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Publication date

2016

Document Version

Final published version

Published in

15th European Conference on the Mathematics of Oil Recovery, ECMOR 2016

Citation (APA)

Khait, M., & Voskov, D. (2016). Operator-based linearization for non-isothermal multiphase compositional flow in porous media. In *15th European Conference on the Mathematics of Oil Recovery, ECMOR 2016* (pp. 1-15). EAGE.

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Operator-based Linearization for Non-isothermal Multiphase Compositional Flow in Porous Media

M. Khait* (TU Delft) & D. Voskov (TU Delft)

SUMMARY

Non-isothermal multiphase compositional simulation is based on the solution of governing equations describing mass and energy transfer in the subsurface. The solution strategy requires a linearization of strongly nonlinear governing equations describing the process. Usually, a Newton-based method is used for the linearization that demands an assembly of a Jacobian matrix and residuals for a fully coupled system of equations. Recently, a new linearization approach was proposed for compositional problems and tested for simulation of binary compositional and low-enthalpy geothermal flow. The key idea of the approach is the transformation of discretised mass conservation equations to an operator form with separate space-dependent and state-dependent components. This transformation provides an opportunity for an approximate representation of exact physics (physical properties) of the problem. Specifically, each term of conservation equations is represented as a product of two different operators. The first operator depends on a current physical state of a system and contains different properties such as density, viscosity, relative permeability, etc. The second operator captures both spatially altered properties such as permeability and the rest of state variables such as pressure in the discrete approximation of the gradient. At the pre-processing stage, all state-dependent operators are uniformly parametrized within the physical space of the problem (pressure-composition intervals). During the simulation process, a multi-linear interpolation is applied to approximate the first type of operators, while the second type of operators is processed based on the conventional approach. In this work, we have extended this approach to general purpose simulation. We introduced the operator-based parametrization of mass and energy conservations equation based on the pressure, composition, temperature, and porosity. In addition, the approach has been extended and tested on truly multi-component systems of practical interest. The accuracy and robustness of the new method have been tested against the results of simulations based on the conventional approach.

Introduction

Numerical simulations are essential for the modern development of hydrocarbon reservoirs (Aziz and Settari, 1979). They are widely used for the evaluation of oil recovery efficiency, a performance analysis, and various optimization problems. Due to the complexity of underlying physical processes and considerable uncertainties in the geological representation of reservoirs, there is a persistent demand for more accurate models. In order to increase the accuracy of a model, one can apply a finer computational grid in space or time, or use a more detailed description of the fluids involved, such as a full compositional formulation. However, this increased accuracy models are counterbalanced by the decrease of the overall simulation performance. In addition, both space and time approximations bring nonlinearity to the system of equations that need to be solved numerically.

After the discretization stage is complete, the nonlinear system needs to be linearized. The particular set of independent variables is defined by the nonlinear formulation of the actual simulation framework (Cao, 2002). Based on the formulation, all properties, and their derivatives need to be determined with respect to nonlinear unknowns. Numerical derivatives provide flexibility in the nonlinear formulation (see Xu et al., 2011 for example), but a simulation based on numerical derivatives may lack robustness and performance (Vanden and Orkwis, 1996). Straightforward hand-differentiation is the state-of-the-art strategy in modern commercial simulators (Schlumberger, 2011). However, this approach requires the introduction of a complicated framework for storing and evaluating derivatives for each physical property which in turn reduces the flexibility of a simulator to incorporate new physical models and increases probability for potential errors.

The development of Automatic Differentiation (AD) techniques allows preserving both flexibility and robustness in derivative computations. In reservoir simulation, the AD-based library (ADETL) was introduced first by Younis (2011), and significantly extended later by Zhou (2012). Using the capabilities of ADETL, an Automatic Differentiation General Purpose Research Simulator (ADGPRS) was developed (Voskov and Tchelepi, 2012). ADGPRS is a unified reservoir simulation framework providing an extensive set of nonlinear formulations (Voskov, 2012; Zaydullin et al., 2013); flexible spatial discretization (Zhou et al., 2011); extended physics models (Iranshahr et al., 2013; Zaydullin et al., 2014a; Garipov et al., 2016); inverse capabilities (Kourounis et al., 2010; Volkov and Voskov, 2016); geothermal formulation (Wong et al., 2015). We use ADGPRS for the implementation and performance comparisons in this study.

The predecessor of the new method described in this work was the Compositional Space Parametrization (CSP) method proposed in Voskov and Tchelepi (2009) and fully developed for compositional simulation by Zaydullin et al. (2013). In this approach, a complex thermodynamic phase behavior is described by a special set of nonlinear unknowns: pressure, phase fractions and tie-line parameters. All properties are defined in a discretized tie-line space, resulting in a piece-wise linear representation of a complex multicomponent thermodynamics based on nonlinear unknowns. This technique reduces expensive phase behavior computations during the course of a simulation.

Inspired by CSP method, the new linearization approach was recently introduced by Khait and Voskov (2016) for geothermal simulation. In this paper, we extend the method to a general purpose reservoir simulation. In the new approach, each term in discretized conservation equations is represented by the product of two operators: state- and space-dependent. The state-dependent operators are adaptively parametrized over the physical space of a simulation problem while space-dependent operators are applied in a conventional manner. During the course of a simulation, the state-dependent operators are calculated based on a multilinear interpolation in a multidimensional space of nonlinear parameters. This approach was applied to the several reservoir simulation problems of practical interest and demonstrated better nonlinear performance with a coarser representation of the physics while the approximation error is controlled by the resolution of the interpolation tables.

Conventional modeling approach

In this section we describe one of the conventional nonlinear formulations for a general purpose thermal-compositional model implemented in ADGPRS (Voskov and Tchelepi, 2012; Zaydullin et al., 2014b) and used in this paper as a reference solution.

Governing equations

Here we describe the flow of energy and mass of a system with n_p phases and n_c components. For this model, n_c component mass conservation equations and a single energy conservation equation need to be written as:

$$\frac{\partial}{\partial t} \left(\phi \sum_{p=1}^{n_p} x_{cp} \rho_p s_p \right) + \operatorname{div} \sum_{p=1}^{n_p} x_{cp} \rho_p \vec{u}_p + \sum_{p=1}^{n_p} x_{cp} \rho_p \tilde{q}_p = 0, \quad c = 1, \dots, n_c, \quad (1)$$

$$\frac{\partial}{\partial t} \left(\phi \sum_{p=1}^{n_p} \rho_p s_p U_p + (1 - \phi) U_r \right) + \operatorname{div} \sum_{p=1}^{n_p} h_p \rho_p \vec{u}_p + \operatorname{div}(\kappa \nabla T) + \sum_{p=1}^{n_p} h_p \rho_p \tilde{q}_p = 0. \quad (2)$$

All terms of the system (1)-(2) can be characterized as functions of the spatial coordinates ξ and physical state ω :

- $\phi(\xi, \omega)$ – effective rock porosity,
- $x_{cp}(\omega)$ – component concentration in phase,
- $\rho_p(\omega)$ – phase molar density,
- $s_p(\omega)$ – phase saturation,
- $\vec{u}_p(\xi, \omega)$ – phase velocity,
- $\tilde{q}_p(\xi, \omega, \mathbf{u})$ – source of phase,
- $U_p(\omega)$ – phase internal energy,
- $U_r(\xi, \omega)$ – rock internal energy,
- $h_p(\omega)$ – phase enthalpy,
- $\kappa(\xi, \omega)$ – thermal conductivity.

The only exception here is the phase source term which also depends on \mathbf{u} - well control variables.

Next, for simplicity we assume that the rock internal energy and thermal conductivity are spatially homogeneous:

$$U_r = f(\omega), \quad \kappa = f(\omega). \quad (3)$$

Phase flow velocity is assumed to follow the Darcy law:

$$\vec{u}_p = - \left(\mathbf{K} \frac{k_{rp}}{\mu_p} (\nabla p_p - \vec{\gamma}_p \nabla D) \right). \quad (4)$$

where:

- $\mathbf{K}(\boldsymbol{\xi})$ – effective permeability tensor,
- $k_{rp}(\boldsymbol{\omega})$ – phase relative permeability,
- $\mu_p(\boldsymbol{\omega})$ – phase viscosity,
- $p_p(\boldsymbol{\omega})$ – phase pressure,
- $\vec{\gamma}_p(\boldsymbol{\omega})$ – gravity vector,
- $D(\boldsymbol{\xi})$ – depth (backward oriented).

After application of a finite-volume discretization on a general unstructured mesh and backward Euler approximation in time we get:

$$V \left(\left(\phi \sum_{p=1}^{n_p} x_{cp} \rho_p s_p \right)^{n+1} - \left(\phi \sum_{p=1}^{n_p} x_{cp} \rho_p s_p \right)^n \right) - \Delta t \sum_l \left(\sum_{p=1}^{n_p} x_{cp}^l \rho_p^l \Gamma_p^l \Delta \psi^l \right) + \Delta t \sum_{p=1}^{n_p} x_{cp} \rho_p \mathbf{q}_p = 0, \quad (5)$$

$$V \left[\left(\phi \sum_{p=1}^{n_p} \rho_p s_p U_p + (1 - \phi) U_r \right)^{n+1} - \left(\phi \sum_{p=1}^{n_p} \rho_p s_p U_p + (1 - \phi) U_r \right)^n \right] - \Delta t \sum_l \left(\sum_{p=1}^{n_p} h_p^l \rho_p^l \Gamma_p^l \Delta \psi^l + \Gamma_c^l \Delta T^l \right) + \Delta t \sum_{p=1}^{n_p} h_p \rho_p \mathbf{q}_p = 0, \quad (6)$$

where V is a control volume of grid cell and $q_p = \tilde{q}_p V$ is a source of phase. Here we have neglected capillarity, gravity and used a Two-Point Flux Approximation (TPFA) with an upstream weighting. Therefore, $\Delta \psi^l$ becomes a simple difference in pressures over the interface l , and similarly ΔT^l is the temperature difference between neighboring blocks. In addition, $\Gamma_p^l = \Gamma^l k_{rp}^l / \mu_p^l$ is a phase transmissibility, with Γ^l assumed to be the space-dependent part of the transmissibility, including permeability and the geometry of the control volume. For the energy conservation equation, an additional term Γ_c^l corresponds to the conductive transmissibility which includes the thermal conductivity of all phases (including solid)

$$\Gamma_c^l = \Gamma^l \left(\phi \left(\sum_{p=1}^{n_p} s_p \kappa_p \right) + (1 - \phi) \kappa_r \right), \quad (7)$$

where

- $\kappa_p(\boldsymbol{\omega})$ – phase thermal conductivity,
- $\kappa_r(\boldsymbol{\omega})$ – rock thermal conductivity.

Nonlinear formulation and linearization

Equations (5) and (6) are approximated in time using a Fully Implicit Method (FIM). The method suggests that the convective flux terms from mass and energy conservation equations as well as the energy conductive flux depend on the values of nonlinear unknowns at the current time step. This introduces nonlinearity into the system, which is further increased by the closure assumption of instantaneous thermodynamic equilibrium. Here we apply a thermal extension of the overall molar formulation (Collins

et al., 1992) for nonlinear solution of the governing equations. In this formulation, an exact thermodynamic equilibrium is required at every nonlinear iteration. Hence, the following system has to be solved for any grid block that contains a multiphase (n_p) multicomponent (n_c) mixture:

$$F_c = z_c - \sum_{p=1}^{n_p} v_p x_{cp} = 0, \quad (8)$$

$$F_{c+n_c} = f_{c1}(p, T, \mathbf{x}_1) - f_{cp}(p, T, \mathbf{x}_p) = 0, \quad (9)$$

$$F_{p+n_c \times n_p} = \sum_{c=1}^{n_c} (x_{c1} - x_{cp}) = 0, \quad (10)$$

$$F_{n_p+n_c \times n_p} = \sum_{p=1}^{n_p} v_p - 1 = 0. \quad (11)$$

In this procedure, which is usually called multiphase flash (Michelsen, 1982), $z_c = \sum_p x_{cp} \rho_p s_p / \sum_p \rho_p s_p$ is the overall composition and $f_{cp}(p, T, x_{cp})$ is the fugacity of component c in phase p . By solving this system we obtain mole fractions for each component x_{cp} and phase fractions v_p for the given overall composition z_c . In the molar formulation the nonlinear unknowns are p, z_c and T (or h), therefore the physical state $\boldsymbol{\omega}$ is completely defined by these variables.

After obtaining the solution of multiphase flash we determine partial derivatives with respect to nonlinear unknowns using the inverse theorem (see Voskov and Tchelepi, 2012 for details) and assemble the Jacobian and residuals. This step is often called linearization. The conventional linearization approach is based on the Newton-Raphson method, which solves on each nonlinear iteration the following linear system of equations:

$$\mathbf{J}(\boldsymbol{\omega}^k)(\boldsymbol{\omega}^{k+1} - \boldsymbol{\omega}^k) + \mathbf{r}(\boldsymbol{\omega}^k) = 0, \quad (12)$$

where $J(\boldsymbol{\omega}^k)$ and $r(\boldsymbol{\omega}^k)$ are the Jacobian and residual defined at the nonlinear iteration k . The conventional approach assumes the numerical representation of rock and fluid properties and their derivatives with respect to nonlinear unknowns. This may require either table interpolation (e.g., for relative permeability) or the solution of a highly nonlinear system (8)-(11) for properties defined by an Equation of State (EoS) in combination with the chain rule and inverse theorem. As a result, a nonlinear solver has to resolve all of the small features of the property descriptions, which can be quite challenging and is often unnecessary due to the numerical nature and uncertainties in property evaluation.

Proposed modeling approach

In this section we describe a multicomponent extension of the approach developed by Khait and Voskov (2016) for low enthalpy geothermal systems.

Computation of partial derivatives during multilinear interpolation

The key advantage of the proposed approach is the extensive usage of piecewise multilinear generalization of piecewise bilinear interpolation for an N -dimensional space at the linearization stage. We chose this approach for its application simplicity in comparison with the approach proposed in Zaydullin et al. (2013) for compositional systems with a large number of components. Both methods have comparable accuracy and performance when applied to systems with a limited number of degrees of freedom, see Weiser and Zarantonello (1988) for details.

An interpolant approximation $A(x_1, \dots, x_N)$ to a function $\alpha(x_1, \dots, x_N)$ can be built using interpolation table values of α :

$$\{\alpha(X_{i_1}, X_{i_2}, \dots, X_{i_N}) : i_1 = 1, \dots, n_1, \dots, i_N = 1, \dots, n_N\}. \quad (13)$$

where n_1, \dots, n_N are the numbers of points along interpolation axes. The first step of the method is to find table intervals $(X_{I_1}, X_{I_1+1}), \dots, (X_{I_N}, X_{I_N+1})$ such that

$$X_{I_1} \leq x_1 \leq X_{I_1+1}, \dots, X_{I_N} \leq x_N \leq X_{I_N+1}$$

In order to further simplify description, we scale each of the intervals to $(0, 1)$. That allows us to reformulate the problem to finding an approximation $\Pi(y_1, \dots, y_N)$ for a function $\pi(y_1, \dots, y_N)$ defined over the unit N-cube:

$$0 \leq y_1 \leq 1, \dots, 0 \leq y_N \leq 1,$$

where

$$y_i = \frac{x_i - X_{I_i}}{X_{I_i+1} - X_{I_i}},$$

using the table values

$$\{\pi(j_1, \dots, j_N) = \alpha(X_{I_1+j_1}, \dots, X_{I_N+j_N}) : j_1 = 0 \text{ or } 1, \dots, j_N = 0 \text{ or } 1\}.$$

The piecewise multilinear approximation is computed in a recursive manner. First, let's define

$$\begin{aligned} \Pi_1^i &= \Pi(j_1, \dots, j_{i-1}, 1, y_{i+1}, \dots, y_N) \\ \Pi_0^i &= \Pi(j_1, \dots, j_{i-1}, 0, y_{i+1}, \dots, y_N) \end{aligned}$$

Then,

$$\begin{aligned} A(x_1, \dots, x_N) &= \Pi(y_1, \dots, y_N), \\ \Pi(j_1, \dots, j_i, y_{i+1}, \dots, y_N) &= \Pi_0^i + y_i(\Pi_1^i - \Pi_0^i), \quad i = 1, \dots, N, \end{aligned}$$

where the table values are

$$\Pi(j_1, \dots, j_N) = \pi(j_1, \dots, j_N).$$

The partial derivatives are determined in a similar way. First,

$$\begin{aligned} \Pi_1^{ki} &= \Pi^k(j_1, \dots, j_{i-1}, 1, y_{i+1}, \dots, y_N) \\ \Pi_0^{ki} &= \Pi^k(j_1, \dots, j_{i-1}, 0, y_{i+1}, \dots, y_N), \end{aligned}$$

and then

$$\begin{aligned} \frac{\delta \alpha}{\delta x_k} &= \frac{\delta A}{\delta x_k} = \Pi^k(y_1, \dots, y_N), \quad k = 1, \dots, N, \\ \Pi^k(j_1, \dots, j_i, y_{i+1}, \dots, y_N) &= \begin{cases} \Pi_0^{ki} + y_i(\Pi_1^{ki} - \Pi_0^{ki}), & i = 1, \dots, k, \\ \frac{\Pi_1^i - \Pi_0^i}{X_{I_i+1} - X_{I_i}}, & i = k, \\ \Pi_0^{ki} + y_i(\Pi_1^{ki} - \Pi_0^{ki}), & i = k+1, \dots, N. \end{cases} \end{aligned}$$

Operator form of the conservation equations

In order to apply the described approximation method we rewrite equations (5) and (6), representing each term as a product of state-dependent and space-dependent operators as in (Khait and Voskov, 2016). In addition, we assume porosity as a pseudo-physical state variable $\phi \in \omega$.

The resulting mass conservation equation is:

$$a(\xi)(\alpha_c(\omega) - \alpha_c(\omega_n)) + \sum_l b(\xi, \omega)\beta_c(\omega) + \theta_c(\xi, \omega, \mathbf{u}) = 0, \quad c = 1, \dots, n_c \quad (14)$$

Here

$$\begin{aligned} a(\xi, \omega) &= \phi V(\xi), \\ \alpha_c(\omega) &= \sum_{p=1}^{n_p} x_{cp} \rho_p s_p, \\ b(\xi, \omega) &= \Delta t \Gamma^l(\xi)(p^b - p^a), \\ \beta_c(\omega) &= \sum_{p=1}^{n_p} x_{cp}^l \rho_p^l \frac{k_{rp}^l}{\mu_p^l}, \\ \theta_m(\xi, \omega, \mathbf{u}) &= \Delta t \sum_{p=1}^{n_p} x_{cp} \rho_p q_p(\xi, \omega, \mathbf{u}). \end{aligned}$$

Here ω and ω_n are nonlinear unknowns on the current and previous time step respectively.

The modified energy conservation equation takes the form:

$$a_e(\xi)(\alpha_e(\omega) - \alpha_e(\omega_n)) + \sum_l b_e(\xi, \omega)\beta_e(\omega) + \sum_l c_e(\xi, \omega)\gamma_e(\omega) + \theta_e(\xi, \omega, \mathbf{u}) = 0, \quad (15)$$

where

$$\begin{aligned} a_e(\xi) &= V(\xi), \\ \alpha_e(\omega) &= \phi \left(\sum_{p=1}^{n_p} \rho_p s_p U_p - U_r \right) + U_r, \\ b_e(\xi, \omega) &= b(\xi, \omega), \\ \beta_e(\omega) &= \sum_{p=1}^{n_p} h_p^l \rho_p^l \frac{k_{rp}^l}{\mu_p^l}, \\ c_e(\xi, \omega) &= \Delta t \Gamma^l(\xi)(T^b - T^a), \\ \gamma_e(\omega) &= \phi \left(\sum_{p=1}^{n_p} s_p \kappa_p - \kappa_r \right) + \kappa_r, \\ \theta_e(\xi, \omega, \mathbf{u}) &= \Delta t \sum_{p=1}^{n_p} h_p \rho_p q_p(\xi, \omega, \mathbf{u}). \end{aligned}$$

In these derivations T^a and T^b are assumed to be the temperatures in the neighboring grid blocks.

This representation allows us to identify and distinguish the physical state dependent operators - $\alpha_c, \beta_c, \alpha_e, \beta_e, \gamma_e$ in both mass (5) and energy (6) conservation equations. The source/sink term can also be processed in a similar manner, but we have left this out of the scope of this work and perform a conventional treatment for this operator.

Operator-based linearization approach

The key idea behind the proposed approach is to simplify the description of fluid and rock properties by building approximation interpolants for the operators $\alpha_c, \beta_c, \alpha_e, \beta_e, \gamma_e$ within the parameter space of a simulation problem. For a general non-isothermal compositional problem with n_c components the method requires $[2n_c + 3]$ operators which depend on $[n_c + 1]$ nonlinear variables $\{p, T, z_1, \dots, z_{n_c-1}\}$. Operators α_e, γ_e also depend on porosity, added as a pseudo-physical state variable according to Khait and Voskov (2016). The values of the operators are fully determined by this set. The pressure and temperature ranges in the compositional parameter space usually can be determined by conditions specified for wells, while the overall composition, as well as porosity, is naturally bounded by the interval $[0,1]$.

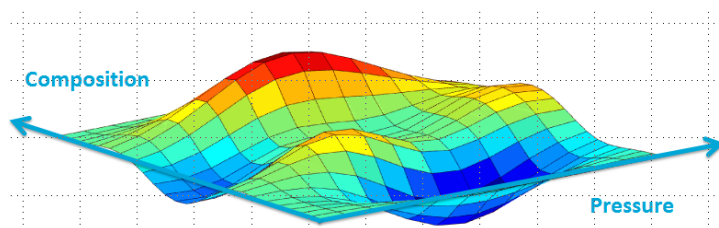


Figure 1 2D parametrization of an abstract operator.

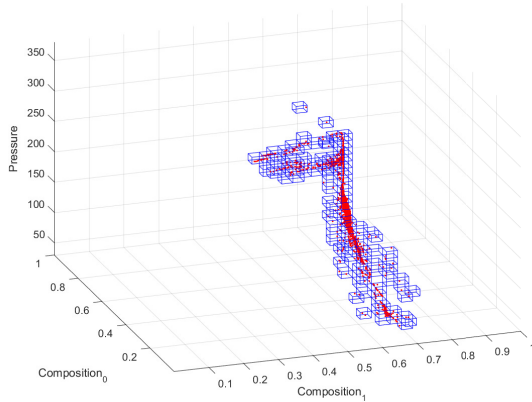
Next we parametrize the interval of each state variable using, for simplicity, the same number $n = n_1 = \dots = n_N$ of uniformly distributed points on the intervals of parameters, according to (13). This results in a set of vectors $(p_i, T_i, z_{1_i}, \dots, z_{n_c-1_i}, \phi_i) : i = 1, \dots, n$ which can be interpreted as a discrete representation of physical space in the simulation. At the pre-processing stage, or adaptively, we can evaluate the operators $\alpha_c, \beta_c, \alpha_e, \beta_e, \gamma_e$ at every point in discrete parameter space and store them in $N_1 = [n_c + 2]$ -dimensional (because of porosity) tables A_e and Γ_e and $N_2 = [n_c + 1]$ -dimensional tables A_c, B_c, B_e . An example for an abstract operator, parametrized in two-dimensional space, is illustrated in Fig. 1. During the simulation we interpolate both values and partial derivatives of all state-dependent operators in mass (14) and energy (15) balance equations, using tables created for each grid block. This provides a continuous description based on the interpolation operator whose accuracy is controlled by the resolution of discretization in parameter space. For an isothermal compositional problem we preserve only mass conservation operators α_c, β_c , defined by $N_3 = [n_c]$ variables $\{p, z_1, \dots, z_{n_c-1}\}$.

This representation simplifies significantly the implementation of complex simulation frameworks. Instead of keeping track of each property and its derivatives with respect to nonlinear unknowns, we can construct an algebraic system of equations with abstract algebraic operators representing the complex physics. The performance of this formulation benefits from the fact that all expensive evaluations can be performed using a limited number of supporting points. Finally, the performance of the nonlinear solver can be improved since the Jacobian is constructed based on a combination of piece-wise linear operators directly dependent on the nonlinear unknowns. In the sections below, we demonstrate the applicability of this approach to several reservoir simulation problems.

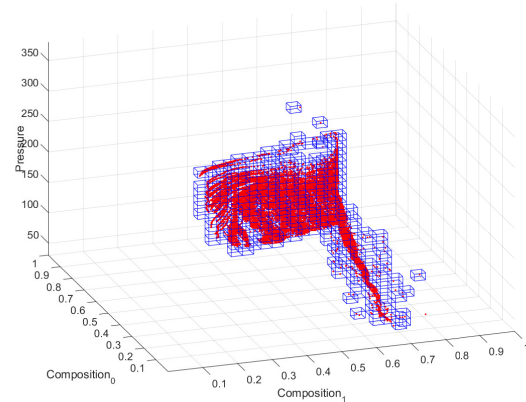
Adaptive operator-based linearization

The total size of the interpolation tables is defined by the number of dimensions N and the number of interpolation points n . While N depends on the number of components and thermal assumptions in the problem of interest, n corresponds to the desired accuracy of the physical representation and can be seen as resolution. Therefore, if parametrization was applied at the pre-processing stage, it would require a substantial amount of memory for the multicomponent systems modeled at a high resolution. Furthermore, the necessity of searching base points for every interpolation in a huge array of data affects the performance of the simulation. Notice, that due to the hyperbolic nature of some variables (e.g. overall compositions), the vast majority of parameter space remains unused (Voskov and Tchelepi, 2009; Zaydullin et al., 2013).

The adaptive approach avoids these disadvantages by removing the need for the entire pre-processing



(a) After 10 days of simulation



(b) After 2000 days of simulation

Figure 2 Adaptive operator-based linearization approach.

stage (Zaydullin et al., 2013). In this approach, base-points are computed whenever they are required by the current physical state of a control volume. The obtained operator values are then employed in the interpolation process and stored for future use. Consequently, every base point involved in interpolation is checked to be pre-computed. If the point was not computed previously, the method adds a new point and performs the computation of appropriate operators. In the end of the simulation, the resulting sparse multi-dimensional table of stored operators represents an actual subspace of physical parameters being used in the process. For example, Fig. 2 shows an adaptive parametrization in the parameter space for a black oil simulation at two different timesteps. The adaptive approach reproduces exact numerical results of the pre-processing method used in Khait and Voskov (2016) with greatly improved overall performance, especially for multicomponent systems.

Numerical results

In this section, we present numerical results for simulations using the adaptive operator-based linearization. A convergence study and an error analysis are provided for different resolutions of the physical parameter space, using simulation results for the conventional linearization approach as a reference solution. To demonstrate the general purpose applicability of the proposed approach, we conduct our study using black-oil, isothermal compositional and non-isothermal compositional problems. All problems are modeled within a single highly-heterogeneous reservoir which is shown in Fig. 3 and represents the 7-th layer of the SPE10 model (Christie and Blunt, 2001) consisting of 60×220 grid cells where the size of every grid cell is $6 \times 3 \times 0.6$ meters. The porosity of the reservoir was defined constantly as $\phi = 0.4$. An injection well is placed in the middle of the reservoir with four producers set at the corners.

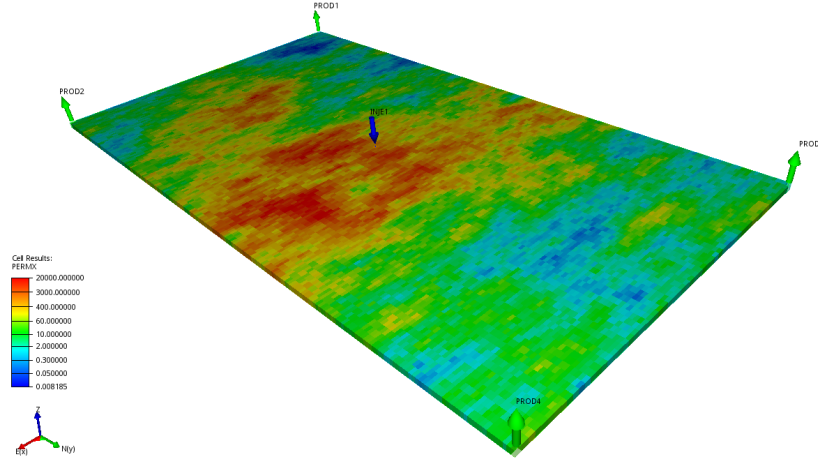


Figure 3: Testcase reservoir permeability along x-axis

Black-oil simulation

Here we used a standard black-oil formulation where only a gas component can dissolve in oil phase. The water injection well operated with Bottom Hole Pressure (BHP) control at a pressure $P_i = 350$ bar and the producer well operated at $P_p = 250$ bar. The reservoir was initialized uniformly with pressure $P_0 = 300$ bar, water saturation $S_w = 0.2$, gas saturation $S_g = 0$ and bubble pressure $P_{bub} = 270$ bar. All simulations were run for 8000 days with a maximum timestep of $\Delta t = 10$ days. The PVT properties, relative permeabilities and capillary pressure tables from SPE 9 test case (Killough, 1995) were used.

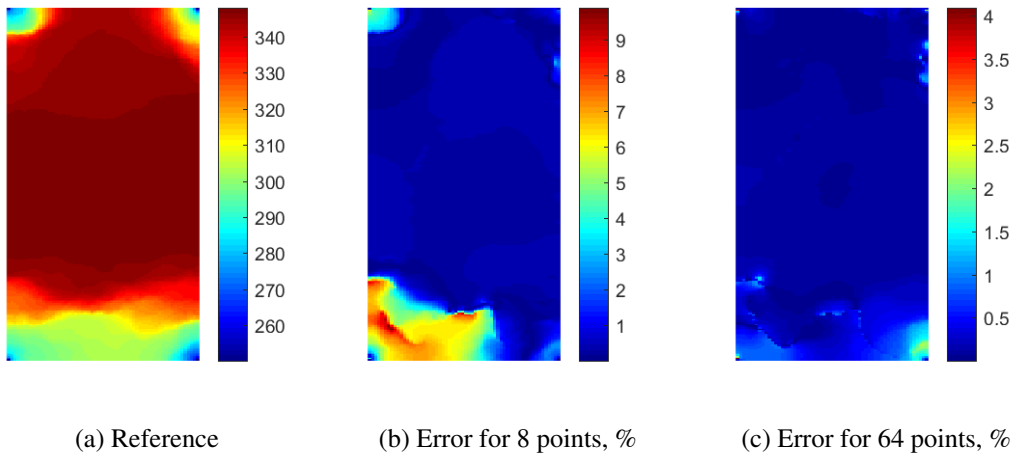


Figure 4: Pressure solution at t=8000 days

Both Figs. 4 and 5 represent a reference solution and an error map at the last timestep for this simulation using an operator-based linearizations with 8- and 64-points. The errors were calculated as the absolute difference between a reference solution and a solution from the proposed approach, normalized by the amplitude of the reference solution. It is easy to see that the error reduces significantly with increasing number of points. Fig. 4 shows pressure solution. Here the error is mainly concentrated near some of the production wells. Composition solution for water is depicted in Fig. 5. In this case, the error reaches its maximum along the displacement front.

To perform a convergence analysis for the new linearization method, the following relation for the error

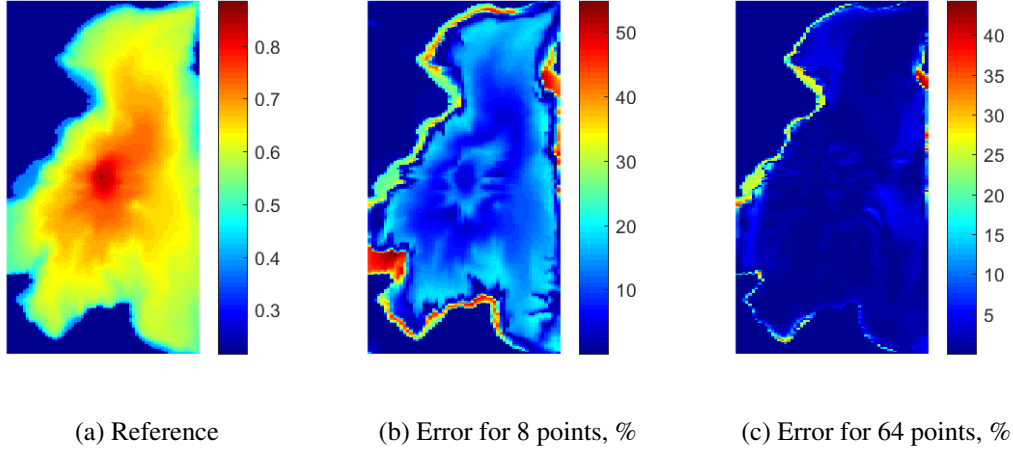


Figure 5: Water composition solution at t=8000 days

was introduced:

$$E = \frac{1}{n_b} \sum_{i=1}^n \frac{|x_{obl}^i - x_{ref}^i|}{(\max(\mathbf{x}_{ref}) - \min(\mathbf{x}_{ref}))} \quad (16)$$

where:

- n_b – number of grid blocks in the model,
- x_{obl}^i – the solution based on operator-based linearization,
- x_{ref}^i – the reference solution.

This error was estimated for every state variable at the end of the simulation. Overall results are shown in Table 1. The resolution of physical space, defined by the number of interpolation points n , is in the first column. The total number of nonlinear iterations is shown in the second column. The next three columns show an estimation error in pressure, composition of gas and composition of oil, respectively. The last column shows the percent of points used for adaptive parametrization of physical space by the operator-based linearization approach.

Table 1 demonstrates that a smaller number of interpolation points results in more linear physics, leading to a smaller number of Newton iterations. The only exception is the 16 points resolution where the number of nonlinear iterations is higher than that for the other resolutions. This reflects the fact that the location of points in current approach was blindly based on a uniform distribution. However even for this case, the number of Newton iterations is significantly less than that for the standard simulation.

Table 1: Results of black oil simulation

Resolution	Iters.	$E_p, \%$	$E_{z_g}, \%$	$E_{z_o}, \%$	Space, %
Std.	6162	-	-	-	-
64	3284	0.15	1.95	2.03	0.789
32	3067	0.27	2.21	2.12	1.965
16	3332	0.47	11.26	3.43	6.238
8	2787	0.99	30.01	6.60	17.188

Isothermal compositional simulation

Next we model an isothermal process of carbon dioxide and methane injection into an oil with composition from Orr Jr. et al. (1995). The initial oil is made of 4 components CO_2 , CH_4 , C_4H_{10} , and $C_{10}H_{22}$ at corresponding compositions: 1% of carbon dioxide, 11% of methane, 38% of n-butane and 50% of decane. We inject a mixture of 80% of CO_2 and 20% of CH_4 at a BHP $P_i = 120$ bar. The production wells operate at BHP $P_p = 60$ bar. The initial pressure is $P_0 = 90$ bars and temperature $T_0 = 350$ K. The simulation period is 4000 days with a maximum time step $\Delta t = 40$ days.

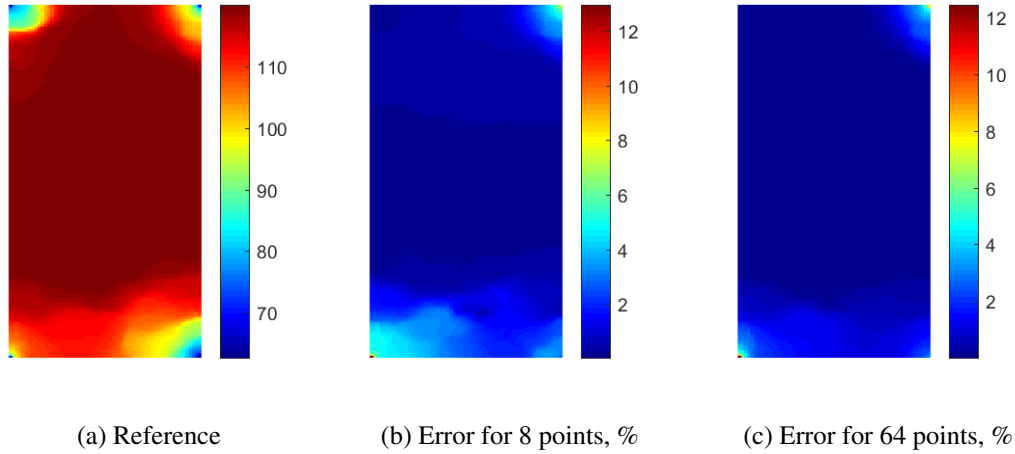


Figure 6: Pressure solution at t=4000 days

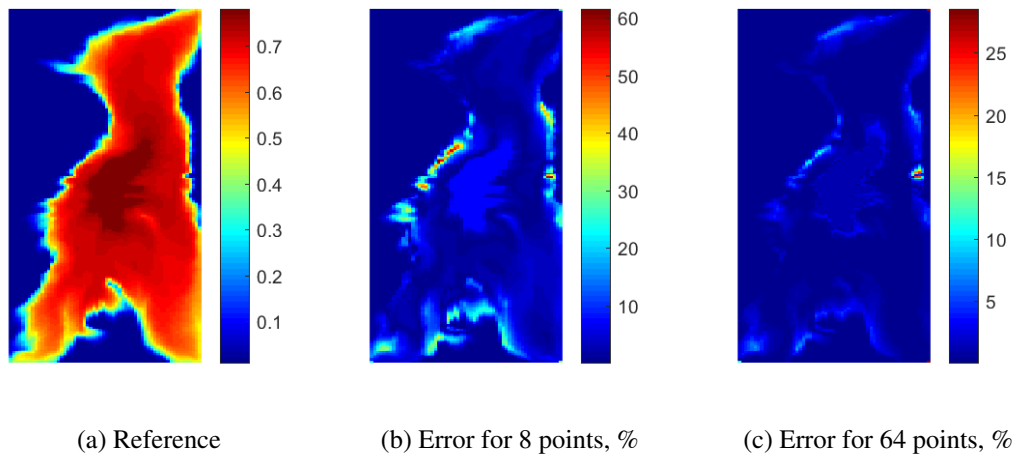


Figure 7: CO_2 composition solution at t=4000 days

Figs. 6 and 7 show pressure and CO_2 composition solutions at the last time step. Unlike in the previous case, the simulation performed with the operator-based linearization converges faster when 8-point and 64-point resolutions are compared. Also, the highest errors in composition solution are still concentrated along the displacement front. Table 2 shows the main results of the isothermal simulation. The difference in the number of Newton iterations number between the standard and operator-based linearization simulations is significantly less than in the previous case, but the trend is similar with an exception now for 8 points.

Table 2: Results of isothermal compositional simulation

Resolution	Iters.	E_p , %	E_{CO_2} , %	E_{CH_4} , %	$E_{C_{10}H_{22}}$, %	Space, %
Std.	710	-	-	-	-	-
64	629	0.29	0.65	1.02	0.76	0.133
32	583	0.30	0.95	1.56	1.17	0.471
16	569	0.32	1.78	2.70	2.17	1.784
8	587	0.72	3.62	5.51	4.52	8.801

Non-isothermal compositional

Our last simulation model is a non-isothermal version of the previous compositional model. The initial and injection conditions of the reservoir are the same except that the injection mixture has a lower temperature of $T = 315$ K. The simulation period is 2000 days with a maximum time step of $\Delta t = 20$ days. Temperature and CO_2 composition distributions at the last time step and corresponding errors are depicted in Figs. 8 and 9. The composition solution behavior remains the same, while the temperature errors are concentrated near the cooling front and the injection well. The latter can be explained by a larger nonlinearity in the energy conservation equation introduced by a correlation for enthalpy.

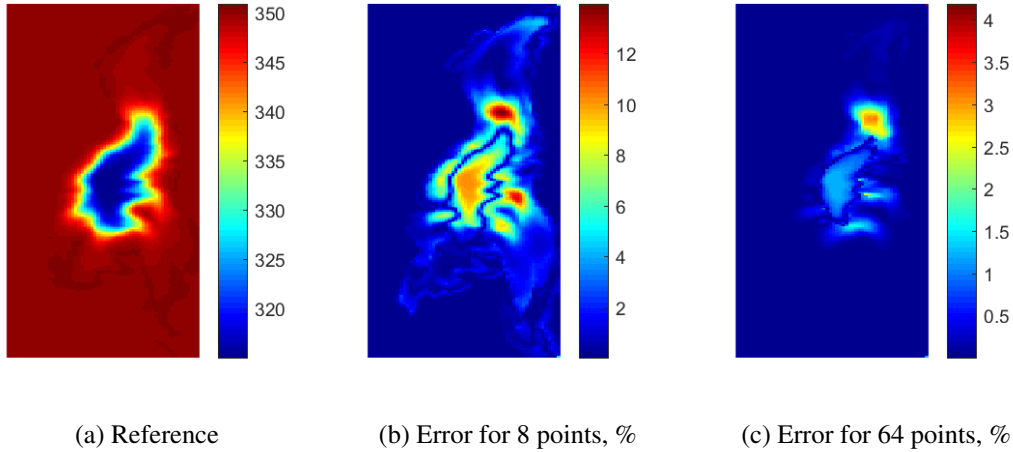


Figure 8: Temperature solution at t=2000 days

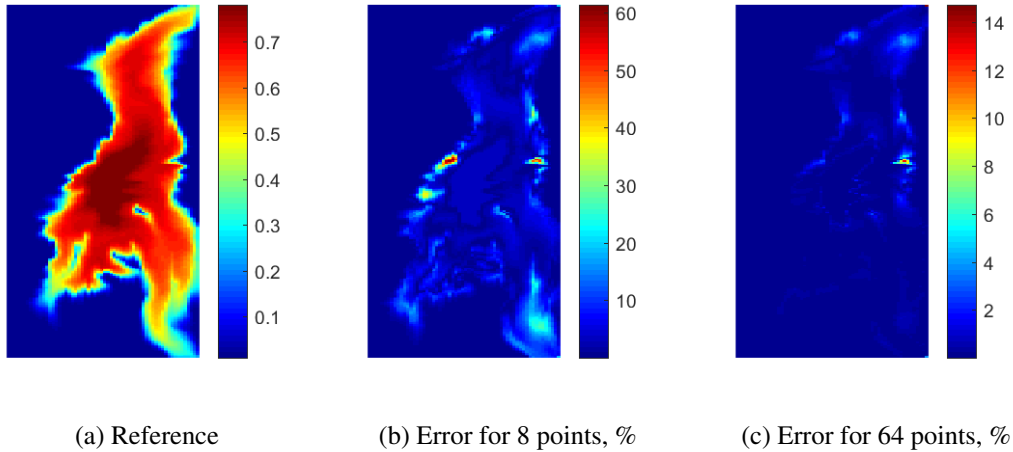


Figure 9: CO_2 composition solution at t=2000 days

Table 3: Results of non-isothermal compositional simulation

Resolution	Iters.	E_p , %	E_T , %	E_{CO_2} , %	E_{CH_4} , %	$C_{10}H_{22}$, %	Space, %
Std.	647	-	-	-	-	-	-
64	587	0.12	0.12	0.19	0.37	0.21	0.005
32	553	0.12	0.27	0.33	0.67	0.37	0.037
16	536	0.14	0.48	1.15	2.02	1.35	0.241
8	555	0.41	1.21	2.79	5.16	3.86	2.371

The convergence results of the non-isothermal simulation are presented in Table 3 and is similar to the isothermal model. In this simulation, the region of adaptive parametrization of physical space drops down to 0.001% which reflects the importance of the adaptive approach for higher dimensional systems.

Conclusions

In this work we presented a new approach for linearization of the general purpose reservoir simulation problem. We applied a new operator-based linearization method where the governing equations are represented in an operator form and each term is the product of two operators: the first is fully defined by the physical state of the problem and the second depends on both spatial and state variables. We introduced a parametrization of the first type of operators using a uniformly distributed mesh in parameter space. The second type of operators was treated in a conventional manner. An adaptive parametrization in the physical space was applied to reduce the memory consumption and increase the efficiency of the interpolation procedure.

We demonstrate the applicability of the new linearization approach for different challenging physical problems of practical interest. In particular, black-oil, isothermal and non-isothermal compositional problems were run in a highly heterogeneous reservoir. We demonstrated that the proposed operator-based linearization approach can reproduce the results of the reference solution on a fine parametrization grid. At the same time, the coarsening of parameter space improves the nonlinear solution while errors in physical approximations remain under control.

The main benefits of the proposed approach are the simplicity of an application, potential improvements in the nonlinear convergence and a generic approach to coarsening the physics in general purpose reservoir simulation. Future work will include an implementation of the operator-based simulator on modern emerging architectures (including GPU), developing advanced nonlinear solvers and balancing errors in spatial, temporal and physical approximation to achieve the best performance and accuracy of reservoir simulations.

Acknowledgments

We acknowledge the Stanford University Petroleum Research Institute for Reservoir Simulation (SUPRI-B) program for the financial support and permission to use ADGPRS in this research.

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