The National IOR Centre of Norway
Post Doc report (Juan Michael Sargado), part of

Adding more physics, chemistry and geological realism into the reservoir simulator

Project 2.6.1

Project manager: Juan Michael Sargado
Other key personnel: Robert Klöfkorn, Tor Harald Sandve
Project duration: November 2019 – July 2020

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Final Project Report

Upscaling of chemo-mechanical compaction to field scale models

Project number and location (UiS, NORCE, IFE): 2.6.4, UiS
Project duration: November 2019 — July 2020
Project manager: Juan Michael Sargado
PhD students and postdocs: Juan Michael Sargado (Postdoc)
Other key personnel: Robert Klöfkorn (NORCE), Tor Harald Sandve (NORCE)

Executive summary

Powerful and accurate simulation tools are vital for realizing safe and profitable commercial production in hydrocarbon reservoirs. It is therefore of paramount importance that these tools incorporate the latest knowledge regarding behavior of reservoir materials, as well as properly model emerging technologies and methods related to reservoir treatment. The current project was aimed extending the capabilities of the Open Porous Media (OPM) software by efficiently coupling to a separate code for handling stress/deformation analysis and incorporating the feedback on flow properties. It was carried out for approximately 8 months out of the originally planned duration of 2 years, during which time work was done on developing a python interface for the OPM flow simulator through which efficient interchange of data can be made with the multiphysics code BROOMStyx for performing mechanical simulations. The latter code was also modified to use the same backend as OPM for constructing and managing grid-associated objects. In addition, research was done on developing efficient discretization schemes and novel constitutive models and formulations for modeling fracture evolution using phase-field approaches. This research has been presented in several international conferences and published in associated proceedings. In particular, an extended abstract describing work done on phase-field modeling of fluid-induced brittle fracture in poroelastic media was chosen as one of five finalists for the 2020 Melosh Medal Competition, a prestigious international graduate-level competition in the field of FEA and computational mechanics.

1 Introduction and background

Compaction effects occur in many reservoirs, and can both be a major driving mechanism towards improved recovery as well as give rise to a number of field operating problems. Experience has shown that these are important phenomena that must be considered when designing reservoir operations. For instance, subsidence of the sea floor in the Ekofisk field due to compaction of the reservoir resulted in the need to perform remediation efforts at considerable expense.

Standard reservoir simulators are mostly built to model flow but not mechanical deformation, and hence lack the capability to simulate reservoir compaction based on the fundamental governing equations. While it is possible to achieve the latter by combining different commercially available simulators, such an approach almost always requires coupling to be done externally, leading to longer execution times for the overall simulation. Furthermore, commercial codes are often limited with regard to the specification or modification of material models, and do not always allow for the use of entirely new user-defined models. As most reservoir rocks exhibit elastoplastic behavior when subject to compaction, the resulting equations become highly

nonlinear and expensive to solve. In order to efficiently incorporate the feedback effect of mechanical deformation in the reservoir flow model, it is necessary to couple together separate codes with minimum overhead.

Furthermore, understanding the evolution of fracture networks in reservoirs as a consequence of mechanical and chemical processes is important both in conventional and unconventional hydrocarbon extraction. In recent years, research on crack initiation and growth within the context of multiphysics settings has garnered a lot of interest thanks to advancements made in fracture modeling algorithms, particularly in a class of methods known as phase-field approaches. While a substantial amount of progress has been made with regard to these methods, many open questions remain especially with regard to applications involving fluid-induced fracture in porous media.

2 Results

2.1 Coupling of OPM with external code for deformation analysis

The main reservoir simulator in the Open Porous Media (OPM) suite is known as `flow`, and is designed for dealing with three-phase black-oil problems via a fully implicit formulation. The resulting nonlinear problem is solved using the Newton-Raphson algorithm together with iterative linear solvers from the Dune Iterative Solver Template Library (`dune-istl`). The simulator employs a cell-centered finite volume formulation based on the two-point flux approximation. This constitutes the current industry standard for flow simulation in porous media, but is not suitable for use with the stress equilibrium equations that govern mechanical deformation.

In the project, preliminary work was done to couple the OPM flow simulator to BROOMStyx [3], an open-source multiphysics framework written in C++ with capabilities to perform mechanical simulations. The main aim is to accomplish efficient two-way coupling, which is important since deformation in the form of compaction and pore collapse can have a significant effect on the reservoir flow properties. This can be achieved by using the Pybind11 library to expose the methods and attributes of the original C++ classes for access within a python environment via lightweight wrapper objects, so that the simulation can be carried out by means of python scripts.

Existing python interfaces to `opm-common` allow parsing of eclipse input decks into data objects. To make use of these, the main function of simulator code was modified to be called via python wrapper that takes the parsed data objects as arguments in place of the original input deck. In collaboration with researchers at the Computational Geosciences and Modelling group at NORCE, this functionality was further extended to allow for timesteps to be articulated within the python script, giving the possibility of changing boundary conditions for specific timesteps from original specifications in the input deck, and providing access to results and internal variables without resorting to deep copying strategies. In order to accomplish this, it was also necessary to modify parts of the backend C++ code in OPM. A new mesh reader class was also written in the BROOMStyx framework for reading mesh files generated by the open-source software Gmsh [1] and constructing the data structures for nodes and cells via the `dune-grid` module. Modifications in the implementation of methods in the `DomainManager` class in BROOMStyx were made in order to allow access to the grid objects from Dune without changing the interface exposed to other classes in the BROOMStyx framework.

Differences in design principles between the two codes give rise to several issues. Dune makes extensive use of template programming, for which parameters such as the problem dimension are required to be known at compile time. On the other hand for the BROOMStyx code, such parameters are expected to be available only at runtime. To remedy this, any necessary parameters needed for the Dune backend are passed via the

variable `CMAKE_FLAGS` specified in the `config.opts` file when building both codes. A generated header file named `config.h` then defines all the template parameters required for compilation. Furthermore, this allows for swapping the actual grid implementation with another at build time without having to make additional changes to the BROOMStyx source code. Another issue concerns the ordering of nodes and faces, as Dune employs its own ordering system for element nodes based on the concept of 'twist', whereas BROOMStyx adopts the ordering system employed by Gmsh. This is dealt with within the `DuneGrid_GmshReader` class in the latter code, where a conversion is made from one system to the other when instantiating the corresponding node and cell objects within BROOMStyx from their Dune counterparts.

2.2 Higher order control volume finite element formulation for phase field brittle fracture

A new control volume finite element formulation for phase-field brittle fracture was developed by the postdoc during the project. It has been shown previously in [4] that a combined formulation utilizing linear finite elements to discretize the displacement field and cell-centered finite volumes based no the two-point flux approximation for the phase-field outperforms a discrete formulation that utilizes linear Lagrange elements for both the displacement and phase-field variables. This can be explained by the fact that TPFA does not assume continuity of the primary variable gradient when calculating the normal derivatives across cell faces. As a result, the FV scheme is better able to model the 'kinks' that occur peaks of the phase-field profile corresponding to fully developed cracks. Nevertheless, the phase-field itself is assumed to be piecewise constant over control volumes, and the combined FE-FV scheme is essentially a P_1-P_0 formulation that achieves the same convergence rate as pure linear finite elements but with the advantage of having smaller absolute errors.

An improvement over the original method was made by performing a linear reconstruction of the phase-field over subcells of the original control volumes based on values at the cell center and the corresponding face midpoint. This implies that the phase-field will generally be discontinuous at subcell boundaries within the control volumes. Said phenomenon has no effect on the discrete form of the stress equilibrium equation as the latter requires only the phase-field value at the cell center. On the other hand, increased accuracy is obtained when integrating the damage over control volumes. This results in a method that exhibits higher order convergence with respect to representing the phase-field profile. Performance of the improved method was investigated for 2D problems by simulating a benchmark problem originally proposed in [2]. It was found that the proposed method is able to achieve similar accuracy to a linear FE formulation but with cells being 4 to 8 times larger in critical regions in comparison with the latter, translating to a reduction in computational time of more than 98%. Results have been presented in various conferences and are published in the proceedings of FVCA IX (see Section 4).

2.3 A new phase-field model for fluid-driven brittle fracture in permeable media

Modeling fluid-driven fracture in a permeable medium involves significant computational challenges within the context of energy applications such as engineered geothermal systems and unconventional hydrocarbon extraction. In addition to a priori unknown crack trajectories, a major issue is scale disparity, in which domain dimensions are in the order of m to km, while fracture apertures are on the order of mm. Competition between different sets of processes with respect to energy dissipation (viscous flow versus crack formation) and fluid balance (storage versus leak-off) gives rise to different regimes, with hydraulic fracturing treatments being initially viscosity- and storage-dominated but evolving towards the leak-off- and toughness-dominated regime.

During the project, an improved numerical framework based on a variationally consistent phase-field model for fluid-driven brittle fracture was developed as a continuation of research conducted while the Postdoc was a PhD fellow at the University of Bergen. The model is based on the framework of Biot poroelasticity, with the key novelty being a consistent regularization of poroelastic parameters with respect to bulk energy degradation. The resulting formulation naturally accounts for the effect of fluid pressure inside fractures, and furthermore does not require any special treatment for imposing force balance at crack faces. To solve the coupled system of equations arising from this model, an efficient numerical framework is devised that combines finite element and control volume concepts. In particular, the phase-field equation is discretized by means of cell-centered finite volumes to better model discontinuities in the phase-field gradient following the discussion in [4]. Performing a proper upscaling of the flow inside fractures enables the use of elements having dimensions more than two orders of magnitude larger than the occurring fracture apertures, as demonstrated through numerical examples. Furthermore, it was shown that the developed framework can successfully model fluid-driven fracture propagation transitioning between different flow and energy dissipation regimes.

2.4 A new unilateral contact model for phase-field brittle fracture

A new model for describing unilateral contact within the context of phase-field approaches was developed, with the aim of incorporating the relaxation of the Poisson effect upon the occurrence of fracture. Similar to the energy splitting scheme introduced by Miehe et al. [2], the proposed model performs a decomposition of the bulk energy based on the principal components of the strain tensor. In [2], the Lamé moduli λ and μ are used in expressing the bulk energy, which is subsequently decomposed as follows:

$$\psi_0^{\pm}(\boldsymbol{\varepsilon}, \boldsymbol{\phi}) = \frac{\lambda}{2} \langle \varepsilon_1 + \varepsilon_2 + \varepsilon_3 \rangle_{\pm}^2 + \mu \left[\langle \varepsilon_1 \rangle_{\pm}^2 + \langle \varepsilon_2 \rangle_{\pm}^2 + \langle \varepsilon_3 \rangle_{\pm}^2 \right] \tag{1}$$

where ε_i $(i = 1, 2, 3)$ denote the principal strain components. Thus λ is degraded based on the sign of the volumetric strain, while the effect of μ along each of the principal directions depends on the sign of its associated strain component. Unfortunately, such a strategy does not properly deal with the Poisson effect, and it can be demonstrated that certain strain states lead to unphysical results. Similarly, a uniform degradation of the Lamé moduli preserves the initial Poisson ratio. As a consequence, alternative splitting schemes have been put forward by subsequent authors such as [5].

In the project, a new model was proposed where the bulk strain energy accounting for damage is instead written in terms of the Young's moduli and Poisson ratios pertaining to the principal directions of strain. These parameters are assumed to be functions of both the strain tensor and the phase-field. Moreover, emphasis is placed on preserving major symmetry of the resulting elasticity tensor in order for the model to be physically meaningful. To accomplish this, an orthotropic formulation is adopted with the directions of orthotropy being made to coincide with the principal orientation of the strain tensor. The compliance tensor

for a linear elastic, orthotropic material can be written as

$$\mathbf{S} = \begin{bmatrix} \frac{1}{E_1} & -\frac{\nu_{21}}{E_2} & -\frac{\nu_{31}}{E_3} & & & \\ -\frac{\nu_{12}}{E_1} & \frac{1}{E_2} & -\frac{\nu_{32}}{E_3} & & & \\ -\frac{\nu_{13}}{E_1} & -\frac{\nu_{23}}{E_2} & \frac{1}{E_3} & & & \\ & & & \frac{1}{G_{23}} & & \\ & & & & \frac{1}{G_{31}} & \\ & & & & & \frac{1}{G_{12}} \end{bmatrix} \tag{2}$$

where E_i and ν_{ij} are the Young's moduli and Poisson ratios associated with the various principal directions. In the this model, the Young's moduli along each direction are selectively scaled by the degradation function based on the sign of their respective associated principal strain component, i.e.

$$\widetilde{E}_i(\boldsymbol{\varepsilon}, \phi) = \begin{cases} g(\phi) E_i, & \varepsilon_i > 0 \\ E_i, & \varepsilon_i \leq 0 \end{cases} \tag{3}$$

To satisfy major symmetry, the components of $\mathbf{S}$ must satisfy the relation $\nu_{ij}/E_i = \nu_{ji}/E_j$. The same restriction applies when said components are modified to account for damage. Hence, the adoption of (3) implies that the Poisson ratios must have the following form:

$$\widetilde{\nu}_{ij}(\boldsymbol{\varepsilon}, \phi) = \begin{cases} g(\phi) \nu_{ij}, & \varepsilon_i > 0 \\ \nu_{ij}, & \varepsilon_i \leq 0 \end{cases} \tag{4}$$

Using the last two expressions, we obtain the bulk elastic energy accounting for damage as $\psi(\boldsymbol{\varepsilon}, \phi) = (1/2)\, \boldsymbol{\varepsilon}^{\mathsf{T}} \mathbf{C}(\boldsymbol{\varepsilon}, \phi)\, \boldsymbol{\varepsilon}$, where the stiffness tensor $\mathbf{C}(\boldsymbol{\varepsilon}, \phi)$ is given by the inverse of $\mathbf{S}$.

As the proposed model requires the strain tensor to be in spectral form, obtaining the 2nd derivatives of the energy with respect to $\boldsymbol{\varepsilon}$ and ϕ are nontrivial. It can be worked out from the above definitions that the dependence of $\mathbf{C}$ on $\boldsymbol{\varepsilon}$ takes the form of step functions. Thus $\partial \mathbf{C}/\partial \boldsymbol{\varepsilon}$ is mostly zero and for practical purposes can be ignored without ill effect. Nevertheless, the other terms arising from the differentiation must be carefully calculated. In particular, the source term in the phase-field equation cannot be expressed in the form $g'(\phi)\, \psi_0^+(\boldsymbol{\varepsilon})$ as is done in existing models. A consequence of this is that irreversibility of crack growth may no longer be imposed via the strategy of using a history variable in place of ψ_0^+ as is commonly done in numerical solution of the phase-field equation.

The model discussed above has been presented at an international conference (See Section 4), and is currently under continuing development. Several important issues are being addressed, such as how to efficiently impose crack growth irreversibility, and also how to incorporate friction for fully developed cracks under compressive-shear loading.

3 Concluding remarks

The project was carried out for only 8 months of the original assigned duration of two years due to resignation of the Postdoc from the position associated with project in July 2020. Nevertheless, preliminary work was done on creating a python interface for running OPM that can serve as a means to efficiently couple the

flow simulator to an external code without either software having to rebuild the discretized geometry and reinitialize variables for each solution step. The BROOMStyx framework was also extended to integrate functionality from dune modules so as to share the same underlying data structures (e.g. for storing the grid) with OPM. Furthermore, several novel contributions were made in the modeling of brittle fracture propagation in solid and porous media via phase-field approaches, which were successfully presented in various international venues. Subsequent to the project, work on the python interface for the OMP blackoil simulator was continued by the Computational Geosciences and Modelling group at NORCE. A version of the BROOMStyx code that has been modified to use the dune-grid backend is also preserved as a separate branch in the online GitHub repository (https://github.com/ broomstyx/broomstyx).

4 Dissemination of results

The work undertaken during the project related to fracture modeling was presented in several international conferences originally scheduled for 2020, and published in an associated proceeding. Additionally, an extended abstract featuring the postdoc's work on phase-field modeling of fluid-induced fracture was selected as one of five finalists at an international competition for PhD students and recent graduates in the field of computational mechanics.

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2. J.M. Sargado. A new unilateral contact model and an efficient discretization scheme for phase-field fracture. *14th World Congress on Computational Mechanics* (Virtual Congress), 11–15 January, 2021. Oral presentation.
3. J.M. Sargado, E. Keilegavlen, I. Berre, J.M. Nordbotten. A novel phase-field model for fluid driven brittle fracture in permeable media based on consistent regularization of poroelastic parameters. *31st Annual Robert J. Melosh Medal Competition* (virtual symposium), 22–23 October, 2020.

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