is defined as the structure or structures of the programming system, which comprise software elements, the externally visible properties of those elements, and the relationships among them [2]. Over the past decades, software architecture has received tremendous attention as an essential field of study in software and its applications. In this section, we review important milestone software architectures and their practical applications. We will then propose a new innovative architecture and discuss its application in reservoir simulations.

6.1. Evolution of Software Architecture. At the very beginning of the software development (say between 1950s and 1970s), the software architecture was one-tier. That is, the developers and users concentrated on the input and output behavior of a program, ignored the internal structure of the software, and treated the entire program as one black box. This model worked for small programs and mainframe computers where all the control functions were centralized and multiple users accessed a computer by terminals. One fatal limitation of the one-tier architecture is that it is not able to easily support programs that are distributed in multiple hosts. In the middle of 1980s, as the development of computer network and distributed computing systems, two-tier software architecture was developed. The two-tier architecture usually consists of multiple clients and one server. Clients and server usually reside at different hosts and coordinately provide the functionality of the application. On the client site, functions such as session, text input, dialog, and display management are usually implemented. The data management functionality is typically realized at server site. The two-tier architecture improves usability, flexibility and scalability as compared to one-tier one. For example, a system with two-tier architecture can easily accommodate hundreds of users (clients) to access a service (server). Many of the web systems today are two-tier based. Nevertheless, the two-tier architecture has its own limitations. The interoperability is limited since the implementation of business logic relies on specific data management systems. When there is need to interoperate with more than one type of data management systems, the application has to be rewritten. The two-tier architecture is also restricted in its maintainability. As part of application logic resides on client, every upgrade or modification must be delivered, installed and tested on each client, increasing workload and costs. Three-tier architecture emerged in the 1990s to overcome the limitations of the two-tier architecture. A third tier (middle tier server) is added between the user interface (client) and the data management (server) components. This middle tier provides process management where rules and business logic are executed and can service more than 100 users with functions such as application execution, queuing and database staging. The three-tier software architecture is most appropriate in an effective distributed client/server environment. Compared to the two-tier, the three-tier architecture provides increased performance, flexibility, maintainability, reusability and scalability while hiding the complexity of distributed processing from the user. Due to these characteristics, the three-tier architecture is a popular choice for network-centric information systems and Internet applications. However, as the size and complexity of the software system grow, the three-tier architecture needs also to be improved as we discuss in the next section.

6.2. Basics of New 2x3 Architecture. For many large and complex software systems, the thee-tier architecture seems to be insufficient. For example, these software systems often require dynamically integration and configuration of multiple heterogeneous applications, and meanwhile handling huge data sets which might be dispersed geographically in different sites. The current available software architectures, such as two-tier, three-tier, cannot meet these requirements because they either mix-up the interface, data sources with application algorithms; or they hardwire the system control with payload data processing. These observations are validated via development of systems such as Virtual Network Laboratory [48], regional data center, reservoir simulation system, etc. We believe that the key issue is separation of control and payload processing. Here, terms "control" and "payload" are borrowed from the field of network communication. Most if not all communication protocols, which are proven to be very successful in the end, have clear separation of controlling processing and payload process. Such separation is essential since it distinguishes "how to do" (control) from "what to do" (payload). Under many circumstances, the payload process, i.e., the logics for solving a specific problem is well understood and developed independently. Control process is often applied to a number available payload processing logics so that a high level problem can be tackled. The separation of control from logic allows changes on control side without the need to change any payload processing logic, and vice versa. In this way, not only are the development and maintenance costs reduced greatly for large and complex software, the flexibility in run-time process change is no longer beyond the possibilities. Based on the principle of control and payload separation, we propose a scheme called 2x3 architecture in which there are two planes: control plan and logic plane. With each plane, there are three tiers, namely interface, business logic, and databases.
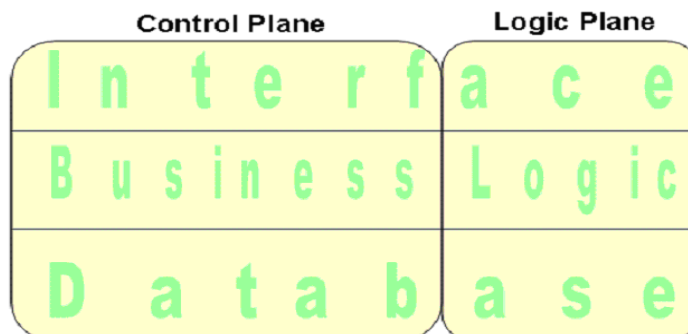

FIGURE 1. The New 2x3 Software Architecture

Our new 2x3 architecture should be able to offer explicit benefits by control and payload separation. Specifically, this architecture allows to

(1) Shortened development cycle and reduced development costs. The 2x3 architecture allows the developer to modify the control process without the need to change the underlying process logics. A new control process may correspond to a new solution to a certain problem. On the other hand, the developers are allowed to update any constituent process logics while the high level control process remains unchanged as long as the interface between the control and logic are kept same. The separation of control from logic let these two parts being taken care of by different groups, thus greatly shortening the software's time-to-shelf and cutting down the involved development costs.

(2) Provide better maintainability. The new 2x3 architecture offers better maintainability since the maintenance workload is separated into the two planes automatically. Moreover, people with domain specific expertise knowledge are allowed to take part in the software maintenance cycle and give domain specific supervision. This is especially true in a large integrated software system where system components are from different domains and dealing with vast different data sources. Some high level expertise need be introduced to monitor the overall control process so that the integration can be accomplished in the least effort and shortest time period.

(3) Improve system reliability. The software reliability is also improved with the 2x3 architecture being enforced. The system errors can be quarantined into different planes and different tiers, and are easier to be identified within the integral software framework.

(4) Increase run-time efficient. The separation of control from logic in the 2x3 architecture also enables run-time process adjustments that are beyond the possibilities of current architectures. It can also be expected that some useful software debugging and testing could be produced and deployed easily within such an architectural framework.

(5) Enhance Reusability. The reusability is enhanced by being possible in both planes: control process and logic process. On the one hand, a single control process, once being set up and verified, can be applied to different sets of logic processes; on the other hand, a single logic process can be incorporated into different control scenarios. Therefore both the control processes and logic processes are reusable with little efforts.

6.3. Application of 2x3 Architecture. At Texas A&M University, we have developed tools and reference systems that allow us to fully leverage the benefits of 2x3 architectures in developing large and complex software systems. Here we describe a reservoir simulation system which is developed by this new methodology. The payload part of the reservoir simulation system consists of multiple application modules which are dynamically configured and integrated under the instruction from the control plane. In our system, workflow is defined as a process that realizes the execution of such integrated multiple applications. As such, our control consists of workflow editor and verifier and workflow execution engine. For detailed description of these components, see [49].

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