A Simulator for Modeling Coupled Thermo-Hydro-Mechanical Processes in Subsurface Geological Media

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Abstract

We present the description of a fully coupled simulator FEHM for modeling coupled thermo-hydro-mechanical (THM) processes in geomedia. 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-Rapshon 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 are 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 applica-

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tion involving fluid injection into an inclined fault zone using a non-orthogonal grid with stress-dependent Young's modulus and permeability.

Keywords: Coupled processes, Finite element, Finite volume, Mechanical deformation, Subsurface modeling, Thermal-hydro-mechanical

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 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 combina-

tion 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 CO_2 . 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 CO_2 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 nonlinear 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 developed to model non-isothermal fluid flow in Hot Dry Rock geothermal reservoirs [23]. FEHM has been developed extensively under projects on conventional/unconventional energy extraction (geothermal, oil, and gas), radionuclide and contaminant transport, watershed management, and CO₂ sequestration. The capabilities of the simulator include non-isothermal, multiphase, multi-component fluid flow and chemical transport in media with dual porosity, dual permeability on unstructured grids. Here, we do not discuss multiphase and multicomponent fluids. FEHM uses an efficient approach for evaluating thermodynamic functions using lookup tables and polynomial approximations to calculate derivatives. FEHM also uses a novel technique of decoupling the material coefficients from the geometric integrals involving shape functions. This allows us to pre-compute the geometric integrals at the beginning of the simulation, saving significant computational resources during iterative solutions of nonlinear problems.

We have incorporated static mechanical force balance equations using the finite element approach. Materials can display linear or nonlinear, elastic or elastic-plastic behavior, and may have anisotropic properties. Spatially varying material properties are mapped from nodes onto finite elements using shape function interpolations. Coupling between the fluid flow, heat transfer and mechanical force balance equations occurs both through the explicit

occurrence of terms in balance equations, e.g., the effective stress and thermal stress, as well as through the dependence of various coefficients on the state variables. Different strategies are needed for handling these couplings depending on the amount of change in the variables and the level of sensitivity of the material parameters to these variations. For instance, injection of cold fluid at high pressures can induce large pressure and temperature changes in the near-field region, requiring a fully coupled scheme to solve the equations; however, on the intermediate scale, these changes may be smaller and an iteratively coupled solution may be adequate. Additionally, in the far-field, explicit coupling schemes may suffice due to longer temporal scales and lesser degree of variations in p , T , and $\boldsymbol{\sigma}$. The direction of our work has been towards developing a simulator capable of handling all three levels of coupling. The state variables computed by the simulator at each node are p , T and displacement components u_x , u_y , and u_z . We discretize the mass and energy balance equations using the control volume (CV) approach, as this is known to lead to good local mass conservation [33]. The mechanical force balance equations are discretized with the finite element (FE) approach. Mapping between the CV and the FE grids is done such that the variables are defined at the same nodes (see Fig. (1)). The reason for this choice is that FE stresses calculated at the Gauss points are known to be of higher order accuracy than average stresses calculated at the nodes [34]. This is important for the applications considered here as there is a strong coupling between the mass-energy and the force balance equations (for example, the permeability can increase by many order of magnitude upon material failure), and failure criteria such as Mohr-Coulomb, Von Mises or Drucker-Prager [35] depend on the state of stress rather than the displacements. In our experience we found that instabilities in the calculation of the stresses at node points become amplified through permeability coupling leading to unphysical solutions. However, this does result in significant memory and CPU costs. For future work it would be desirable to consider the development of a CV method for calculating nodal stresses that is stable for inhomogeneous material properties.

3. Governing equations

3.1. Balance equations

The balance of mass for a single phase fluid is given as follows (note that boldface symbols in the equations represent vectors/tensors):

$$\frac{\partial}{\partial t}(\rho\phi) + \nabla \cdot \mathbf{q} = Q_m, \quad (1)$$

$$\mathbf{q} = -\frac{k\rho}{\mu} \nabla (p - \rho g z), \quad (2)$$

where ρ is the density of the fluid, k is the permeability, ϕ is the porosity, p is the pressure, μ is the viscosity of the fluid, g is the acceleration due to gravity, z is the height in the vertical direction, $\mathbf{q}$ is the Darcy flux and Q_m is the mass source/sink term. Although not presented here, FEHM has the capability of solving multicomponent, multiphase flow equations.

The balance of energy for the fluid-rock mixture, assuming local thermal equilibrium between fluid and rock, and neglecting the dissipation of mechanical energy due to deformation of the solid, is given by [36]:

$$\frac{\partial}{\partial t}(\rho U \phi + (1 - \phi)\rho_r C_r T) + \nabla \cdot (\mathbf{q} \rho H) - \nabla \cdot (\kappa \nabla T) = Q_e, \quad (3)$$

where U is the specific internal energy of the fluid, H is the specific enthalpy, ρ_r is the density of the rock, T is the temperature of the fluid-rock mixture, C_r is the specific heat of the rock, κ is the thermal conductivity of the rock-fluid mixture and Q_e is the external energy source. For water, FEHM uses polynomial approximations for U , H , ρ , μ as functions of temperature and pressure. These approximations are derived from National Institute of Standards and Technology (NIST) databases and facilitate efficient evaluation of analytical derivatives [44].

The static force balance for the fluid-rock mixture is given by (assuming quasi-steady state):

$$\nabla \cdot \boldsymbol{\sigma} + \rho_r \mathbf{b} = \mathbf{0}, \quad (4)$$

where $\boldsymbol{\sigma}$ is the stress tensor, $\mathbf{b}$ is the body force vector, $\mathbf{0}$ is a vector of zeros.

3.2. Constitutive equations

3.2.1. Stress-strain relationship

Assuming infinitesimal strains, the stress-strain relationship is given by

$$\boldsymbol{\sigma} = \mathcal{D}\boldsymbol{\varepsilon}, \quad (5)$$

where $\mathcal{D}$ is the fourth-order elasticity tensor, and $\boldsymbol{\varepsilon}$ is the second-order strain tensor given by

$$\boldsymbol{\varepsilon} = \frac{1}{2} \left[\nabla \mathbf{u} + (\nabla \mathbf{u})^T \right], \quad (6)$$

with $\mathbf{u}$ being the displacement of the rock, $(\mathbf{A})^T$ being the transpose of any second-order tensor $\mathbf{A}$. In FEHM one can input a more generalized form of $\mathcal{D}$, such as for a transversely isotropic medium; however, for the work presented here we shall assume that the rock is isotropic, i.e., the tensor $\mathcal{D}$ can be expressed in the index notation as follows:

$$\mathcal{D}_{ijkl} = \lambda \delta_{ij} \delta_{kl} + 2G \delta_{ik} \delta_{jl}, \quad (7)$$

where λ , G are the Lamé parameters, δ is the Kronecker delta. Additionally, FEHM can handle spatial variation in $\mathcal{D}$ as well as functional dependence of $\mathcal{D}$ on p , T , and $\boldsymbol{\sigma}$. Equations (7) and (5) with thermal stress and pore pressure effects reduce to [37]:

$$\boldsymbol{\sigma} = \lambda \text{tr}(\boldsymbol{\varepsilon}) \mathbf{I} + 2G \boldsymbol{\varepsilon} - K (\beta \Delta p + \alpha \Delta T) \mathbf{I}, \quad (8)$$

where β is Biot's coefficient, α is the coefficient of linear thermal expansion, $\mathbf{I}$ is the second order identity tensor and $\text{tr}(\)$ is the trace operator, K is the bulk modulus. Note that Eqns. (5) and (8) are written based on the convention that stresses are positive in tension. Plasticity models such as von Mises and Drucker-Prager have been incorporated in FEHM, however, their details are not discussed here.

3.2.2. Permeability-stress/deformation relations

Permeability in fault dominated reservoirs is perhaps the parameter most sensitive to variations in p , T , and $\boldsymbol{\sigma}$ (or $\mathbf{u}$). For example, Evans [10] noted a 15-fold increase in the

injectivity upon hydraulic stimulation at the Soultz EGS reservoir in France. Sensitivity of fracture permeability to normal opening is well recognized [38, 39, 40]. Laboratory tests have shown as much as two orders of magnitude increase in fracture permeability upon shear displacement [41]. We have incorporated in the simulator several models of fracture aperture and stress/deformation behavior combined with permeability relationships. These models are as follows:

Permeability-stress model with a tensile failure criterion: We have incorporated a simplified model of permeability enhancement resulting from tensile opening of flowing fractures. The conceptual model comprises three sets of fractures, in each of the x_1x_2 , x_2x_3 , and x_3x_1 coordinate planes. Let σ_l be the component of stress normal to the x_ix_j plane, where $\sigma_l < 0$ indicates a state of tension. Then the permeabilities k_η ($\eta = i, j$) in the x_η ($\eta = i, j$) directions are calculated according to

$$k_\eta = \begin{cases} k_{\eta 0}, & \sigma_l \geq -T, \\ k_{\eta 0} + \frac{k_{\eta 0}(\gamma_\eta - 1)}{-W} (\sigma_l + T), & -W - T \leq \sigma_l \leq -T, \\ k_{\eta 0}\gamma_\eta, & \sigma_l \leq -W - T, \end{cases} \quad (9)$$

with T, W being positive. In these equations, γ_η are user defined maximum factors by which to multiply the permeabilities, T is the amount which the absolute value of the tensile stress must exceed in order for material failure to occur, and W is the amount of stress in excess of T at which the $k_{i,j}$ become $\gamma_{i,j}k_{i,j}$. As an illustration, consider a situation where the σ_1 component of the stress tensor becomes tensile and less than $-T$. In this case the k_2 and k_3 components of the permeability will be increased along a linear ramp of width W , ending at the values γ_2k_2 and γ_3k_3 . Nonlinear material behavior can also be approximated by reducing the Young's moduli in the coordinate directions by user-specified factors.

Permeability-stress model with a Mohr-Coulomb failure criterion: We have developed a general framework for modeling permeability variation as a function of shear failure. Within this framework, shear failure can occur either along pre-existing user-defined fault planes or along the plane of maximum excess shear τ_{ex} given by

$$\tau_{ex} = |\tau| - S_0 - \Gamma\sigma, \quad (10)$$

where $|\tau|$ is the absolute value of shear stress on a plane, σ is the effective stress normal to that plane, S_0 is the cohesion and Γ is the coefficient of static friction in the plane. Failure occurs when the excess shear is greater than zero. The maximum value of excess shear $\tau_{ex,max}$ is given as [35]

$$\tau_{ex,max} = \frac{1}{2}(\sigma_1 - \sigma_3)(\Gamma^2 + 1)^{1/2} - \frac{1}{2}\Gamma(\sigma_1 + \sigma_3) - S_0, \quad (11)$$

where σ_1 is the maximum principal stress, σ_3 is the minimum principal stress. The maximum excess shear occurs at the angle β with respect to the direction of σ_1 where

$$\tan(2\beta) = -\frac{1}{\Gamma}. \quad (12)$$

Consider a coordinate system ζ, η, θ such that ζ and η lie in the plane determined by β , and θ is orthogonal to this plane. The components of permeability k_i in the ζ, η , and θ directions are modified by user-specified multipliers given as

$$k_i = \begin{cases} k_{i0}, & \tau_{ex} \leq 0, \\ k_{i0} + \frac{k_{\eta 0}(\gamma_i - 1)}{\tau_{ex, \gamma}} \tau_{ex}, & 0 \leq \tau_{ex} \leq \tau_{ex, \gamma}, \\ k_{i0} \gamma_i, & \tau_{ex} \geq \tau_{ex, \gamma}. \end{cases} \quad (13)$$

where k_{i0} is the initial permeability, γ_i is a user defined multiplier, and $\tau_{ex, \gamma}$ is the user defined value of excess shear at which the initial permeability is multiplied by γ . Equation (13) describes a ramp starting at k_{i0} when $\tau_{ex} = 0$ and ending at $\gamma_i k_{i0}$ when $\tau_{ex} \geq \tau_{ex, \gamma}$. The modified permeability tensor is then rotated back to the grid co-ordinates x, y, z . In the current version of FEHM, while the permeabilities are allowed to be different in x, y, z directions, full tensor permeability is not handled. It is possible to develop various schemes to approximate the full tensor, although, currently we retain only the diagonal components.

Gangi model: A bed of nails model [39] that evaluates permeability and fracture stiffness as a function of the effective normal stress across a rough fracture

$$k(p) = k_0 \left[1 - \left(\frac{p}{p_l} \right)^m \right]^3, \quad (14)$$

where p is normal confining pressure, $k(p)$ is the permeability at the confining pressure p , k_0 is the permeability at zero pressure, p_l is the effective modulus of asperities, and m is a parameter such that $0 < m < 1$.

Fracture sets model as proposed by Bai et al., [42] and Elsworth and Xiang [43] based on orthogonal sets of parallel fractures subjected to normal and shear stresses are also included in FEHM.

4. Solution methodology

FEHM adopts a finite volume (FV) formulation of the coupled equations for flow and energy transport because FV formulation is known to preserve local mass balance [33], and a finite element (FE) formulation for the mechanical force balance equations.

4.1. Mass and thermal energy balance equations

Temporal discretization is performed in FEHM using the Backward Euler method. The following numerical analogue of the mass balance equation (1) is solved:

$$V_i \frac{(\rho\phi)_i^{n+1} - (\rho\phi)_i^n}{\Delta t} - \sum_{\text{neighbor cells}} \left\{ k_{har} \left(\frac{\rho}{\mu} \right)_{ij} \left(\frac{A_{ij}}{\Delta d_{ij}} \right) [(p_j - p_i) - (\rho g)_{ij}(z_j - z_i)] \right\}^{n+1} = Q_m^{n+1}, \quad (15)$$

where n refers to the time-step index. The summation refers to neighboring nodes, j , connected to node i . Here $\left(\frac{\rho}{\mu} \right)_{ij}$ represents an inter nodal average of $\frac{\rho}{\mu}$ between node i and j . The term k_{har} refers to harmonic weighting of the intrinsic permeability of nodes i and j . The term V_i is the volume of the control volume surrounding node i . The area factor $(A_{ij}/\Delta d_{ij})$ refers to the internodal area divided by distance between nodes i and j . In FEHM, harmonic, arithmetic, and (flow) upwinded internodal evaluations are available for averaging of the $(.)_{ij}$ term.

Similarly the numerical analogue of the energy balance equation (3) is

$$V_i \frac{(\rho U \phi + (1 - \phi) \rho_r C_r T)_i^{n+1} - (\rho U \phi + (1 - \phi) \rho_r C_r T)_i^n}{\Delta t} + I_2 + I_3 = Q_e^{n+1}, \quad (16)$$

267 where

$$I_2 = \sum_{\text{neighbor cells}} \left\{ k_{har} \left(\frac{\rho^2 H}{\mu} \right)_{ij} \left(\frac{A_{ij}}{\Delta d_{ij}} \right) [(p_j - p_i) - (\rho g)_{ij}(z_j - z_i)] \right\}^{n+1}, \quad (17)$$

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$$I_3 = \sum_{\text{neighbor cells}} \left\{ \kappa_{har} \left(\frac{A_{ij}}{\Delta d_{ij}} \right) (T_j - T_i) \right\}^{n+1}, \quad (18)$$

269 where the term κ_{har} represents the harmonic weighting of the thermal conductivity of rock
270 in nodes i and j .

271 4.2. Mechanical force balance equations

272 For the mechanical force balance, there is an option of using either a control volume based
273 formulation or a finite element formulation. In traditional quadrature-based finite element
274 methods, the global stiffness matrix is assembled during every iteration by performing a sum-
275 mation of the integral over the quadrature points in the element. The discretized mechanical
276 force balance equation takes the form (for the x_l direction is shown, similar equations can
277 be written for the other directions)

$$\begin{aligned} & \sum_i \left\{ \int \left[\frac{\partial N_j}{\partial x_l} (\lambda + 2\mu) \frac{\partial N_i}{\partial x_l} + \frac{\partial N_j}{\partial x_m} \mu \frac{\partial N_i}{\partial x_m} + \frac{\partial N_j}{\partial x_n} \mu \frac{\partial N_i}{\partial x_n} \right] dv \right\} U_{li} + \\ & \sum_i \left\{ \int \left[\frac{\partial N_j}{\partial x_l} \lambda \frac{\partial N_j}{\partial x_m} + \frac{\partial N_j}{\partial x_m} \mu \frac{\partial N_i}{\partial x_l} \right] dv \right\} U_{mi} + \\ & \sum_i \left\{ \int \left[\frac{\partial N_j}{\partial x_l} \lambda \frac{\partial N_j}{\partial x_n} + \frac{\partial N_j}{\partial x_n} \mu \frac{\partial N_j}{\partial x_l} \right] dv \right\} U_{ni} - \\ & \sum_i \left\{ \int \left[N_j \frac{\partial N_i}{\partial x_l} K \beta \right] dv \right\} \Delta p_i - \sum_i \left\{ \int \left[N_j \frac{\partial N_i}{\partial x_l} K \alpha \right] dv \right\} \Delta T_i + \sum_i \left\{ \int \mathbf{b} N_i dv \right\} = 0, \end{aligned} \quad (19)$$

278 where $\mathbf{b}$ is the body force vector as given in Eq. (4), N_i are the finite shape functions, x_l , x_m ,
279 x_n are the coordinates, U_l , U_m , U_n are the nodal displacements in the coordinate directions,
280 with the integration performed over the volume of an element while the summation is over
281 the nodes.

282 The algorithm is simplified considerably in FEHM where the elasticity tensor is factored
283 out, and the integrals over the shape functions are pre-computed to save a significant amount

of computation. This increase in computational speed is obtained at the cost of increased memory usage for saving the integrals at every node. However, in most finite element meshes, a large number of nodes have very similar nodal connectivity patterns and savings in memory can be achieved by saving the integrals only once for each class of elements with a similar connectivity structure.

4.3. Coupling of the THM equations

The coupling between the fluid flow-heat transfer equations and the deformation equation occurs through: 1) explicit occurrence of the pressure and temperature terms in the force balance equation (Eq. (4)), 2) through the dependence of material coefficients in the force balance equation (i.e., Young's modulus) on pore pressure and temperature, 3) dependence of the porosity and permeability on rock deformation, as well as on pore pressure. Permeability of rocks is known to change dramatically upon rock failure. The criteria used for computing rock failure (e.g., Mohr-Coulomb criteria) depend on the state of the local stress, rather than the displacements or the strains. Hence it is necessary to calculate nodal stresses for estimating permeabilities in coupled THM formulation. In finite element formulation the computed stresses are element based, defined by integration over the element volume of derivatives of element shape functions. Gradients calculated by the FEM can be discontinuous across element boundaries; hence stresses can change discontinuously from element to element. Since a given node may belong to multiple elements, multiple stress values are possible at the node. Gauss point stresses within each element are interpolated to nodes using shape functions and volume-weighted average over all the elements connected to a given node is used. This is the approach used in the present work. This average stress is then used for estimating permeabilities (and porosities) in the coupled formulation. When stress changes are large (for e.g., due to plasticity), this approach can lead to instabilities. To circumvent this, we have formulated a novel approach for mapping element properties on control volumes used in the flow and energy balance equations which will be presented in a subsequent paper.

4.4. Assembly and solution of the equations

The simultaneous set of mass, energy and mechanical balance equations are solved iteratively to compute pressure, temperature and deformations at each node at each time step. FEHM employs a Newton-Raphson iteration with analytically computed Jacobians to solve the nonlinear equations. Within each Newton-Raphson iteration, there is an option to perform an algebraic reduction in the effective degrees of freedom per node to “precondition” the linear system solution and improve efficiency. FEHM employs iterative solvers such as GMRES and BiCGSTAB [45] for linear system solution.

5. Verification

Many functionalities of the simulator have been verified against commercially available simulators [25, 46]. A comparison between FEHM and a commercially available simulator has been reported by Kelkar et al., [25] to test results for permeability as a function of the average effective stress including coupling between pore pressure and stress using poroelasticity theory. We present here two examples comparing FEHM with analytical results. The first one shows comparison against steady state solution in a one-dimensional domain where permeability is a function of pore pressure. The second verification is for transient compaction problem including porosity changes with deformation. Then we present an example with Young’s modulus as a function of temperature comparing thermal stresses modeled by FEHM against those from the commercial code Abaqus.

5.1. Permeability as a function of pressure

We compare FEHM capabilities against an analytical solution for the case of a one-dimensional domain where permeability is a function of pore pressure. To make the problem analytically tractable, we consider the Richard’s equation under saturated, steady-state condition, for a horizontal one-dimensional domain and without a mass source:

$$\frac{\partial}{\partial x} \left(k \frac{\partial p}{\partial x} \right) = 0 \Rightarrow k \frac{\partial p}{\partial x} = c, \quad (20)$$

where c is a constant.

Now, assuming that a constant uniaxial horizontal stress σ_0 is applied with no body forces, we shall couple the stress and the flow equation by choosing a form for the permeability k as follows:

$$k = A(\sigma_0 - \beta p), \quad (21)$$

where A is a constant. Using (21) in (20), we get

$$A\sigma_0 p - A\beta \frac{p^2}{2} = qx + C_1, \quad (22)$$

where C_1 is a constant. Assuming the boundary conditions that $p = p_1$ at $x = 0$ and $p = p_2$ at $x = 10$, we arrive at the following quadratic equation for pressure

$$p^2 - \frac{2\sigma_0}{\beta}p + \frac{2\sigma_0}{\beta} \left[(p_2 - p_1) \frac{x}{10} + p_1 \right] - \left[(p_2^2 - p_1^2) \frac{x}{10} + p_1^2 \right] = 0. \quad (23)$$

For comparison with FEHM solution, the following values were chosen: $p_1 = 10$ MPa, $p_2 = 11$ MPa, $\sigma_0 = -10$ MPa, permeability = 10^{-15} m², $\rho_r = 2000$ kg/m³, $C_1 = 1000$. The numerical grid consists of 21 equally spaced nodes. A good match between FEHM and the analytical solution was found as seen in Fig. (2).

5.2. Transient coupled pore pressure and deformation test

In this example, we consider a transient compaction problem with porosity as a function of strain. Consider a 100 m long, fully saturated, one-dimensional horizontal column in the x direction. The right hand side is held fixed in the x direction, while a compressive load of 1 MPa rightward is applied instantaneously at the left side. No fluid flow is allowed out the right side, and the pressure is held constant on the left side. The load on the left results in compression of the column, lowering of the void space available to the fluid, and expulsion of fluid at the left boundary. The analytical solution for the fluid pore pressure p during this process is given by

$$p(x, t) = p_0 \left[\frac{4b}{\pi} \sum_{n=0}^{\infty} \frac{e^{-\left[\frac{\pi(2n+1)}{2}\right]^2 ct}}{(2n+1)} \sin \left[\frac{(2n+1)\pi x}{2L} \right] + 1 \right], \quad (24)$$

355 where

$$a \equiv \rho_0 \phi \beta_w E + \rho \alpha, \quad (25)$$

356

$$b \equiv \frac{\rho \alpha \sigma_l}{p_0 a}, \quad (26)$$

357 and

$$c \equiv \frac{\rho k E}{\mu a L^2}. \quad (27)$$

358 In the above equations x is the distance from the left boundary, t is time, α is a constant
 359 rate of change of porosity with respect to strain, σ_l is the load magnitude, p_0 is the initial
 360 column pressure, ϕ is the porosity, β_w is the compressibility of water, E is Young's modulus,
 361 and L is the length of the column. The derivation for the (24) is given as follows:

362 There are two governing equations and three material relationships describing the be-
 363 havior of the system described in section (5.2). First, for a one-dimensional fluid saturated
 364 porous medium, mass conservation of the fluid phase is given as

$$\frac{\partial(\phi \rho)}{\partial t} - \frac{\partial}{\partial x} \left(\frac{k \rho}{\mu} \frac{\partial p}{\partial x} \right) = 0, \quad (28)$$

365 where ϕ is the porosity, ρ is the fluid density, k is the permeability, μ is the fluid dynamic
 366 viscosity, and p is the pressure. In the following, we consider pressure as the independent
 367 variable; we take k and μ as constants. Second, the force balance is given by

$$\frac{\partial \sigma}{\partial x} = 0. \quad (29)$$

368 In addition to the governing equations, there are three material relations. The first material
 369 relationship gives the porosity as a function of strain

$$\phi = \phi_0 + \alpha \epsilon, \quad (30)$$

370 where ϕ_0 is the uniform initial column porosity and α is a constant. Second, the equation
 371 of state for density is

$$\rho = \rho_0 [1 + \beta_w (p - p_0)], \quad (31)$$

where β_w is the compressibility of water and ρ_0 is the uniform initial fluid density. Third, the constitutive law relating stress and strain is

$$p - \sigma = E\epsilon, \quad (32)$$

where E is Young's modulus and $\sigma > 0$ corresponds to a state of compression. Equation (29) implies that the stress could depend at most on time. Therefore, the total stress at all points in the column is at all times equal to that at the left boundary. For a step loading of magnitude σ_l on the left side of the column at time zero, we therefore have

$$\sigma = \sigma_l \theta(t) + p_0, \quad (33)$$

where θ is the Heaviside step function. Putting (30) and (31) into (28) leads to

$$\frac{\partial p}{\partial t} - \frac{k\rho E}{\mu a} \frac{\partial^2 p}{\partial x^2} - \frac{k\rho_0\beta_w E}{\mu a} \left(\frac{\partial p}{\partial x} \right)^2 = \frac{\rho\alpha}{a} \frac{\partial \sigma}{\partial t}, \quad (34)$$

where a is given in Eq. (25). This equation is to be solved with the boundary conditions

$$p(0, t) = p_0, \quad (35)$$

$$\frac{\partial p}{\partial x}(L, t) = 0,$$

and the initial condition

$$p(x, 0) = p_0. \quad (36)$$

We now nondimensionalize the problem via the transformations

$$\chi \equiv \frac{x}{L},$$

$$\tau \equiv \frac{k\rho Et}{\mu L^2 a} \equiv ct, \quad (37)$$

$$\mathcal{P} \equiv \frac{p - p_0}{p_0}.$$

Equation (34) then becomes

$$\frac{\partial \mathcal{P}}{\partial \tau} - \frac{\partial^2 \mathcal{P}}{\partial \chi^2} - \frac{p_0 \rho_0 \beta_w}{\rho} \left(\frac{\partial \mathcal{P}}{\partial \chi} \right)^2 = \frac{\rho \alpha \sigma_l \delta(\tau)}{p_0 a}, \quad (38)$$

where $\delta(\tau)$ is the Dirac delta function. For the values given in Table (1), the coefficient of $\delta(\tau)$ is on order unity, while that of the quadratic term on the left hand side is on order $10^{-4} \ll 1$. Therefore, the balance described by the equation is dominated by terms other than the quadratic and the latter may be neglected. The problem to be solved becomes

$$\frac{\partial \mathcal{P}}{\partial \tau} - \frac{\partial^2 \mathcal{P}}{\partial \chi^2} = b\delta(\tau), \quad (39)$$

where b is given in Eq. (26).

The boundary conditions become

$$\mathcal{P}(0, \tau) = 0, \quad (40)$$

$$\frac{\partial \mathcal{P}}{\partial \chi}(1, \tau) = 0, \quad (41)$$

and the initial condition is now

$$\mathcal{P}(\chi, 0) = 0. \quad (42)$$

Although the densities appearing in the definitions of τ , b , and a are not constant, we shall solve the problem assuming an average value $\rho \approx \rho_0$. This assumption is justified because it results in very small differences between τ, b , and a relative to each other and relative to unity.

For a solution, we start by expanding the inhomogeneous term in a weighted sum of normalized eigenfunctions of the operator $-\partial^2/\partial\chi^2$ with eigenvalues λ_n :

$$\phi_n(\chi) = \sqrt{2} \sin(\sqrt{\lambda_n}\chi), \quad (43)$$

396

$$\lambda_n = \left[\frac{\pi(2n+1)}{2} \right]^2, \quad (44)$$

397

$$b\delta(\tau) = b\delta(\tau) \sum_{n=0}^{\infty} \sqrt{\frac{2}{\lambda_n}} \phi_n(\chi), \quad (45)$$

where the ϕ_n and λ_n have been chosen such that the ϕ_n satisfy (40). Note that the sum on the right hand side of (45) is approximately equal to unity for $0 \leq \chi \leq 1$. We now assume

400 that $\mathcal{P}$ takes the separated form

$$\mathcal{P} = \sum_{n=0}^{\infty} \mathcal{P}_n(\tau) \phi_n(\chi), \quad (46)$$

401 and substitute (46) and (45) into (39). This substitution yields a differential equation in the
402 $\mathcal{P}_n$, which has the solution

$$\mathcal{P}_n(\tau) = \left(c_n + b \sqrt{\frac{2}{\lambda_n}} \right) e^{-\lambda_n \tau}, \quad (47)$$

403 for $\tau > 0$ and where the c_n are constants to be determined from the initial conditions.
404 Equation (42) implies that $c_n = 0$ for all n . Therefore, the solution takes the form

$$\mathcal{P}(\chi, \tau) = b \sqrt{2} \sum_{n=0}^{\infty} \frac{e^{-\lambda_n \tau}}{\sqrt{\lambda_n}} \phi_n(\chi). \quad (48)$$

405 Returning to dimensional quantities and using the definitions of the eigenfunctions and
406 eigenvalues leads to Eq. (24).

407 Table (1) gives the values of the parameters used for this comparison. For convenience,
408 a constant value for μ has been chosen in this verification test. In general, FEHM uses
409 polynomial relations for viscosity as a function of temperature and pressure that are fit to
410 NIST database [44]. Figure (3) shows the pore pressures given by equation (24) in blue and
411 those from the corresponding FEHM simulation in red. 101 equally spaced nodes were used
412 for the FEHM results. An excellent agreement is noted for the time evolution of pressure
413 profile.

414 Using this example, convergence of the simulator is studied and Fig. (4) shows the log of
415 the error (based on L2 norm) as a function of negative log of the grid spacing. It is seen that
416 as the grid spacing decreases, the error also decreases. In addition, numerical stability of the
417 simulator is studied in Fig. (5). Pressure as a function of time for the node farthest from
418 the outflow boundary is shown for time-step sizes ranging from 10^{-6} day to 1 day. Excellent
419 stability is noted and as expected inaccuracy increases as the time-step size increases.

420 5.3. Young's modulus as a function of temperature

421 We compare the FEHM capability for temperature dependent Young's modulus compar-
422 ing thermal stresses modeled by FEHM against those from the commercial code Abaqus [47].

A problem was solved to compare FEHM thermal stress calculations with Young's modulus as a function of temperature with those from Abaqus in which a three-dimensional grid was chosen with 16302 nodes, 10 m in the x direction, and 100 m in the y direction and 51 m in the z direction. The grid spacing was uniform 1 m everywhere in the x direction. The grid spacing away from the heater was 2 m in the y and z directions, while being refined to 0.1 m in y and z near the heater. The parameters used for this problem are shown in Table (2) and the domain used is shown in Fig. (6).

Heat was applied at the $y = 0$ face over a strip 1 m wide in the z direction. All other model boundaries had zero heat flux across them. The face of the model at $y = 50$ was pinned with zero displacement in all directions, and the sides were placed on rollers, with zero x -displacement at $x = 0$ and $x = 10$ m faces, and zero y -displacement at $y = 0$ and $y = 50$ m faces. Young's modulus decreased by nearly an order of magnitude from cold to hot end of the problem domain. Figures (7), (8)(A) show the comparison of the stresses and temperature as a function of distance from the heater after 90 days of heating obtained from Abaqus and FEHM, and a good match can be seen. It is interesting to note a peak in the stress curves near the heated end due to the competing effects of increasing temperature rise and decreasing Young's modulus. The relation between Young's modulus and temperature used is shown in Fig. (8)(B).

6. Applications

In this section, we show a good match of FEHM results with field data from Desert Peak geothermal area in Nevada, USA demonstrating FEHM capabilities to model non-linear permeability-stress relationship with shear failure including thermal stress. This is followed by a demonstration example involving a large-scale three-dimensional domain with an inclined fault using a non-orthogonal grid. In this problem, we model non-isothermal fluid injection incorporating gravitational effects and stress-dependent Young's modulus and permeability.

6.1. Geothermal problem

This example shows a validation of FEHM results with field data from Desert Peak geothermal area in Nevada, USA demonstrating FEHM capabilities to model non-linear permeability-stress relationship with shear failure including thermal stress. Field data are available in published literature [48] for a shear stimulation treatment conducted by injecting cooler water into hot formation at the Desert Peak geothermal field in Nevada, USA. The geological setting has been described by Faulds et al., [49], fracture characteristics and state of stress has been studied by Hickman and Davatzes [50]. This was modeled using a domain of $2 \text{ km} \times 2 \text{ km}$ in the horizontal directions and 1 km in the vertical direction (Fig. (9)). The z axis was aligned with the maximum principal stress, which was taken to be vertical. The x axis was taken to be horizontal and aligned with the least principal stress. There were a total of 79,365 computational nodes. Injection was at a point at the center of the x and z dimensions, and $\frac{1}{4}$ of the way from the boundary along the y axis (coordinates of the injector are (0,-500,500) m). The grid spacing was decreased near the injection point to improve model resolution.

The example discussed here assumes isotropic values for the permeability multipliers, although the FEHM model is capable of handling more general cases. The parameters used for this model are shown in Table (3). Fluid flow boundary conditions were chosen to be such that pressure was held at the constant initial value on the exterior faces of the model volume, and a constant specified pressure of 13.1 MPa was applied at the injection point. Temperature of injected fluid (170°C) was lower than the initial formation temperature (190°C). The heat flow boundary conditions were taken to be no flow of heat at the external boundaries of the model volume. The mechanical boundary conditions were chosen as follows: The axis were chosen so that the z axis was pointed vertically upwards and the x and y axis were oriented in a horizontal plane. The bottom, left and back faces of the model were placed on rollers. On the top face of the model a vertically downward normal stress of 22.6 MPa was applied to simulate the overburden. On the right face of the model a compressive normal stress of 13.8 MPa, and that on the front of the model of 18.1 MPa were applied to simulate the

477 minimum and median principal horizontal stresses respectively.

478 The rationale for the choice of boundary conditions and parameter values are discussed
479 in [51]. The permeability-stress model with shear failure given in Eqns. (10)–(13) was used
480 and a permeability multiplier (i.e., the increase in permeability realized upon shearing) of 60
481 was found to match the data quite well, as seen in Fig. (10). As the injection proceeded, the
482 rock cooled over time and the normal stresses decreased. This combined with reduction in
483 normal effective stress due to pore pressure led to Mohr-Coulomb criteria (Eq. (10)) being
484 satisfied after about 5 days of injection. The permeability then starts increasing leading
485 to an increase in injection rates. The value of the multiplier is higher than that measured
486 by Lutz et al., [52] but falls below the enhancement in fracture permeability upon shearing
487 measured by Lee and Cho [41].

488 6.2. Inclined fault simulations

489 This example involves a large-scale three-dimensional domain with an inclined fault using
490 a non-orthogonal grid. We model non-isothermal fluid injection incorporating gravitational
491 effects and stress-dependent Young’s modulus and permeability. Fluid is injected into a 1000
492 m high slab of rock in which is embedded a 30 m wide fault inclined at $\sim 19^\circ$ relative to
493 the vertical. The slab is composed of three horizontal layers, each having different elastic
494 moduli, with an across-fault offset of 100 m (Fig. (11)). The permeability is equal to 10^{-15}
495 m^2 everywhere except in the fault zone, where it is 10^{-14} m^2 . Both permeabilities and elastic
496 moduli are isotropic. In this simulation, fluid is injected at a rate of 10^{-3} kg/s at a location
497 inside the fault ($x = 5 \text{ m}$, $y = 500 \text{ m}$, $z = 500 \text{ m}$) while a constant pressure of 9 MPa is
498 maintained at another location inside the fault ($x = 5 \text{ m}$, $y = -500 \text{ m}$, $z = 500 \text{ m}$). The
499 injected fluid has a temperature of 40°C while that of the in situ fluid is 150°C . The boundary
500 conditions are as follows: The axes are chosen so that the z axis points vertically upwards
501 and the x and y axis are oriented in a horizontal plane. The external boundaries of the model
502 domain have no flow boundary conditions for the flow and heat transfer equations. For the
503 mechanical boundary conditions, the bottom of the model is placed on rollers, and a normal
504 compressive stress of 33 MPa oriented vertically downwards is applied on the top of the

model. A normal compressive stress of 25 MPa in the horizontal directions is applied on the remaining four vertical faces of the model. The Mohr-Coulomb failure criterion is employed in the entire solution domain, with permeabilities increasing by a factor of 10 and Young's moduli decreasing by a factor of 5 under conditions of maximum failure. The right side of Fig. (13) shows results after 10 years of simulation time in a plane perpendicular to the fault and containing the injection point. For comparison, the left side of Fig. (13) shows results from a similar simulation with no coupling between deformation and fluid flow. In addition to enhanced permeability and mechanical weakening in the fault zone, flow and stress coupling leads to laterally heterogeneous deepening of surface topography outside the fault zone. In practice, such a change in topography may be detectable via, e.g., satellite altimetry. Note that due to the combined effect of gravity and stress-dependent permeability the fluid has a tendency to migrate downwards, as indicated by the temperature and permeability contours in Fig. (13).

7. Conclusion

In this paper, we have described the coupled THM modeling capabilities of the subsurface flow and transport simulator FEHM developed at Los Alamos National Laboratory. These capabilities have been developed to address problems in subsurface flow and transport associated with emerging areas such as enhanced geothermal systems, CO₂ sequestration, unconventional oil and gas recovery. Several analytical solutions have been developed and used to benchmark different aspects of the THM coupling. We have presented comparisons of a subset of FEHM capabilities with other commercially available simulators. We have also demonstrated a good fit of simulator results based on a permeability-stress model to field data from Desert Peak, Nevada. All the examples presented here involve loose coupling among the THM processes using the semi-implicit coupling approach. On the other hand, there are many cases of interest where solving the balance equations implicitly is likely necessary. For example, if permeability and Young's modulus contrasts in the inclined fault example were higher, then thermal effects would be convected farther before each update of the system stress state, and the converged time step size would decrease relative to the

case of lower permeability; if for such a system finer grid resolution is desired, computational times could become impractical. Such possibilities provide strong motivation for the idea of having a single simulator, as opposed to a number of inter-communicating codes, with the capability to solve the THM governing equations fully implicitly, especially for problems involving a large number of grid cells. In a forthcoming paper, we shall show results based on fully implicit coupling and we shall also perform a comparison between explicit, semi-implicit and fully implicit coupling.

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Table 1: Parameters used in the transient deformation test.

parameter	value	parameter	value
β_w	$4.4 \times 10^{-10} \text{ Pa}^{-1}$	E	10^{10} Pa
ρ	990 kg/m^3	k	10^{-13} m^2
μ	$0.66 \times 10^{-3} \text{ Pa}\cdot\text{s}$	ϕ_0	0.1
α	0.1	σ_l	10^6 Pa
β	1.0	p_0	10^5 Pa

Table 2: Parameter values for comparing thermal stresses between Abaqus and FEHM.

parameter	value
Poissons ratio	0.25
Thermal Expansion (linear)	$1.8 \times 10^{-5} / ^\circ\text{C}$
Rock thermal conductivity	1 W/m/ $^\circ\text{C}$
Rock density	2200 (kg/m ³)
Rock specific heat	1256.04 (J/kg/K)
Rock porosity	0

Table 3: Parameters used in the Desert Peak geothermal problem (see Fig. (9)).

parameter	value
Formation temperature	190 °C
Initial pore pressure	9 MPa
Bottom hole injection pressure	13.1 MPa
Injection temperature	170 °C
Principal in situ stress Maximum	22.6 MPa (vertical)
Principal in situ stress Intermediate	18.1 MPa
Principal in situ stress Minimum	13.8 MPa
Thermal conductivity	3 W/m/K
Heat capacity	820 J/kg/K
Porosity	10%
Initial permeability $\times$ thickness	9 md.m
Friction Coefficient	0.8
Cohesion	2 MPa
Permeability multiplier (all directions)	60
Young's modulus	30 GPa
Poisson' ratio	0.15
Coefficient of Thermal Expansion	10-4 /°C
Biot poroelastic parameter	0.5

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Figure 1: Schematic illustrating the mapping between the finite volume and finite element grids. Dots show the nodes, thick solid black lines show nodal connections and gray region shows the control volume.

Figure 2: Comparison of analytical and FEHM solutions for 1D steady problem.

Figure 3: Comparison between FEHM (red dots) and analytic solution (blue curves) for a one-dimensional transient loading problem. The top curve is the pore pressure at ≈ 1 s and the bottom curve is that at ≈ 6600 s of simulation time. The horizontal axis shows the distance from the outflow boundary.

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(a) σ_{yy} vs distance

(b) σ_{zz} vs distance

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(a) T vs distance

(b) Young's modulus vs T

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Figure 13: Temperature, permeability, and vertical displacements after 10 years of simulation time in a plane perpendicular to the fault and containing the injection point. The left figures show simulation results without coupling between fluid flow and deformation, while the right figures show result with coupling.