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GDSA Framework: High-Performance Safety Assessment Software to Support the Safety Case

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Summary

Siting, construction, and waste operations of a deep geologic repository for commercial spent nuclear fuel (SNF) is expected to take multiple decades. During this multi-decade timeline, geologic site and engineering data, as well as computer hardware and software, will advance significantly. An objective of the US effort is to develop a post-closure safety assessment capability that is flexible enough to take advantage of these advances. This capability is based on a massively parallel, high-performance computing (HPC) environment. The US effort also has the objective of improving transparency in model development and application, and is developing the new post-closure safety assessment capability in an open-source licensing format. This new Geologic Disposal Safety Assessment (GDSA) Framework *consists of two main open-source software components that are optimized for parallel computations in an HPC environment: PFLOTRAN for multi-physics domain simulation and Dakota for uncertainty quantification and sensitivity analyses. To increase confidence and transparency in the repository safety case, the development philosophy for* GDSA Framework *is based on (1) increasingly mechanistic representations of multi-physics couplings; (2) realistic three-dimensional spatial resolution of features and processes, including explicit representation of all emplaced waste packages; and (3) appropriate quantification and propagation of uncertainties. The work described here summarizes the capabilities of* GDSA Framework *and its application to a generic repository concept for waste disposal in a crystalline host rock.*

Introduction

Throughout the expected decades-long timeframe for geologic repository development, it is anticipated that conceptual models, numerical models, computer hardware, and computer software will evolve significantly through various knowledge gathering and R&D efforts, as indicated schematically in Figure 1. This evolution from generic models during the Concept Evaluation stage (the current stage in the U.S.) to site-specific models (after final site selection) demands that total system safety assessment, or performance assessment (PA), be flexible enough to accommodate concomitant software and hardware advances. This is an important motivating factor for the current effort in the U.S. to build a high-performance PA modelling capability based on the most advanced and flexible hardware and software architectures currently available. Flexibility, as well as transparency, are also the motivation for developing system PA software in an open-source format (Hammond et al. 2014). Development of this high-performance software, *Geologic Disposal Safety Assessment (GDSA) Framework* (https://pa.sandia.gov), for modelling deep geologic disposal of SNF and HLW, has been ongoing for several years in the U.S. repository program [Sevougian et al. 2015; Mariner et al. 2016; Sevougian et al. 2016].

A repository safety case (or licensing case) also evolves during the decades-long siting and development process of a repository project (Figure 1); and at each major milestone or stage in such a project, the primary elements of the project and its safety case are updated based on the most recent information available. Figure 2 shows typical elements of a safety case for documenting and building confidence in the technical feasibility, safety, and performance of any deep geologic repository. With respect to satisfying health and environmental safety regulations for the long-term (post-closure) performance of the disposal system, periodic project updates primarily involve the interplay between Elements 3.3 and 4.2 of the Safety Case shown in Figure 2, i.e., the evolving technical (knowledge/engineering) bases and the latest safety assessment analyses, as previously shown in Figure 1. This interplay between technical-basis knowledge, safety assessment, and future R&D is shown in more detail in Figure 3, as a relational or flow diagram, for a single stage (or iteration) of the repository project (Sevougian et al. 2017).

Figure 1: Illustrative timeline for evolution of a repository project and its associated safety case, as well as the temporal iteration among knowledge gathering (technical bases), safety assessment, and R&D prioritization decisions

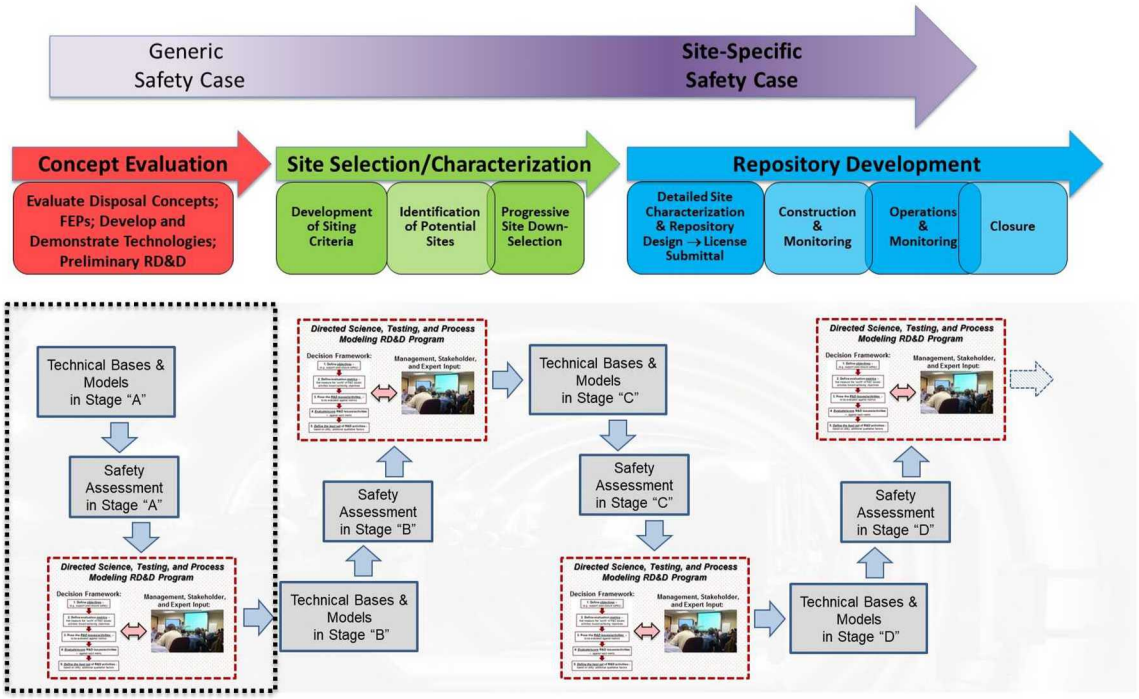
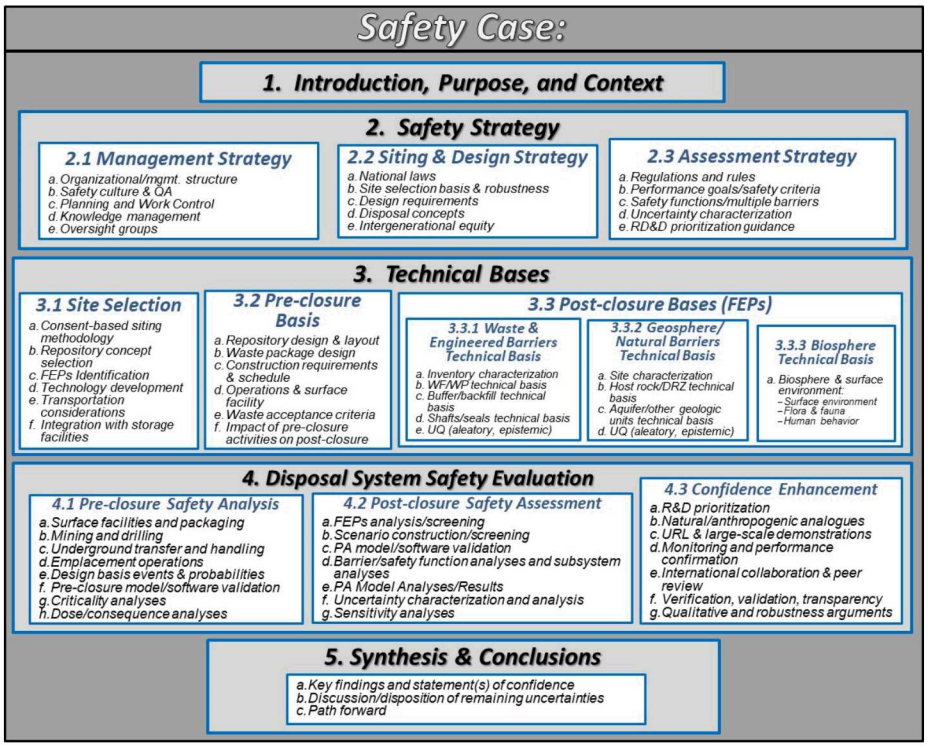


Figure 2: Major elements of the Safety Case



GDSA Framework Architecture

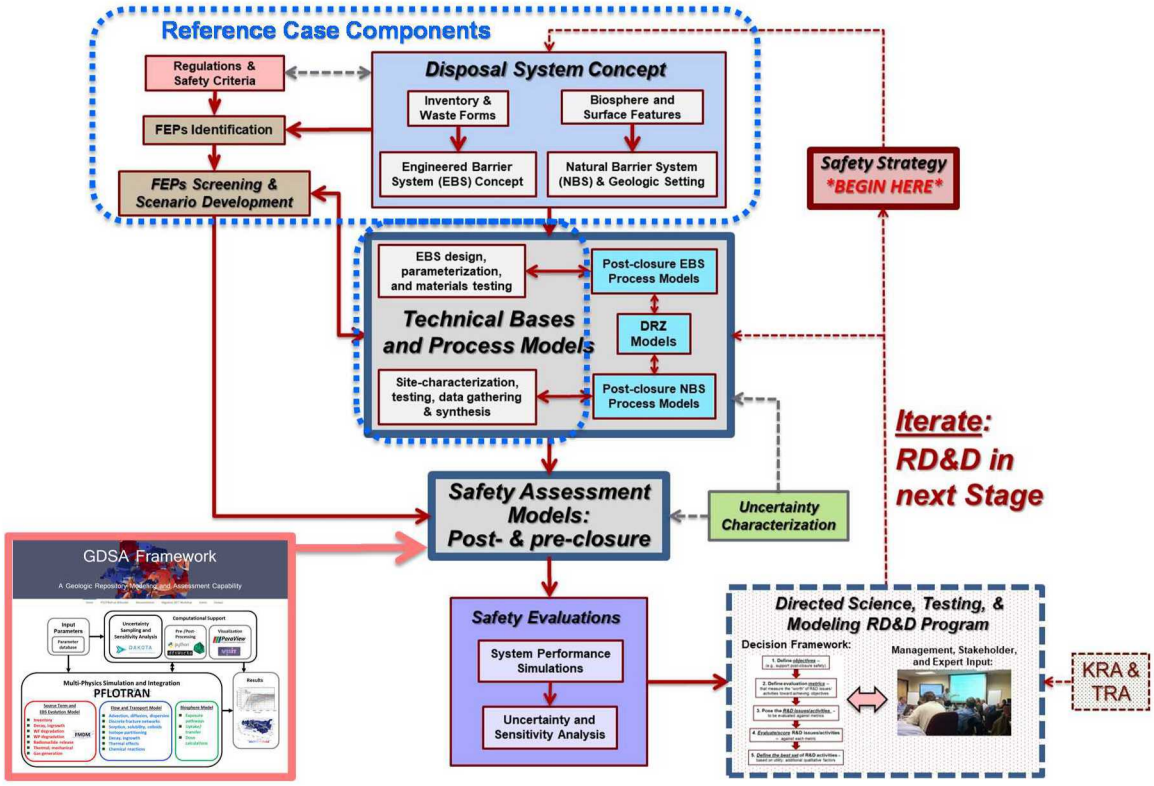
During the evolution from generic safety assessments to later site-specific safety assessments (Figure 1), the associated PA model and software has three primary, ongoing roles:

1. Quantitatively evaluate potential disposal concepts and sites in various host-rock media
2. Build confidence in the repository safety case—first generic, then site-specific
3. Help prioritize R&D activities through multiple stages of the repository program

These three roles are facilitated by building confidence in the quantitative evaluations of total system performance over long regulatory time frames. Two desired capabilities of the PA model are helpful in this regard: (1) less reliance on assumptions, simplifications, and process abstractions, i.e., more direct (or mechanistic) representation of multi-physics couplings over a large heterogeneous three-dimensional domain, including explicit representation of all emplaced waste packages when appropriate; and (2) a numerical solution and code architecture that can evolve throughout the repository lifecycle and is able from the outset to use the most advanced hardware and numerical solvers available. Overlying these capabilities is the necessity for reliable quantification and propagation of uncertainties, both aleatory and epistemic, from input to output.

Figure 3: Evolution and iteration of technical bases and performance assessment

{Reference case components are enclosed by blue dotted boxes. KRA & TRA are explained in Sevougian and MacKinnon (2017).}



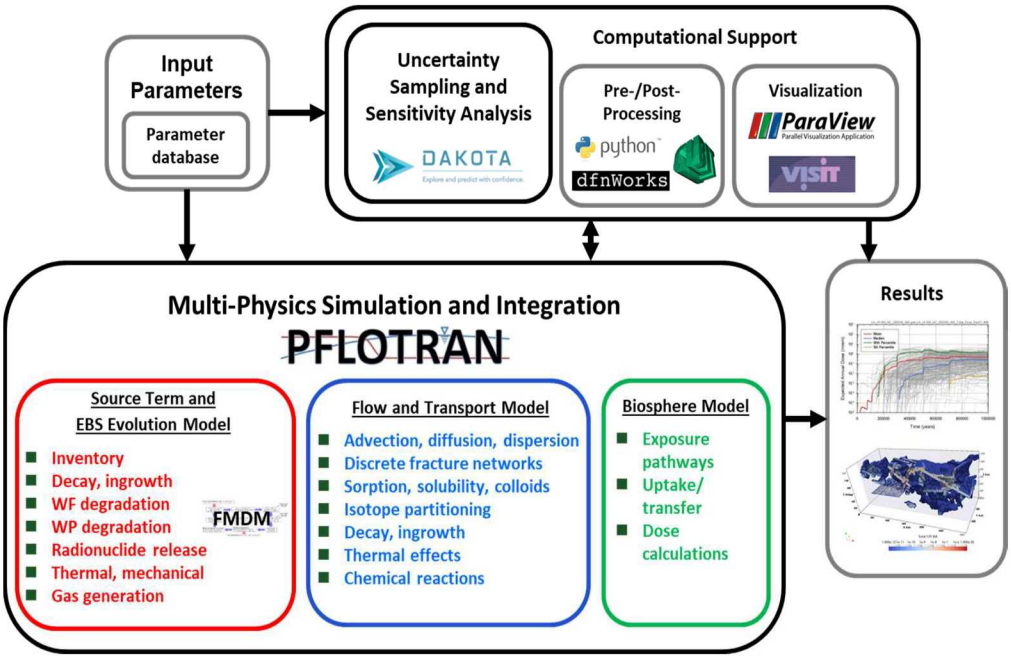
In light of the above three roles and desired capabilities of the PA model, *GDSA Framework* is built on the following key components:

- A numerically scalable reactive multiphase flow and transport code (PFLOTRAN at https://bitbucket.org/pflotran/pflotran), working in concert with coupled process model codes

- Open-source statistical software for sampling, sensitivity analysis, and uncertainty quantification (Dakota at https://dakota.sandia.org)
- Open-source computational support software and scripts for workflow, and for processing and visualizing results (e.g., Python, ParaView, VisIt)
- Free but licensed software for mesh generation (CUBIT at https://cubit.sandia.gov)

These key components are schematically depicted in Figure 4. In a probabilistic PA simulation, Dakota generates a set of parameter input vectors based on random sampling of the uncertainty distributions defined in the input set. The sampled input vectors are used by PFLOTRAN and any coupled process models to simulate source-term release, engineered barrier system (EBS) evolution, flow and transport through the EBS and natural barrier system (NBS), and uptake in the biosphere. After the simulation, various software packages may be used to analyze and visualize the output time histories of parameters and performance metrics. Dakota may also be used to evaluate the effects of parameter uncertainty on specific outputs, such as dose.

Figure 4: Schematic depiction of *GDSA Framework* architecture



PFLOTRAN [Hammond et al. 2011; Lichtner and Hammond 2012; Lichtner et al. 2018] is an open source (https://documentation.pflotran.org; https://bitbucket.org/pflotran/pflotran), reactive multi-phase flow and transport simulator designed to leverage massively-parallel high-performance computing (HPC) to simulate subsurface earth system processes. PFLOTRAN has been employed on peta-scale leadership-class DOE computing resources to simulate thermal-hydrologic-chemical (THC) processes at the Nevada Test Site [Mills et al. 2007], multi-phase CO_2-H_2O flow for carbon sequestration [Lu and Lichtner 2007], CO_2 leakage within shallow aquifers [Navarre-Sitchler et al. 2013], and uranium fate and transport at the Hanford 300 Area [Chen et al. 2013].

PFLOTRAN solves the non-linear partial differential equations describing mass, momentum, and energy transport in porous media. Parallelization is achieved through domain decomposition using the Portable Extensible Toolkit for Scientific Computation (PETSc) [Balay et al. 2013]. PETSc provides a flexible interface to data structures and solvers that facilitates the use of parallel computing. PFLOTRAN is written in Fortran 2003/2008 and leverages state-of-the-art Fortran programming (i.e. Fortran classes, pointers to procedures, etc.) to support its object-oriented design. PFLOTRAN employs a single, unified framework for simulating multi-physics processes on both structured and unstructured grid discretizations. The code requires a small,

select set of third-party libraries (e.g., MPI, PETSc, BLAS/LAPACK, HDF5, Metis/Parmetis). Both the unified structured/unstructured framework and the limited number of third-party libraries greatly facilitate usability for the end user. PFLOTRAN scales well to over 10,000 processes or cores (Hammond et al. 2014).

PFLOTRAN provides "factories" (code that constructs data structures, linkages, etc.) within which the developer can integrate a custom set of process models and time integrators for simulating surface and subsurface multi-physics processes. Within the execution step, any number of process models can be coupled and run at identical or dissimilar time scales. The "Process Model Coupler" or PMC class enables this flexibility (Sevougian et al. 2016; Hammond and Frederick 2017).

The Dakota software toolkit is open-source software developed and supported at Sandia National Laboratories (Adams et al. 2013). It is intended as a flexible, extensible interface between simulation codes and a variety of iterative systems analysis methods, including optimization, uncertainty quantification, nonlinear least squares methods, and sensitivity/variance analysis. *GDSA Framework* uses Dakota as the interface between input parameters and PFLOTRAN. Dakota is also used to analyze the effects of uncertainty in parameter values on repository performance. Specific Dakota capabilities important to *GDSA Framework* include: (1) scalable parallel computations on HPC clusters, (2) uncertainty sampling and propagation, (3) and probabilistic sensitivity analysis methods.

Despite the robustness of the HPC and open-source concept used by *GDSA Framework*, computer hardware limitations will still be a consideration for the foreseeable future given the large spatial-temporal scales, complex coupled processes, and multiple uncertainty distributions necessary to represent post-closure repository evolution over perhaps one million years. Thus, scale averaging methods and surrogate models must be analyzed and applied for some parts of the spatial-temporal domain, at least during the current early repository stages, prior to final site-selection.

Application of *GDSA Framework* to an SNF Repository in a Generic Crystalline Host Rock

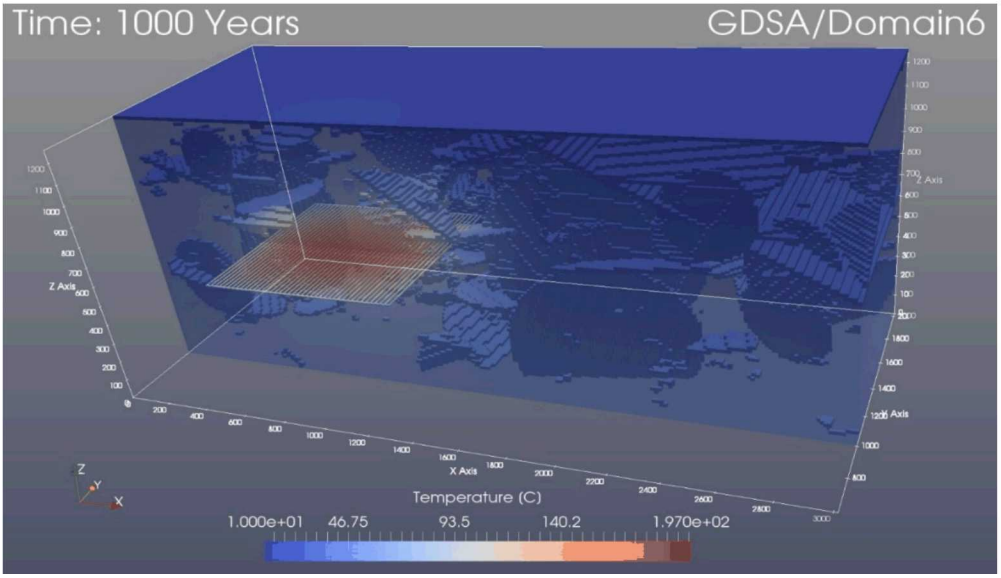
In the current Concept Evaluation stage of repository development in the U.S. (Figure 1), generic "reference cases" are used to represent potential repositories in various host-rock media, based on typical geologies and properties for clay/shale, salt, or granite/crystalline host rock in the U.S., along with generic engineered designed concepts that are appropriate for these host rocks. A reference case is a representative "surrogate" for site- and design-specific information not yet available during the current Concept Evaluation stage, but which can be used to *demonstrate capabilities* of the PA model/software framework, in preparation for its use during site screening and site evaluation. Detailed characteristics, parameters, and analyses associated with the generic crystalline host-rock reference case are briefly summarized below, but fully documented in Mariner et al. (2016).

The crystalline reference case calls for a mined repository located at about 600 m below land surface in a fractured crystalline rock. It is assumed that this repository would hold 70,000 MTHM of commercial SNF. Within cylindrical disposal drifts, waste packages are centered in a buffer consisting of compacted bentonite pellets or bricks. The bentonite buffer serves as an impermeable barrier to bulk movement of pore water, effectively isolating the waste container (and its radionuclide inventory) from connection with possible fractures in the host rock and in the disturbed rock zone (DRZ) surrounding the drift excavation.

The representation of fractured crystalline rock in the generic reference case is based primarily on the well-characterized, sparsely fractured metagranite at Forsmark, Sweden (Follin et al. 2014). Conceptually, the crystalline host rock is comprised of two media: fractures and rock matrix. Numerically it is simulated in *GDSA Framework* with two types of grid cells: those containing a fracture or fractures and those without fractures (the matrix). The fracture networks in these simulations are originally generated as discrete fracture networks (DFNs), which are sets of two-dimensional planes distributed in a three-dimensional domain (Figure 5). The method used in *GDSA Framework* maps the stochastically generated DFN to an equivalent continuous porous medium (ECPM) domain that allows for the simulation of coupled heat flow, fluid flow, and radionuclide transport, including heat conduction through the matrix of the fractured rock, which are *coupled* processes not easily modelled in an explicit DFN model. Computational efficiency is also greatly enhanced using the ECPM method, allowing for multi-realization PA analyses in a reasonable wall-clock time on an HPC cluster (Stein et al. 2017).

Figure 5: Transparent view of the generic crystalline repository model domain at 1000 years after repository closure

{Colored by temperature and indicating major structural features (upper right) and disk-shaped fractures, as well as the repository emplacement drifts, for a single realization of the uncertain fracture network (Domain6).}



PA simulations were divided into two sets: (1) a set of 15 "fracture realizations," i.e., 15 simulations of the repository system, each with a different realization of the uncertain fracture network, but with the same sampling of other uncertain parameters such as buffer porosity, aquifer permeability, et al.; and (2) a set of 50 realizations based on a single fracture network (Domain6) but using a 50-vector random sample of other uncertain input parameters. Both sets were run using *GDSA Framework* on an unstructured mesh in three dimensions. The unstructured mesh was constructed with CUBIT (Blacker et al. 2016). DFNs were generated with dfnWorks (Hyman et al. 2015) and mapped to an ECPM domain with a Python script. The ECPM domain contains 4,848,260 cells; of these, approximately 2.5 million are smaller grid cells in and around the repository. Sensitivity analyses (Speakman rank correlation coefficients of maximum [^{129}I] over 1,000,000 years versus the distributions of the eight sampled input parameters) were conducted using the second set of 50 realizations and indicated, as might be expected, a strong positive correlation of ^{129}I concentration with aquifer permeability and waste package degradation rate (Mariner et al. 2016).

Thermal output of the SNF must be considered in the simulations and can influence the rate and timing of waste package failure and waste form degradation, as well as fluid flux due to thermal expansion around the repository horizon. Temperatures peak just below 200 °C at approximately 200 years after waste emplacement but the repository remains warmer than background for about 10,000 years (Mariner et al. 2016). Figure 5 is a transparent view of the generic crystalline repository model domain at 1000 years after repository closure, colored by temperature, for one specific realization of the heterogeneous distribution of fractures (called "Domain6"). Figure 6 shows the spatial distribution of the conservative tracer ^{129}I at 400 years after repository closure (after about 3% of the waste packages have been breached by general corrosion processes) for this same fracture network (Domain6) and for typical ("deterministic") values of the uncertain model input parameters, i.e., the same fixed parameter values used in the 15-realization fracture simulation set described above. At this time of 400 years, transport in highly permeable connected fractures has carried ^{129}I to the east (right) face of the model domain, 1.5 km from the repository. Also indicated in this figure is the process of ^{129}I diffusion from the repository, as well as from fractures into the crystalline rock matrix.

Time histories of ^{129}I concentration are plotted in Figure 7 for both sets of simulations, at an "observation point" in the sediments (glacial till) at the top of the model domain. Figure 7 (left) shows ^{129}I concentration at observation point "glacial2" for the 15 different realizations of the stochastic fracture network. Differing

degrees of fracture distribution, size, and permeability result in significantly different transport times for ^{129}I through the crystalline host rock to the surface (i.e., to the biosphere), because of the randomness of fracture network connectivity (and resulting transport time) to the surface. This wide variation in transport times, based on fracture-distribution uncertainty alone, may be contrasted with the more uniformity of transport time through the host rock (Figure 7, right) for the 50-realization simulation set, which is based only on uncertainties in several underlying rock, fluid, waste, and EBS parameters, such as bentonite porosity, aquifer permeability, and SNF degradation rate (Mariner et al. 2016), for a single fracture domain (Domain6).

Figure 6: ^{129}I concentration at 400 years in the deterministic simulation of Fracture Domain6

{Concentration is contoured on a log scale at intervals of 10^{-12} mol/L to 10^{-5} mol/L; contours are colored by ^{129}I concentration.}

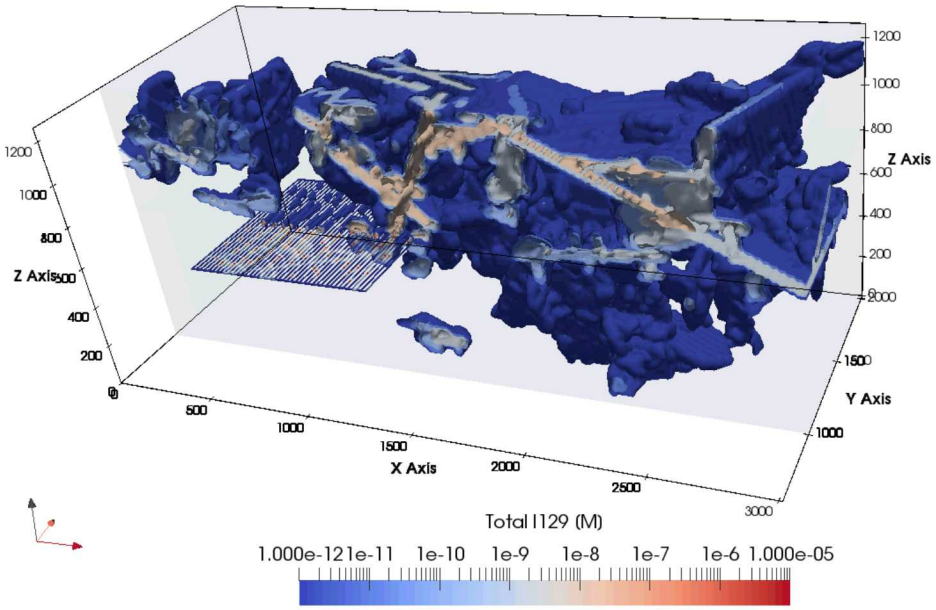
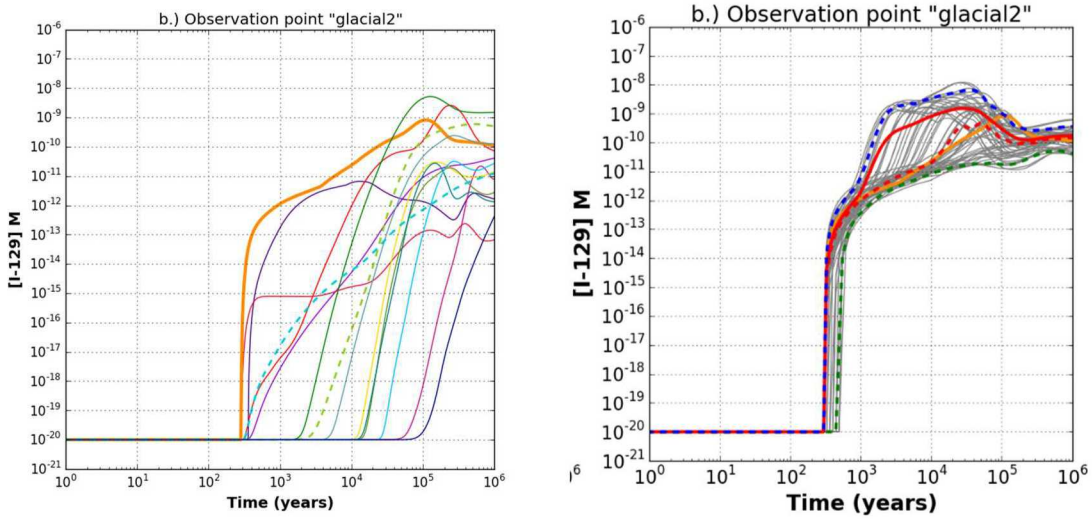


Figure 7: (*left*) Predicted ^{129}I concentration versus time at observation point "glacial2" for 15 fracture-network realizations—the heavy orange line is Domain6. (*right*) Predicted ^{129}I concentration versus time for 50 sampled realizations of uncertain parameters at observation point "glacial2" for fracture network Domain6.



Summary and Conclusions

Development of an enhanced performance assessment (PA) capability for geologic disposal of SNF and HLW has been ongoing for several years in the U.S. repository program. The new *GDSA Framework* software is intended to be flexible enough to evolve through the various stages of repository activities, beginning with generic PA activities in the current Concept Evaluation stage to site-specific PA modelling in the Repository Development stage. *GDSA Framework* utilizes modern software and hardware capabilities by being based on open-source software architecture and being configured to run in a massively parallel, high-performance computing (HPC) environment. It consists of two main components, the open-source Dakota uncertainty sampling and analysis software and the PFLOTRAN reactive multi-phase flow and transport simulator.

Reference cases or "generic repositories" have been, and are being developed, based on typical properties for potential salt, clay, and granite host-rock formations and corresponding engineered design concepts for each medium, in order to demonstrate the capabilities of the new PA software and to prepare for future repository stages, such as site screening and site evaluation.

Progress in the development of *GDSA Framework* continues to affirm that HPC-capable codes can be used to simulate important multi-physics couplings directly in a total system performance assessment of a deep geologic repository. The generic repository applications modelled to date indicate that the developing capability can simulate complex coupled processes in a multi-kilometer domain, while simultaneously simulating the coupled behavior of meter-scale features, including every waste package within the domain.

References

Adams, B.M., M.S. Ebeida, M.S. Eldred, J.D. Jakeman, L.P. Swiler, W.J. Bohnhoff, K.R. Dalbey, J.P. Eddy, K.T. Hu, D.M. Vigil, L.E. Baumann, and P.D. Hough. 2013a. *Dakota, a Multilevel Parallel Object-Oriented Framework for Design Optimization, Parameter Estimation, Uncertainty Quantification, and Sensitivity Analysis, Version 5.3.1+ User's Manual.* SAND2010-2183, Updated May 22, 2013. Sandia National Laboratories, Albuquerque, NM. (http://dakota.sandia.gov/).

Balay S., J. Brown, K. Buschelman, V. Eijkhout, W.D. Gropp, D. Kaushik, M.G. Knepley, L. Curfman McInnes, B.F. Smith and H. Zhang. 2013. PETSc Users Manual, ANL-95/11 – Revision 3.4, Argonne National Laboratory, Argonne IL.

Chen, X., G. Hammond, C. Murray, M. Rockhold, V. Vermeul and J. Zachara. 2013. "Applications of Ensemble-based Data Assimilation Techniques for Aquifer Characterization using Tracer Data at Hanford 300 Area", Water Resources Research, 49, doi:10.1002/2012WR013285

Follin, S., L. Hartley, I. Rhen, P. Jackson, S. Joyce, D. Roberts, and B. Swift 2014. "A methodology to constrain the parameters of a hydrogeological discrete fracture network model for sparsely fractured crystalline rock, exemplified by data from the proposed high-level nuclear waste repository site at Forsmark, Sweden," Hydrogeology Journal, 22(2), 313-331. doi: 10.1007/s10040-013-1080-2.

Hammond, G.E. and J.M. Frederick 2017. "Minimizing the Impact of Software Evolution on Radioactive Waste Management," in Proceedings of the International High-Level Radioactive Waste Management (IHLRWM 2017) Conference, April 9 – 13, 2017, Charlotte, NC, SAND2016-12458C.

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", in F. Zhang, G.T. Yeh, and J. Parker (ed.) Groundwater Reactive Transport Models, Bentham Science Publishers.

Hammond, G.E., P.C. Lichtner, and R.T. Mills 2014. "Evaluating the Performance of Parallel Subsurface Simulators: An Illustrative Example with PFLOTRAN", Water Resources Research, 50, 208-228, doi:10.1002/2012WR013483.

Hyman, J. D., S. Karra, N. Makedonska, C. W. Gable, S. L. Painter and H. S. Viswanathan 2015. "DFNWorks: A discrete fracture network framework for modeling subsurface flow and transport," Computers & Geoscience, 84:10-19.

Lichtner, P.C. and G.E. Hammond. 2012. Quick Reference Guide: PFLOTRAN 2.0 (LA-CC-09-047) Multiphase-Multicomponent-Multiscale Massively Parallel Reactive Transport Code. DRAFT LA-UR-06-7048. December 8, 2012. Los Alamos National Laboratory, Los Alamos, NM.

Lichtner, P. C., G. E. Hammond, C. Lu, S. Karra, G. Bisht, B. Andre, R. Mills, J. Kumar, and J.M. Frederick 2018. PFLOTRAN Documentation, Release 1.1, https://www.pflotran.org/documentation/index.html.

Lu, C. and P.C. Lichtner. 2007. "High resolution numerical investigation on the effect of convective instability on long term CO2 storage in saline aquifers", Journal of Physics Conference Series, 78, doi:10.1088/1742-6596/78/1/012042.

Mariner, P. E., E. R. Stein, J. M. Frederick, S. D. Sevougian, G. E. Hammond, and D. G. Fascitelli 2016. Advances in Geologic Disposal System Modeling and Application to Crystalline Rock, FCRD-UFD-2016-000440, SAND2016-96107R. Sandia National Laboratories, Albuquerque, NM, September 22, 2016.

Mills, R., C. Lu, P.C. Lichtner, and G. Hammond. 2007. Simulating Subsurface Flow and Transport on Ultrascale Computers using PFLOTRAN, Journal of Physics Conference Series, 78, 012051 doi:10.1088/1742-6596/78/1/012051.

Navarre-Sitchler, A., R.M. Maxwell, E.R. Siirila, G.E. Hammond and P.C. Lichtner. 2013. "Elucidating geochemical response of shallow heterogeneous aquifers to CO2 leakage using high-performance computing: implications for monitoring CO2 sequestration", Advances in Water Resources, v53, pp. 45-55, doi:10.1016/j.advwatres.2012.10.005.

Sevougian, S. D. and R. J. MacKinnon 2017. "Technology Readiness Assessment Process Adapted to Geologic Disposal of HLW/SNF," in Proceedings of the International High-Level Radioactive Waste Management (IHLRWM 2017) Conference, April 9 – 13, 2017, Charlotte, NC, SAND2017-0179C

Sevougian, S. D., G. A. Freeze, W. P. Gardner, G. E. Hammond, P. Mariner, and R. J. MacKinnon. 2015. "Performance Assessment Modeling of a Generic SNF/HLW Repository in Salt with Coupled Thermal-Hydrologic Effects – 15423," in Proceedings of the WM2015 Conference, March 15 – 19, 2015, Phoenix, Arizona USA.

Sevougian, S. D., E. R. Stein, G. E. Hammond, P. E. Mariner, and W. P. Gardner 2016. "Enhanced Performance Assessment Models for Generic Deep Geologic Repositories for High-Level Waste and Spent Nuclear Fuel – 16223," in Proceedings of the WM2016 Conference, March 6 – 10, 2016, Phoenix, Arizona USA.

Sevougian, S. D., E. R. Stein, M. B. Gross, G. E. Hammond, J. M. Frederick, and P. E. Mariner 2017. "Performance Assessment of a Generic Repository for Defense-Related HLW/SNF in Fractured Crystalline Host Rock – 17059," in Proceedings of the WM2017 Conference, March 5 – 9, 2017, Phoenix, Arizona USA, SAND2016-11750C.

Stein, E. R., J. M. Frederick, G. E. Hammond, K. L. Kuhlman, P. E. Mariner, and S. D. Sevougian 2017. "Modeling Coupled Reactive Flow Processes in Fractured Crystalline Rock," in Proceedings of the International High-Level Radioactive Waste Management (IHLRWM 2017) Conference, April 9 – 13, 2017, Charlotte, NC.

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