ELSEVIER

Advances in Water Resources 25 (2002) 1147–1173

Advances in Water Resources

www.elsevier.com/locate/advwatres

Computational engineering and science methodologies for modeling and simulation of subsurface applications

Mary F. Wheeler *, Małgorzata Peszyńska

Texas Institute for Computational and Applied Mathematics, University of Texas, Austin, TX 78712, USA

Abstract

We discuss computational engineering and science (CES) methodologies and tools applicable to a variety of subsurface models and their couplings. First we overview both basic and widely recognized multiphase and multicomponent models. In the CES methodologies area we focus on accurate and robust numerical algorithms and linear and nonlinear solvers with parallel scalability. In the CES tools area, we discuss a few representative programming tools and technologies. We present several simulation examples which reflect the experiences of the research group at the Center for Subsurface Modeling at The University of Texas at Austin.

1. Introduction

The emergence of terascale computing capabilities and web technologies has given promise to significant advances in computational engineering and science. In theory, such capabilities and technologies should make possible simulations of physical phenomena of unprecedented sophistication and detail, depicting events that occur in many different spatial and temporal scales, that involve diverse physics and which involve interrogative and interactive collaborations among researchers at distinct and distant locations. It is expected that the 21st Century will bring the integration of system software, programming tools, and the seamless coupling of and communication between state-of-the-art simulation tools for use in a wide range of porous media applications. These include data structures and scalable software tools for adaptive modeling and meshing of coupled simulations, all complying with modern standards for verification of code and models. The purpose of this paper is to identify and briefly review a few of the currently promising computational engineering and science (CES) methodologies and information technology (IT) tools applicable to a variety of subsurface models and their couplings. Our selection of certain methodologies and tools reflects our own research experiences at the Center for Subsurface Modeling (CSM) at The University of Texas at Austin. We realize that most likely, we have neglected important results from other research groups; however, a broader perspective requires a monograph.

We start in Section 2 by recalling a few basic and widely recognized multiphase and multicomponent models of flow and transport in the subsurface. These form the basis for our subsequent discussion of selected numerical methods and IT tools. In addition, we discuss some new and important nonlinear extensions of these models, including couplings of models commonly called *multiphysics* couplings. There are two major types of such couplings. The first type is concerned with multiple phenomena occuring simultaneously in one domain; for example, flow and geomechanics must be coupled when modeling subsidence occuring from pumping water or hydrocarbons from a reservoir. The second type is concerned with phenomena occuring in separate continua which are interacting with each other through an interface; such splitting is defined in order to increase the speed of computations. Finally, we discuss additional modeling elements which form a *multiphysics computational framework* for general subsurface applications.

The numerical discretization of these models and the *multiphysics* couplings gives rise to major algorithmic challenges. These challenges include the issues of stability and accuracy of spatial and temporal discretizations. We are concerned with the robustness, efficiency and scalability, of the implementation of individual models and their couplings. In Section 3 we present results of our research on relevant algorithms. In particular, we focus

* Corresponding author.
E-mail address: mfw@ticam.utexas.edu (M.F. Wheeler).

0309-1708/02/$ - see front matter
PII: S0309-1708(02)00105-7

on two of the advanced discretization methods: (i) the *expanded mixed methods* applicable to multiblock nonmatching grids and the couplings of multiphase flow models, and (ii) the application of the Discontinuous Galerkin method for reactive transport. Furthermore, we discuss (iii) time-stepping issues and (iv) relevant findings in linear and nonlinear solvers; these issues are critical to the success of any simulation and, in particular, to those involving multiple models. Finally, we motivate and address the aspects of parallel implementation of the underlying algorithms.

Consider now a scientist or an engineer who, on an everyday basis, deals with the simulation of complex subsurface phenomena occuring at multiple scales with data coming from real-life applications. From their perspective, the models and discretizations, albeit fundamental to simulation, may be taken for granted, and their selection takes but a fraction of the total simulation time. The majority of their time is spent on general pre- and post-processing of simulation input and output data. Traditional tasks include mesh generation, incorporation of data from reservoir characterization, data management and manipulation, data exploration, visualization and interpretation. We devote Section 4 to modern dynamic IT tools which are beginning to replace, or to complement, traditional "manual" tasks. Specifically, we briefly discuss an example in which a few IT tools and technologies have been coupled to our simulator for application specification, program composition and optimization, adaptive runtime application management, collaborative and interactive application monitoring and steering, and active data management. This choice is, again, very particular, as it reflects our own research experience.

Our presentation of the ideas presented in this paper is accompanied by illustrations which demonstrate the capabilities of simulation tools developed at CSM. These illustrations are included in an attempt to motivate the presentation. Unfortunately, detailed discussion of these simulation results is outside the scope of this paper.

Last, but not least, we would like to mention several active research directions which are not, for lack of space, covered in this paper. These include in particular a range of multiscale algorithms. Here we refer the reader to research on mortar spaces [126] and other techniques of *upscaling* for example those in [15,74]. In the area of IT tools, we neglect several important areas; *mesh generation and refinement* tools, parallel performance analyses, verification and validation tools.

2. Modeling elements of a computational framework

Physical models are fundamental to any simulation. In the past, popular groundwater simulators like MODFLOW, FEMWATER or MT3D were built with one specific model in mind. In addition, it was commonly believed that most of the subsurface phenomena of interest occur in fully saturated formations below the water table. Discoveries of hazardous and radioactive chemicals transported through unsaturated zones [6], as well as high-profile disasters involving dams, earthquakes, and land subsidence due to groundwater pumping [129,188], have changed many such assumptions and have posed challenges to researchers designing and building subsurface simulators. It is now postulated [6] that such simulators should take into account a plethora of geological, geomechanical, hydrological, thermal, chemical and biological processes. In the meantime, similar challenges have affected simulators in the petroleum and gas industries. In particular, the use of sophisticated geomechanics models coupled to flow as opposed to the use of constant compressibility coefficients, is now considered to be a correct way to account for subsidence, cavity generation and other phenomena [59,114,116,151]. In general, since modeling of coupled phenomena is poorly understood, the simulators must allow for easy inclusion of new processes as well as the incorporation and assimilation of new data.

These are the motivations for the construction of a *multiphysics computational framework* which is intended for general purpose subsurface applications, including both environmental and resource recovery. With the emergence of new computational methodologies and with dramatic increases in computational power, such general purpose simulators with multiphase multicomponent physical models motivated by diverse applications are becoming popular in industry, government and academic research centers. These include: oil industry simulators Eclipse [148,149], Powers [66], VIP [92], and ACRES [2], as well as environmental simulators like TOUGH2 [130] STOMP [101,181] and UTCHEM [10] and many others not listed here. However, in spite of the progress in modeling and in computational techniques, frequently, still, only simple and, at times outdated, models are used to simulate a wide range of phenomenona (see discussion in [7]). In practice, users comfortable with the terminology, units system, and input/output tools of an established simulation tool are likely to remain loyal to that tool in spite of its limited computational capabilities.

To overcome some of these constraints and leverage resources, several groups have created general purpose computational frameworks, or PSE (Problem Solving Environments), which were developed with a broad scope of applications in mind. Models and applications are built on top of a set of common building blocks which handle memory management as well as I/O and visualization, provide parallel communication tools and a suite of solvers etc. Examples include general-purpose simulators like Sierra [5] or UG [26]. In our group we

have developed the IPARS framework (Integrated Parallel Accurate Reservoir Simulator) [119,166,177] which is equipped with general multiphysics multiblock capabilities and was designed for subsurface applications [104,125,126].

The fundamental modeling elements of such a computational framework are described below. First, we recall a few models of flow and transport in the subsurface which provide a background for the advanced discretization methods discussed in Section 3. Second, we motivate and discuss the concept of model couplings which we refer to as *multiphysics* and which can be split into two categories: (A) couplings of models defined in separate domains which interact across a common interface and (B) couplings of models defined in the same or, in general, in overlapping domains. Finally, we discuss other elements of a general purpose computational framework for subsurface applications in which multiple physical models can coexist and be coupled in various ways. Our exposition is illustrated by simulation examples which were obtained with our framework IPARS [119,166,177].

2.1. Models

Consider a porous medium of porosity ϕ with general anisotropic nonhomogeneous (intrinsic) permeability tensor $\mathbf{K}$. Other measurable quantities like *hydraulic conductivity* can be used instead of $\mathbf{K}$, and porosity can be combined with the *moisture content* variable. Here D denotes depth and G is the gravity constant. For simplicity we assume isothermal conditions. Multiple flowing phases are denoted by the subscript m, each with associated pressure P_m, density ρ_m, saturation S_m, relative permeability k_m and viscosity μ_m, with mobility $\lambda_m = (k_m/\mu_m)$. Note that $\sum_m S_m = 1$. Dissolved and flowing multiple components are denoted with subscript M. Since a component can exist in more than one phase, we define n_{mM} as the mass fraction of component M in phase m and the total concentration of a component as $N_M = \sum_m \rho_m S_m n_{mM}$. Also, since one phase can consist of more than one component we have $\sum_M n_{mM} = 1$. This is a standard formulation which is discussed in [48,98,121] (see also review [145]).

Assuming isothermal and local equilibrium conditions, the conservation of mass is written for each component as follows:

$$\frac{\partial(\phi N_M)}{\partial t} + \nabla \cdot \boldsymbol{V}_M = q_M + \sum_m \phi S_m R_{mM}. \tag{1}$$

The source term q_M represents injection/production wells; the terms R_{mM} denote chemical reactions. Flux $\boldsymbol{V}_M$ is the overall mass flux of component M,

$$\boldsymbol{V}_M = \sum_m \rho_m (n_{mM}\boldsymbol{U}_m - \phi S_m \boldsymbol{D}_{mM} \nabla n_{mM}), \tag{2}$$

where $\boldsymbol{U}_m$ is the velocity of phase m, and the remaining term is diffusive/dispersive flux. The definition of $\boldsymbol{U}_m$ comes from momentum conservation which is given by either Darcy's law

$$\boldsymbol{U}_m = -\mathbf{K}\lambda_m(\nabla P_m - \rho_m G \nabla D), \tag{3}$$

Forchheimer, Navier–Stokes, or yet another law, e.g. [85].

The system is closed by adding capillary pressure relationships $P_{cm_1m_2} = P_{m_1} - P_{m_2}$ with $P_{cm_1m_2}$ determined experimentally along with relative permeabilities k_m, both typically fluid and rock-type specific functions of saturation. Note that $k_m(S_m)$ is typically a nondecreasing function. Additionally, equations of state (constitutive laws) specify the dependence of density ρ_m and viscosity μ_m on pressure P_m and composition n_{mM}.

A standard approach for including complicated equilibrium and nonequilibrium adsorption in the system (1) and (2) is to make species in a stationary phase assume a new identity M' different from one (denoted by M) that they have in flowing phases. To this end one needs to rewrite (1) for a stationary phase with ϕ replaced by $1-\phi$. Obviously, $\boldsymbol{V}_{M'} = \mathbf{0}$ and $q_{M'} = 0$. With this convention the adsorption, desorption, dissolution and precipitation, or any other exchange between stationary and flowing phases, are modeled by reaction terms [22].

A specific physical model arises from general Eqs. (1) and (2) by adding assumptions, modifications, or simplifications. Examples follow:

2.1.1. Two-phase flow model

For a simple two-phase (oil–water or air–water or oil–gas) flow model we assume that reactive terms in (1), as well as dispersive terms in (2), are zero. Furthermore, we assume immiscibility or, in other words, that "phase" is identified with "component" for both the wetting fluid ($w \equiv W$) and the nonwetting fluid ($n \equiv N$) and therefore that $n_{nN} = 1, n_{wW} = 1, n_{nW} = 0, n_{wN} = 0$. The mass conservation equation following (1) is

$$\frac{\partial(\phi N_W)}{\partial t} + \nabla \cdot (\rho_w \boldsymbol{U}_w) = q_W, \tag{4}$$

$$\frac{\partial(\phi N_N)}{\partial t} + \nabla \cdot (\rho_n \boldsymbol{U}_n) = q_N. \tag{5}$$

Definition of phase velocities follows Eq. (3) or is modified to account for high gas velocities. Application specific parameters and terminology, e.g. *hydraulic head* instead of pressure, *suction* instead of capillary pressure, or *moisture content* instead of saturation times porosity, can be defined and applied. Values of relative permeabilities and capillary pressure as well as the scale of a problem are strongly dependent on a given application. Still, the main difference between the two-phase models discussed here comes from state equations for liquids

(oil, water) and gases (air, hydrocarbon gas). For example, the water phase is incompressible or slightly compressible whereas air can be assumed to satisfy the real gas law. Some models assume that the air phase is under atmospheric pressure and derive Richards equation [135] which collapses the system (4) and (5) to one nonlinear equation. In addition, the choice of units for each N_M may be critical in implementation: the gas phase/component may be three orders of magnitude lighter than liquid phases. As a result, the residuals formed in the linear/nonlinear solution process may differ by orders of magnitude. To make them compatible, one may simply divide equations (4) and (5) by standard (reference) density values. Concentration variables are modified as $N_M \mapsto \overline{N}_M = (N_M/\rho_{m,\mathrm{ref}})$. Remaining terms are changed as well, for example $q_M \mapsto \overline{q}_M = (q_M/\rho_{m,\mathrm{ref}})$, and one may use the notion of pressure (and in general, composition) dependent on *formation volume factors* $B_m = (\rho_{m,\mathrm{ref}}/\rho_m)$. As a result, we obtain

$$\frac{\partial(\phi\overline{N}_W)}{\partial t} + \nabla\cdot\left(\frac{1}{B_w}\boldsymbol{U}_w\right) = \overline{q}_W, \tag{6}$$

$$\frac{\partial(\phi\overline{N}_N)}{\partial t} + \nabla\cdot\left(\frac{1}{B_n}\boldsymbol{U}_n\right) = \overline{q}_N. \tag{7}$$

Applications of this two-phase model are multi-fold as they apply to the unsaturated zone (air–water) or waterflooding in high pressure oil reservoirs or to low pressure gas reservoirs. See Fig. 1 for simulation results in an oil–water reservoir and Fig. 4 for results of coupling this model with reactive transport.

2.1.2. Three-phase model

A more complex example is the three-phase model which accounts for the flow of three distinct phases: water, liquid (mainly hydrocarbon components) and gaseous (air or hydrocarbon). The easiest such model is *immiscible*, and it is composed of the system (6) and (7), where the nonwetting phase N is the liquid phase identified with the nonwetting component n, which is complemented with the gas component equation

$$\frac{\partial(\phi\overline{N}_G)}{\partial t} + \nabla\cdot\left(\frac{1}{B_g}\boldsymbol{U}_g\right) = \overline{q}_G. \tag{8}$$

In this model, the gas component is identified with the gas phase. Appropriate models for three-phase relative permeabilities and capillary pressures [60] which exploit existing two-phase data complement the system (see [86,100]).

In this paper we are interested in more general three-phase flow models which are relevant to the following two significant applications: (i) the *water–NAPL–air* model [86,101,181] used for the simulation of oil spills and associated remediation efforts, and (ii) the *black-oil* (*water–oil–gas*) model popular in the petroleum industry [31,48,98,110,121,162]. In these applications there can be several components, including aqueous W, heavy hydrocarbon O, light hydrocarbon G or air A, which can exist in multiple phases. For example, the water component can exist in the liquid (water) phase as well as in the vapor phase which is mixed with air and/or hydrocarbons. In general, the components become *fully* or *partially miscible* with others depending upon the prevailing pressure and temperature conditions. This dependence is quantified by thermodynamic equations of state specific to the application [160]. In addition, viscosities can be made composition dependent.

In some cases, some of the three phases may disappear in some parts of the reservoir. For example, consider the black-oil model (Fig. 2) and assume that $n_{wW} = 1$, $n_{gG} = 1$, $n_{oW} = 0$ [98,104,106]. This model can be cast in the form similar to (6) and (7) with $N = O, n = o$, which is complemented by the gas component equation

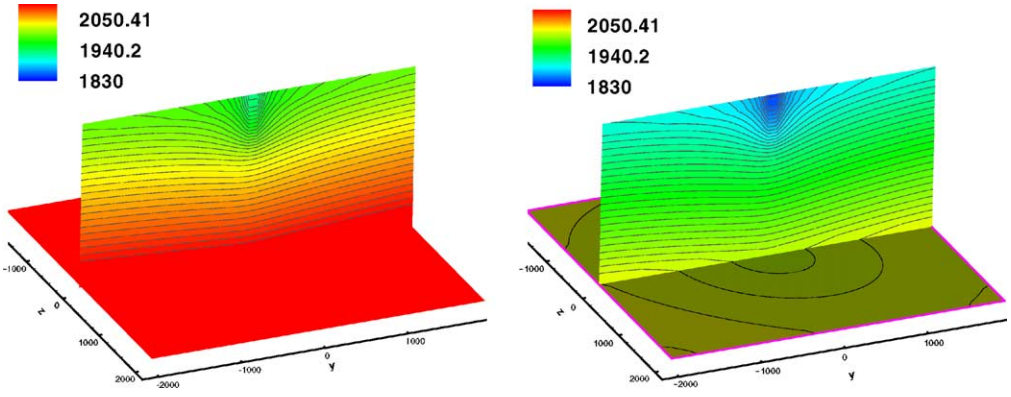

Fig. 1. Pressure contours for the simulation of (two-phase) primary depletion from a reservoir. Reservoir (A) is in contact with an aquifer that is represented by the Dirichlet condition (left) and (B) is situated over impermeable strata which are represented by the Neumann no-flow condition (right). The same contour levels are used for both cases.

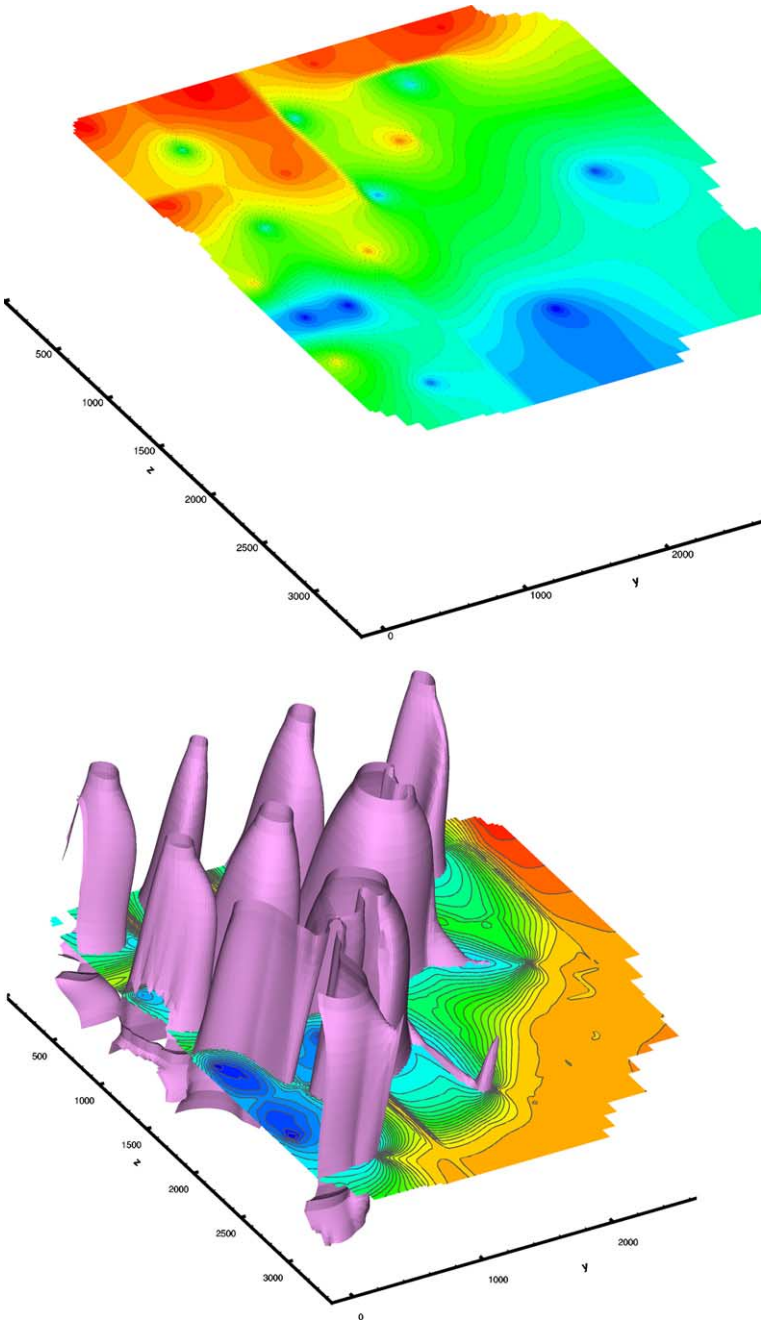

Fig. 2. Water pressure contours (top) and oil concentration contours (bottom) superimposed over isosurfaces of gas saturation in a black-oil reservoir with 20 wells. Simulation uses black-oil model and 501,401 unknowns. Note the position of 10 injection wells (high pressure = red) and of 10 production wells (low pressure = blue). Visible are coning effects as well as influence of impermeable faults: one fault is located to the right of the well in the lower left corner, another is between two wells closest to the right upper corner.

$$\frac{\partial(\phi\overline{N}_G)}{\partial t} + \nabla\cdot\left(\frac{1}{B_g}\boldsymbol{U}_g + R_o\frac{1}{B_o}\boldsymbol{U}_o\right) = \overline{q}_G. \tag{9}$$

Here we use an auxiliary thermodynamic quantity R_o to denote the ratio of dissolved gas amount to oil amount. At pressures higher than the *bubble pressure*, the gas is entirely miscible in the oil phase with $R_o = \overline{N_G}/\overline{N_O}$ and $S_g = 0$, from which it follows that $k_g = 0$ and $\boldsymbol{U}_g = 0$ (two-phase conditions).

In some cases, the appearance and disappearance of the phases can be predicted. In other words, it can be localized in space and in time. In such cases it is advantageous to use a reduced model locally. This concept of local reduction of a model is exploited in our *multiphysics* couplings described in Section 2.2.

2.1.3. Reactive transport in saturated zones

Here we consider a single phase multicomponent reactive transport model, in which the dependence of the density of the water phase on pressure and composition is ignored, i.e. $\rho_w = \rho_{w,\mathrm{ref}}$. Water can be treated as one of the components, but since it is the only phase, the notion of saturation S_w and of relative permeabilities k_w is obsolete. Darcy's law then is written using $\mu = \mu_w$, $P = P_w$, $\rho = \rho_w$, as

$$\boldsymbol{U} = -\mathbf{K}\frac{1}{\mu}(\nabla P - \rho G \nabla D) \tag{10}$$

Furthermore, if the rock formation is incompressible ($\partial\phi/\partial t = 0$) we obtain the following mass conservation equation for water, with $q_W \mapsto \overline{q_W} = (1/\rho_{w,\mathrm{ref}})q_W = \overline{q}$:

$$\nabla \cdot \boldsymbol{U} = -\nabla \cdot \mathbf{K}\frac{1}{\mu}(\nabla P - \rho G \nabla D) = \overline{q}. \tag{11}$$

Effects of adsorption, dispersion, as well as chemical reaction, are modeled by the following equation written for concentration of each species $c_M = n_{wM}\rho_w$ (not including the water component):

$$\phi\frac{\partial c_M}{\partial t} + \nabla \cdot (\boldsymbol{U}c_M - \phi \boldsymbol{D}_M \nabla c_M) = q_M + \phi R_M. \tag{12}$$

In general, the diffusion–dispersion tensor $\boldsymbol{D}_M = \boldsymbol{D}_{wM}$ is dependent upon the velocity $\boldsymbol{U} = \boldsymbol{U}_w$, and it includes molecular and Fickian diffusion as well as transverse and longitudinal dispersion. Eq. (12) is a well-known reactive transport model used to simulate the transport and fate of chemicals, remediation and biodegradation (see [145,183] and references therein).

2.2. Multiphysics

As explained above, it has been recognized that simulation of flow and transport in the subsurface must be accompanied by simulation of all the coupled phenomena that influence, or are influenced by, the flow and transport [6,188]. The strength of the coupling between some phenomena can become apparent only at some particular spatial and temporal scales or only in some special application-dependent cases. In addition, some of the most complicated phenomena may be very localized. Therefore it is important to design a simulator which allows for the selection of simpler local models whenever appropriate, and, at the same time, would enable couplings whenever necessary. These days, as an alternative to large comprehensive models which account for all of the phenomena at once, one sees the emergence of the *multiphysics* couplings which enable the local-in-space or local-in-time couplings of individual models which sometimes can be considered "black boxes". At times, these "black boxes" can arise as (parts of) legacy code capable of simulating certain individual isolated processes. They can be incorporated in the multiphysics simulator without the need to invest major resources in the development of a comprehensive model. Such a general modular strategy allows for incremental updates to the simulator whenever new measurements and theory become available. Finally, the multiphysics couplings can be used as a first step in deriving a comprehensive model to gather information on how to tune its individual pieces.

Research on combining local-in-space and local-in-time couplings is underway. However, in this paper, we divide multiphysics couplings into two types. First, in Section 2.2.1, we discuss the local-in-time couplings of models which are defined in the same domain or in general, in overlapping domains. Next, in Section 2.2.2 we discuss the local-in-space phenomena which practically means that the models can be defined in adjacent domains with physically meaningful conservation properties specified across their interface. Discretization in space and time as well as solvers are a challenge here (see Sections 3.1.1 and 3.5 for discussion). Both types of couplings can be realized in a loose (staggered-in-time) fashion or more tightly, where a solution is obtained by iterating between models. Time-stepping challenges arising in these couplings are discussed in Section 3.3. Parallel scaling and launching of different models on different remote platforms poses challenges (see Section 3.4).

2.2.1. Couplings in the same domain

Various geoscience applications have relied upon couplings of codes which operate in more or less the same or overlapping computational domains. These include 3D or 4D seismic models coupled to flow models which deliver information about permeability and other basic reservoir data. On the other hand, history-matching of reservoir simulation results relies on the coupling of flow models with sophisticated optimization packages [67,107,110]. Here we give two examples of couplings in the same domain: (i) geomechanics + flow and (ii) reactive transport + multiphase flow. Both can be thought of as a form of "operator-splitting" and as such, are subject to many delicate time-stepping problems.

The two couplings are similar in that they both involve a multiphase flow model. The major difference is that in case (i) an iterative (tight) two-way coupling between models is used whereas in case (ii) one-way coupling is used (flow influences the transport but not vice-versa).

Geomechanics + flow: It is well known that the state of stress affects the flow in porous reservoirs and that the fluid flow influences the mechanical behaviour of the rock formation. The basic models for coupled flow and geomechanics come from the classical theory of poroelasticity. The *Biot model* [33] of diffusion in elastic media describes laminar flow of a single-phase, slightly

compressible fluid through a purely elastic structure. Such models were historically developed in soil science and have been refined considerably for the increasingly more demanding needs of engineering and geophysics. The traditional use of a constant rock compressibility can be seen as a very special case of the Biot model but it has been shown to be inadequate for modeling the subsidence, fracturing and collapse of the structure.

In particular, a major subsidence research effort by the US Geological Survey [129] paralleled unprecedented growth in the use of ground water in North America, especially in California, Texas, and Arizona. Air–water systems coupled with geomechanics have been shown to be extremely important in applications to dam behavior during earthquakes, and the results are generally relevant to water transport in the vadose zone of soils [188]. In oil and gas reservoirs, the prediction of reservoir subsidence and formation of cavities is a highly nonlinear and difficult problem, and it requires plasticity models.

Numerical models of coupled flow + geomechanics involve one-way or staggered-in-time computations; see [62,102,113,115,116,150,151,172] (see also analysis in [152–154]). See Fig. 3 for an example of results from geomechanics + flow coupling which was run using an IPARS black-oil flow model and a geomechanics model in two-way coupling. In our approach, both models, the multiphase flow and the geomechanics model, can be seen as "black-boxes" which are accompanied by routines necessary to realize the two-way coupling.

Reactive transport + multiphase flow: In order to model the transport and fate of chemicals in the vadose zone, a reactive transport model has to be coupled to a multiphase flow model. Developments of this kind were discussed in excellent review papers [145,183]. Our model is based on our prior work [18,22,120,128].

In many instances, the assumption of (constant) equilibrium partitioning of components between multiple phases is valid. In such cases, a phase-summed (or other) model for reactive transport can be derived and coupled to any multiphase flow model. A phase-summed reactive transport model has a generic structure similar to the one in (12). Therefore both models, the multiphase flow model, and the reactive transport model, can be assumed to be "black-boxes". Obviously, additional post-processing and driver routines have to be added. An example of the results of such a coupling is shown in Fig. 4.

It turns out that such a coupling of an existing and complex multiphase flow model with a reactive transport model is a convenient way to investigate and test many modeling assumptions and numerical techniques. One of its features is that it allows for separate time-stepping. Moreover, it allows for the use of different grids, approximations and solvers for flow and transport (see discussion in Section 3.2.1).

Finally, the coupling allows the investigation of various types of feedback between reactive transport and flow. In particular, porosity, or permeability of the porous medium, may be affected by the transported reactive components (weak feedback). Moreover, the viscosity and density of the flowing phases may be dependent upon the concentration of the fluid (strong feedback).

2.2.2. Couplings across an interface

Couplings of models or codes across interfaces has become a research topic in several disciplines, including aerospace and engineering mechanics [34,79] and biomedical applications [30]. Such couplings are frequently referred to as "heterogeneous domain decomposition" [131]. In geosciences, such couplings have been used in regional climate models. Another important area is that of couplings of hydrodynamics (shallow water) with groundwater models of saturated or unsaturated zones [64,112,175]. Another example arises in resource recovery applications; namely, high-velocity pipe flow models and near-wellbore models are coupled to reservoir simulation models [103,163].

The main motivation behind this type of coupling is the expected reduction of overall computational cost of the simulation by individually selecting the most

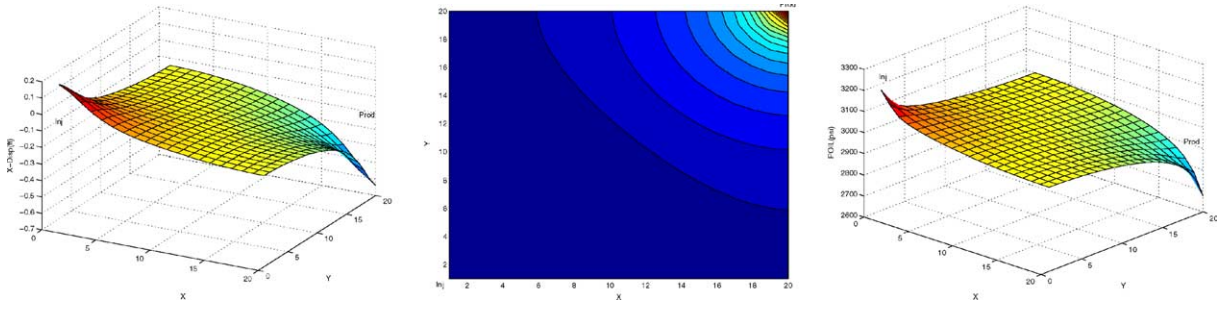

Fig. 3. Results of geomechanics + flow coupling in a reservoir with an injection well in the lower left corner and a production well in upper right corner. Shown are displacement (left), gas saturation contours (middle), and pressure (right), in one of the middle layers of the reservoir after one year of production. The maximum absolute displacement shown is 3% of the reservoir dimensions and may cause well or reservoir damage.

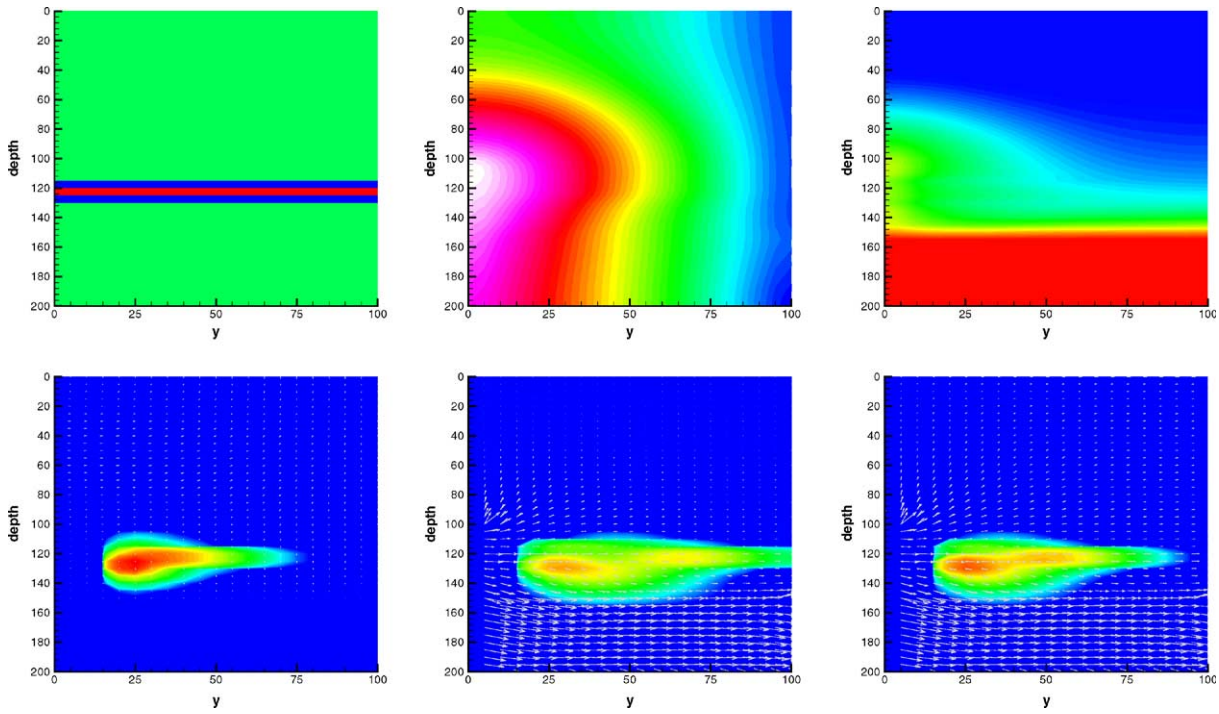

Fig. 4. Transport in an unsaturated zone: 2D domain with high permeability zone around depth 125 ft (top left) subject to water table at depth 150 ft raised to 100 ft on left-hand side. Pressure head and saturation contours after 1000 days are shown on the top center and the top right figure. A conservative tracer plume is initially in the variable permeability zones at depths between 120 and 130 and at $20 \leqslant y \leqslant 25$. It is advected in three different equilibrium partitioning scenarios. Bottom: tracer profiles and phase-summed velocity after 1000 days for tracer soluble in nonwetting phase only (left), tracer soluble in wetting phase only (middle), and tracer evenly partitioned between nonwetting and wetting phase (right). Note that the nonwetting phase travels left and up while the wetting phase travels left and down.

appropriate code to be executed in a given subdomain. In our reseach we have coupled different multiphase flow models. Fig. 5 shows a simulation using the coupling of a black-oil model, a two-phase model and of a single-phase model. The reservoir is nonuniformly dipping with layered permeability. Shown are grid and distribution of fluids and pressure and concentration contours initially, and after 2000 days of simulation. The initial (equilibrium) distribution of fluids follows the gravity direction: oil and gas prevail in upper parts of the reservoir and disappear towards the bottom where mostly water is present. Oil and gas in this reservoir are produced from the top, and several water injection wells are placed in the bottom part of the reservoir. The single-phase model denoted by "1" is assigned to the bottom part, the two-phase model denoted by "2" and the black-oil model denoted by "3" are assigned to the middle and the top part, respectively. The models are coupled across interfaces which are located in the regions where one or more phases are absent, or where because of residual conditions it is legitimate to consider a simpler model on one side and a more complex one on the other. Furthermore, in the assumed production conditions, the overall direction of the flow during the simulation stays fixed so that these residual conditions are not violated. If the flow direction changes, the model assignments can be changed and solver parameters can be adaptively modified.

The coupling conditions imposed on the interface come from physical principles of conservation of momentum and mass. Note that the interfaces between the subdomains are "artificial" and that they arise only as a computational concept, therefore the matching of quantities across an interface arises naturally. This would not be the case if the interfaces were "real" and arose between two distinctly different media. The coupling conditions are realized, respectively, by the matching of phase pressures (or some other variables) and by the matching of component mass fluxes (see formulation in Section 3.1.1). The system is tightly coupled and is solved by iteration, with sophisticated discretization methods, time-stepping strategies [124,172] and solver techniques [186,187]. In addition, several modeling issues are handled: these include the matching of constitutive relationships and state equations on the interface, including proper initialization, and the choice of primary unknowns [104,105,123,125, 171] (see also Section 3.5).

The solutions obtained with the multiphysics procedure can be validated by comparison to results obtained from solving the above problem on the same grid (with or without domain decomposition) with one model only

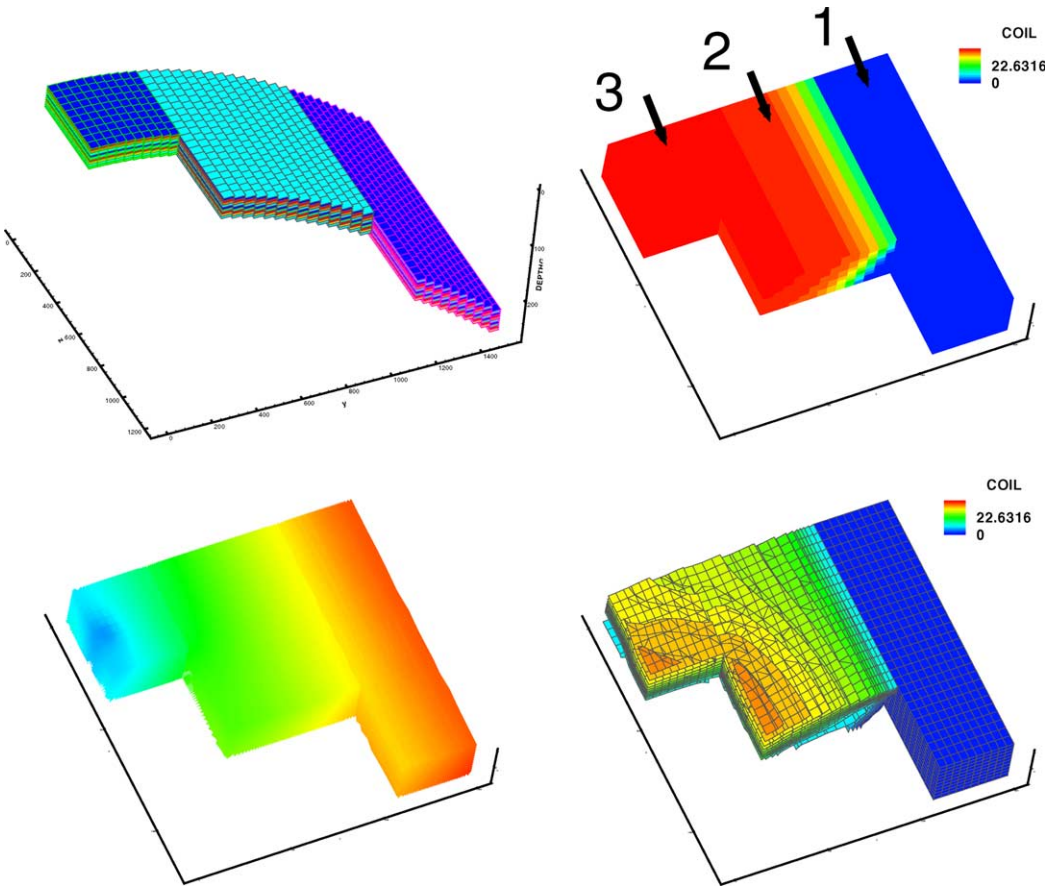

Fig. 5. Multiphysics simulation of oil recovery in a dipping reservoir. Grid, domain decomposition and nonuniform dipping character of the field are shown on top left. Initial oil concentration is shown on top right. Pressure and oil concentration contours shown bottom left and right. For technical reasons, dip cannot be shown for pictures other than the first.

(in this case with black-oil model "3" which includes all of the other models). While pointwise values of primary unknowns can be difficult to compare, well production and injection rates are an excellent basis for validation, see discussion in [126] and results in [104,125].

2.3. Multiphysics computational framework for subsurface applications

In this Section we discuss several modeling concepts which are useful in the construction of general purpose subsurface simulators designed for general applications.

First, as mentioned above, a general subsurface simulator should allow for modular inclusions of multiple models as well as additional processes and features which are important for either one of the intended applications. Important examples include such phenomena as density-driven flows important for environmental applications, non-Darcy flows important in high-velocity regions in gas reservoirs, and hysteresis, which should be accounted for both environmental and energy applications.

As another example, relative permeability and capillary pressure relationships are frequently assumed to have a fixed functional form (van-Genuchten or Brooks–Corey) whose parameters are determined by least-squares fitting of experimental data. The exclusive use of such functional relationships may limit the applicability of the simulator. For example, the entry-pressure data, which is important in simulating flow through rock formations of different types, cannot be used with van-Genuchten curves. Moreover, the use of such rational expressions verbatim with noninteger powers is not computationally efficient. As an alternative, one may use piecewise splines which offer a desired level of smoothness, and, at the same time, can be made to fit data exactly, are not computationally expensive, and can include, as special cases, any of the desired functional forms [170].

Moreover, one of the primary differences between the capabilities of simulators is in how they initialize variables and interact with source terms. Researchers involved with the modeling of environmental problems impose various boundary conditions to drive the flow in the unsaturated zone. At the same time, they frequently treat wells as point sources. This may lead to inaccurate flow path predictions if the pressure drop in the wells, rather than the volume or mass rate, is specified. On

the other hand, in petroleum reservoirs and other energy applications, boundaries are usually ill-defined and no-flow boundary conditions are used while the source terms are typically associated with wells. We believe that simultaneous inclusion of well models, as well as of boundary conditions, is desired. This facilitates validation with analytical or analytical/experimental results and numerical studies as well as simulation of cases from both energy and environment applications.

2.3.1. Initialization

Most problems derived from the general Eqs. (1) and (2) are transient. Therefore, it is necessary to define the initial condition of a reservoir, A specific numerical model needs to initialize its primary unknowns as well as its auxiliary variables. In general, there are two approaches to initialization: the first one assumes that the reservoir is in hydrostatic equilibrium under given pressure and fluid content conditions from which the values of primary unknowns are computed; the second allows for ad-hoc values of the primary unknowns. While the latter is easier to implement and it makes comparison and validation studies of different models and simulators easier, it assigns the responsibility of defining a physically meaningful problem to the user. On the other hand, implementation of hydrostatic equilibrium may be tedious. Its advantage is that it initiates a model in a manner consistent with the physics, and therefore the problem is consequently easier to solve. For example, in a realistic model with a gravity component, it is unlikely that the initial pressure of the reservoir is higher at the top than it is at the bottom. Such specification will make the pressure solution work unnecessarily hard in order to find the correct physical solution.

In general, it is useful to have both options—eqilibirium and nonequilibrium—available to the user of the simulator. In all examples shown in this section we assume hydrostatic equilibrium at the beginning of the simulation.

2.3.2. Boundary conditions

For incompressible single-phase flow problems as in Eq. (11), the most commonly used boundary conditions are of Dirichlet or Neumann types. These generally (in smooth domains) lead to well-posed problems if (smooth enough) Dirichlet pressure data is specified on at least one part of the boundary, or if the net flux is zero and pressure at a point (or its average) is given.

For general compressible multiple flowing phases (e.g. the two-phase flow problem described by the Eqs. (4) and (5)), the well-posedness has only been established for a few special cases, [13,16,41] and there is no theory for the black-oil model (4), (5) and (9). Therefore, the question of appropriateness of given boundary conditions is answered on a case-by-case basis. The difficulties arise from the hyperbolic nature of the problem and from the nonlinearities involved. For example, specification of two of the phase pressures as boundary conditions may be incorrect if, for example, their difference falls outside the capillary pressure range. On the other hand, the parabolic terms in the multiphase problems, which arise from compressibility components, may help to smooth the solutions locally. For example, in a reservoir which is not initially at hydrostatic equilibrium and which is governed by two-phase flow model, the no-flow boundary conditions may lead to physically meaningful solutions.

A separate issue arises in convection-dominated problems where incorrect specification of boundary conditions can induce artificial boundary layers. Specification of boundary conditions is especially tricky for nonlinear convection problems as it is generally difficult to predict the position of the saturation or concentration front or the location of the *free boundary* or the *seepage boundary*.

These difficulties are amplified by the fact that boundary conditions of interest to an applications group may be fairly sophisticated and may lead to numerically difficult problems (see [32,127,165]). Therefore, the question of what kind of conditions should be made available to the users of a simulator need to be evaluated for each model and each *multiphysics* coupling separately. Again, the responsibility to ensure that these conditions are physically meaningful may have to be left to the user.

2.3.3. Wells

In order to accurately describe the predominantly radial character of the flow(s) in the vicinity of wells, *well models* are required. These are frequently based on the well-known *Peaceman correction* [122]. Such well models, or *well boundary conditions* take into account the actual geometrical parameters of a well—its radius, so called "skin" etc.—and they are directly applicable to single-phase flow models and finite differences, or equivalently mixed FEM discretizations. Extensions exist for different discretizations and nonstandard flow models [63,78]. Multiphase flow well models based on Peaceman correction have been derived and tied to reservoir models to account for different types of injection and production wells which are either pressure- or rate- (volume or mass) specified or which impose constraints on both pressure and rate [3]. Also, there exist new models applicable to horizontal or multilateral wells [40], and there is research underway on *smart and intelligent wells* [163].

2.3.4. Simulation examples

In this Section we present simulation examples to illustrate some of the modeling concepts discussed above. All were obtained with IPARS [119,166,177].

Multiphysics examples are shown in Figs. 3–5, demonstrating the couplings of geomechanics + flow, reactive transport + multiphase flow, and of multiphase models coupled across interface, respectively. An example of the use of boundary conditions in a two-phase flow model is in Fig. 4. Both boundary conditions and wells are used in the example shown in Fig. 1 which demonstrates primary recovery production in a two-phase reservoir which is either connected to an aquifer or isolated. An example of the use of wells in a black-oil model is in Fig. 2.

3. Computational engineering and science methodologies

It is widely recognized that one cannot achieve simulation goals merely through increases in hardware systems or advances in computers alone and that smart methods and algorithms are a key ingredient. In this section we will describe a collection of locally conservative algorithms, namely, mixed finite element (MFE) and discontinuous Galerkin (DG) methods, which have been employed for treating flow and reactive transport in porous media. Clearly there exist other well known schemes such as higher order Godunov, Muscle, ENO, control volume, collocation, and characteristic Galerkin methods that have been applied to subsurface flow and transport problems. In general, the latter schemes possess one or more major deficiencies. They either have not been extendable to unstructured and/or nonconforming grids, are at best second order convergent in regions with smooth solutions, involve dual grids which are very complicated in three dimensional simulations, or are not locally conservative. On the other hand MFE and DG methods can be defined such that they do not have any of these deficiencies. The results presented in this paper reflect that we have more experience with MFE than with the DG methods.

Other topics addressed in this section include the use of mortar spaces for coupling multiphysics multinumerics MFE applications, linear and nonlinear iterative solvers for solving the discrete systems, and parallel scalability of algorithms on terascale computers.

3.1. Mixed and hybrid finite element methods

Mixed and hybrid finite element (MFE) methods [36] are based on a variational principle expressing an equilibrium (saddle point) condition that can be satisfied locally on each finite element. In particular for elliptic problems, the MFE formulation involves solving for both the scalar variable and the flux. Approximating spaces for the MFE method can be chosen to satisfy three important properities: local mass conservation, continuous fluxes, and the same order of convergence, and in some cases superconvergence, for both the scalar variable and the flux [77,117].

The application of MFE methods to modeling unstable miscible displacement in porous media was first introduced and analyzed in [69,70]. In [89] MFE and conforming Galerkin methods were compared for computing saturated groundwater flow in a heterogeneous porous media; results demonstrated that the Galerkin method can yield nonphysical behavior, i.e. streamlines end on the no-flow boundaries, whereas the MFE scheme produced physically meaningful results. Major reasons for this difference in behaviour of the two methods can be attributed to the fact that unlike conforming Galerkin, the MFE method is locally conservative and fluxes are continuous. Namely, the appropriate physics is satisfied for the MFE method even on coarse grids. Similar results were observed in [142] for the DG method, which is described below. The DG method is also locally conservative and has averaged fluxes which are continuous. Mixed methods have been successfully applied to many applications including mass conservation equations in multiphase flow [124,125,127], Stokes flow [36] and electromagnetics [61].

The MFE procedure is also used as a projection method for constructing mass conservative velocity fields from one grid to another [44]. This is extremely important in modeling of environmental surface and subsurface flow problems. For example, flow and multispecies transport are often solved separately using completely different numerical methods and grids due to differences in length and time scales of the phenomena involved. For accurate transport, it is desirable for the velocities to be locally conservative on the transport grid.

There is a well established relationship between the MFE on rectangular meshes and cell-centered finite differences (CCFD) for diffusion problems [146,167]; namely, the two are equivalent "modulo the use of appropriate numerical quadrature". This observation provides a useful approach of applying well models from CCFD formulations, which are used extensively in the petroleum industry, to MFE formulations and as well as using MFE formulations for tensor coefficients and general boundary conditions to CCFD methods [20].

For example, consider discretization of Eq. (10) with the lowest order Raviart Thomas space RT0 [161] on a rectangular grid in 3D whose elements are indexed by ijk with cell dimensions denoted by δx_i, δy_j, δz_k, respectively. Phase pressures $P = P_m$ are approximated by discontinuous piecewise constants in each cell. The phase velocity $\boldsymbol{U}$ is approximated by the tensor product of discontinuous piecewise constants and continuous piecewise linears with the requirement that the corresponding fluxes be continuous—the x (y, z) component is a continuous piecewise linear in x (y, z) and a

discontinuous constant in both y and z (x and z, x and y). For example, choose a test function $v_{i+1/2,j,k}$ satisfying these requirements, which is continuous in x direction over cells i,j,k and $i+1,j,k$, and discontinuous in j,k direction. We multiply (10) rewritten as $\mu\mathbf{K}^{-1}\boldsymbol{U} = -(\nabla P - \rho G\nabla D)$ by $v_{i+1/2,j,k}$ and integrate by parts. Spatial integrals are approximated using a trapezoidal quadrature rule which results in a CCFD scheme for the velocity component in the x direction on the edge between cells i,j,k and $i+1,j,k$:

$$\mu\delta y_j\delta z_k\delta x_{i+1/2,jk}K^{-1}_{i+1/2,jk}U_{i+1/2,jk} = \delta y_j\delta z_k(P_{i+1,jk} - P_{ijk} - G\rho_{i+1/2,jk}(D_{i+1,jk} - D_{ijk})), \tag{13}$$

where $\delta x_{i+1/2,jk}, \rho_{i+1/2,jk}$ are arithmetic averages and $K_{i+1/2,jk}$ is a harmonic average of $\mathbf{K}$ between these cells as in

$$\frac{K_{i+1/2,jk}}{\delta x_{i+1/2,jk}} = 2\left(\frac{\delta x_i}{\mathbf{K}_{ijk}} + \frac{\delta x_{i+1}}{\mathbf{K}_{i+1,jk}}\right)^{-1}. \tag{14}$$

Of course, this formula assumes $\mathbf{K}$ is invertible and therefore it cannot be applied directly to general subsurface problems and, in particular, to multiphase problems. An extension of the mixed method referred to as the *expanded mixed method* [104,106,119,125,172,177] bypasses these difficulties by introducing extra "velocity-like" unknowns which in practical calculations are eliminated. Extensions, also to full tensor coefficients, general geometry, and nonmatching multiblock grids are treated in [17,19,20] respectively. The hybrid form is quite similar to the so-called local discontinuous Galerkin method (LDG) [39,49]. In addition, a new coupling approach to discretizing flow in porous media via mixed finite element methods on nonmatching multiblock grids has been formulated and analyzed [168,177]; this can be viewed as an enhanced velocity interface coupling. The velocity space along the interfaces is enhanced to give a flux-continuous approximation. No additional matching conditions need to be imposed. The computational complexity of the resulting multiblock algebraic problem is comparable to a single block case. This method yields optimal convergence for pressures and interior velocities but no superconvergence.

Consider now the three-phase model of flow given by (6)–(8). Extensions to black-oil model or water–NAPL–air models are immediate. The appropriate modification of (13) is for $m = w,n,g$

$$\delta x_{i+1/2,jk}U_{m,i+1/2,jk} = K_{i+1/2,jk}\lambda_m(P_{m,i+1,jk} - P_{m,ijk} - G\rho_{m,i+1/2,jk}(D_{i+1,jk} - D_{ijk})), \tag{15}$$

where λ_m is the mobility of phase m evaluated at $i+1/2,jk$ by upwinding, that is, from the values of saturations at i,j,k or $i+1,j,k$ depending on the gradient of potential [169]. Here we adopt the convention that, if $\mathbf{K}$ is zero on a cell i,j,k, then $U_{m,i+1/2,jk}$ and $U_{m,i-1/2,jk}$ are set to zero. This is a standard CCFD formulation for multiphase flow which can be shown to be equivalent to the expanded mixed formulation [127].

The complete set of discrete equations for the general three-phase flow model (6)–(8). is obtained by multiplying each of them by a piecewise constant test function and integrating. Also, discretization in time is applied. Here we use the backward Euler method in time. The discrete form reads

$$\delta x_i\delta y_j\delta z_k(\phi\overline{N}_M)^{n+1}_{ijk} + \delta t^{n+1}\int_{\Omega_{ijk}}\nabla\cdot\left(\frac{1}{B_m}\boldsymbol{U}_m\right)^{n+1} = \delta t^{n+1}\overline{q}^{n+1}_{M,ijk} + \delta x_i\delta y_j\delta z_k(\phi\overline{N}_M)^n_{ijk} \tag{16}$$

for $m = w,n,g$ as corresponds to Eqs. (6)–(8), respectively. For black-oil equations, modification to include R_o as in (9) is immediate.

This system, complemented by all the necessary auxiliary relationships including capillary pressure and volume balance $\sum_m S_m = 1$, is solved for a set of primary unknowns. These can be chosen in many ways, for example, for the black-oil model, we consider $(P_w, \overline{N}_N, \overline{N}_G)$. Such a choice of unknowns of one pressure and two other unknowns, such as concentrations or saturations, is a popular choice for mixed elliptic–parabolic–hyperbolic problems in reservoir simulation. The coupled system is linearized by Newton's method. A *GMRES* solver with multi-level preconditioner [53,96,97], or an *LSOR* is then applied to solve the linear system at every Newton step (see discussion on solvers in Section 3.5).

In the next section, we describe a mortar mixed formulation for three phase flow.

3.1.1. Multiblock mixed mortar method for three-phase flow

Consider now a three-dimensional reservoir domain Ω which has been divided into n_{bl} nonoverlapping subdomains (blocks) Ω_k, $k = 1,\ldots,n_{bl}$. These blocks can be chosen to approximate geological faults, geometry irregularities, variations of rock properties, physical/chemical properties of flow, and distribution and types of wells, etc. A grid is constructed locally on each block and can be nonmatching on the interfaces between neighboring blocks. Fig. 6 illustrates a typical geometry of a three dimensional domain decomposition. The interfaces between blocks are filled with "mortars", elements of a finite element space called the *mortar space,* which is constructed on the two dimensional interfaces. While our formulation permits the treatment of general rock properties and geometries, we will assume for convenience that the reservoir has only one rock type and that it consists of a union of rectangular blocks, each having it own smooth rectangular tensor product grid as shown in Fig. 6. In addition, for the sake of

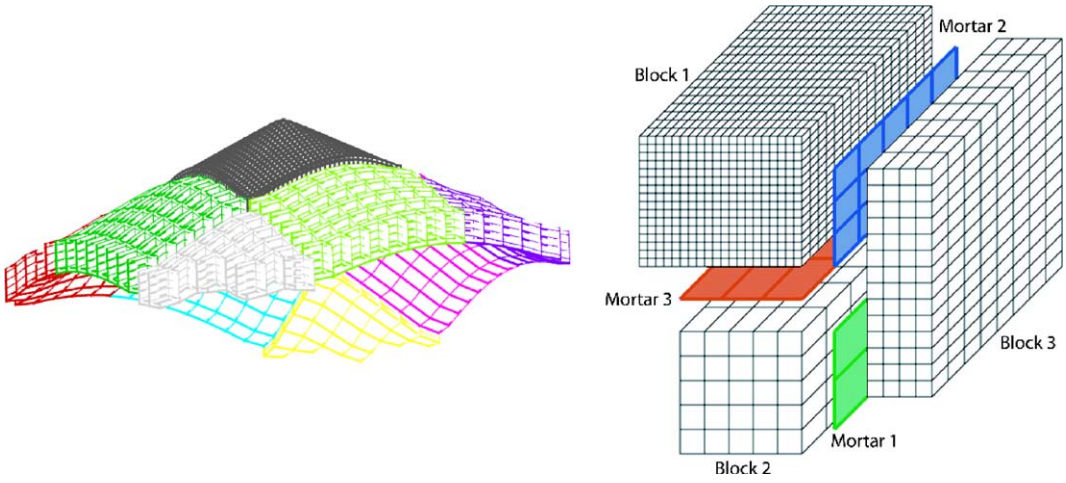

Fig. 6. Multiblock decomposition: actual grid used in one of simulations (left), idealization with three blocks and with mortars between blocks (right).

simplicity, we do not take into account the occurence of hysteresis or other nonlocal in time effects.

Each subdomain Ω_k can have associated with it a different physical or numerical model which could be one of the models in Section 2.1 or some other model which can be fully implicit, sequential or explicit in time. In order to couple the subdomain problems, additional equations are required for ensuring mass and momentum conservation across the interfaces. This is done, respectively, by imposing matching conditions both on the phase pressures and the component fluxes. Specifically, on each interface $\Gamma_{kl}, 1 \leqslant k < l \leqslant n_{bl}$, we impose

$$P_m|_{\Omega_k} = P_m|_{\Omega_l}, \quad m = w, o, g \tag{17}$$

$$[\boldsymbol{V}_M \cdot \nu]_{\Gamma_{kl}} =: \boldsymbol{V}_M|_{\Omega_k} \cdot \nu_k + \boldsymbol{V}_M|_{\Omega_i} \cdot \nu_l = 0, \quad M = W, O, G \tag{18}$$

This approach is motivated by a domain decomposition algorithm for single-phase flow developed originally for conforming grids [83], and later generalized to nonmatching grids coupled with *mortars* [17,185], and used for multiphase models [104,106,119,125,172,177].

The conditions (17) and (18) can be reformulated as "find the value of $\psi = (P_w, P_o, P_g)$ at every point of Γ_{kl} so that $B(\psi) = ([\boldsymbol{V}_W \cdot \nu], [\boldsymbol{V}_O \cdot \nu], [\boldsymbol{V}_G \cdot \nu]) = 0$". In the discrete form, these conditions are imposed in the weak sense and are discretized using the *mortar spaces* constructed on the grids defined on all Γ_{kl}. The use of mortar spaces amounts in practice to averaging of the interface primary unknowns ψ and of the jumps in the fluxes $B(\psi)$. In implementation, these averaging operations are handled by inexpensive projections between mortar grids and subdomain grids.

Multiple scales: Obviously, since the grids on subdomains do not need to match across Γ_{kl}, the mortar approach is well suited for handling locally refined grids around wells or in other regions where one wants to capture fine scale phenomena.

Moreover, the choice of mortar grid Γ_{kl} has consequences for the accuracy of the overall problem and thereby, in addition to subdomain grid size, it introduces another discretization parameter associated with the mortar space. On the other hand, very fine mortar grid has many degrees of freedom on the interface for which the interface problem is solved. Therefore, the presence of mortar grid introduces *multiscale resolution*, and leads to a novel approach to *upscaling* [126]. Adaptivity of mortar grids is currently under research.

Interface primary unknowns: Because of the assumed homogeneity of rock type and the lack of nonlocal-in-time effects, the equality of phase pressures (17) on Γ_{kl}, which is an "artificial" interface, is equivalent to the equality of all phase saturations across that interface. This means that, in order to express momentum conservation, instead of pressures as in Eq. (17), we can match a different set of variables, for example, we can use ψ similar to the set of primary unknowns of the three-phase model or of the black-oil model: $\psi = (P_w, \overline{N}_O, \overline{N}_G)$. We remark that, in the general case of different rock properties, the pressure and fluxes would still be continuous; however, instead of one, two mortar spaces should be used for saturations to reflect saturation discontinuities.

In summary, the (discrete) subdomain problems (15) and (16) are coupled with a nonlinear (discrete) interface problem $B(\psi) = 0$ (we supress the discrete notation on ψ and $B(\psi)$). This interface problem is solved for ψ by the following iterative procedure. It assumes an initial guess for ψ on the interface to be used after projection as a Dirichlet boundary condition on subdomains. The subdomain problems are then solved and the jump in the component fluxes is calculated on the interface. If the jump is less than a given tolerance, the current time

step is completed; otherwise, the interface unknowns ψ are updated and the procedure is repeated until convergence. More precisely, the interface problem is solved by an inexact Newton method [53,76,91] in which derivatives are computed using a forward difference GMRES iteration. More details and results can be found in [119,126,172,174,184,186,187] (see also discussion in Section 3.5).

Coupling of models: The formulation presented in this Section can be extended to the coupling of different physical or numerical models. An example and related modeling issues have been discussed in Section 2.2.2. In particular, in the case of coupling different multiphase models, the treatment of the missing phase must be handled. Mortar finite elements also lend themselves to *multinumerics*, (e.g. different time steps in different domains, coupling of implicit and explicit approaches etc. [124]).

Also of interest are coupling approaches which do not require mortar spaces. In particular, the DG methods described below may be used in conjunction with mixed finite element or continuous finite element methods, for the purpose of coupling different physical phenomena and/or different grids [55,137]. Here one can take advantage of the fact that DG methods do not require element interfaces to align, to allow for nonmatching grids at the interface between methods.

3.2. Discontinuous Galerkin methods

There are a variety of methods based on the use of discontinuous approximating spaces. Examples include the Basey and Rebay method [25] and the LDG [12,49] methods, the Oden, Babuska, Bauman [118] method, and the interior penalty Galerkin methods [180], and the NIPG methods [143]. In [23] a general framework of these methods is presented. Application of these methods to a wide variety of problems can be found in [4].

DG methods are of interest because they have several appealing properties: (1) they are element-wise conservative; (2) they support local approximations of high order; (3) they are robust and nonoscillatory in the presence of high gradients; (4) they are implementable on unstructured and even nonmatching meshes; and, (5) with the appropriate meshing, they are capable of delivering exponential rates of convergence. As an example, Fig. 7 demonstrates the ability of DG methods to compute solutions on nonmatching grids; here we have computed the solution of an elliptic equation like (11) using a DG method which is highly refined on part of the domain. Notice that the symmetry of the solution is maintained.

DG methods are of particular interest for multiscale, parallel implementation. They allow for varying the order of approximation over an element, thus they are capable of resolving multiple scales within the element. Moreover, they are highly local: typical DG methods only require communication between elements which share faces, thus they are well-suited for parallel computation. CSM researchers have developed, analyzed, and implemented DG methods for a variety of problems and applications, including single and two-phase flow in porous media [136,138,143,144], contaminant transport [12,40,52], shallow water flow [11], and elastic and acoustic wave propagation [141].

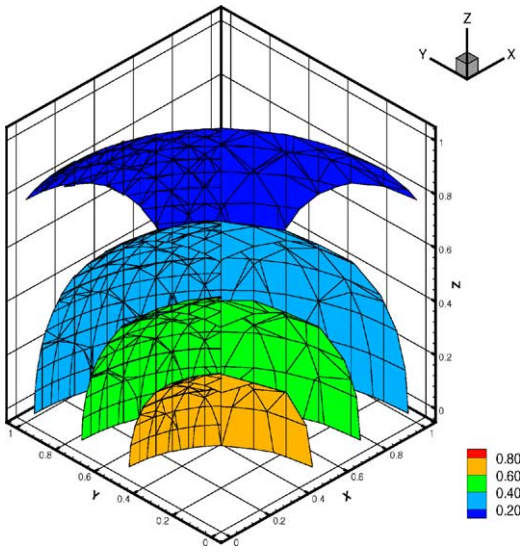

Fig. 7. DG solution to an elliptic model problem on a nonmatching grid.

An important porous media application where DG methods could prove important is reactive transport. When dealing with general chemistry and transport, it is imperative that the transport operators be monotone and conservative. While a number of monotone finite difference methods have been proposed for structured grids, many of these approaches have not been extended to unstructured grids. With the use of appropriate numerical fluxes, approximate Riemann solvers and stability post-processing (slope-limiting), DG methods can be used to construct discretizations which are conservative and monotone.

3.2.1. DG transport formulation

We now briefly describe the DG method for modeling reactive transport. Let Ω be a polygonal domain bounded in $\mathbb{R}^d$, $d = 2, 3$ and let $\boldsymbol{U}$ be a velocity field that satisfies (11). We decompose the boundary of the domain into an inflow part Γ_{in} and an outflow part Γ_{out}, $\partial\Omega = \Gamma_{\text{in}} \cup \Gamma_{\text{out}}$, where $\Gamma_{\text{in}} = \{x \in \partial\Omega : \boldsymbol{U} \cdot \boldsymbol{n} < 0\}$, and $\Gamma_{\text{out}} = \{x \in \partial\Omega : \boldsymbol{U} \cdot \boldsymbol{n} \geqslant 0\}$. The transport of a contaminant through a porous medium is modeled by the following equation which is a special case of Eq. (12), with boundary and initial conditions completing the system:

$$\phi c_t + \nabla \cdot (\boldsymbol{U}c - D(\boldsymbol{U})\nabla c) = f(c), \quad \text{in } \Omega \times (0,T], \tag{19}$$

$$(\boldsymbol{U}c - D(\boldsymbol{U})\nabla c)\cdot \boldsymbol{n} = \boldsymbol{U}\ c_{\text{in}} \cdot \boldsymbol{n}, \quad \text{on } \Gamma_{\text{in}} \times (0,T], \tag{20}$$

$$-D(\boldsymbol{U})\nabla c \cdot \boldsymbol{n} = 0, \quad \text{on } \Gamma_{\text{out}} \times (0,T], \tag{21}$$

$$c(0,\cdot) = c_0, \quad \text{in } \Omega. \tag{22}$$

Corresponding to (12) $c = c_M$ is the concentration of the contaminant, $f(c) = q_M + \phi R_M$ a general nonlinear reaction source function, $D(\boldsymbol{U})$ a diffusion–dispersion tensor lumped with porosity ϕ.

We now establish some notation for the spatial discretization. Let $\mathscr{E}_h = \{E\}_E$ be a nondegenerate subdivision of Ω, made of triangles in 2D and tetrahedra in 3D. We allow for a nonconforming partition of the domain. Let h be the maximum diameter of the elements. Let Γ be the skeleton of the mesh of Ω, that is the union of the open sets that coincide with interior edges (or faces) of elements. We also associate with each set γ_k in Γ, a unit normal vector $\boldsymbol{n}_k$. For γ_k in $\partial\Omega$, the vector $\boldsymbol{n}_k$ is outward to $\partial\Omega$.

As shown in Fig. 8, we define for w sufficiently smooth, the jump $[w]$ and the upwind w_* value. We assume below that $\boldsymbol{n}_k$ is outward to E_k^1.

$$\{w\} = \tfrac{1}{2}(w|_{E_k^1}) + \tfrac{1}{2}(w|_{E_k^2}), \quad [w] = (w|_{E_k^1}) - (w|_{E_k^2}),$$
$$\forall \gamma_k = \partial E_k^1 \cap \partial E_k^2,$$
$$\{w\} = (w|_{E_k^1}), \quad [w] = (w|_{E_k^1}),$$
$$\forall \gamma_k = \partial E_k^1 \cap \partial\Omega,$$

$$w_* = \begin{cases} w|_{E_k^1} & \text{if } \boldsymbol{u}\cdot\boldsymbol{n}_k \geqslant 0, \\ w|_{E_k^2} & \text{if } \boldsymbol{u}\cdot\boldsymbol{n}_k < 0. \end{cases} \quad \forall \gamma_k = \partial E_k^1 \cap \partial E_k^2.$$

Let r be an integer. The finite element subspace consists of discontinuous piecewise polynomials:

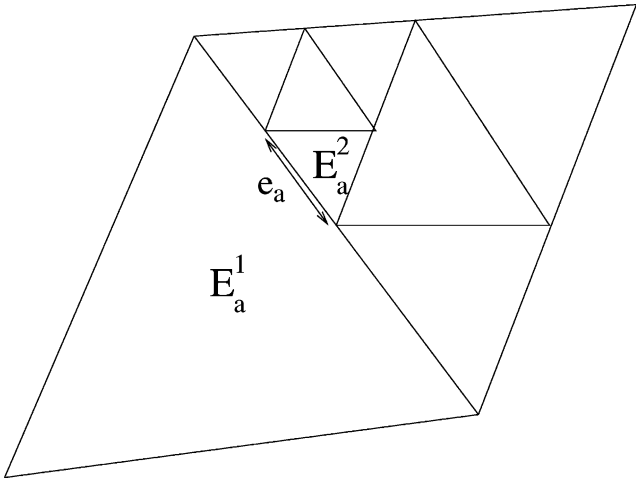

Fig. 8. DG jump.

$$\mathscr{D}_r(\mathscr{E}_h) = \{v : v|_E \in P_r(E) \quad \forall E \in \mathscr{E}_h\},$$

where $P_r(E)$ is a discrete space containing the set of polynomials of total degree less than or equal to r on E.

We introduce the bilinear form $b_{NS} : H^s(\mathscr{E}_h) \times H^s(\mathscr{E}_h) \to \mathbf{R}$, $s > 3/2$, and the linear form $L : L^2(\Omega) \to \mathbf{R}$:

$$\begin{aligned} b_{NS}(\mathbf{U};\mathbf{w},\mathbf{v}) = {} & \sum_{E\in\mathscr{E}_h}\int_E D(\boldsymbol{U})\nabla w\cdot\nabla v - \sum_{E\in\mathscr{E}_h}\int_E \boldsymbol{U}w\cdot\nabla v \\ & - \sum_{\gamma_k\in\Gamma}\int_{\gamma_k}\{D(\boldsymbol{U})\nabla w\cdot\boldsymbol{n}_k\}[v] \\ & + \sum_{\gamma_k\in\Gamma}\int_{\gamma_k}\{D(\boldsymbol{U})\nabla v\cdot\boldsymbol{n}_k\}[w] \\ & + \sum_{\gamma_k\in\Gamma}\int_{\gamma_k}\boldsymbol{U}\cdot\boldsymbol{n}_k w_*[v] + \sum_{\gamma_k\in\Gamma_{\text{out}}}\int_{\gamma_k}\boldsymbol{U}\cdot\boldsymbol{n}_k wv. \end{aligned} \tag{23}$$

$$L(c;v) = \int_\Omega f(c)v - \sum_{\gamma_k\in\Gamma_{\text{in}}}\int_{\gamma_k}\boldsymbol{u}\cdot\boldsymbol{n}_k c_{\text{in}} v. \tag{24}$$

The discontinuous Galerkin approximation C_{DG} in $L^2(0,T;\mathscr{D}_r(\mathscr{E}_h))$ satisfies the formulation:

$$\left(\phi\frac{\partial C_{\text{DG}}}{\partial t}, v\right) + b_{NS}(\boldsymbol{U};C_{\text{DG}},v) = L(C_{\text{DG}},v), \quad t>0, \quad \forall v\in\mathscr{D}_r(\mathscr{E}_h), \tag{25}$$

$$(C_{\text{DG}}(0),v) = (c_0,v), \quad \forall v\in\mathscr{D}_r(\mathscr{E}_h). \tag{26}$$

Remark. It should be noted that the approximation of the concentration satisfies on each element E the following mass balance

$$\int_E \phi\frac{\partial C_{\text{DG}}}{\partial t} - \int_{\partial E}\{D(\boldsymbol{U})\nabla C_{\text{DG}}\}\cdot\boldsymbol{n}_E + \int_{\partial E}\boldsymbol{U}\cdot\boldsymbol{n}_E C_*^{\text{DG}} = \int_E f(C^{\text{DG}}).$$

This property is a unique feature of the DG methods.

DG *hp* error estimates involving mesh size h and degree of approximation p were established in [143] for elliptic problems and in [139,140] for an upwinded scheme for modeling transport with nonlinear reaction. In both papers, optimal rates of convergence in the energy norm were obtained for meshes which can be nonconforming and for approximations that can vary locally over each element. In the transport paper, both continuous time (semidiscrete problem) and discrete time procedures were considered.

3.2.2. DG simulation examples

Two numerical examples are presented in this section. The first example involves simulating flow in the geological L-site, that is located in the south-eastern United States. The L-site consists of a large fly ash disposal

pond located adjacent to a river. A cross section is given in Fig. 9. There are five different types of rocks. The hydraulic conductivity ranges from 0.31 m/day to 17.2 m/day.

The flow is modeled using a quadratic approximation, or $r = 2$. The boundary conditions are the following: no flow on the top and bottom boundaries and Dirichlet boundary conditions on the vertical boundaries. We impose a constant pressure at the inlet that is higher than the one at the outlet. For this problem with D defined to be the absolute permeability in Eq. (23) the DG solution satisfies:

$$b_{NS}(\mathbf{0};\mathbf{P},\mathbf{v}) = \int_{\Omega} fv \quad \forall v \in \mathscr{D}_r(\mathscr{E}_h) \tag{27}$$

The pressure solution is shown in Fig. 10. Details regarding this computation as well as applying an *hp* adaptive procedure are discussed in [142].

A second example is a linear transport benchmark problem. Here we compare the DG method with three well known transport schemes, Godunov (first and higher order) and the characteristic mixed method. Results are shown in Fig. 11. Note that sharpest contours are obtained with DG.

3.3. Time stepping approaches

Effective time stepping schemes are essential for multiphysics applications and coupled systems. This is a topic that has not received adequate attention in either research or in application areas. It is critical to modeling large scale coupled multiphysics problems accurately and efficiently. Practical questions arise concerning global and local time step control, the use of different spatial grids and time steps in subdomains, and the use of different timesteps for different physical models defined on different subdomains. Preservation of conservation of material volumes across the space-time boundaries as well as conservation of mass and similar properties also effect the time step.

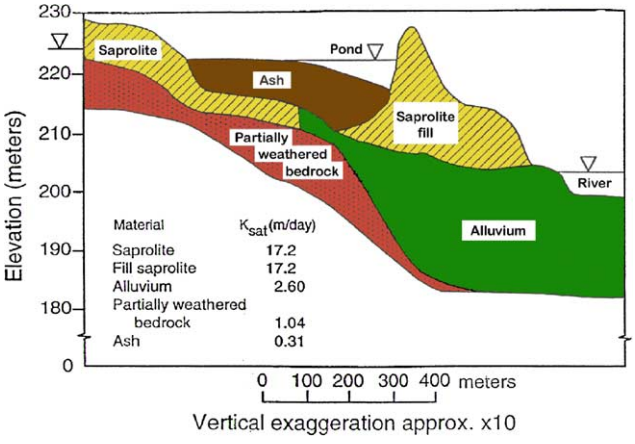

Fig. 9. Geology of the L-site.

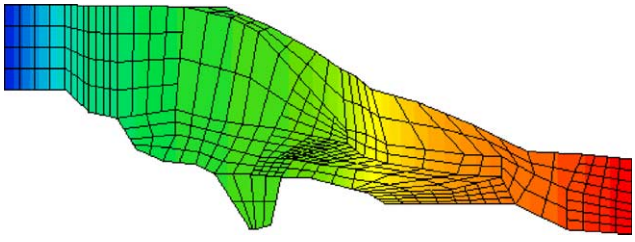

Fig. 10. Quadratic approximation of the pressure field.

3.3.1. Fully implicit and time-split approaches

Numerous scientific papers on reactive transport in porous media have appeared in the literature, in particular in *Water Resources Research* and *Journal of Contaminant Hydrology*. In general, these papers emphasize computational and experimental results. The authors wish however to point several papers which address theoretical issues. In [57,173] a priori error estimates both in space and time for an operator splitting technique modeling advection, diffusion, and reaction systems were established and, in [58], the effectiveness of this approach for treating in situ biodegradation problems in porous media was demonstrated. This theoretical work was extended to treating nonequilibrium adsorption kinetics in [56]. In addition, this approach to kinetic and local equilibrium using an interior point method was extended in [147]. More recently, a consistent split algorithm for semi-discrete nonlinear reactive transport problems was analyzed in [90].

In reactive transport, it is not clear a priori how tightly equations should be coupled. In particular an adaptive time-implicit/time-split approach may be warranted, whereby certain terms are adaptively modeled either fully implicitly or through a split step. This type of adaptive approach could vary spatially as well; i.e., the method of time-stepping may vary across the physical domain. Research on the use of various adaptive, higher order, and local time-stepping for the advection/reaction/diffusion schemes is clearly needed.

In many energy and environmental applications, large systems of coupled partial differential equations arise, such as geomechanical reservoir simulation and 4D seismic. Depending on the nature or time scales of these equations and the feedback between equations, these couplings can be "loosely" or "tightly" coupled in time. For loosely coupled models, in many cases it is appropriate to time-lag or time-split the equations, whereby certain terms are evaluated at previous time-levels, or split off from the equations and solved in a separate step. An example for such time-splitting is the coupling of IPARS and the SNL mechanics code JAS3D. For tightly coupled models, such time-lagging or splitting may lead to severe temporal errors. In these

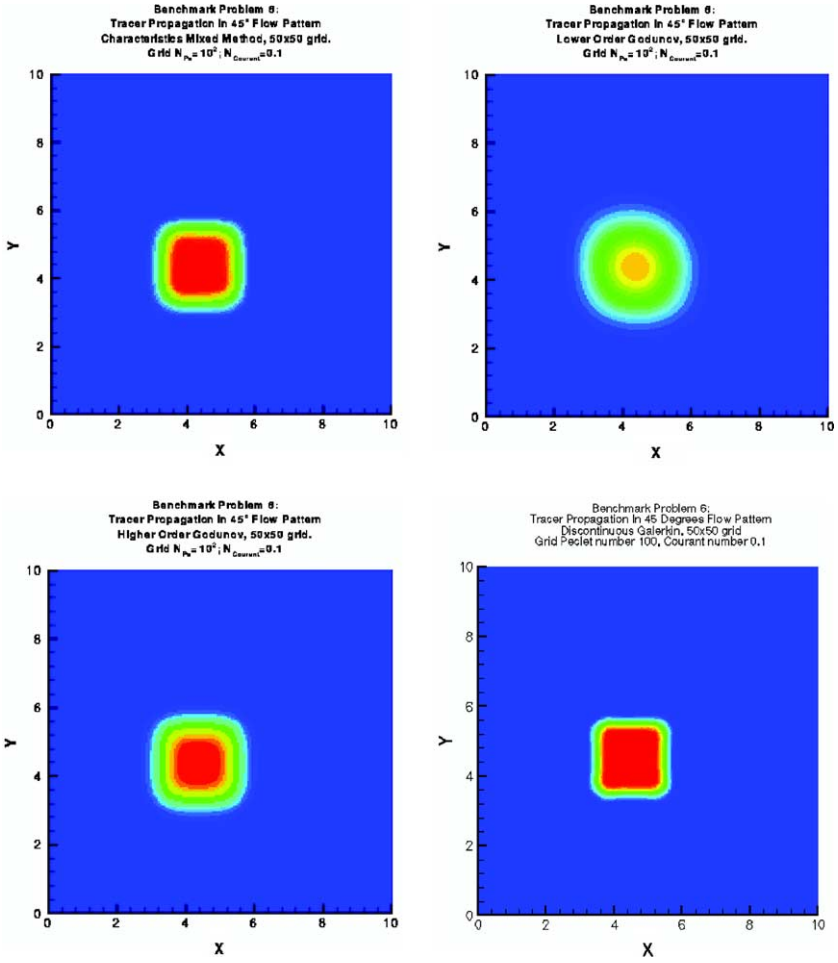

Fig. 11. Simulation of tracer propagation using characteristic mixed method, first order Godunov, higher order Godunov and DG methods (from left to right, top to bottom). Peclet number $= 10^2$. Same grid 50×50 used in all examples.

cases, a more fully implicit approach may be warranted. Thus sophisticated linear and nonlinear solution techniques must be developed.

In a similar fashion it is a standard practice to decouple the system of multiphase flow equations into a pressure equation and a system of concentration equations. Examples of such approaches are IMPES (implicit pressure and explicit saturation), streamlines (saturations solved along flow streamlines), and sequential (implicit pressure and implicit saturation). These techniques can also be employed as preconditioners for the fully implicit system as discussed below.

Similar to IMPES or sequential techniques for multiphase flow are the Chorin [46,47] and Glowinski [82] splittings for the incompressible Navier–Stokes equations which involve decoupling the system into transport and second order elliptic (pressure) equations, and splitting techniques for transport [134] and Stokes equations [132]. The former approach has also been used as a preconditioner for the fully implicit system.

3.4. Parallel solution techniques

The advances in computing technologies have given promise to all disciplines in computational engineering and science. In recent years, the processing speed of workstations has been increasing at the rate predicted by Moore's law which states that, every 18 months, the data density on integrated circuits doubles; this trend is expected to hold for at least another decade. In fact, individual workstations available these days, off-the-shelf, have an associated peak performance of several GFlops as measured by standard benchmark tests based on Linpack [68]. On the other end of the spectrum, the peak performance of computing equipment is measured these days in Teraflops, and it comes mainly from massively parallel systems [111]. While these systems are not necessarily accessible to geoscientists on a daily basis, their structure, contrary to that of supercomputers of yesterday, is similar from applications point of view to the structure of low-cost configurations available to many research groups.

Along with the increase in the processor speeds of individual machines, came the improved ability and interest in putting them together in "do-it-yourself", inexpensive, Beowulf clusters or other parallel configurations. While parallel computing is not a new concept, the ability to get supercomputer-like performance from low-cost machines is relatively recent [24]. As a measure of the success of the cluster approach, the prestigious Gordon Bell prize in computing in 1997 was awarded to a project developed on a 16 processor Intel cluster (http://research.microsoft.com/gbell). Finally, the concept of Grid [1] as well as of the *peer-to-peer computing* at www.seti.org provide another paradigm of low-cost parallel computing. In summary, it is not clear what future will bring to computing, but it appears that parallel processing will remain its essential component.

As it has been confirmed in the past, advances in hardware alone and in particular, in processor speed only, do not guarantee dramatic reductions in computational time. In general, parallel performance of a code depends on the efficiency of hardware, the communication software of a given (parallel) platform, and the performance of the numerical algorithms implemented. The development of parallel scalable algorithms is an essential ingredient of any large-scale computing project. The notion of scalability [14] is related to the expectation that the computational time necessary to solve a given problem should decrease with an increasing number of processors. More precisely, it is expected that *speedup*—defined as the ratio of computational time on one processor to the computational time on p processors—in an "ideal" case should be *linear*, that is, equal p. In practice, thanks to the *caching* of some of the processor data, the speedup can be *superlinear*. Obviously, the time spent on computations versus the time spent on communication between processors, as predicted by Amdahl's law [14], constrain the speedup. In fact, close-to-linear speedup is obtained only for large enough problems such that communication costs are much smaller than computation costs. In another direction, a notion of *scaled speedup* is considered, in which the problem size is increased linearly along with the number of processors. In an ideal case, such scaled speedup would be equal to 1 [87].

Information on the scalability of a given computing system is based on various benchmark tests. The most widely applied benchmarks use linear algebra package Linpack [68] which, among other features, has the advantage of being easily portable between different machines. Unfortunately, efficiency measures obtained with Linpack cannot be extrapolated in a straightforward way. In particular, in subsurface applications, the complexity of computational algorithms is rarely a linear function of the number of unknowns, and the increase in the problem size is frequently local and/or associated with a change in the physics of the problem. A typical example is a convective front travelling with a given velocity. Some local phenomena (reactions etc.) may be associated whose computational complexity remains fixed regardless of the size of the reservoir. On the other hand, if the size of the reservoir is fixed but the computational grid is refined, we do not only increase the number of unknowns but we also change the conditioning of the associated linear and nonlinear system. In summary, there is a need for the development of new and improved parallel computational techniques for subsurface applications as well as for the development of performance measures tailored to these applications.

Our group has over a decade of experience in the parallel computation and the development of scalable parallel algorithms. This expertise includes the development of domain decomposition methods for the solution of elliptic and parabolic equations [50], parallel iterative solvers for multiphase flow [53], development of parallel shallow water and water quality simulators [45,54], development of parallel contaminant transport simulators [18,22,45] and the development of the multiphase multicomponent simulator framework IPARS [119,124,125,166,172,177]. In recent studies, we evaluated the scalability of IPARS for problems of fixed size with increasing number of processors for both single-block simulations [176] as well as for multiblock simulations [126]. Here we include some scalability results which are shown in Fig. 12.

3.5. Linear and nonlinear solvers

The choice of linear and nonlinear solvers is clearly dependent on the time stepping and/or time splitting chosen for the coupled system. If the time splitting involves breaking up the coupled system into a sequential system involving modeling either elliptic and/or transport equations, then robust and efficient solution techniques can be applied to each equation. For transport dominated problems explicit time stepping is frequently employed and for diffusion dominated problems if the time step is not too large, block preconditioning techniques. In the case of the elliptic equations (incompressible), it is well known that for accuracy and efficiency the corresponding discrete system must be solved implicitly.

Beginning with the first international domain decomposition conference in Paris in January 1987, there has been an extensive development of robust parallel domain decomposition techniques based on Krylov subspace or multilevel preconditioners for elliptic scalar equations. Both overlapping domain decomposition algorithms such as additive Schwarz, multiplicative Schwarz, BPX, BEPS [156] and nonoverlapping domain decomposition such as Balancing [50] and multigrid on the interface [179] have been investigated both theoretically and computationally. It has been shown that for

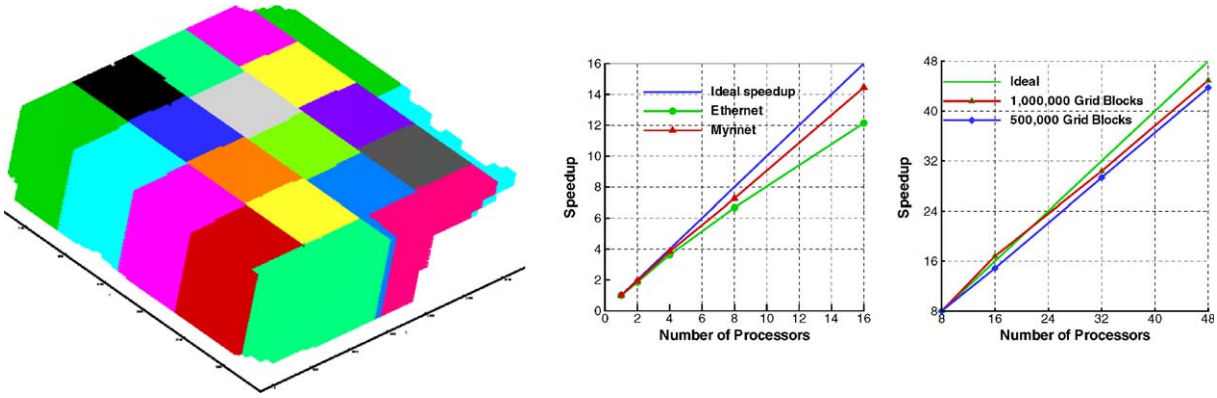

Fig. 12. Parallel scaling of black-oil model in IPARS on parallel Linux cluster with (fast) Myrinet switch or (relatively slow) Ethernet switch. Figure on the left shows decomposition of the computational domain between 20 processors for the grid from Fig. 2. Figures in the center and on the right show speed-up = computational time on one processor divided by time on p processors vs number of processors p for two cases: 500,000 cells and 1,000,000 cells (1.5 M and 3 M unknowns, respectively). Center: speed-up for 500 K cells with Myrinet and Ethernet. Right: speed-up for 500 K and 1 M cells and only Myrinet. Close to ideal (linear) speed-up is achieved for large problems and with fast network Myrinet switch.

problems with coefficients that are not "too rough" the condition number for these methods behaves like $C(\log(1+H/h))$ where H is diameter of the domain and h denotes the mesh size and C is a constant independent of H and h. Thus by fixing H/h, i.e. the number of subdomains grows as the number of unknowns grows, the condition number remains constant and thus the number of conjugate gradient iterations remains constant.

In this section we discuss two terascale linear solver approaches, preconditioned Krylov subspace methods and multilevel/multigrid methods, for solving the fully implicit in time discretized coupled nonlinear multiphase system. We assume the system has been linearized by a Newton or inexact Newton method. While fully implicit time-stepping schemes are the most robust, they are the most expensive in the subsurface flow simulation since they result in nonlinear systems being solved at each time step. Thus one is confronted with solving many times very large nonlinear nonsymmetric systems which are ill-conditioned. However, good initial guesses for system are generally available; namely, either the last time step solution or a guess obtained by extrapolation over previous time steps.

For simplicity we will assume that the underlying discretization method of a given multiphase flow model like the one discussed in Section 2 is implicit Euler in time and mixed finite element or cell-centered finite differences in space. In addition we shall restrict our attention to the preconditioned generalized minimum residual (GMRES) approach in which the preconditioner is based on a family of two-stage decoupling techniques.

The first scheme is based on two-stage preconditioning techniques. At the first stage a decoupling preconditioner is introduced which decouples a given pressure from saturations or concentrations. This decoupling allows for a second stage, a preconditioning of the diagonal pressure block of the Jacobian independently of the saturation blocks. Different techniques for decoupling and pressure block preconditioning have been considered and implemented. The set of available pressure block preconditioners comprises LSOR and truncated Neumann series methods based on the red-black ordering, parallel solvers for a discrete separable operator, and algebraic multigrid methods [96,97].

The second approach [97] is based on algebraic and geometric multigrid (agglomeration) method [35,88,109, 164] for the fully implicit and IMPES schemes [75,96, 169]. This approach employs a super coarsening strategy to obtain the coarsest level mesh. The finest grid is three dimensional. The next grid is obtained by using a two-by-two coarsening of the areal cross section of the original grid; i.e. the two dimensional points are obtained by a vertical averaging of the columns. The nongradual coarsening from grid one to grid two requires an efficient smoother which was chosen to be line SOR with vertical blocking. The remaining intermediate and coarse grids are obtained by two-by-two coarsening of the previous grid. This multigrid approach can also be applied as a preconditioner.

Both of these approaches share a low arithmetical complexity per iteration (optimal or nearly optimal order with respect to the number of unknowns) and a good convergence rate. In [97] parallel numerical results obtained with these solvers for modeling three phase flow with vertical wells is presented.

Interface solvers and preconditioners: There are two main approaches for solving the multiblock algebraic system: (1) reduction of the global system to a mortar interface problem as described in Section 3.1.1 and (2) solution of the coupled subdomain-mortar system. The

main advantage of the former approach, which involves solving both subdomain problems and an interface problem and which is currently implemented in IPARS, is that the subdomains are loosely coupled and it is easy to implement in parallel couplings of different physical and numerical models. The solution of the interface problem may, however, be expensive, especially for nonlinear problems, due to several nested iteration loops. On the other hand, solving the coupled system eliminates one of the loops and is potentially faster, but is less flexible.

In the case of single phase flow the interface problem leads to a symmetric positive definite linear system and an efficient multigrid solver with conjugate gradient (CG) smoothing has been developed and analyzed [179]. Various types of preconditioners for CG on the interface have been developed for matching grids, including balancing and Neumann–Neumann domain decomposition [50,51,99,108], Robin-type algorithms [9,21,71,73], three-field formulations [37,95], and approximation of the Steklov–Poincaré operator [8,182].

Our current approach in the multiphase flow case [178] leads to a nonlinear interface problem which provides the loosest subdomain coupling and greatest flexibility (see Section 3.1.1 for its description). This algorithm can be viewed as a nonoverlapping counterpart of some overlapping nonlinear domain decomposition methods [38,72,158]. Some efficient interface multilevel Newton-GMRES solvers and preconditioners have been developed [184,186,187]. Although these methods behave well in practice, some theoretical questions regarding their convergence are still open. An additional complication here is due to the coupling of different physical models. Choosing primary interface variables and imposing correct matching conditions are critical in this case [123].

4. Information technology tools

With the increase of computational speed came the increase in the size and resolution of simulation data. While the amount of time that is spent on computations may decrease, or may stay fixed at worst, the amount and complexity of operations on simulation data and adapting the underlying physical and numerical models has increased at least linearly. Hence the need for sophisticated IT tools which address tasks beyond simple pre- and post-processing of simulation data. This need has been recognized by a number of leading groups in computer and computational sciences throughout the world.

One objective of the IT tools effort is the realization of a collaborative software environment. Such an environment may enable scientists and engineers to collectively and collaboratively specify, compose, configure, manage, and visualize a new generation of accurate, adaptive, interactive and immersive simulations. Specifying, composing and managing these applications is nontrivial. Furthermore, managing, accessing, and manipulating the large volumes of distributed multiresolution data associated with these applications is a significant challenge. Both these issues require the development of an integrated software infrastructure providing tools and technologies that can support application developers.

Below we first give an example of how selected IT tools can benefit subsurface simulations. Next we give a few details and references on a few selected IT tools which were used.

Example of the coupling of IPARS with IT tools: In general, geological data necessary for simulation have been traditionally extremely difficult to obtain, as information has been limited to well logs and generally low resolution seismic information restricted to the position of faults, pinchouts and fractures. However, modern 3D and 4D seismic and sensor technologies are beginning to deliver not only high resolution permeability and porosity data but also details on the presure, temperature and composition of fluids present in a field. Still, large data uncertainties, which require stochastic studies, remain. For example, hundreds or thousands of Monte Carlo simulations may be performed for which the permeability data is generated with geostatistics and which incorporate all the available well log, seismic and other "real" field data. Simulation results can help to identify the best or the worst well pattern or to find an expected economic yield from a given field; all of this is with an assigned uncertainty level.

As an example (see Fig. 13), we consider a relatively simple data set [93]. The permeability field in this set is geostatistically generated. This relatively coarse data set has 9000 cells but, when hundreds of geostatistical realizations are run, possibly terabytes of data are possibly generated. Such data is analyzed in order to determine for example the "worst" and "best" recovery scenarios and an "average" economic value of a field. The amount of data that needs to be processed is overwhelming for an individual and therefore the use of the data management tool such as active data repository (ADR) is very useful (see description below).

Furthermore, assume that geological data about a field is given and that we wish to optimize recovery from such a field, or to play "what-if" scenarios. In such a case, we may run multiple cases and collect all the data as explained above. Or, we can interact with the simulation and change some of the parameters "on-the-fly". Such actions may need to be coordinated between different scientists collaborating on the same project. In this direction, the use of interactive steering software such as DISCOVER portal proved to be promising. We implemented the coupling between IPARS and DIS-

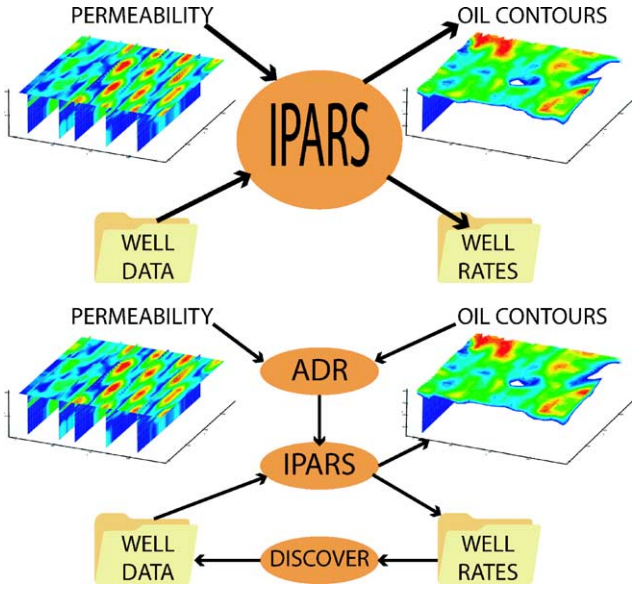

Fig. 13. Top: traditional set up of simulations. Bottom: coupling of a reservoir simulator (IPARS) with data managenent tools (ADR) and interactive sterring software (DISCOVER). Data shown: geostatistical permeability field associated with the SPE9 data problem (left) and simulated oil contours (right) after 1000 days of recovery. Note correlation of preferential water paths (right, blue spots) and oil pockets (right, red spots) with high (left, red) and low (left, blue) permeability regions.

COVER and explored "what-if" scenarios by changing well parameters.

Programming environments and application development tools: Programming environments enable scientists and engineers to specify and compose applications at a high-level using "keywords" and programming abstractions. It is a major motivation in the development of the UG software at the University of Heidelberg [26–29], the SIERRA system at Sandia National Laboratories (SNL) [5] and much of the work at the Texas Institute for Computational and Applied Mathematics (TICAM) at The University of Texas, in particular, the work on IPARS.

Adaptive computational engines: The goal of adaptive computational engines is to provide a unifying substrate to enable interoperability between application frameworks and solution methodologies. Parallel and distributed implementations of these techniques lead to interesting problems in dynamic data-distribution, load balancing, communications and coordination, and resource management. Furthermore, complex simulation on highly irregular domains may require hybrid techniques combining multiple adaptive solution methods and, correspondingly, different data-structures in different parts of the domain. Prototypes for this work are GrACE/MACE (www.caip.rutgers.edu/TASSL/Projects/ACE/) adaptive computation engines which are currently being used to support large scale adaptive simulations in subsurface modeling, computational fluid dynamics, geophyiscs, numerical relativity, and relativistic hydrodynamics. In particular, MACE was used for IPARS multiblock data structures and has achieved excellent parallel scaling [126].

Adaptive runtime management for dynamic applications: Adaptive runtime management infrastructure manages and optimizes application execution using current system and application states, and predictive models for system behavior and application performance: see work on the Armada framework [133,155,157] (www.caip.rutgers.edu/TASSL/arm.html) that provides system and application sensitive adaptive runtime support for adaptive mesh refinement applications.

Distributed interactive steering and collaborative visualization environment (DISCOVER): DISCOVER is an attempt to develop a generic framework that will enable interactive steering of scientific applications and also allow for collaborative visualization of data sets generated by such simulations. It leads to the development of a computational infrastructure that will have the potential of transforming large-scale distributed scientific and engineering simulations into interactive and collaborative simulations where numerous scientists, geographically distributed, will monitor, analyse and steer scientific computations. IPARS has been coupled with the DISCOVER framework, and it has served as a prototype implementation that has the following features: (1) IPARS application control from remote, geographically distributed clients monitoring the application; (2) Central server that bridged the connection between distributed clients and the IPARS application; (3) Collaboration among clients; (4) Regular and automatic updates from the application about the global computation parameters to all clients; (5) Plots of well data for various well parameters at the clients' desktops. Other work in this direction includes [65,81].

Active data repository: An example of a software tool for data-management and manipulation techniques for assimilating, interpreting, disseminating, and interacting with very large (petabyte), diverse and multi-resolution datasets is the ADR [80,94]. In ADR, datasets can be described by a multidimensional coordinate system. In some cases, datasets may be viewed as structured or unstructured grids; in other cases (e.g. multiscale or multiresolution problems), datasets are hierarchical with varying levels of coarse or fine meshes describing the same spatial region. ADR is designed to make it possible to carry out data aggregation on processors that are tightly coupled to disks. Since the output of a data aggregation is typically much smaller than the input, the use of ADR can significantly reduce the overhead associated with obtaining postprocessed results from large datasets. In a project underway, ADR is being used to combine an existing fluid dynamics (shallow water) code with an existing groundwater model under the IPARS framework. Modeling challenges include accounting for

the flux of phases between domains (e.g. overland flow of water seeping into the vadose zone and then into an aquifer) and flux of species between domains, since the transport mechanisms can change at domain boundaries. Moreover, different chemical reactions may be important in different parts of the domain.

Visualization: There is a need for a range of visualization techniques and tools for exploring multi-resolution data including high quality images and animations, "desktop" analysis tools for runtime data interpretation, and collaborative "portal-based" visualization for global access, real-time monitoring and control. Note that with today's technology and today's commercial software it takes hours to postprocess and produce complicated images like the one in Fig. 2. Still, these images may not yet possess the quality or the resolution adequate for high-end visualization hardware. On the other hand, images of well rates as in Fig. 1 or images of low resolution 2D slices through a field, as in Fig. 4, can be obtained fast enough so that they can even be displayed in real-time in remote locations. These issues are the subject of current research [42,43,159].

5. Conclusions

The future holds many exciting computational challenges. Huge increases in computational power provide an opportunity for developing an understanding of the correct physical description of certain phenomena at various scales. Computing hardware, systems software, and simulation tools and algorithms, can be utilized in accounting for a wide range of physical processes in a model. The need for close cooperation and collaboration among interdisciplinary teams of engineers and scientists, computational scientists, and applied mathematicians for treating multiscale and multiphysics problems has been recognized by a number of leading groups in computer and computational sciences throughout the country.

In this paper we have provided examples, mathematical and computational, demonstrating the coupling of various codes and algorithms for modeling multidomain, multiphysics applications in porous media. In addition, we have noted that there is a commonality of many multiphysics applications. e.g. time splitting involving diffusion, transport and reactions. Moreover, we have discussed the creation of comprehensive frameworks which allow the integration of system software, programming tools, and the seamless coupling of and communication between state-of-the-art simulation tools.

Acknowledgements

We would like to thank several colleagues affiliated with Center for Subsurface Modeling. Beatrice Rivière and Krzysztof Banas provided DG examples, and Xiuli Gai provided the geomechanics + flow examples and the parallel scaling results. Qin Lu, Manish Parashar and Ivan Yotov were involved in code development for the multiblock capabilities of the IPARS framework and Shuyu Sun was involved in the implementation of a reactive transport model coupled to multiphase flow. Ryan Martino was involved in the coupling of IPARS with ADR. John Wheeler provided the foundation for the IPARS framework and a lot of insight and expertise in the area of multiphase flow. Supported partially by grants DOE: DE-FG03-99ER25371, DOD: PET2/UTA01-347, and the NSF grants: SBR 9873326, ITR EIA-0121523, NPACI 10181410.

References

[1] Advanced Programming Models Working Group of the Global Grid Forum. Available from: http://www.eece.unm.edu/apm/.
[2] ACRES reference manual. Technical report, Atlantic Richfield Company, September 1998.
[3] IPARS User's Manual. Technical report, Center for Subsurface Modeling, Texas Institute for Computational and Applied Mathematics, University of Texas at Austin, 1998–2000.
[4] Cockburn B, Karniadakis GE, Shu C-W, editors. Lecture notes in computational science and engineering. Springer-Verlag;2000.
[5] SIERRA Common Code Architecture, 2002. Available from: http://www.sandia.gov/ASCI/apps/SIERRA.html.
[6] A national roadmap for vadose zone science and technology. doe/ID-10871, Available from: http://www.inel.gov/vadosezon, August 2001.
[7] Dawson CD, Holder AW, Bedient PB. FLOTRAN, a three dimensional ground water model, with comparisons to analytical solutions and other models 2000;23:517–530.
[8] Achdou Y, Nataf F. Preconditioners for the mortar method based on local approximations of the Steklov–Poincaré operator. Math Models Meth Appl Sci 1995;5(7):967–97.
[9] Achdou Y, Nataf F. A Robin–Robin preconditioner for an advection–diffusion problem. CR Acad Sci Paris Sér I Math 1997;325(11):1211–6.
[10] Agca C, Pope GA, Sepehrnoori K. Modelling and analysis of tracer flow in oil reservoirs. J Petrol Sci Eng 1990;4(1):3–19.
[11] Aizinger V, Dawson C. A discontinuous Galerkin method for two-dimensional flow and transport in shallow water. Adv Water Resour 2002;25:67–84.
[12] Aizinger V, Dawson CN, Cockburn B, Castillo P. The local discontinuous Galerkin method for contaminant transport. Adv Water Resour 2000;24:73–87.
[13] Alt HW, di Benedetto E. Nonsteady flow of water and oil through inhomogeneous porous media. Ann Scuola Norm Sup Pisa Cl Sci 4 1985;12(3):335–92.
[14] Amdahl G. Validity of the single-processor approach to achieving large-scale computing capabilities. AFIPS Press; 1967.
[15] An L, Glimm J, Sharp D, Zhang Q. Scale up of flow in porous media. In: Bourgeat AP, Carasso C, Luckhaus S, Mikelić A, editors. Mathematical modeling of flow through porous media. World Scientific; 1995. p. 26–44.
[16] Arbogast T. The existence of weak solutions to single porosity and simple dual-porosity models of two-phase incompressible flow. Nonlinear Anal Theor Meth Appl 1992;19:1009–31.
[17] Arbogast T, Cowsar LC, Wheeler MF, Yotov I. Mixed finite element methods on non-matching multiblock grids. SIAM J Numer Anal 2000;37:1295–315.

[18] Arbogast T, Dawson C, Wheeler MF. A parallel algorithm for two phase multicomponent contaminant transport. Appl Math 1995;40:163–74.
[19] Arbogast T, Dawson CN, Keenan PT, Wheeler MF, Yotov I. Enhanced cell-centered finite differences for elliptic equations on general geometry. SIAM J Sci Comput 1998;19(2):404–25.
[20] Arbogast T, Wheeler MF, Yotov I. Mixed finite elements for elliptic problems with tensor coefficients as cell-centered finite differences. SIAM J Numer Anal 1997;34(2):828–52.
[21] Arbogast T, Yotov I. A non-mortar mixed finite element method for elliptic problems on non-matching multiblock grids. Comput Meth Appl Mech Eng 1997;149:255–65.
[22] Arbogast T, Bryant S, Dawson C, Saaf F, Wang C, Wheeler M. Computational methods for multiphase flow and reactive transport problems arising in subsurface contaminant remediation. J Comput Appl Math 1996;74:19–32 [TICAM Symposium, Austin, TX, 1995].
[23] Arnold D, Brezzi F, Cockburn C, Marini D. Discontinuous Galerkin methods for elliptic problems. In: Karniadakis GE, Cockburn B, Shu C-W, editors. First International Symposium on Discontinuous Galerkin Methods, vol. 11 of Lecture Notes in Computational Science and Engineering. Springer-Verlag, 2000, p. 89–101.
[24] Baker M, editor. Cluster Computing White Paper. Available from: http://www.dcs.port.ac.uk/ mab/tfcc/WhitePaper, 2000.
[25] Bassi F, Rebay S. A high-order accurate discontinuous finite element method for the numerical solution of the compressible Navier–Stokes equations. J Comput Phys 1997;131:267–79.
[26] Bastian P, Birken K, Lang S, Johannsen K, Neuss N, Rentzreichert H, et al. UG: A flexible software toolbox for solving partial differential equations. Comput Visualization Sci 1997;1.
[27] Bastian P, Hackbusch W, Wittum G. Additive and multiplicative multi-grid—a comparison. Computing 1998;60(4):345–64.
[28] Bastian P. Load balancing for adaptive multigrid methods. SIAM J Sci Comput 1998;19(4):1303–21 [electronic].
[29] Bastian P, Lang S, Eckstein K. Parallel adaptive multigrid methods in plane linear elasticity problems. Numer Linear Algebra Appl 1997;4(3):153–76.
[30] Bathe M, Kamm RD. Fluid-structure interaction finite element analysis of pulsatile blood flow through a compliant stenotic artery. J Biomech Eng 1999:361–9.
[31] Bergamaschi L, Mantica S, Manzini G. A mixed finite element-finite volume formulation of the black-oil model. SIAM J Sci Comput 1998;20(3):970–97.
[32] Binning P, Celia M. Practical implementation of the fractional flow approach to multi-phase flow simulation. Adv Water Resour 1999;22(5):461–78.
[33] Biot M. General theory of three-dimensional consolidation. J Appl Phys 1941;12:155–64.
[34] Birnbaum NK, Francis NJ, Gerber BI. Coupled techniques for the simulation of fluid-structure and impact problems. In: 8th International Conference on Numerical Mathematics and Computational Mechanics, 1999.
[35] Brezina M, Vanek P. A black-box iterative solver based on a two-level Schwarz method. Computing 1999;63:233–63.
[36] Brezzi F, Fortin M. Mixed and hybrid finite element methods. New York: Springer-Verlag; 1991.
[37] Brezzi F, Marini LD. Macro hybrid elements and domain decomposition methods. In: Optimisation et controle, Sophia-Antipolis, 1992. Cepadues, Toulouse, 1993, p. 89–96.
[38] Cai XC, Dryja M. Domain decomposition methods for monotone nonlinear elliptic problems. In: Keyes D, editor. Contemporary mathematics, vol. 180. American Mathematical Society; 1994. p. 21–7.
[39] Castillo P, Cockburn B, Perugia I, Schötzau D. An a priori error analysis of the local discontinuous Galerkin method for elliptic problems. SIAM J Numer Anal 2000;38(5):1676–706 [electronic].
[40] Chen W, Zhu D, Hill AD. A comprehensive model of multilateral well deliverability. In paper SPE 64751, presented at the SPE International Oil & Gas Conference and Exhibition in China, 7–10 November 2000. p. 200.
[41] Chen Z, Khlopina NL. Degenerate two-phase incompressible flow problems. i. regularization and numerical results. Commun Appl Anal 2001;5(3):319–34.
[42] Childers L, Disz T, Olson R, Papka ME, Stevens R, Udeshi T. Access grid: immersive group-to-group collaborative visualization. In: Proceedings of the Fourth International Immersive Projection Technology Workshop, June 2000.
[43] Childers L, Disz TL, Hereld M, Hudson R, Judson I, Olson R, Papka ME, Paris J, Stevens R. Activespaces on the grid: the construction of advanced visualization and interaction environments. In: Parallelldatorcentrum Kungl Tekniska Högskolan Seventh Annual Conference, Stockholm, Sweden, 1999.
[44] Chippada S, Dawson CN, Martinez M, Wheeler MF. A projection method for constructing a mass conservative velocity field. Comp Meth Appl Mech Eng 1998;157:1–10.
[45] Chippada S, Dawson CN, Martinez M, Wheeler MF. Finite element approximations to the system of shallow water equations, part ii: Discrete time a priori error estimates. SIAM J Numer Anal 1999;36(1):226–50.
[46] Chorin AJ. Numerical solution of the Navier–Stokes equations. Math Comp 1968;22:745–62.
[47] Chorin AJ. On the convergence of discrete approximations to the Navier–Stokes equations. Math Comp 1969;23:341–53.
[48] Coats KH, Thomas LK, Pierson RG. Compositional and black oil reservoir simulator, In: 13th SPE Symposium on Reservoir Simulation, San Antonio, Texas, 12–15 February 1995.
[49] Cockburn B, Shu C-W. The local discontinuous Galerkin method for time-dependent convection–diffusion systems. SIAM J Numer Anal 1998;35(6):2440–63 [electronic].
[50] Cowsar LC, Mandel J, Wheeler MF. Balancing domain decomposition for mixed finite elements. Math Comp 1995;64:989–1015.
[51] Cowsar LC, Weiser A, Wheeler MF. Parallel multigrid and domain decomposition algorithms for elliptic equations. In: Keyes DE et al., editors. Fifth International Symposium on Domain Decomposition Methods for Partial Differential Equations. Philadelphia: SIAM; 1992. p. 376–85.
[52] Dawson CN, Aizinger V, Cockburn B. Local discontinuous Galerkin methods for problems in contaminant transport. In: Cockburn B, Karniadakis GE, Shu CW, editors. First International Symposium on Discontinuous Galerkin Methods, vol. 11 of Lecture Notes in Computational Science and Engineering. Springer-Verlag; 2000. p. 309–14.
[53] Dawson CN, Klie H, Wheeler MF, Woodward C. A parallel, implicit, cell-centered method for two-phase flow with a preconditioned Newton–Krylov solver. Comput Geosci 1997;1:215–49.
[54] Dawson CN, Parr VJ, Wheeler MF. Issues in parallel computation of flow and transport in surface waters. In: Arabnia HR, editor. Proceedings of the International Conference on Parallel and Distributed Processing Techniques and Applications, Las Vegas, NV, 26–29 June, vol. 1. CSREA Press; 2000. p. 21–7.
[55] Dawson CN, Proft J. Coupling local discontinuous Galerkin and continuous Galerkin methods for transport equations. Comp Meth Appl Mech Eng 2002;191:3213–31.
[56] Dawson CN, van Duijn CJ, Wheeler MF. Characteristic-Galerkin methods for contaminant transport with nonequilibrium adsorption kinetics. SIAM J Numer Anal 1994;31(4):982–99.
[57] Dawson CN, Wheeler MF. Time-splitting methods for advection–diffusion–reaction equations arising in contaminant transport. In: O'Malley RE, editor. Proceedings of the Second International Conference on Industrial and Applied Mathematics ICIAM'91, Philadelphia. SIAM; 1991. p. 71–82.

[58] Dawson CN, Wheeler MF, Chiang CY. Modeling in-situ biorestoration of organic compounds in groundwater. Transp Porous Media 1991;6:667–702.
[59] Dean R. A poroelastic multicompent reservoir simulator, submitted for publication.
[60] Delshad M, Pope GA. Comparison of the three-phase oil relative permeability models. Transp Porous Media 1989;4:59–83.
[61] Demkowicz L, Vardapetyan L. Modeling of electromagnetic absorption/scattering problems using hp-adaptive finite elements. Comp Meth Appl Mech Eng 1998;152(1–2):103–24.
[62] Desai CS. Modelling and testing: implementation of numerical models and their application in practice. In: Desai CS, Gioda G, editors. Numerical methods and constitutuve modelling in geomechanics. New York: Springer-Verlag; 1990. p. 1–168.
[63] Ding Y, Renard G. A new representation of wells in numerical reservoir simulation. SPE Reservoir Eng 1994:140–4.
[64] Discacciati M, Miglio E, Quarteroni A. Mathematical and numerical models for coupling surface and groundwater flows. Appl Numer Math, submitted for publication.
[65] Disz TL, Evard R, Henderson MW, Nickless W, Olson R, Papka ME, et al. Designing the future of collaborative science: Argonne's futures laboratory. IEEE Parallel Distributed Technol Sys Appl 1995:14–21.
[66] Dogru AH, Li KG, Sunaidi HA, Habiballah WA, Fung L, Al-Zamil N, Shin D, McDonald AE, Srivastava NK. Massively parallel reservoir simulator for large scale reservoir simulation. In: Proceedings of the SPE Symposium on Reservoir Simulation, Proceedings of the 1999 15th Symposium on Reservoir Simulation, 14–17 February 1999. p. 73–92.
[67] Dogru AH. Megacell reservoir simulation. J Petrol Technol 2000;52(5).
[68] Dongarra JJ, Duff IS, Sorensen DC, van der Vorst HA. Numerical linear algebra for high-performance computers. Philadelphia, PA: Society for Industrial and Applied Mathematics (SIAM); 1998.
[69] Douglas Jr J, Ewing RE, Wheeler MF. The approximation of the pressure by a mixed method in the simulation of miscible displacement. RAIRO Anal Numér 1983;17(1):17–33.
[70] Douglas Jr J, Ewing RE, Wheeler MF. A time-discretization procedure for a mixed finite element approximation of miscible displacement in porous media. RAIRO Anal Numér 1983;17(3):249–65.
[71] Douglas Jr J, Paes Leme PJ, Roberts JE, Wang J. A parallel iterative procedure applicable to the approximate solution of second order partial differential equations by mixed finite element methods. Numer Math 1993;65(1):95–108.
[72] Dryja M, Hackbusch W. On the nonlinear domain decomposition method. BIT 1997;37(2):296–311.
[73] Dureisseix D, Ladevèze P. A multi-level and parallel strategy for structural analysis. In: Owen DRJ, Onate E, Hinton E, editors. Computational plasticity, fundamentals and applications. Barcelonne: CIMNE; 1997. p. 1790–7.
[74] Durlofsky LJ. Numerical calculation of equivalent grid block permeability tensors for heterogeneous porous media. Water Resour Res 1991;27(5):699–708.
[75] Eaton J. A multigrid preconditioner for two-phase flow in porous media. PhD thesis, The University of Texas at Austin, 2001.
[76] Eigenstat SC, Walker HF. Globally convergent inexact Newton method. SIAM J Sci Optim 1994;4:393–422.
[77] Ewing RE, Lazarov RD, Wang J. Superconvergence of the velocity along the gauss lines in mixed finite element methods. SIAM J Numer Anal 1991;28:1015–29.
[78] Ewing RE, Lazarov RD, Lyons SL, Papavassiliou DV, Pasciak J, Qin G. Numerical well model for non-Darcy flow through isotropic porous media. Comput Geosci 1999;3(3–4):185–204.
[79] Farhat C, Lesoinne M. Two efficient staggered algorithms for the serial and parallel solution of three-dimensional nonlinear transient aeroelastic problems. Comp Meth Appl Mech Eng 2000;182:499–515.
[80] Ferreira R, Kurc T, Beynon M, Chang C, Sussman A, Saltz J. Object-relational queries into multidimensional databases with the active data repository. Parallel Process Lett 1999;9(2):173–95.
[81] Foster I, Papka ME, Stevens R. Tools for distributed collaborative environments: a research agenda. In: High Performance Distributed Computing Focus Workshop on Multimedia and Collaborative Environments, 1996.
[82] Glowinski R, Mantel B, Périaux J. Numerical methods for the time dependent Navier–Stokes equations for incompressible viscous fluids by finite-element and alternating direction methods, 1982.
[83] Glowinski R, Wheeler MF. Domain decomposition and mixed finite element methods for elliptic problems. In: Glowinski R, Golub GH, Meurant GA, Periaux J, editors. First International Symposium on Domain Decomposition Methods for Partial Differential Equations. Philadelphia: SIAM; 1988. p. 144–72.
[85] Grigg RB, Hwang MK. High velocity gas flow effects in porous gas–water system. SPE 1998;39978:203–14.
[86] Helmig R. Multiphase flow and transport processes in the subsurface. Springer; 1997.
[87] Foster I. Designing and building parallel programs. Addision-Wesley; 1995.
[88] Jenkins EW, Kelley CT, Kees CE, Miller CT. An aggregation-based domain decomposition preconditioner for groundwater flow. SIAM J Sci Comput 2001;23(2):430–41.
[89] Kaasschieter ES. Mixed finite elements for accurate particle tracking in saturated groundwater flow. Adv Water Resour 1995;18:277–94.
[90] Kanney J, Miller CT, Kelley CT. Convergence of iterative split-operator approaches for approximating nonlinear reactive transport problems. Preprint.
[91] Kelley CT. Iterative methods for linear and nonlinear equations. Philadelphia: SIAM; 1995.
[92] Killough J, Commander D. Scalable parallel reservoir simulation on a Windows NT-based workstation cluster. In: SPE paper 51883 presented at the Fifteenth SPE Symposium on Reservoir Simulation, February, 1999. p. 41–50.
[93] Killough JE. Ninth SPE comparative solution projection: a reexamination of black-oil simulation. In: The 13th Symposium on Reservoir Simulation, San Antonio, Texas, February 1995, SPE 29110. p. 135–47.
[94] Kurc T, Chang C, Ferreira R, Sussman A, Saltz J. Querying very large multi-dimensional datasets in adr. In: Proceedings of SC'99, Portland, Oregon, 13–19 November 1999.
[95] Kuznetsov YA, Wheeler MF. Optimal order substructuring preconditioners for mixed finite element methods on non-matching grids. East–West J Numer Math 1995;3(2):127–43.
[96] Lacroix S, Vassilevski Y, Wheeler MF. Iterative solvers of the implicit parallel accurate reservoir simulator (IPARS). Numer Linear Algebra Appl 2001;4:537–49.
[97] Lacroix S, Vassilevski Yu, Wheeler JA, Wheeler MF. Iterative solution methods for modeling multiphase show in porous media fully implicitly, submitted for publication.
[98] Lake LW. Enhanced oil recovery. Englewood Cliffs, NJ: Prentice-Hall; 1989.
[99] Le Tallec P. Neumann–Neumann domain decomposition algorithms for solving 2D elliptic problems with nonmatching grids. East–West J Numer Math 1993;1(2):129–46.
[100] Lenhard RJ, Parker JC. Measurement and prediction of saturation–pressure relationships in three-phase porous media systems. J Contam Hydrol 1987;1:407–24.
[101] Lenhard RJ, Oostrom M, White MD. Modeling fluid flow and transport in variably saturated porous media with the stomp simulator. 2. Verification and validation exercises. Adv Water Resour 1995;18(6).

[102] Lewis RW, Sukirman Y. Finite element modelling for simulating the surface subsidence above a compacting hydrocarbon reservoir. Int J Analytic Numer Meth Geomech 1993;18:619–39.
[103] Litvak ML, Wang CH. Simplified phase-equilibrium calculations in integrated reservoir and surface-pipeline-network models. SPE J 2000;5(2):236–41.
[104] Lu Q, Peszynska M, Wheeler MF. A parallel multi-block black-oil model in multi-model implementation. SPE J 2002;7(3):278–87.
[105] Lu Q, Parashar M, Peszynska M, Wheeler MF. Parallel implementation of multi-physics/multi-block for multi-phased flow in subsurface, in preparation.
[106] Lu Q. A parallel multi-block/multi-physics approach for multiphase flow in porous media. PhD thesis, University of Texas at Austin, Austin, Texas, 2000.
[107] MacMillan DJ, Pletcher JL, Bourgeois SA. Practical tools to assist history matching. In: Proceedings of the 1999 15th Symposium on Reservoir Simulation, 14–17 February 1999. p. 107–17.
[108] Mandel J, Brezina M. Balancing domain decomposition for problems with large jumps in coefficients. Math Comp 1996; 65(216):1387–401.
[109] Mandel J, McCormick S, Ruge J. An algebraic theory for multigrid methods for variational problems. SIAM J Numer Anal 1988;25:91–110.
[110] Mattax CC, Dalton RL. Reservoir simulation. In: SPE monograph series, vol. 13. Richardson, Texas, 1990.
[111] Meuer HW, Strohmaier E, Dongarra J. Top 500 report 1996. Supercomputer 1997;13(1).
[112] Miglio E, Quarteroni A, Saleri F. On the coupling of free surface and groundwater flows. Comput Fluids, submitted for publication.
[113] Minkoff S, Stone C, Arguello J, Bryant S, Eaton J, Peszynska M, Wheeler M. Coupled geomechanics and flow simulation for time-lapse seismic modeling. In: Expanded Abstracts, Soc Expl Geophys, 1999. p. 1667–70.
[114] Minkoff S, Stone CM, Arguello JG, Bryant S, Eaton J, Peszynska M, Wheeler MF. Staggered in time coupling of reservoir flow simulation and geomechanical deformation: step 1—one-way coupling. In: 1999 SPE Symposium on Reservoir Simulation, Houston, Texas, 1999, SPE 51920.
[115] Minkoff S, Stone CM, Arguello JG, Bryant S, Eaton J, Peszynska M, Wheeler MF. Staggered in time coupling of reservoir flow simulation and geomechanical deformation: step 1—one-way coupling. In: 1999 SPE Symposium on Reservoir Simulation, Houston, Texas, 1999, SPE 51920.
[116] Minkoff S, Stone CM, Bryant S, Peszynska M, Wheeler MF. A loose coupling algorithm for fluid flow and geomechanical deformation modeling, submitted for publication.
[117] Nakata M, Weiser A, Wheeler MF. Some superconvergence results for mixed finite element methods for elliptic problems on rectangular domains. In: Whiteman JR, editor. The mathematics of finite elements and applications V. Academic Press; 1985. p. 367–89.
[118] Oden JT, Babuška I, Baumann CE. A discontinuous hp finite element method for diffusion problems. J Comput Phys 1998; 146:491–516.
[119] Parashar M, Wheeler JA, Pope G, Wang K, Wang P. A new generation EOS compositional reservoir simulator. Part II: framework and multiprocessing. In: Fourteenth SPE Symposium on Reservoir Simulation, Dallas, Texas. Society of Petroleum Engineers; June 1997. p. 31–8.
[120] Parker JC. Multiphase flow and transport in porous media. Rev Geophys 1989;27(3):311–28.
[121] Peaceman DW. Fundamentals of numerical reservoir simulation. 1st ed. Amsterdam, Oxford, New York: Elsevier Scientific Publishing Company; 1977.
[122] Peaceman DW. Interpretation of well-block pressure in numerical reservior simulation with non-square grid blocks and anisotropic permeability. Trans AIME 1983;275:10–22.
[123] Peszynska M. Advanced techniques and algorithms for reservoir simulation III. Multiphysics coupling for two phase flow in degenerate conditions. In: Chadam J, Al Cunningham, Ewing RE, Ortoleva P, Wheeler MF, editors. IMA Volumes in Mathematics and its Applications, vol. 131: Resource recovery, confinement, and remediation of environmental hazards. Springer; 2002. p. 21–40.
[124] Peszynska M, Lu Q, Wheeler MF. Coupling different numerical algorithms for two phase fluid flow. In: Whiteman JR, editor. MAFELAP Proceedings of Mathematics of Finite Elements and Applications, Brunel University, Uxbridge, UK, 1999. p. 205–14.
[125] Peszynska M, Lu Q, Wheeler MF. Multiphysics coupling of codes. In: Bentley LR, Sykes JF, Brebbia CA, Gray WG, Pinder GF, editors. Computational methods in water resources. A.A. Balkema; 2000. p. 175–82.
[126] Peszynska M, Wheeler MF, Yotov I. Mortar upscaling for multiphase flow in porous media. Comput Geosci 2002;6:73–100.
[127] Peszynska M, Jenkins E, Wheeler MF. Boundary conditions for fully implicit two-phase flow model. In: Feng X, Schulze T-P, editors. Recent advances in numerical methods for partial differential equations and applications. AMS Contemporary Mathematics Series, 2002.
[128] Peszynska M, Sun S. Reactive transport model coupled to multiphase flow models. In: Hassanizadeh S-M, Schotting RJ, Gray WG, Pinder GF, editors. Computational methods in water resources. Elsevier; 2002. p. 923–30 .
[129] Poland GH, Davis J. Land subsidence due to withdrawal of fluids. Geolog Soc Amer Rev Eng Geol 1969;2:187–269.
[130] Pruess K. TOUGH2—a general-purpose numerical simulator for multiphase fluid andheat flow. Technical Report LBL 29400, Lawrence Berkeley Laboratory, University of California, Berkeley, Calif, 1991.
[131] Quarteroni A, Pasquarelli F, Valli A. Heterogeneous domain decomposition: principles, algorithms, applications. In: Keyes DE et al., editors, Fifth International Symposium on Domain Decomposition Methods for Partial Differential Equations. Philadelphia: SIAM; 1992. p. 129–50.
[132] Quarteroni A, Saleri F, Veneziani A. Factorization methods for the numerical approximation of Navier–Stokes equations. Comput Methods Appl Mech Eng 2000;188(1–3):505–26.
[133] Ramanathan S, Parashar M. A multi-threaded communication engine for distributed adaptive applications. In: 2001 International Conference on Parallel and Distributed Processing Techniques and Applications (PDPTA 2001), Nevada, USA. Computer Science Research, Education, and Applications (CSREA) Press; 2001.
[134] Rannacher R. On Chorin's projection method for the incompressible Navier–Stokes equations. In: The Navier–Stokes equations II – theory and numerical methods, Oberwolfach, 1991. Berlin: Springer; 1992. p. 167–183.
[135] Richards LA. Capillary conduction of liquids through porous media. Physics 1931;1:318–33.
[136] Rivière B. Discontinuous Galerkin finite element methods for solving the miscible displacement problem in porous media. PhD thesis, The University of Texas at Austin, 2000.
[137] Rivière B, Wheeler MF. Coupling locally conservative methods for single phase flow. Comput Geosci, in press.
[138] Rivière B, Wheeler MF. A discontinuous Galerkin method for two-phase flow in porous media, in preparation.
[139] Rivière B, Wheeler MF. Discontinuous Galerkin methods for flow and transport in porous media. Comm Numer Meth Eng 2002;18:63–80.

[140] Rivière B, Wheeler MF. Non conforming methods for transport with nonlinear reaction. TICAM report 01-29, 2001, submitted for publication.
[141] Rivière B, Wheeler MF. Discontinuous finite element methods for acoustic and elastic wave problems. Part I: Semidiscrete error estimates. Technical Report 01-04, Texas Institute for Computational and Applied Mathematics, The University of Texas at Austin, 2001, submitted for publication.
[142] Riviere B, Wheeler MF, Banas K. Part II: Discontinuous Galerkin method applied to a single-phase flow in porous media. Comput Geosci 2000;4:337–49.
[143] Riviere B, Wheeler MF, Girault V. Part I: Improved energy estimates for interior penalty, constrained and discontinuous Galerkin methods for elliptic problems. Comput Geosci 1999;3:337–60.
[144] Riviere B, Wheeler MF. A discontinuous Galerkin method applied to nonlinear parabolic equations. Discontinuous Galerkin methods: theory, computation and applications. Comput Sci Eng 1999;5:231–44.
[145] Russell T. Modeling of multiphase multicontaminant transport in the subsurface. Rev Geophys 1995;33.
[146] Wheeler MF, Russell TF. Finite element and finite difference methods for continuous flows in porous media. In: Ewing RE, editor. The mathematics of reservoir simulation. Philadelphia: SIAM; 1983. p. 35–106.
[147] Saaf F. A study of reactive transport phenomena in porous media. PhD thesis, Rice University, 1996.
[148] Schlumberger Technology Corporation. Eclipse-100, Reference Manual, 1998.
[149] Schlumberger Technology Corporation. Eclipse-100, Technical Description, 1998.
[150] Settari A, Mourits FM. Coupling of geomechanics and reservoir simulation models. In: Siriwardane, Zaman, editors. Computer methods and advances in geomechanics. Rotterdam: Balkema; 1994. p. 2151–8.
[151] Settari A, Walters D. Advances in coupled geomechanical and reservoir modeling with applications to reservoir compaction. In: Exp. Abst., SPE 51927, SPE, 1999. p. 345–57.
[152] Showalter R. Diffusion in poro-elastic media. J Math Anal Appl 2000;251:310–40.
[153] Showalter R, Momken B. Single-phase flow in composite poroelastic media. Math Meth Appl Sci 2002;25:115–39.
[154] Showalter R, Su N. Partially saturated flow in a poroelastic medium. Discrete Contin Dynam Syst—Ser B 2001;1:403–20.
[155] Sinha S, Parashar M. System sensitive runtime management of adaptive applications on heterogeneous environments. In: Proceedings of the 15th International Parallel and Distributed Computing Symposium (IEEE, ACM), 10th Heterogeneous Computing Workshop, San Francisco, CA. IEEE Computer Society Press, 2001. CD-ROM.
[156] Smith BF, Bjørstad PE, Gropp WD. Domain decomposition. Parallel multilevel methods for elliptic partial differential equations. Cambridge: Cambridge University Press; 1996.
[157] Steensland J, Chandra S, Thun'e M, Parashar M. Characterization of domain-based partitioners for parallel SAMR applications. In: IASTED International Conference on Parallel and Distributed Computing and Systems, 2000.
[158] Tai X-C, Espedal M. Rate of convergence of some space decomposition methods for linear and nonlinear problems. SIAM J Numer Anal 1998;35(4):1558–70.
[159] Taylor VE, Chen J, Disz TL, Papka ME, Stevens R. Immersive visualization of supercomputer applications: Exploring the end-to-eng lag of different applications. IEEE Comput Sci Eng 1996;3(4):46–54.
[160] Tester JW, Modell M. Thermodynamics and its applications. 3rd ed. Prentice-Hall; 1997.
[161] Thomas JM. These de Doctorat d'etat. 'a l'Universite Pierre et Marie Curie, 1977.
[162] Trangenstein JA, Bell JB. Mathematical structure of the black-oil model for petroleum reservoir simulation. SIAM J Appl Math 1989;49(3):749–83.
[163] van Delden R, Jalali Y. Subsea production control systems; mature technology facing demands for performance enhancement and embedded intelligence. In: Presentation at Offshore Europe 2001: Oil and Gas Exhibition Conference, 4–7 September 2001, Aberdeen, SPE 71823, 2001.
[164] Vanek P, Mandel J, Brezina M. Algebraic multigrid by smoothed aggregation for second and fourth order elliptic problems. Computing 1996;56:179–96.
[165] Vauclin M, Khanji D, Vachaud G. Experimental and numerical study of a transient, two-dimensional unsaturated-saturated watwer table recharge problem. Water Resour Res 1979;15(5):1089–101.
[166] Wang P, Yotov I, Wheeler MF, Arbogast T, Dawson CN, Parashar M, Sepehrnoori K. A new generation EOS compositional reservoir simulator. Part I: Formulation and discretization. In: Fourteenth SPE Symposium on Reservoir Simulation, Dalas, Texas, Society of Petroleum Engineers, June 1997. p. 55–64.
[167] Weiser A, Wheeler MF. On convergence of block-centered finite differences for elliptic problems. SIAM J Numer Anal 1988;25(2):351–75.
[168] Wheeler J, Wheeler MF, Yotov I. Enhanced velocity mixed finite element methods for flow in multiblock domains. Comput Geosci, submitted for publication.
[169] Wheeler JA, Smith RA. Reservoir simulation on a hypercube. SPE Reservoir Eng 1990:544–8.
[170] Wheeler JA. Private communications.
[171] Wheeler MF. Advanced techniques and algorithms for reservoir simulation, II: The multiblock approach in the integrated parallel accurate reservoir simulator (IPARS). In: Chadam J, Al Cunningham, Ewing RE, Ortoleva P, Wheeler MF, editors. IMA volumes in mathematics and its applications, vol. 131: resource recovery, confinement, and remediation of environmental hazards. Springer, 2002.
[172] Wheeler MF, Arbogast T, Bryant S, Eaton J, Lu Q, Peszynska M, Yotov I. A parallel multiblock/multidomain approach to reservoir simulation. In: Fifteenth SPE Symposium on Reservoir Simulation, Houston, Texas, Society of Petroleum Engineers, 1999, SPE 51884. p. 51–62.
[173] Wheeler MF, Dawson CN. An operator-splitting method for advection-diffusion-reaction problems. In: Whiteman JR, editor. The mathematics of finite elements and applications VI. London: Academic Press; 1987. p. 382–463.
[174] Wheeler MF, Yotov I. Mortar mixed finite element approximations for elliptic and parabolic equations. In: Chui CK, Schumaker LL, editors. Approximation theory IX. Nashville, TN: Vanderbilt University Press; 1998. p. 377–92.
[175] Wheeler MF, Peszynska M, Dawson CN. Multiphysics couplings for environmental problems. In: Proceedings of the DOD Users Group Conference, Albuquerque, New Mexico, 2000.
[176] Wheeler MF, Peszynska M, Gai X, El-Domeiri O. Modeling subsurface flow on PC cluster. In: Tentner A, editor. High performance computing. SCS; 2000. p. 318–23.
[177] Wheeler MF, Wheeler JA, Peszynska M. A distributed computing portal for coupling multi-physics and multiple domains in porous media. In: Bentley LR, Sykes JF, Brebbia CA, Gray WG, Pinder GF, editors. Computational methods in water resources. A.A. Balkema; 2000. p. 167–74.
[178] Wheeler MF, Yotov I. Physical and computational domain decompositions for modeling subsurface flows. In: Mandel J, et al., editors. Tenth International Conference on Domain Decomposition Methods, Contemporary Mathematics, vol. 218. American Mathematical Society; 1998. p. 217–28.

[179] Wheeler MF, Yotov I. Multigrid on the interface for mortar mixed finite element methods for elliptic problems. Comput Meth Appl Mech Eng 2000;184:287–302.
[180] Wheeler MF. An elliptic collocation-finite element method with interior penalties. SIAM J Numer Anal 1978;15(1):152–61.
[181] White MD, Oostrom M, Lenhard RJ. Modeling fluid flow and transport in variably saturated porous media with the stomp simulator. 1. Nonvolatile three-phase model description. Adv Water Resour 1995;18(6).
[182] Xu J, Zhang S. Preconditioning the Poincaré–Steklov operator by using Green's function. Math Comp 1997;66(217):125–38.
[183] Yeh GT, Tripathi VS. A critical evaluation of recent developments in hydrogeochemical transport models of reactive multichemical components. Water Resour Res 1989;25:93–108.
[184] Yotov I. A multilevel Newton–Krylov interface solver for multiphysics couplings of flow in porous media. Numer Linear Algebra Appl, in press.
[185] Yotov I. Mixed finite element methods for flow in porous media. PhD thesis, Rice University, Houston, Texas, 1996. TR96-09, Dept. Comp. Appl. Math., Rice University and TICAM report 96-23, University of Texas at Austin.
[186] Yotov I. Interface solvers and preconditioners of domain decomposition type for multiphase flow in multiblock porous media. In: Minev P, Lin Y, Wong YS, editors. Advances in computation: theory and practice. Nova Science Books and Journals; 2000.
[187] Yotov I. Advanced techniques and algorithms for reservoirsimulation IV. Multiblock solvers and preconditioners. In: Chadam J, Al Cunningham, Ewing RE, Ortoleva P, Wheeler MF, editors. IMA volumes in mathematics and its applications, vol. 131: resource recovery, confinement, and remediation of environmental hazards. Springer; 2002.
[188] Zienkiewicz OC, Chan AHC, Pastor M, Schrefler BA, Shiomi T. Computational geomechanics. Chichester: Wiley; 1999.