Multiscale Modeling in PFLOTRAN for Geologic Repository Performance Assessment

Emily R. Stein, Glenn E. Hammond, and Carlos Jove Colon
ergiamb@sandia.gov, Sandia National Laboratories, Albuquerque, NM

Problem

Performance assessment of a deep geologic repository for nuclear waste requires simulation of radionuclide concentrations at kilometer-scale distances from the repository and simulation of processes occurring at meter and centimeter scales, such as repository resaturation and nearfield reactive transport. Even with high performance computing, the computation can become prohibitively expensive.

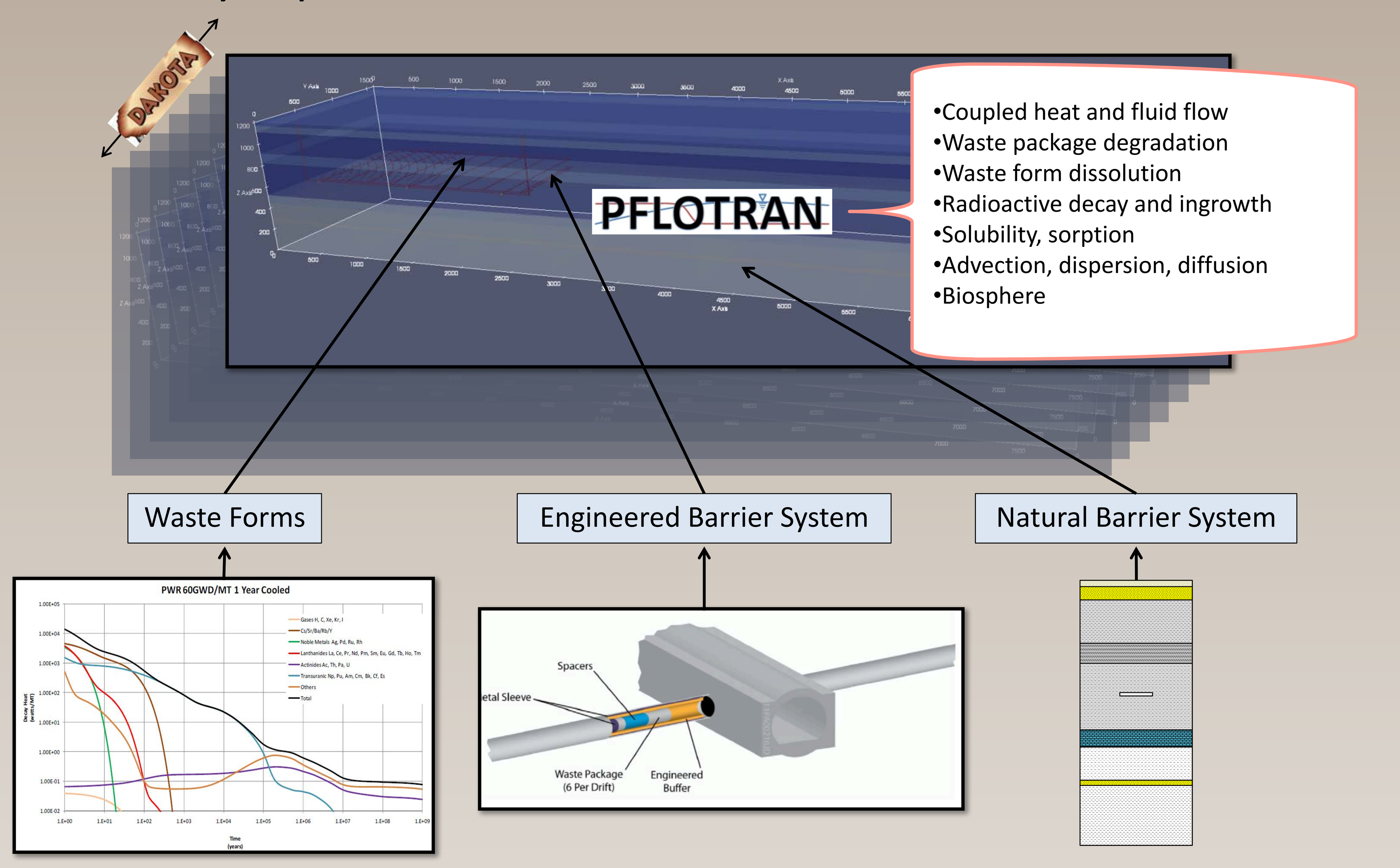

Figure 1. Performance assessment simulations are performed with *GDSA (Geologic Disposal Safety Assessment) Framework* [1], which uses PFLOTRAN [2] to couple multiphase fluid flow, reactive transport, and other process models, and Dakota [3] to sample input parameters and generate multiple realizations for uncertainty quantification and sensitivity analysis.

Model

Multi-scale modeling that uses fully-coupled, finely-discretized one-dimensional (1D) continua embedded in a three-dimensional (3D) model domain achieves subgrid-scale refinement in and around each waste package, enabling resolution of cm-scale processes affecting radionuclide fluxes from a repository in a kilometer-scale model domain.

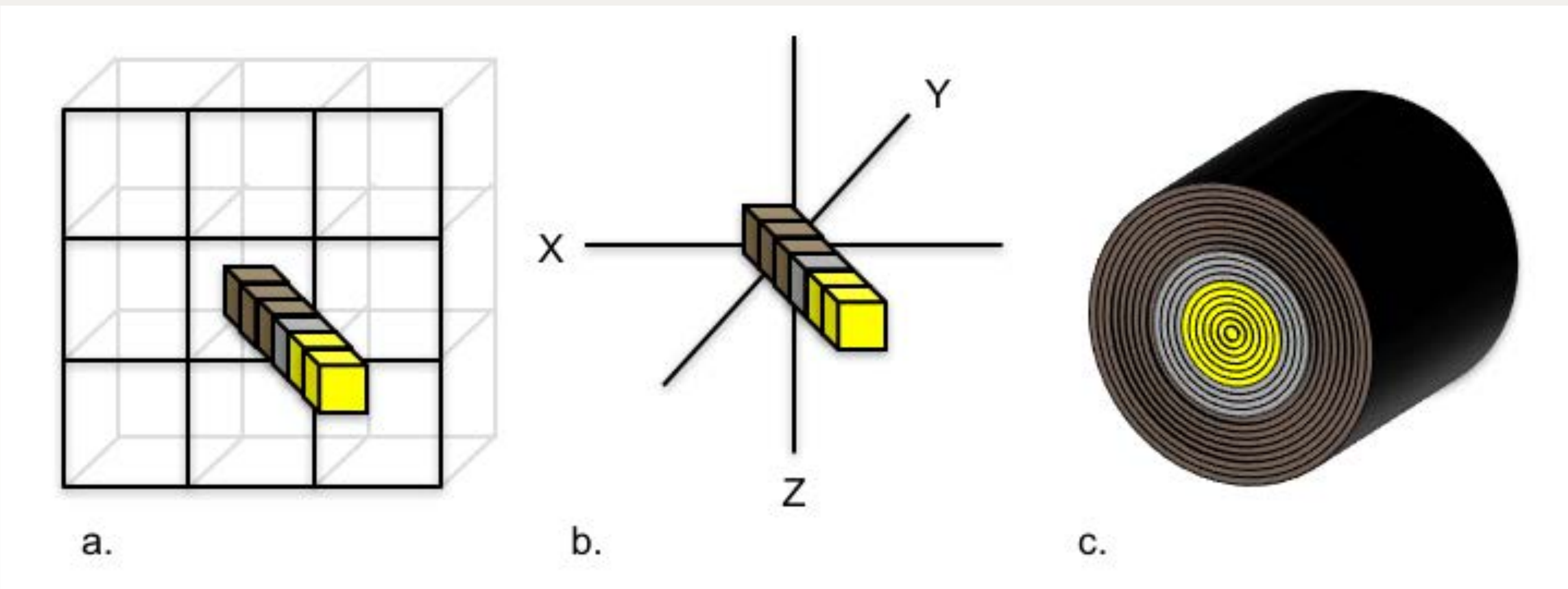

Figure 2. Schematic illustration of embedded 1D continuum. a) The 1D continuum is embedded in a 3D grid that occupies the X, Y, and Z dimensions. b) The 1D continuum occupies a virtual 4th dimension. c) Each 1D continuum represents a cylindrical waste package and the surrounding cylindrical volume of engineered materials (such as steel waste package overpack, bentonite buffer, cement liner) between the waste package and the wall of the emplacement drift. The 1D continuum is discretized into volumes representing concentric cylindrical shells, and the location of the outermost volume coincides with the location of the 3D grid cell in which the 1D continuum is embedded.

Simulations

A comparison of a 1D embedded continuum to various discretizations in 3D was made using a simulation of heat conduction. Accurate thermal modeling is important because temperature influences reaction constants. Numerically, heat conduction is the same as diffusion of a conservative tracer.

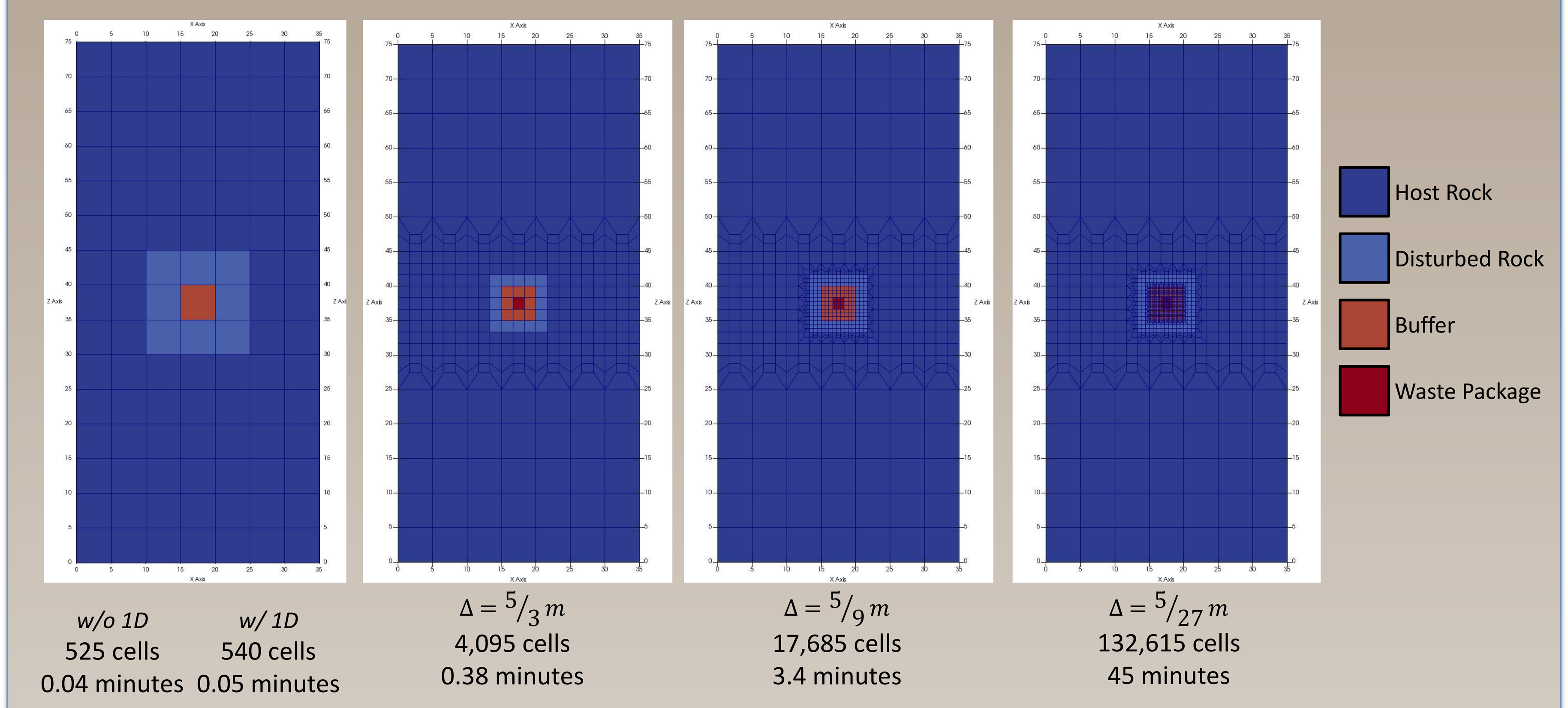

Figure 3. Five simulations of a hot spent nuclear fuel waste package in a buffer-filled drift were run, each with different discretization and identical waste package and buffer volume, heat source, and material properties. Cells in the 3D discretizations ranged from 5 m to 5/27 m on a side. The 1D continuum was discretized into 15 cells and embedded in a 5-m cell.

Results

The 1D continuum acts as a perfect heat source to the 3D cell. The buffer temperature predicted by the 1D continuum simulation corresponds almost exactly to the temperature predicted in the 3D simulation with 5-m discretization (Figure 4b). However, the 1D continuum simulation predicts temperatures about 30 degrees warmer in both the waste package center and the buffer than predicted by the finely discretized 3D simulations.

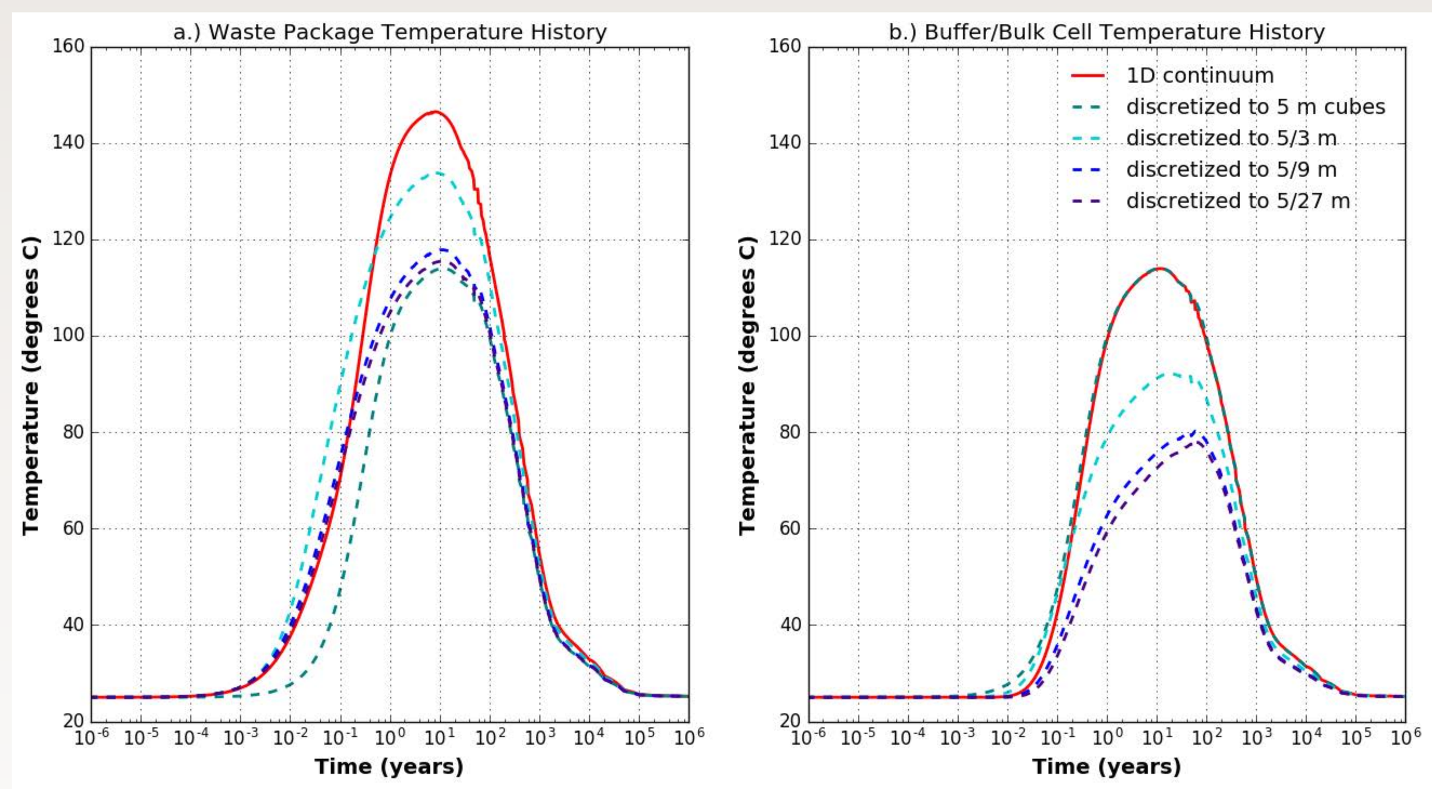

Figure 4. Temperature versus time in (a) the waste package center and (b) the buffer adjacent to the waste package.

Future Work

Over-prediction of temperatures within the 1D continuum (waste package) and the associated 3D cell (buffer) is due to the coarse grid resolution in the 3D domain adjacent to the 1D continuum. In the future, a more sophisticated interface with the 3D domain will be developed.

References

1. SNL (2017). GDSA Framework: A Geologic Disposal Safety Assessment Modeling Capability. Open Source. Available from: pa.sandia.gov.
2. Hammond, G. E., P. C. Lichtner, C. Lu and R. T. Mills (2011). "PFLOTRAN: Reactive Flow and Transport Code for Use on Laptops to Leadership-Class Supercomputers." Groundwater Reactive Transport Models. F. Zhang, G. T. Yeh and J. Parker. Bentham Science Publishers.
3. Adams, B. M., K. R. Dalbey, M. S. Eldred, L. P. Swiler, W. J. Bohnhoff, J. P. Eddy, D. M. Vigil, P. D. Hough and S. Lefantzi (2012). DAKOTA, A Multilevel Parallel Object-Oriented Framework for Design Optimization, Parameter Estimation, Uncertainty Quantification, and Sensitivity Analysis: Version 5.2+ User's Manual. SAND2010-2183. Sandia National Laboratories, Albuquerque, New Mexico.

Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

SAND2017-9395C