High-performance Reservoir Simulator for Energy Transition Applications

Khait, M.; Wang, Y.; Lyu, X.; Voskov, D.

DOI
10.3997/2214-4609.202121066

Publication date
2021

Document Version
Final published version

Published in
2nd Geoscience and Engineering in Energy Transition Conference, GET 2021

High-performance Reservoir Simulator for Energy Transition Applications

M. Khait[1], Y. Wang[1], X. Lyu[1], D. Voskov[1,2]

[1] Delft University of Technology, [2] Stanford University

Summary

Alternative to CPU computing architectures, such as GPU, continue to evolve increasing the gap in peak memory bandwidth achievable on a conventional workstation or laptop. Such architectures are attractive for reservoir simulation, which performance is generally bounded by system memory bandwidth. However, to harvest the benefit of a new architecture, the source code must be inevitably rewritten, sometimes almost completely. One of the biggest challenges here is to refactor the Jacobian assembly which typically involves large volumes of code and complex data processing. We demonstrate an effective and general way to simplify the linearization stage extracting complex physics-related computations from the main simulation loop and leaving only an algebraic multi-linear interpolation kernel instead. In this work, we provide the detailed description of simulation performance benefits from execution of the entire nonlinear loop on the GPU platform. We evaluate the computational performance of Delft Advanced Research Terra Simulator (DARTS) for various energy transition subsurface applications of practical interest on both CPU and GPU platforms, comparing particular workflow phases including Jacobian assembly and linear system solution with both stages of the Constraint Pressure Residual preconditioner.

Introduction

Fully implicit methods (FIM) are conventionally used in reservoir simulation because of their unconditional stability (Aziz and Settari, 1979). On the other hand, after discretization is applied to governing Partial Differential Equations (PDE) of a problem, the resulting nonlinear system represents different tightly coupled physical processes, which is difficult to solve. Usually, a Newton-based iterative method is applied, which demands assembly of the Jacobian and the residual for the combined system of equations (i.e., linearization) at every iteration forming often ill-conditioned linear system of equal size. The solution of such systems takes the majority of the simulation time in most practical applications.

A novel linearization approach called Operator-Based Linearization (OBL) was proposed by Voskov (2017).It could be seen as an extension of the idea to abstract the representation of properties from the governing equations, suggested in Zaydullin et al. (2013) and Haugen and Beckner (2015). In the OBL approach, the parameterization is performed based on the conventional molar variables. All properties involved in the governing equations are lumped in a few operators, which are parameterized in the physical space of the simulation problem either in advance or adaptively during the simulation process. The control on the size of parameterization hypercube helps to preserve the balance between the accuracy of the approximation and the performance of nonlinear solver (Khait and Voskov, 2017).

Delft Advanced Research Terra Simulator (DARTS) was introduced and described by Khait (2019). It exploits the OBL approach to decouple the computations of physical properties from the main simulator core. Jacobian assembly in DARTS is therefore simplified and generalized increasing its portability to alternative computational architectures, such as GPU. We evaluate the computational performance of DARTS for two subsurface applications relevant to energy transition on both CPU and GPU platforms.

Method

We consider mass and energy transport for a system with n_p phases and n_c components. For this model, the n_c component mass and energy conservation equations can be written as

$$\frac{\partial m_c(\boldsymbol{\xi},\boldsymbol{\omega})}{\partial t} + \operatorname{div} f_c(\boldsymbol{\xi},\boldsymbol{\omega}) + q_c(\boldsymbol{\xi},\boldsymbol{\omega},\mathbf{u}) = 0, \quad c = 1,\ldots,n_c+1. \tag{1}$$

Here, $\boldsymbol{\xi}$ are space-dependent parameters, $\boldsymbol{\omega}$ are state-dependent parameters, $\boldsymbol{u}$ are control variables, and

$$m_c(\boldsymbol{\xi},\boldsymbol{\omega}) = \phi \sum_{j=1}^{n_p} x_{cj}\rho_p s_j, \quad c = 1,\ldots,n_c, \tag{2}$$

$$m_c(\boldsymbol{\xi},\boldsymbol{\omega}) = \phi \sum_{j=1}^{n_p} \rho_p s_j u_j + (1-\phi)u_r, \quad c = n_c+1, \tag{3}$$

where t is time, φ is effective rock porosity, x_{cj} is component c concentration in phase j, ρ_j denotes phase j molar density, s_j is saturation of phase j and u_j is phase internal energy. Similarly,

$$f_c(\boldsymbol{\xi},\boldsymbol{\omega}) = \sum_{j=1}^{n_p} x_{cj}\rho_j\vec{v}_j + s_j\rho_j\mathbf{J}_{cj}, \quad c = 1,\ldots,n_c, \tag{4}$$

$$f_c(\boldsymbol{\xi},\boldsymbol{\omega}) = \sum_{j=1}^{n_p} h_j\rho_j\vec{v}_j - \left(\phi \sum_{j=1}^{n_p} \kappa_j s_j + (1-\phi)\kappa_r\right)\nabla T, \quad c = n_c+1, \tag{5}$$

where h_j is the phase enthalpy, κ_j is phase thermal conduction, $\vec{v}_j$ is Darcy velocity and $\boldsymbol{J}_{cj}$ is Fick's diffusion flux. Also, $\boldsymbol{K}$ is the effective permeability tensor, k_{rj} is relative permeability, μ_j is phase viscosity, p_j is phase pressure, γ_j is hydrostatic gradient, and D is depth.

According to the Operator Based Linearization (OBL) method proposed in Voskov (2017), all terms in the Equation 1 are written as functions of a physical state $\boldsymbol{\omega}$ and a spatial coordinate $\boldsymbol{\xi}$. The physical state represents a unification of all state variables (i.e., nonlinear unknowns: pressure, temperature/enthalpy, saturations/compositions, etc.) of a single control volume. In the overall molar formulation, the nonlinear unknowns are pressure p, fluid enthalpy h and overall composition z_c,

therefore the physical state $\boldsymbol{\omega}$ is completely defined by these variables. The spatial coordinate $\boldsymbol{\xi}$ defines the location of a given control volume which reflects the distribution of heterogeneous rock properties (e.g., porosity, thermal conduction) and elements of space discretization (e.g., transmissibility). Besides, well control variable $\boldsymbol{u}$ is introduced to represent various well management strategies. Equation 1 is discretized in space using finite-volume two-point flux approximation and in time using backward Euler approximation. The applied Fully Implicit Method (FIM) yields that the convective flux term depends on the values of nonlinear unknowns at the current time step. Next, we rewrite Equation 1 neglecting for simplicity buoyancy and capillary forces (see more general treatment in Khait and Voskov, 2018a; Lyu et al., 2021a), and represent each term as a product space-dependent properties and of state-dependent operators (Khait and Voskov, 2018b). The resulting conservation equations read

$$\frac{V\phi_0}{\Delta t}\left(\alpha_c(\boldsymbol{\omega})-\alpha_c(\boldsymbol{\omega}^n)\right) - \sum_l \left[\beta_c^l(\boldsymbol{\omega})\Gamma^l(\boldsymbol{\xi})\Delta\Phi_j - \gamma_{cj}^l(\boldsymbol{\omega})\Gamma_d^l(\boldsymbol{\xi})\Delta x_{cj}\right] - \beta_c^w(\boldsymbol{\omega},\mathbf{u})\Gamma^w(\boldsymbol{\xi})\Delta p^w = 0, \quad c=1,\ldots,n_c, \tag{6}$$

$$\frac{V}{\Delta t}\Big[\phi_0\left(\alpha_e(\boldsymbol{\omega})-\alpha_e(\boldsymbol{\omega}^n)\right) + (1-\phi_0)u_r(\boldsymbol{\xi})\left(\alpha_r(\boldsymbol{\omega})-\alpha_r(\boldsymbol{\omega}^n)\right)\Big] - \sum_l \beta_h^l(\boldsymbol{\omega})\Gamma^l(\boldsymbol{\xi})\Delta\Phi_j - \sum_l \Gamma_r^l(\boldsymbol{\xi})\Big[\phi_0\beta_e^l(\boldsymbol{\omega})+(1-\phi_0)\kappa_r\alpha_r(\boldsymbol{\omega})\Big]\Delta T^l - \beta_h^w(\boldsymbol{\omega},\mathbf{u})\Gamma^w(\boldsymbol{\xi})\Delta p^w = 0, \tag{7}$$

where V is the volume of mesh grid block, φ_0 is rock porosity at the reference pressure, Γ_l, Γ_{ld} and Γ_{lr} are the space-dependent part of convective, diffusive and conductive transmissibility respectively, Φ_j is phase potential. The nonlinear operators α, β, γ represents nonlinear operators based on governing properties of PDEs, see more details in Lyu et al. (2021b).

Delft Advanced Research Terra Simulator (DARTS) implements the equations described above for both CPU and GPU platforms. From the perspective of the simulation nonlinear loop, the operator interpolation replaces properties calculations during the Jacobian assembly. Besides, it also 'shadows' physical phenomena behind the operators, leaving out only the values of supporting points, which are rarely computed but utilized all the time during interpolation for Jacobian and residual evaluation. This allows to detach fluid and rock properties calculations (now only performed during operator evaluation at supporting points) from the main nonlinear loop, as well as to relax the performance requirements for such calculations.

Results

Geological storage of CO_2 is critically important for the reduction of greenhouse gas emissions. Due to the buoyant characteristic of injected gas and the complex geology of subsurface reservoirs, most injected CO2 rapidly migrates to the top of the reservoir. The detailed behavior of gravity-induced instabilities can be modelled using two-phase flow with gravity currents and convective dissolution in the presence of the capillary transition zone (CTZ), see details in Lyu et al. (2021b).

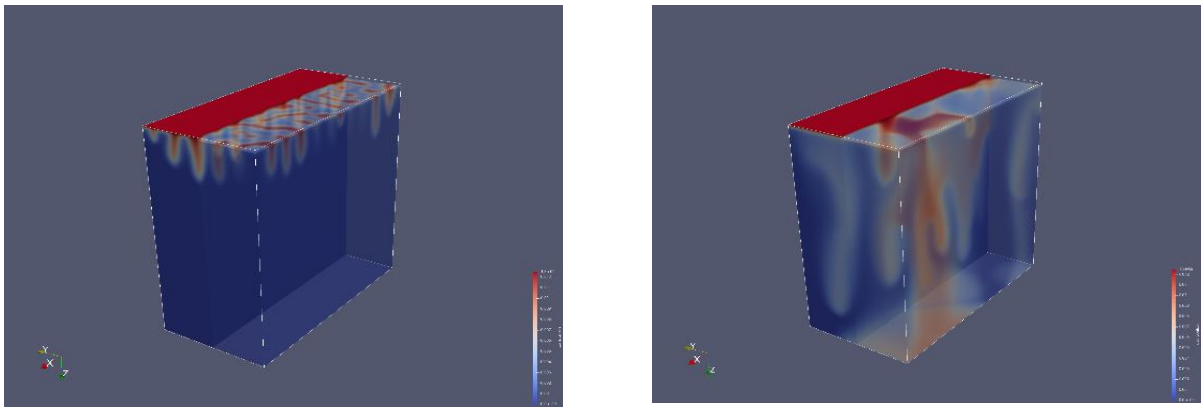

Figure 1 *CO_2 concentration in brine during sequestration after 100 (left) and 400 years(right)*

Figure 1 demonstrates the CO_2 concentration for the simulation with single-phase brine after 100 and 400 years of CO_2 injection. The model is based on an unstructured triangular extruded mesh with 100 layers and 1.1million grid blocks in total. The top layer was initialized with constant CO_2 composition of 0.0125 (dissolution limit), while pure brine filled the rest of the reservoir. The model was simulated for 3000 years with a maximum timestep of 365 days. Simulation timings can be found in Table 1, where CPU1(s) represents sequential run on Intel Core i7-8086K; CPU2(20) – parallel run with 20 threads on 2 x IntelXeon E5-2640 v4; GPU – NVidia GeForce RTX2080 Ti.

Table 1 *Overall simulation performance of carbon dioxide storage model on different platforms*

Platform	TS	NI	LI	Init, s	Jacobian, s	Setup, s	Solve, s	Total, s
CPU1 (s)	3015	6696	57726	25.4	3523.0	24193.9	20110.4	48400.1
CPU2 (20)	3015	6790	61438	35.4	623.7	3761.3	8363.8	13682.3
GPU	3015	6725	57487	37.5	204.1	1114.1	1183.1	3333.9

The geothermal reservoir under investigation is located in the West Netherlands Basin (WNB), which is an inverted rift basin in the Netherlands. The reservoir properties of Delft Sandstone have been extensively studied before by Willems et al. (2016, 2017). Figure 2) shows the porosity distribution at the geological resolution of the target reservoir scaled vertically by a factor of 3. The model includes intersections of sandstone and shale facies. The facies distribution corresponds to circa 0.8 million grid blocks for the sandstone and 2.4 million blocks for shale facies. Even though the water mainly flows through the sandstone formation, for thermal simulation it is crucially important to take shale facies into account too, as was shown in the recent benchmark study by Wang et al. (2020). The presence of the shale layers in the simulation allows the use of higher discharge rates that result in high energy production for an equivalent system lifetime. The predicted lifetime of both doublets is significantly extended when the shale layers are included in the model. Using the full model with 3.2 million cells, we computed the forecast for 100 years of two geothermal doublets production with the maximum time step of 365 days. The simulation results (cold water plums distribution) can be seen in Figure 2. Simulation performance of this model is shown in Table 2.

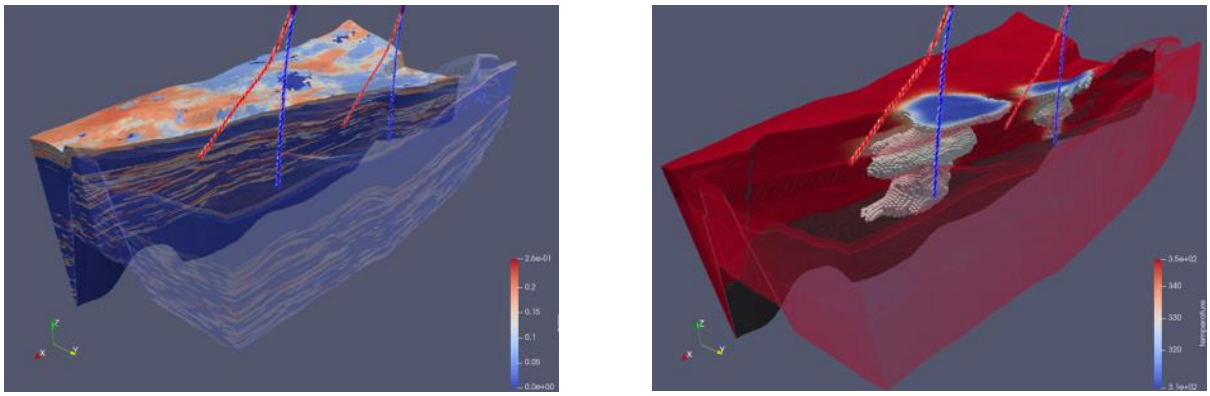

Figure 2 *Geothermal reservoir initial porosity (left) and temperature distribution after 100 years*

Table 2 *Overall simulation performance of geothermal model on different platforms*

Platform	TS	NI	LI	Init, s	Jacobian, s	Setup, s	Solve, s	Total, s
CPU1 (s)	107	287	4819	78.88	219.99	819.40	3885.12	5019.17
CPU2 (20)	107	291	4916	103.04	35.21	305.41	1506.01	1976.64
GPU	107	288	5161	78.12	18.03	18.03	276.98	486.60

Conclusions

Delft Advanced Research Terra Simulator (DARTS) framework is built on top of the Operator-Based Linearization approach. It substantially simplifies Jacobian construction and reduces the time required for porting simulation code to different architectures, such as GPU. Proving this claim, we demonstrated

two examples of fully offloaded GPU simulations relevant to energy transition: a carbon dioxide long-term storage and a realistic model of geothermal energy production. To the best of our knowledge, these are the first simulations of these applications fully offloaded to a GPU device. Compared to sequential execution on a high-frequency modern desktop CPU, the multithread version reduces simulation time by 2-4 folds on a server node with two sockets, depending on a particular application. At the same time, the GPU version demonstrated overall improvement in the range of 8-14 (10-14 without time for sequential initialization stage). DARTS provides a forecast for 100 years with a 3.2 million grid blocks geological model in only 8 minutes, while the forecast for 3000 years for carbon dioxide sequestration scenario on a 1.1 million unstructured mesh takes less than an hour. The fastest results were achieved on a regular workstation equipped with a gaming GPU graphics card.

References

Aziz, K. and Settari, T. [1979]. Petroleum Reservoir Simulation. *Applied Science Publishers*.

Christie, M. and Blunt, M. [2001]. Tenth spe comparative solution project: A comparison of upscaling techniques. *SPE Reservoir Evaluation and Engineering*, 4(4):308–316.

DARTS [2019]. Delft Advanced Research Terra Simulator.https://darts.citg.tudelft.nl.

Esler, K. et al. [2014]. Realizing the potential of GPUs for reservoir simulation. *ECMOR XIV-14th European Conference on the Mathematics of Oil Recovery*.

Haugen, K. and Beckner, B. [2015]. A general flow equation framework. *SPE Reservoir Simulation Symposium 2015*,2:1310–1318.

Khait, M. [2019]. Delft Advanced Research Terra Simulator: General Purpose Reservoir Simulator with Operator-Based Linearization. *PhD thesis, TU Delft*.

Khait, M. and Voskov, D. V. [2017]. Operator-based linearization for general purpose reservoir simulation. *Journal of Petroleum Science and Engineering*, 157:990 – 998.

Khait, M. and Voskov, D. [2018a]. Adaptive parameterization for solving of thermal/compositional nonlinear flow and transport with buoyancy. *SPE Journal*, 23:522–534.

Khait, M. and Voskov, D. [2018b]. Operator-based linearization for efficient modeling of geothermal processes. *Geothermics*,74:7–18.202

Lyu, X., Khait, M., and Voskov, D. [2021a]. Operator-based linearization approach for modelling of multiphase flow with buoyancy and capillarity. *SPE Journal*, 1-18.

Lyu, X., Voskov, D., and Rossen, W. R. [2021b]. Numerical investigations of foam-assisted CO_2 storage in saline aquifers. *International Journal of Greenhouse Gas Control*, 108:103314.

Voskov, D. V. [2017]. Operator-based linearization approach for modeling of multiphase multi-component flow in porous media. *Journal of Computational Physics*, 337:275–288.

Wang, Y., Voskov, D., Khait, M., and Bruhn, D. [2020]. An efficient numerical simulator for geothermal simulation: A benchmark study. *Applied Energy*, 264.

Willems, C. J. L., Goense, T., Nick, H. M., and Bruhn, D. F. [2016]. The relation between well spacing and net present value in fluvial hot sedimentary aquifer geothermal doublets; a West Netherlands Basin case study. *Workshop on Geothermal Reservoir Engineering*

Willems, C., Nick, H., Weltje, G., and Bruhn, D. [2017]. An evaluation of interferences in heat production from low enthalpy geothermal doublets systems. *Energy*, 135:500–512.

Zaydullin, R., Voskov, D., and Tchelepi, H. [2013]. Nonlinear formulation based on an equation-of-state free method for compositional flow simulation. *SPE Journal*, 18(2):264–273.