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Advancements in High-Performance Multi-physics Simulation Capabilities for the Geologic Disposal Safety Assessment Framework

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INTRODUCTION

Performance assessment for geologic radioactive waste repositories can include coupled simulation of highly nonlinear physical phenomena including heterogeneous multiphase fluid flow, thermal propagation, radionuclide transport (e.g., advection, dispersion, sorption, decay, ingrowth), and sophisticated models for waste package degradation. Furthermore, PA simulations typically account for a vast range of length scales from the sub-meter scale (single waste package) in the near-field of a repository to the multi-kilometer far-field. As part of the Geologic Disposal Safety Assessment (GDSA) program, simulation capabilities are being developed in the high-performance subsurface flow and transport simulator PFLOTRAN specifically for modeling these physical phenomena. This work presents a summary of recent code development efforts and a look at the future direction of the software framework.

This year marked the release of PFLOTRAN Version 4.0, which included a series of performance improvements to more efficiently solve increasingly complex nonlinear systems of equations, such as capillary pressure/relative permeability smoothing and new nonlinear solution search methods (see [1] and [2]). A new Material Transform process model has been added to the code which allows the user to flexibly apply new material augmentations from a menu of options such as illitization. These models can be used to alter material properties (e.g., porosity, permeability, k_d) as a function of PFLOTRAN state variables. PFLOTRAN's dual porosity model for matrix/fracture flow has been upgraded to allow the user to employ the UFD Decay process model to simulate radionuclide sorption, partitioning, decay, and ingrowth in the rock matrix (secondary continuum). Verification of this capability is being undertaken as part of the DECOVALEX international collaboration. Furthermore, the code has been modified to include more robust modeling of salt host rock formations with updated equations of state and a preliminary update to PFLOTRAN's GENERAL mode to add a mass balance for a soluble rock matrix (see [3]). Developments in progress include the GDSA QA testing framework, advanced algorithms for interpreting constitutive relationships like capillary pressure functions from datasets, and code performance enhancements. More details on the developments described here can be found in Nole et al. (2022) [4]. PFLOTRAN users are directed to doc-dev.pflotran.org for the latest documentation of available software capabilities.

MATERIAL TRANSFORM MODULE

The material transform module was added to PFLOTRAN in order to provide a flexible and modular means by which to model transient material properties in a simulation domain as a function of available state variables. The module was designed as its own process model in the code, meaning it can make use of its own time-stepper if iterations are required to solve a given material transformation. The process model is sequentially coupled to other process models in PFLOTRAN as a "child" of the flow process model and a "peer" of the transport model. In PFLOTRAN, "peer" process models proceed independently and "children" sync with their "parent" at the timestep size of the parent.

For example, the material transform module currently supports a reduced order model for high-temperature smectite illitization. In this model, the user can choose from two options (Huang et al. [1993] [5] or Cuadros and Linares [1996] [6]) whereby when given an initial concentration of smectite among other tuning parameters, the rate of change of smectite to illite is computed as a function of temperature. The amount of smectite in a given material is tracked over time to ultimately achieve an irreversible illitization process (Figure 1).

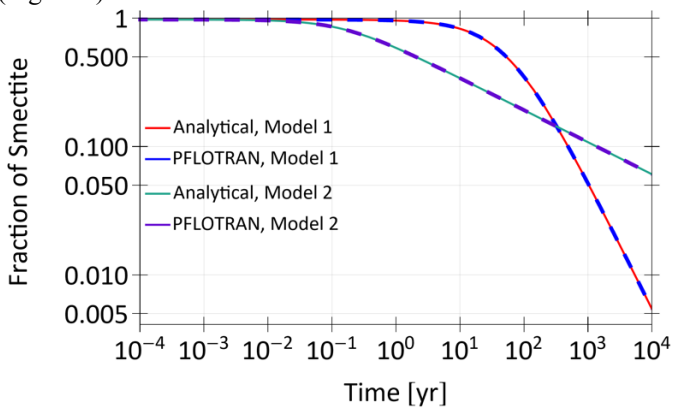

Figure 1. Smectite fraction vs time for a given temperature history, using 1) the Huang et al. (1993) illitization model Cuardos and Linares (1996) illitization model.

The consequence of smectite illitization is a reduced sorption coefficient (k_d) and an increase in material permeability, which can potentially affect fluid flow and transport of radionuclides in the subsurface away from a geologic radioactive waste repository. Due to the nature of

the material transform process model being a "child" of the flow process model, the flow process model will receive updated k_d and permeability values at each flow time step.

This type of model is particularly useful for applications such as argillite-hosted repository systems where a bentonite backfill material can undergo smectite illitization if the temperature and chemical conditions are favorable. Slated for future development is a material transformation that considers buffer erosion near high-velocity flow paths in fractured geologic media, a process which is considered in some international safety cases involving radioactive waste disposal in crystalline host rocks.

FULLY COUPLED SOLUTE TRANSPORT

In typical freshwater aquifers, aqueous chemical species are typically light enough and found in low enough concentrations as to not significantly affect the flow properties of the water solvent, like density and viscosity. This concept forms the basis of a justification for sequentially coupling fluid flow and reactive transport in PFLOTRAN. If the transport primary solution variables do not significantly affect the flow primary solution variables, then solving both the flow and transport solutions can oftentimes be more effectively achieved through sequential coupling.

One exception to this is the case of a brine pore water system. If the pore water contains salt (as exemplified by pore water contained in a salt host rock where the rock itself can dissolve into the water), salt typically dissolves in high enough concentrations to meaningfully affect the density, viscosity, and saturation pressure of the pore water. Considering this feedback between the solute and the liquid flow properties is therefore very important. Until now, modeling salinity effects on flow properties required modeling salinity as part of the transport equations and then handing off updated salinity to the flow solution at sync points under the standard sequential flow and transport coupling scheme. Since these two systems are much more tightly coupled when salt is a solute, sequential coupling in this manner requires taking very small time steps in order to avoid numerical artifacts.

A solute mass balance has been developed in PFLOTRAN's GENERAL mode which solves conservation of solute mass in the same fully implicit system of equations for solving water mass, air mass, and energy conservation. This formulation is flexible to consider salt transport in soluble (salt) and insoluble porous media. Thus far, performance of the fully implicit model has been compared to the sequentially coupled model on the Elder problem [7], a well-studied density-driven flow problem (Figure 2).

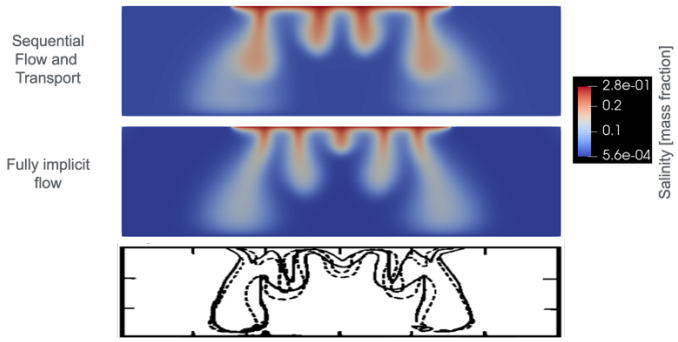

Figure 2. Comparison of salinity distribution between sequentially and fully coupled flow and salt transport after 4 years of the Elder problem.

The fully implicit formulation generally shows much better agreement with published solutions of the Elder problem than the sequentially-coupled formulation, and it is also able to take larger time steps than the sequentially coupled formulation without generating numerical artifacts, making this formulation much more desirable for simulations run to long times.

MULTICONTINUUM RADIONUCLIDE DECAY

PFLOTRAN's multiple continuum (MULTICONTINUUM) transport mode solves for reactive transport using a dual continuum disconnected matrix model (DCDM), where a fractured porous medium can be represented as two interacting continua representing the fracture network (the primary continuum) and the rock matrix (the secondary continuum). These two continua are connected by a mass transfer coupling term. The formulation in PFLOTRAN is similar to a dual porosity model, where flow takes place in the fracture network but fracture-matrix transfer and intra-matrix fluxes are diffusive, and each fracture cell is associated with its own set of matrix cells which do not communicate with other sets of matrix cells.

Development of this transport mode is being advanced as part of the DECOVALEX international model validation project, where in Task F participants are comparing performance assessment metrics for a crystalline geologic repository reference case. The MULTICONTINUUM transport mode has been updated for this application to consider radionuclide sorption, partitioning, decay, and ingrowth in the rock matrix by linking with PFLOTRAN's UFD Decay process model which has been developed specifically for geologic radioactive waste disposal applications. We demonstrate the capability by comparing concentration of ^{241}Am in the fracture (Figure 3) and the matrix (Figure 4) at 2 different times against concentration of a non-decaying tracer.

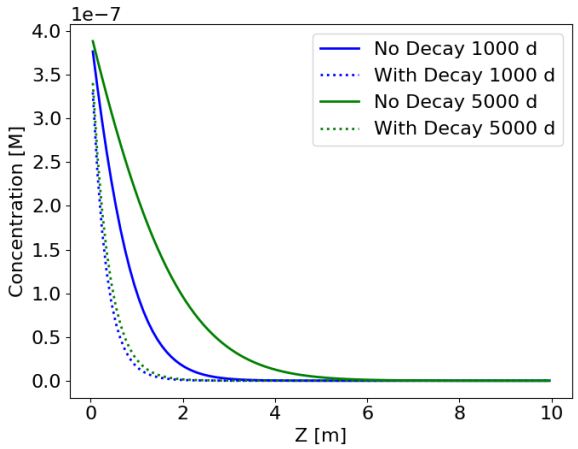

Figure 3. Concentration in the fracture with a decaying isotope (dotted line) versus non decaying tracer (solid line)

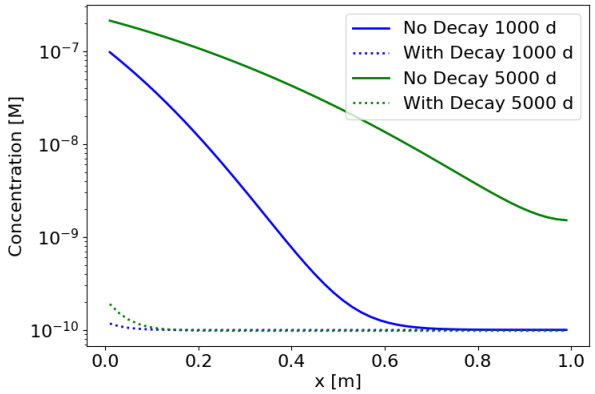

Figure 4. Concentration in the matrix with a decaying isotope (dotted line) versus non decaying tracer (single line)

In the fracture, the concentration profile of tracer throughout the fracture moves further and further from the concentration profile of the decaying isotope. In the matrix, transport of the decaying isotope is similarly significantly retarded in comparison to the tracer due to a combination of decay and sorption by the matrix. Radionuclide decay, sorption, partitioning, and ingrowth are therefore very important processes to consider when modeling matrix diffusion because these processes can interact in ways that both retard transport in the fracture pathways but also can reduce diffusive flux into the rock matrix which could act as radionuclide containment.

NONLINEAR SOLVERS

Simulating coupled thermal-hydrologic-chemical processes in subsurface engineered radioactive waste repository systems can often involve solving discrete systems with extreme variation in grid length scales (high resolution in the nearfield of a repository, low resolution in the far field host rock environment), heterogeneity in physical properties (rock properties vs engineered barrier properties vs open tunnel properties), and phase transitions. Coupling all of these processes together can be extremely computationally burdensome due to poor matrix conditioning as well as extreme transient nonlinearities that can be introduced.

PFLOTRAN's default nonlinear solver uses a traditional Jacobian-based Newton-Raphson method to solve nonlinear systems of partial differential equations. This method has been shown to be very effective for a broad range of subsurface flow and transport modeling applications, but requirements for modeling systems at higher resolution and with more nonlinear coupled processes have led the PFLOTRAN development team to develop more efficient solvers for multiphase and high temperature applications.

PFLOTRAN and PETSc, the solver library upon which PFLOTRAN is built, were recently updated to have the option of using a new trust region-based nonlinear solver, called the Newton Trust Region Dogleg Cauchy solver (NTRDC; see Park et al. [2021] [8]). Development of this solver and promising preliminary performance achievements were detailed in Nole et al. (2021) [9].

Here, we show a more thorough exploration of NTRDC performance on a repository-scale performance assessment model in unsaturated alluvium considering heat sources from 12 PWR, 24 PWR, and 37 PWR waste packages (see also [2]). Using PFLOTRAN's GENERAL mode, each waste package type is respectively associated with increasing thermal loading, which adds progressively stronger nonlinearity to the overall system through an increased prevalence of phase changes. It should be noted here that this particular simulation failed to complete using the default Newton Raphson nonlinear solver for waste packages larger than 12 PWR.

When run on a set number of cores (144), the 12, 24, and 37 PWR cases all performed around the same in terms of computation time (Figure 5). However, there were some differences in linear iterations, nonlinear iterations, and time step cuts. The 12, 24, and 37 PWR cases experienced 2.7M, 4.3M, and 9.4M phase state changes (liquid to two-phase, two-phase to gas, vice versa) in the domain throughout the simulation, respectively. The 37 PWR produced three times as many state changes, increasing the number of Newton iterations and restricting time step size (i.e., through more time step cuts).

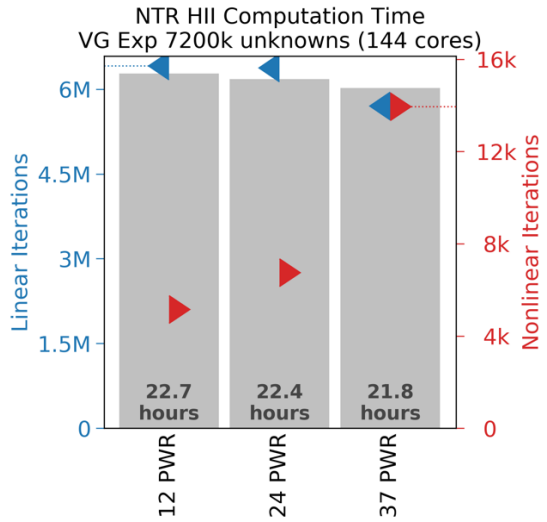

Figure 5. Wall clock time, Newton, and linear solver iteration counts for an unsaturated alluvium model run with the three (12, 24, 37) different PWR cases on 144 cores using NTR-HII.

The 12 PWR and 24 PWR cases had substantially fewer nonlinear iterations and time step cuts (Figure 6), yet the computation time was slightly greater than the 37 PWR case. The slightly lower number of linear solver iterations for 37 PWR may be explained by the larger number of time steps and conversely, the smaller average time step size, which produced linear systems that were more diagonally dominant and easier to solve.

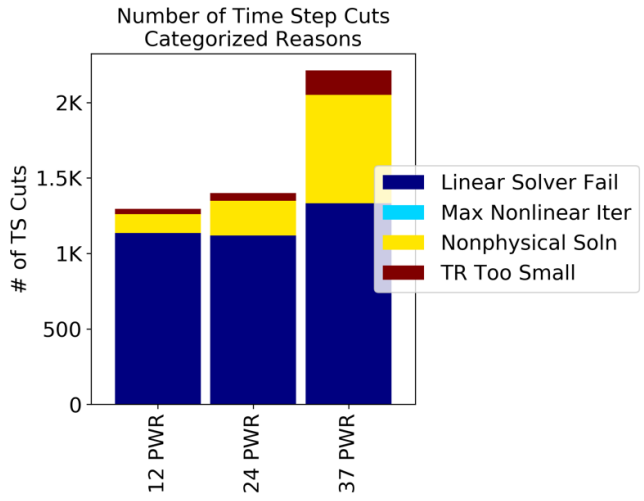

Figure 6. Time step cut counts for an unsaturated alluvium model run with the three (12, 24, 37) different PWR cases on 144 cores using NTR-HII.

This new nonlinear solver has shown a lot of promise in efficiently solving tightly coupled systems with strong nonlinearities, especially on problems where a traditional Newton Raphson algorithm must cut its time stepping to such small time step sizes that simulations would not finish in an acceptable timeframe. Work is ongoing to test this solver on broader model test cases and to tailor the solver to all flow and transport modes in PFLOTRAN.

CONCLUSIONS

Recent software developments have significantly advanced the state of modeling capabilities available in PFLOTRAN to geologic radioactive waste disposal modelers. These developments include code performance improvements for strongly nonlinear problems by introducing a new nonlinear solver (NTRDC); a new module for adding material transformation reduced order process models to the code such as high-temperature smectite illitization; full coupling of a salt solute to the fluid flow solution in GENERAL mode; and consideration of radionuclide sorption, partitioning, decay, and ingrowth in PFLOTRAN's multicontinuum model. All of these code improvements facilitate flexibility in process model selection and higher fidelity modeling for applications relevant to the GDSA project and radioactive waste containment modeling generally.

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REFERENCES

[1] M. PAUL, et al. "Modeling Geologic Waste Repository Systems Below Residual Saturation." 2022 International High Level Radioactive Waste Management Conference. Phoenix, AZ (2022).

[2] H. PARK, et al. "Newton Trust Region methods for Nuclear Waste Repository Porous Media Flow Simulations." 2022 International High Level Radioactive Waste Management Conference. Phoenix, AZ (2022).

[3] D. FUKUYAMA and Nole, M. "Development of a Fully Implicit Flow and Solute Transport Model in PFLOTRAN." 2022 International High Level Radioactive Waste Management Conference. Phoenix, AZ (2022).

[4] M. NOLE, et al. "PFLOTRAN Development FY2022." Sandia National Laboratories, Albuquerque, NM, USA (2022).

[5] W.L. HUANG., et al. “An experimentally derived kinetic model for smectite-to-illite conversion and its use as a geothermometer.” Clays and Clay Minerals 41(2), 162-177(1993). https://doi.org/10.1346/CCMN.1993.0410205

[6] J. CUADROS, and Linares, J. “Experimental kinetic study of the smectite-to-illite transformation.” Geochimica et Cosmochimica Acta 60(3), 439-453 (1996). https://doi.org/10.1016/0016-7037(95)00407-6

[7] W.R. SOUZA, and Voss, C. I. “Analysis of an anisotropic coastal aquifer system using variable-density flow and solute transport simulation.” *Journal of Hydrology*, *92*(1-2), 17-41 (1987).

[8] H.D. PARK, et al. “Linear and nonlinear solvers for simulating multiphase flow within large-scale engineered subsurface systems.” *Advances in Water Resources*, *156*, 104029 (2021).

[9] M. NOLE, et al. *PFLOTRAN Development FY2021* (No. SAND2021-8709R). Albuquerque, NM, Sandia National Labs (2021).