



Contents lists available at ScienceDirect

International Journal of Rock Mechanics & Mining Sciences

journal homepage: www.elsevier.com/locate/ijrmms

A simulator for modeling coupled thermo-hydro-mechanical processes in subsurface geological media

S. Kelkar^a, K. Lewis^{a,1}, S. Karra^{a,*}, G. Zyvoloski^a, S. Rapaka^{a,2}, H. Viswanathan^a,
P.K. Mishra^{a,3}, S. Chu^a, D. Coblentz^b, R. Pawar^a

^a Computational Earth Science Group (EES-16), MS T003, Earth and Environmental Sciences Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA

^b Geophysics Group, Earth and Environmental Sciences Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA

ARTICLE INFO

Article history:

Received 1 March 2013

Received in revised form

19 June 2014

Accepted 23 June 2014

Available online 17 July 2014

Keywords:

Coupled processes

Finite element

Finite volume

Mechanical deformation

Subsurface modeling

Thermal-hydro-mechanical

ABSTRACT

We present the description of a fully coupled simulator FEHM for modeling coupled thermo-hydro-mechanical (THM) processes in geomechanics. The coupled equations for fluid flow and energy transport are implemented using finite volume whereas Galerkin finite element method is used for mechanical force balance. The simulator is designed to address spatial scales on the order of tens of centimeters to tens of kilometers, and time scales on the order of hours to tens of years. The governing coupled nonlinear equations are solved using a Newton–Raphson scheme with analytically or numerically computed Jacobians. A suite of models is available for coupling flow and mechanical deformation via permeability–deformation relationships. The coupled simulator is verified by comparing with several analytical solutions developed for this purpose. A subset of the simulator capabilities is benchmarked against commercially available simulators. We also demonstrate a good match with data from Desert Peak geothermal field in Nevada, USA. This validation required the use of a shear failure model with non-linear permeability–stress relationship. In addition, we present another application involving fluid injection into an inclined fault zone using a non-orthogonal grid with stress-dependent Young's modulus and permeability.

Published by Elsevier Ltd.

1. Introduction

The importance of coupled thermal, hydrological and mechanical processes (THM) in geological media in the context of engineering is well recognized [1,2]. Areas of application where THM processes are of importance include nuclear waste isolation [3,4], geological sequestration of CO₂ [5,6], production of fossil fuels [7], underground gas storage [8], geothermal energy [9,10], and Arctic landscape [11]. Coupled chemical and biological processes are important as well, however, the work described here is limited to THM processes.

Due to the recent advances in available computational power and the development of robust algorithms, computational methods have

begun to play an increasingly important role complementing experimental and theoretical approaches. Field experiments and measurements are difficult and expensive to perform, hence available data are sparse. Additionally, it is necessary to estimate project performance for varied operational scenarios on spatial and temporal scales far exceeding those at which direct measurements are possible. Simulations also play a critical role in estimating the risk of low-probability, high-impact scenarios, where experiments are too risky; for example, leakage from nuclear waste repositories and induced seismicity due to large-scale fluid injection/withdrawal. The processes involved are complex and depend on many factors, including (i) type and state of the rock formations, (ii) nature, composition and phases of the pore fluids, (iii) in situ conditions of pressure (p), temperature (T) and stress (σ), and (iv) nature and extent of disturbances introduced by the engineering applications and their evolution over the life cycle of the project.

Coupled THM processes have been modeled using a number of different approaches, each approach presenting specific benefits for intended applications. There are a large number of publications, discussing many different codes using a variety of methods and approaches. Without attempting to provide a comprehensive literature review, we will note some of these efforts. Wang and

* Corresponding author. Tel.: +1 505 606 1894.

E-mail address: satkarra@lanl.gov (S. Karra).

¹ Present address: School of Science, Monmouth University, 400 Cedar Avenue, West Long Branch, NJ 07764, USA.

² Present address: Siemens Corporate Research, 755 College Road, East Princeton, NJ 08540, USA.

³ Present address: Department of Civil and Environmental Engineering, 800 N. State College Blvd, California State University Fullerton, CA 92834, USA.

Kolditz [12] present the details of designing and implementing an object-oriented finite element code, and later on describe the parallel implementation of such a framework in Geosys/Rockflow [13]. Zhou and Ghassemi [14] developed a finite element model for fully coupled thermo-hydro-mechanical-chemical (THMC) processes to study wellbore dynamics in shale. Nishimura et al. [11] developed a fully coupled THM finite element (FE) formulation for freezing and thawing in water-saturated soils. Podgorney et al. [15] discuss a parallel code under development for simulating the mass and energy balance equations. McClure and Horne [16] use a DFN model to investigate induced seismicity. A detailed review of the THMC literature can be found in [17].

Sequential coupling using different codes allows flexibility in software development and a degree of choice in pairing mechanical and flow simulators [18]. Generally this results in more sophisticated stress–displacement relationships being available such as plasticity and large-displacement formulations. Fu et al. [19] discuss a distinct element code combined sequentially with a fluid flow code. There have also been other THM codes developed that use sequential coupling for subsurface applications such as TOUGHFLAC [20] and IPARS-JAS3D [21]. Recently, Taron et al. [22] have proposed a method to couple TOUGHREACT and FLAC3D codes for modeling THMC processes in deformable, fractured porous media.

We have developed a THM simulator in a single integrated code, FEHM, with the option of solving a THM problem using explicit or implicit coupling. By explicit coupling we mean that the derivatives of the mass and energy balance equations with respect to the displacement variables and the derivatives of the force balance equations with respect to the pressure and temperature do not appear in the Jacobian matrix. The mass and energy balance equations are solved simultaneously and sequentially coupled to the force balance equation. On the other hand, implicit coupling involves solving the mass, energy and force balance equations simultaneously with a full Jacobian. In this work, we use an intermediate iterative approach, where at each Newton–Raphson iteration within each timestep a partial Jacobian is constructed without the derivatives of mass and energy balance equations with respect to displacements. We shall call this approach semi-implicit. The simulator uses a combination of finite element (for mechanical) and finite volume (for thermo-hydro) methods, and is capable of representing complex geometries using unstructured meshes to solve multi-phase flow of water, air and CO₂. FEHM has had a long history of simulating subsurface flow and transport problems. Initial FEHM development for coupled THM processes was started in the 1980s and was directed towards problems concerning enhanced geothermal systems [23]. Later on, thermo-hydro-chemical simulations of radionuclide transport involving multicomponent reactions from proposed geologic repositories were conducted [24]. The simulator has since been applied to a variety of problems including unconventional oil extraction [25], environmental management [26], geothermal energy [27], nuclear waste isolation [28] and methane hydrates [29]. Recently, FEHM has been used to solve multi-phase flow problems concerning CO₂ sequestration [30]. To efficiently explore the effect of coupled processes, it is beneficial to have the flexibility to solve a problem through both explicit and implicit coupling. For cases in which coupling is weak, sequential explicit coupling leads to memory and computational savings. However, strongly coupled processes often require more computationally intensive implicit coupling to obtain accurate results [31]. Furthermore, the ability to solve the coupled THM equations in a single simulator reduces communication and input/output (I/O) times compared to solving mass and energy equations in one code and sequentially coupling to another code for solving force balance equations. Therefore, a single simulator with the option to implicitly or explicitly solve THM while minimizing I/O and memory requirements has been a goal for FEHM development.

The problems under consideration range from the near-wellbore region to the basin scale, involving spatial scales from tens of centimeters to tens of kilometers, and temporal scales from hours to decades. In such cases, large variations in fluid pressure, temperature and stresses are expected. The geomechanics may be fracture-dominated and inhomogeneous with large changes in material properties. Material properties such as permeability and Young's modulus can vary by several orders of magnitude as highly non-linear functions of pressure, temperature, fluid saturations, stresses, and deformations. FEHM also has the capability of solving THM problems with strong non-linearities in material parameters, for instance, permeability as a non-linear function of stress/deformations or Young's modulus as a function of temperature.

For weakly coupled cases, FEHM can solve THM problems using a sequential explicit algorithm. Advantages of this approach are memory and computational savings. However, in general, the solutions obtained from solving explicitly depend on the time step size, with the difference between solutions approaching zero as the time step size approaches zero. In many cases, however, the time step size below which solutions converge within an acceptable tolerance is large enough to allow practical computation times. On the other hand, when the relevant physical processes are tightly coupled, solution convergence can place unacceptable limits on the time step size. In FEHM, for systems in which implicit coupling is required, the user can select, in the order of increasing computational cost, semi-implicit or fully implicit method to obtain accurate solutions. Our fully integrated simulator is optimized to reduce the amount of communication and I/O to provide the flexibility in choosing more or less memory based on the nature of the coupling in the THM based application.

We have developed and implemented in FEHM a methodology suitable for simulating fully coupled THM processes of interest in reservoir engineering applications in geological media. In this paper, we shall focus on examples that demonstrate semi-implicit coupling. We present verification of FEHM by comparing against analytical solutions for a steady state problem with permeability as a function of fluid pressure, and a transient problem with porosity as a function of strain. Simple geometry is chosen in these examples to facilitate analytical treatment. We benchmark a subset of FEHM capabilities using more complicated examples in three dimensions with stress dependent permeability and temperature dependent Young's modulus by comparing against commercially available simulators. Next we present examples that go beyond the capabilities of commercially available simulators. We demonstrate that FEHM results compare well with field data for an enhanced geothermal system (EGS) from Nevada, USA. In this demonstration we show that to get a match with the field data, it is necessary to allow permeability to be a function of shear stress. Finally, we present another THM model with stress-dependent Young's modulus and permeability on a non-orthogonal grid embedding an inclined fault including thermal and gravitational effects.

The outline of this paper is as follows: we describe our general approach in Section 2. In Section 3, we present the governing equations used for our modeling. A brief description of the solution methodology is given in Section 4. The verification studies and two large scale applications of FEHM with THM processes are shown in Sections 5 and 6, respectively. Final remarks are noted in Section 7.

2. Approach

We have built an integrated simulator capable of solving fully coupled nonlinear continuum equations of mass and energy balance, and mechanical deformation in fractured porous media using a Newton–Raphson scheme with a complete Jacobian and efficient linear equation solvers. The simulator FEHM [32] was originally

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