

A DISTRIBUTED COMPUTING PORTAL FOR COUPLING MULTI-PHYSICS AND MULTIPLE DOMAINS IN POROUS MEDIA

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ABSTRACT. We describe a computing framework or portal called IPARS for modeling multi-phase, multi-physics flow in porous media, suitable for massively parallel computers or clusters of workstations. The framework provides all the memory management, message passing, table lookup, solvers and input/output so that a developer only needs to code the relevant physics. This software permits rigorous, physically representative coupling of different physical and numerical flow models in different parts of the domain and accounts for structural discontinuities. In addition, different formulations or physical models can exist on different subdomains. The framework also permits non-matching grids between subdomains for handling geological faults using either a *mortar* or a *dual* formulation. In this paper we discuss single-, two-, and three-phase flow models that have been implemented within the framework based upon a fully coupled *dual* interface formulation for coupling of subdomains. A brief discussion of multi-physics using the *mortar* formulation can be found in [16] of this proceedings.

1. INTRODUCTION

Cost-effective management of oil and gas reservoirs is driving development of a new generation of reservoir simulators. The central challenge is to maximize economic benefit from a resource whose properties are only poorly known and in which a variety of complex chemical and physical phenomena take place. Three areas of research are converging to address this challenge: multi-physics multi-numerics models, improved reservoir description, and production optimization.

The heart of this effort must be a robust reservoir simulator. This will comprise coupled programs that together account for multi-component, multi-phase flow and transport through heterogeneous geological structures (porous media) and through wells, and surface facilities. The coupled programs must accommodate different physical processes occurring simultaneously in different parts of the domain, and for computational efficiency, should also accommodate multiple numerical schemes.

A prerequisite for effective reservoir simulation is a high quality description of the reservoir properties that govern fluid flow. Recent advances in seismic profiling, well

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logging, continuous data telemetry, pressure transient testing, geostatistics, chemical tracers, and automated history matching offer great potential for better defining these reservoir properties. These techniques yield a heterogeneous set of data structures that represent different geological features at different levels of spatial resolution. Thus the practical integration of these new, multi-scale, static and dynamic data sources presents a huge data management challenge. After a reservoir is brought onstream this difficulty is compounded by a feedback loop between flow rates predicted by the simulator and those observed in the field. This feedback demands continuous updating of reservoir properties through history matching.

In contrast to the properties of the reservoir, the number, locations and flow rates of injection and production wells are entirely determined by the operator. The problem is to find the optimal recovery strategy within an extremely large space of possible strategies against the backdrop of uncertainty in the reservoir description. The ability to carry out comparative computations and quantify uncertainty in many multi-scale, multi-resolution datasets obtained from reservoir description and reservoir simulation models is essential for solving this problem. Moreover, it is an economic imperative to define a recovery strategy as soon as possible at the appraisal stage, and to refine that strategy in real time as new wells are drilled and new data obtained.

Implementing cost-effective groundwater remediation strategies poses similar challenges to those described above for petroleum reservoir production. Both applications involve complex, difficult-to-characterize geological structures and require selection of an optimum strategy from a large set of possibilities. The environmental application presents special additional difficulties, a primary one being that the location and duration of a contamination source are often poorly constrained. Furthermore, in contrast to petroleum reservoirs, there is no revenue stream with which to balance the cost of obtaining additional information. Hence groundwater remediation places a premium on realization management, i.e., being able to carry out a very large number of conditional simulations in order to maximize the value of existing information and to guide the collection of new data.

Based on the needs described above, a new generation framework or portal called IPARS (Integrated Parallel Accurate Reservoir Simulator) suitable for single processor and massively parallel computers and clusters of workstations has been developed at the Center for Subsurface Modeling (CSM) at The University of Texas at Austin. The IPARS framework provides all the memory management, well management, message passing, table lookup and input/output management, so that the developer only needs to code the relevant physics. The portal is designed for portability on a collection of machines with no special adaptation of the code between machines.

In the past, porous-media simulators have been developed with a focus on a particular physical process, e.g. single-phase flow, Richard's equation, or steam stimulation. As field development strategies become more complex, several recovery processes often occur simultaneously within the same aquifer or reservoir. Through the development of the multi-block paradigm, we have broken the restraint of traditional

“one-process-at-a-time” simulators that cannot couple the different domains in such fields. The IPARS framework permits rigorous, physically representative coupling of different models in different parts of the domain. A discussion of interface couplings based on mortar spaces can be found in [1, 20, 19, 15] and in these proceedings in [16]. Both the mortar and dual approaches have advantages and disadvantages which are currently under investigation at CSM.

In addition, different formulations or physical models can exist on different subdomains. In this direction, IPARS has been loosely coupled with the Sandia geomechanical model JAS3D [12]. This coupling allows for large nonlinear deformations, contacts, sliding surfaces, and inelastic responses in the geology.

The outline of this paper is as follows: In Section 2, we briefly describe the IPARS framework. In Section 3, we define single-phase, two-phase hydrology, and three-phase black-oil models implemented under IPARS. For description of an air-water model as well as computational results see [11]. A formulation of the dual interface approximation is given in Section 4. In Section 5, computational results are presented.

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2. THE IPARS SIMULATION FRAMEWORK

The development of a subsurface simulator framework suitable for research and with possible commercial applications has been an ongoing project for the past four years at CSM. The IPARS framework [18, 13] runs on parallel and single processor computers, solves problems involving a million or more grid elements, and supports a variety of physical and mathematical models and in the future generalized well management.

The simulator framework supports three dimensional transient flow of multiple phases containing multiple components plus immobile phases (rock and adsorbed components). Phase densities and viscosities may be arbitrary functions of pressure and composition or may be represented by simpler functions. The initial system is isothermal, but nonisothermal calculations may be added later.

Porosity and permeability may vary with location in an arbitrary manner. Relative permeability and capillary pressure are functions of saturations and rock type. The framework allows for general two-phase and three-phase formulations. Any dependence of relative permeability and capillary pressure on composition and pressure is left to the individual physical model.

The subsurface reservoir/aquifer consists of one or more geological fault blocks. Each fault block has an independent user-defined coordinate system and gravity vector. Flow between fault blocks however, can occur only through a common face. The primary grid imposed on each fault block is a logical cube with variable grid spacing. Irregular geometries are represented by keying out (removing) selected grid elements.

Currently, the framework supports logically rectangular grids. Dynamic grid refinement of the primary grid on each fault block is supported by the framework but also must be supported by individual physical models.

The IPARS framework supports an arbitrary number of wells each with one or more completion intervals. A well may penetrate more than one fault block but a completion interval must occur in a single fault block. On parallel machines, well grid elements may be assigned to more than one processor. The framework assigns primary responsibility for a well calculation to one of these processors and communicates well data between processors.

Discretizations that have been employed in the framework are cell-centered finite differences or mixed finite elements based on the RT0 spaces and backward differences in time. Provision has been made for higher order approximations. The framework has also been designed to handle dynamic grid refinement but this is not currently implemented.

The nonlinear algebraic equations are solved by either fully implicit or semi-implicit techniques. The simulator has the capability of updating quantities that do not strongly influence the primary unknowns both between Newtonian iterations and between time steps. For example, tracer calculations may be made between time steps. Both mass balance and volume balance formulations are supported. The framework supports multiple linear solvers such as line SOR, Petsc, and multi-stage preconditioners [8, 5]. Currently, there are five separate solvers in IPARS.

Portability of the simulator is emphasized as well as ease of implementation. In particular, the object oriented framework has modules written in Fortran, C, and C++. The basic idea has been to code in the language most appropriate for a given calculation. The code is portable across several serial and parallel platforms including Linus (clusters), SGI, RS6000, T3E, and Windows (DOS). The parallel portion of the simulator is formulated for a distributed memory, message passing machine. MPI was selected for the base code but the framework is organized to facilitate incorporation of any reasonable message passing system.

Internally, the simulator uses a single set of units chosen to minimize multiplication by conversion factors and facilitate interpretation of debug output. Externally, the user may choose any physically correct and consistent units. The simulator will determine and apply the appropriate conversion factors. The simulator provides default sets of external units.

Free form keyword input is used for data input to the computation stage of the simulator. The keyword input file is explicitly defined to serve as an output file for a graphical front end or geostatistical grid and property generator. Work on web launching of IPARS is ongoing and preliminary results using NETSOLVE have been encouraging [2].

Multiple levels of output with visualization are provided in the simulator. These range from selective memory dumps for debugging or restart to minimal output for automatic history matching. Present research involves the coupling of IPARS with

ADR (Active Data Repository) [3, 9] for exploration of history matching scenarios with uncertainty in the geological data. ADR enables integration of storage, retrieval, and processing of multidimensional multiple datasets on parallel machines and provides support for spatial queries and complex data aggregations.

3. PHYSICAL MODELS IN IPARS

In the IPARS multi-block setting, each of the faultblocks can have a different *physical model* associated with it. Traditionally, a physical model is a set of differential equations (conservation and constitutive laws) describing a particular physical process, e.g., single-phase or multi-phase flow. Additionally, for a given physical process, there can be multiple discretizations and numerical algorithms implemented. For example, an algorithm for the two-phase flow can be solved in an implicit, semi-implicit, or explicit fashion. A physical model is then the set of specific discrete equations which are to be solved.

There are currently eight physical models in IPARS:

- Implicit hydrology model (two liquid phases)
- IMPES hydrology model (two liquid phases)
- Two implicit black-oil models (different primary unknowns)
- Implicit air-water model
- Two single-phase models (implicit and explicit)
- Compositional model

The differential equations for each model typically form a subset of the following general set of equations. Consider isothermal flow in the absence of reactions, dispersion and adsorption. The conservation of mass is specified for each component denoted with subscript M as follows [4, 10, 14]:

$$(1) \quad \frac{\partial(\phi W_M)}{\partial t} - \nabla \cdot F_M = q_M.$$

Here W_M is the total component concentration which is equal to the sum of $\rho_m S_m n_{mM}$ over all phases m , with ρ_m, S_m denoting density and saturation of phase m , respectively, and n_{mM} denoting mass fraction of component M in phase m . Note that, for every given phase m , the sum of n_{mM} over all components is equal to 1 [10]. The source term representing the injection/production wells is denoted by q_M , and F_M is the overall mass flux of this component, equal to the sum

$$(2) \quad F_M = \sum_m \rho_m n_{mM} V_m,$$

where V_m is the velocity of phase m . The definition of V_m comes from the momentum conservation which is given by either Darcy's law

$$(3) \quad V_m = K \frac{k_m}{\mu_m} (\nabla P_m - \rho_m G \nabla D),$$

or by Forchheimer law, or by some other non-Darcy equations extensions, [7]. Note that P_m, k_m, μ_m denote the pressure of phase m , its relative permeability and viscosity, respectively. K is a general permeability tensor, D denotes the depth and G is the gravity constant.

The system is closed by adding capillary pressure relationships defining pressure difference between phases as function of saturations. Additionally one requires that the sum of all saturations be 1 and one adds an equation of state (constitutive law) for each phase which specifies the dependence of density ρ_m on pressure and composition n_{mM} .

The general equations 1–3 are made specific for a given physical model adding assumptions and simplifications. The notation as well as the units adopted are those commonly used for such a model. Below we discuss three examples: first two-phase models, then single-phase models and then black-oil models.

3.1. The two-phase model. We assume here that only two phases $m = w, o$, are present and that they can be identified with the components $M = W, O$ (water and oil). In other words, the fluids are immiscible and so $n_{oW} = n_{wO} = 0$ and $n_{wW} = 1, n_{oO} = 1$. We use $N_M = W_M$ and $U_M = F_M$. The equations 1–3 simplify to

$$(4) \quad \frac{\partial(\phi N_W)}{\partial t} - \nabla \cdot U_W = q_W,$$

$$(5) \quad \frac{\partial(\phi N_O)}{\partial t} - \nabla \cdot U_O = q_O,$$

$$(6) \quad U_W = \rho_w V_w = \rho_w K \frac{k_w}{\mu_w} (\nabla P_w - \rho_w G \nabla D)$$

$$(7) \quad U_O = \rho_o V_o = \rho_o K \frac{k_o}{\mu_o} (\nabla P_o - \rho_o G \nabla D)$$

Additionally, the pressures P_w, P_o are related to each other by the capillary pressure function $P_{cow} = P_o - P_w$ which is given as a function of saturation.

Although we specified the above equations for an water–oil system, the same set is used for an air–water model. What sets these apart is the equation of state. For hydrology model it is assumed that both fluid phases are slightly compressible, i.e., they are characterized by constant compressibility and reference density values. For the air–water model, a simple gas law is used [11].

For the numerical solution, the set of differential equations for the hydrology model 4–7 is discretized in space and time. The latter, time discretization, takes two forms: the implicit form, in which the resulting nonlinear system is solved for P_o, N_O , and the sequential (IMPES) form. In the sequential formulation first a pressure equation is solved for P_w and then a saturation equation is solved for S_w [15].

3.2. The single-phase model. The single-phase model equations are a subset of the two-phase equations. We assume that only one phase w and only one component W are present. This makes the notion of saturation S_w obsolete with $N_W = \rho_w$ and the equation 4 is rewritten as

$$(8) \quad \frac{\partial(\phi\rho_w)}{\partial t} - \nabla \cdot U_w = q_W.$$

Darcy's law is rewritten for single phase, since relative permeability is irrelevant:

$$(9) \quad U_W = \rho_w K \frac{1}{\mu_w} (\nabla P_w - \rho_w G \nabla D).$$

The fluid is slightly compressible as in the two-phase model.

After discretization in space and time, the above system can be solved implicitly or explicitly.

3.3. The black-oil model. The black-oil model is a three component / three phase (water, oil and gas) system subject to the following commonly used restrictions [14, 17]: 1) the water component exists only in the water phase and it is the only component in that phase, 2) the gas phase contains only the gas component and may be absent if pressure is high enough, and 3) the oil phase may contain both oil and gas components.

These restrictions imply

$$\begin{aligned} n_{wW} &= 1, \quad n_{wO} = 0, \quad n_{wG} = 0 \\ n_{oW} &= 0, \quad n_{oO} + n_{oG} = 1 \\ n_{gW} &= 0, \quad n_{gO} = 0, \quad n_{gG} = 1. \end{aligned}$$

Further, we introduce reference densities $\rho_w^{ref}, \rho_o^{ref}, \rho_g^{ref}$ and define the formation volume factors B_w, B_o, B_g as well as the solution gas-oil ratio R_s :

$$\begin{aligned} B_w &= \frac{\rho_w^{ref}}{\rho_w}, \quad B_o = \frac{\rho_o^{ref}}{n_{oO}\rho_o}, \quad B_g = \frac{\rho_g^{ref}}{\rho_g}, \\ R_s &= \frac{n_{oG}\rho_o^{ref}}{n_{oO}\rho_g^{ref}}. \end{aligned}$$

The above is a common notation: the typical measurements of B_w, B_o, B_g and R_s are given in the engineering literature [14, 10, 6]. Next, in order to use the stock tank units, we divide the component equations by the reference densities and define $N_W = \frac{W_W}{\rho_w^{ref}}, N_O = \frac{W_O}{\rho_o^{ref}}$ and $N_G = \frac{W_G}{\rho_g^{ref}}$. Equivalently,

$$N_W = \frac{S_w}{B_w}, \quad N_O = \frac{S_o}{B_o}, \quad N_G = \frac{S_g}{B_g} + R_s \frac{S_o}{B_o}.$$

New source terms $\bar{q}_M = \frac{q_m}{\rho_m^{ref}}$ are defined. Also, we use

$$U_W = \frac{V_w}{B_w}, \quad U_O = \frac{V_o}{B_o}, \quad U_G = \frac{V_g}{B_g},$$

where velocities V_m are defined by 3. This implies

$$\frac{F_W}{\rho_w^{ref}} = U_W, \quad \frac{F_O}{\rho_o^{ref}} = U_O, \quad \frac{F_G}{\rho_g^{ref}} = U_G + R_s U_O.$$

In summary, the mass conservation for the black-oil model is described by

$$(10) \quad \frac{\partial(\phi N_W)}{\partial t} - \nabla \cdot U_w = \bar{q}_W,$$

$$(11) \quad \frac{\partial(\phi N_O)}{\partial t} - \nabla \cdot U_O = \bar{q}_O,$$

$$(12) \quad \frac{\partial(\phi N_G)}{\partial t} - \nabla \cdot (U_G + R_s U_O) = \bar{q}_G,$$

with fluxes and velocities defined as above.

The phase behavior in the black-oil model is described by the following criterion involving the reservoir pressure. If the oil pressure is high enough (above the *bubble point*), then all of the gas component is dissolved in the oil phase. If $N_G > R_s N_O$, then all three phases are present. Conversely, $S_g = 0$ and $N_G \leq R_s N_O$. Additionally, the phase pressures are related to one another by capillary pressure relationships.

The set of discrete equations corresponding to 10–12 can be solved implicitly or explicitly. The two black-oil models in IPARS are both implicit. One uses P_w, N_O, N_G as primary variables and the other one uses P_o, N_O, N_G .

4. DUAL FORMULATION

In subsurface modeling, there are many reasons for introducing grid discontinuities. Local grid refinement may be required near a well and geological faults and fissures produce discontinuities in the strata that must be matched by the grid.

In this section we describe an algorithm for calculating fluxes between fault blocks or subdomains with possibly non-matching grids. The equations described below deal only with fluxes between blocks having the same physical model but can be modified to treat interfaces between different physical models. We define the procedure assuming non-matching grids on the interface between two fault blocks A and B . Let the subscript a denote the index of an element in fault block A and b that of fault block B . Recall from previous section that subscript m denotes phase m . We note from Figure 1 that for each element a in block A , there may be several elements b in block B that couple to element a . We define the mass flux of phase m from element a to

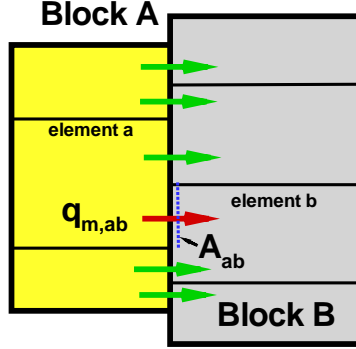


FIGURE 1. Mechanism of dual representation.

element b by

$$q_{m,ab} = T_{m,ab} \left[P_{m,a} - P_{m,b} - \frac{1}{2} G(\rho_{m,a} + \rho_{m,b})(D_a - D_b) \right]$$

where the transmissibility from element a to element b is given by

$$(13) \quad T_{m,a} = \left(\frac{\rho k}{\mu} \right)_{m,ab} A_{ab} 2 \left(\frac{\Delta x_a}{K_a} + \frac{\Delta x_b}{K_b} \right)^{-1}$$

Here the area shared by surfaces of elements a and b is denoted by A_{ab} and the distance from the center of the element a to the plane of the intersection of elements a and b by Δx_a .

Let the total flux from element a to block B be denoted by

$$(14) \quad q_{m,a} = \sum_b q_{m,ab}$$

If we denote by $\alpha_{j,a}^k$ the primary variable j evaluated in element a at the Newton iterant k and set

$$(15) \quad \Delta \alpha_{j,a}^{k+1} = \alpha_{j,a}^{k+1} - \alpha_{j,a}^k$$

we obtain the Newtonian approximation for the intrablock flux as

$$\begin{aligned} q_{m,a}^{k+1} \approx q_{m,a}^k &+ \sum_j \left(\frac{\partial q_{m,a}}{\partial \alpha_{j,a}} \right)^k \Delta \alpha_{j,a}^{k+1} \\ &+ \sum_{j,b} \left(\frac{\partial q_{m,a}}{\partial \alpha_{j,b}} \right)^k \Delta \alpha_{j,b}^{k+1}. \end{aligned}$$

We remark that several elements b may be coupled to one element a , which can complicate the matrix structure of the Jacobian. This can be avoided by making a change of variable at the interface such that the regular structure of the Jacobian is preserved. Details regarding this system will appear in a forthcoming paper.

5. COMPUTATIONAL RESULTS

In this section we present some computational results for the multi-block implementation in dual or mortar version. For simplicity, the implicit two-phase model is used. We discuss accuracy and efficiency of the two formulations for the multi-domain case with the two-phase model. Multi-physics examples will be presented elsewhere.

The results shown here are essentially the first such results presented for the dual formulation. The intension of the comparison is to signal a trend rather than infer about absolute applicability or efficiency of either of the two formulations. In particular, the codes for the dual and mortar formulation have not yet been optimized for parallel performance, i.e., highest accuracy at smallest cost.

5.1. *Description of simulation cases.* For the sake of comparison we consider a relatively small quarter five spot problem of dimensions 324' x 324' x 16'. The wells are located at (1,1) and (323, 323) and penetrate through all vertical layers. The vertical permeability is 200 md with a layer of 50 md of thickness 2' in the middle of the reservoir. The ratio of vertical to horizontal permeability is .1. The compressibility constants are 0.4000E-04, 0.3300E-05 for oil and water, respectively. The reservoir initially is in hydrostatic equilibrium with an oil pressure of 500 psi and a water saturation of 22% at the top of reservoir. The injection pressure is 510 psi and it is dropped at production well initially to 480 psi and down to 350 psi at 30 days. The simulation of the waterflood is 500 days: the water front arrives at the production well around 300 days. Variable time steps from 1 day to 15 days are used. Convergence tolerance for the Newton solver is chosen to keep material balances exact to 5 or 6 significant figures.

Several spatial discretizations are considered with no special refinement around wells. Grids range from 6x6x8 (coarse) to 18x18x8 (medium), and 54x54x8 (fine) for the computational area. The multi-block cases include

- A. single block case which serves as a basis for comparison,
- D. three blocks with matching grids,
- E. three blocks with nonmatching grids (grid in the middle block is offset by half of original gridblock size).

The pointwise values of primary variables as well as of profiles of saturations etc. can be obtained during the simulation by memory dumps at selected time steps. For example, saturation profiles at 500 days are shown in Figure 2. Note the effect of low permeability layer in the middle of reservoir and the water front that has reached the

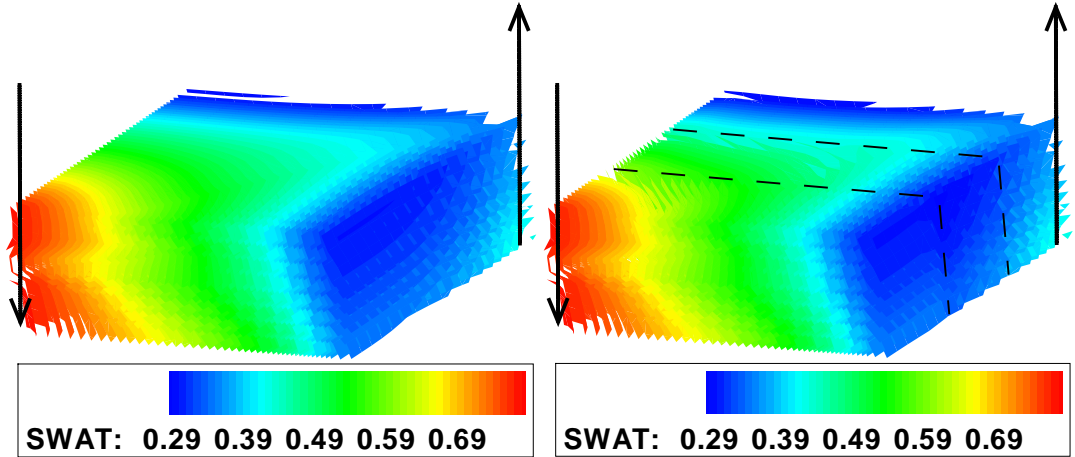


FIGURE 2. Saturation profiles at 500 days of simulation for medium grid, case A (left) and E (right). Position of wells (injection and production) is marked with arrows and interface is marked with dashed line.

bottom of the production well. Also note the grids for multi-block cases D and E in Figure 3.

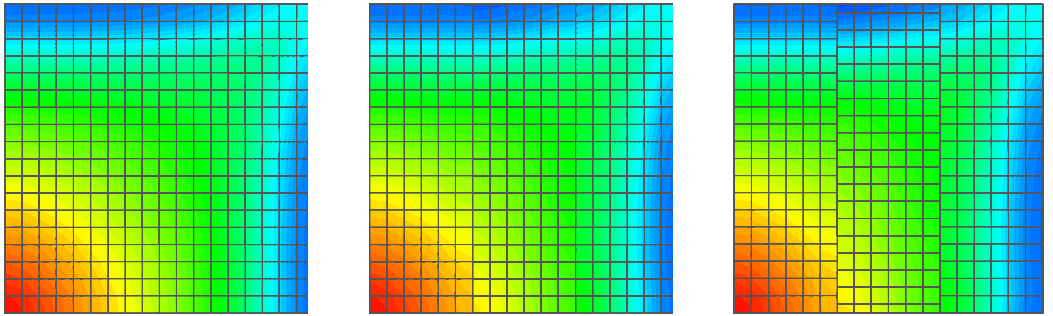


FIGURE 3. Aerial projection of saturation profiles at 500 days for medium grid for case A (left), D (middle) and E (right).

5.2. Comparison of results for mortar and dual formulations. The qualitative information from the profiles as seen above is quite instructive. However, for the sake of comparison of mortar and dual formulation, it is difficult to use the pointwise values especially for large cases and nonmatching grids. Instead, we use well output

which is inexpensive to compute and which provides the essential information for a reservoir engineer.

Note that the cases A and D should yield quantitatively the same results as A, as the grid over the whole computational region is the same, and that the results for case E should be close to those for A and D. On the other hand, when grids are refined, the gridblock containing the well has different dimensions for each refinement case and the Peaceman correction “moves” the well to the center of the gridblock where it appears which has profound effect on well rates, see Figure 4.

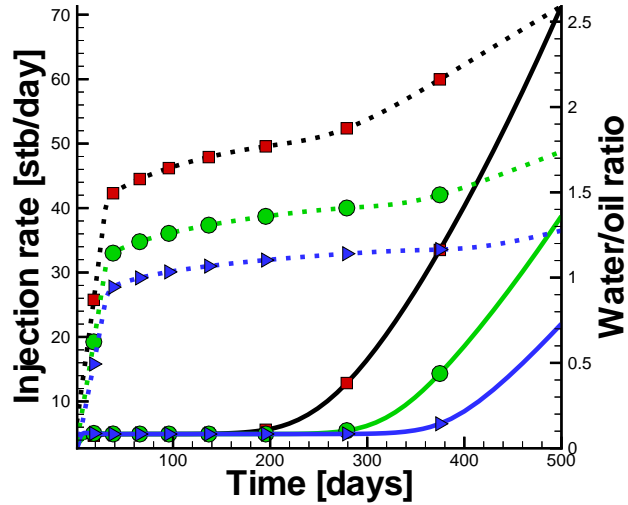


FIGURE 4. Injection rate (dotted) and water/oil ratio (solid) for case A, various grid sizes: coarse (squares), medium (circles), fine (triangles).

The well rates for cases A, D, and E and medium grid are shown in Figure 5. Each plot contains 5 distinct lines but they appear indistinguishable.

More precisely, when compared to the case A, the well rates for D using dual formulation are identical. This is because for matching grids the fully discrete implicit problem solved in case D is exactly equivalent to the problem solved in case A. Next, the well rates for case E using the dual formulation show loss of some digits. The difference between A and E for dual formulation is of maximum 20% for coarse grid case, of no more than 7% for medium case, and about 1% for fine grid case.

On the other hand, the mortar formulation requires outer interface and inner subdomain iterations as well as projections between the grids and the mortar grid. During these operations, some digits are lost even in the case of matching grids. However, high convergence of the mortar formulation makes the difference between A and D,

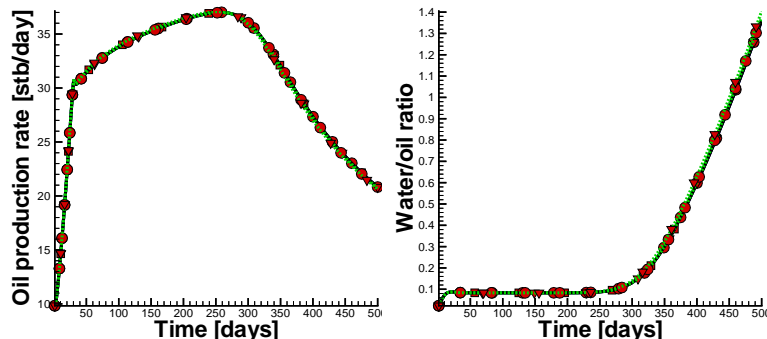


FIGURE 5. Comparison of oil production rate (top), and water/oil ratio (bottom) for cases A (squares), D (circles) and E (diamonds) for mortar (solid) and dual formulation (dotted).

E small: the results show agreement to up to 0.3%, 0.1% and 0.05% for the coarse, medium and the fine grid case, respectively, between A and both cases D and E.

As concerns the computational cost, the dual formulation takes of no more than 20% longer for case D or E relative to A. This makes the dual code much faster than the mortar code which typically requires several subdomain solves and nontrivial interface preconditioners. However, the mortar formulation allows for different type of mortar grids, which determine the accuracy as well as the efficiency of the computations. The results discussed above were obtained with the finest mortar grid available. However, if the goal were to meet the accuracy attained by the dual, the execution time could be cut down by choosing a coarser mortar grid.

The agreement discussed above for both formulations is sufficiently close for practical purposes. This is in view of the influence of the gridblock size over well rates as demonstrated in Figure 4.

6. CONCLUSIONS

A distributed computing portal for modeling multi-domain multi-phase flow has been described. Computational results using this framework have been presented in these proceedings and elsewhere.

The results of the simulation exhibit convergence for both dual and mortar formulation even on coarse grids. These approaches show promise for modeling multi-domain multi-physics applications.

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