Impact of High Performance Computing on the Detailed Simulation of Subsurface Flow and Contaminant Transport Using eSTOMP – 16341

Vicky Freedman[1], Diana Bacon[1], Mark Rockhold[1] and Kearn (Pat) Lee[2]
[1]Pacific Northwest National Laboratory
[2]AREVA Federal Services

ABSTRACT

The ability to model subsurface processes at the field-scale is essential to site closure and remedial action decisions. Field-scale models often require high-performance computing to meet the computational demands associated with complex systems, model calibration, and uncertainty quantification. eSTOMP, a parallel version of STOMP, is an analytical tool that meets the need for investigating coupled processes in the subsurface involving regional multifluid flow and biogeochemistry. The scalability of eSTOMP makes it ideal for simulating contaminant and geochemical reactive transport when long run times result from execution of a serial code. To demonstrate the impact of high-performance computation on subsurface analyses, the application of eSTOMP is presented for two sites. The first site involves uranium surface complexation within a highly dynamic, variably saturated flow field. The use of this model in conjunction with continued field monitoring is expected to provide a rigorous basis for developing operational strategies for field remediation and for defining defensible remediation endpoints. The second site involves the long-term dissolution of low-level radioactive glass emplaced within a near-surface repository. The waste form release rate is evaluated by modeling the basic physical and chemical processes that are known to control the waste form dissolution behavior, including pH and composition of the fluid contacting the glass. Simulations demonstrate that glass dissolution rates vary both in time and as a function of position within the disposal system, and that a "leach rate" or radionuclide release rate parameter can only be estimated after identifying these impacts in a dynamic system.

INTRODUCTION

Cleanup and closure of U.S. Department of Energy (DOE) Office of Environmental Management (EM) waste sites requires the evaluation of remedial alternatives, including risk-informed approaches to manage residual contamination. Predictive modeling is essential for establishing the technical justification for remediation decisions, evaluation of risks associated with contaminants left in place, and the long-term management of EM sites. However, simplifying assumptions that diminish technical credibility are too often applied to models without adequate justification for their use. This may result in costly, technically impractical site closure requirements that are not protective of human health and the environment.

Representing the physical and chemical complexity of many sites requires coupling multiple fluid phases and geochemical components at multiple scales in highly heterogeneous systems (e.g., [1-2]). This increased complexity brings a

concomitant need for more computational power that exceeds the processing power of a typical desktop computer. The advent of high-performance computation (HPC) not only meets this need, but also provides the resources to further increase complexity and sophistication of subsurface models. However, complexity is not the end-goal of modeling. Rather, the primary objective is to understand what is important in determining system behavior, and representing those features, events, and processes in pursuit of model parsimony.

Fig. 1. Hanford Site location.

Not all modeling problems would benefit from HPC, but it can improve modeling by providing the ability to 1) use larger and more detailed computational grids; 2) incorporate uncertainty into contaminant transport predictions; 3) perform inverse modeling on multiple parameters at the field scale; and 4) develop more complete computational models of coupled multiphase and geochemical processes. In this paper, two examples of applications using HPC are presented using eSTOMP (extreme-scale Subsurface Transport Over Multiple Phases) [3], an HPC simulator based on STOMP [4-5]. The first application focuses on a persistent uranium plume in the 300 Area at the Hanford Site, located in southeastern Washington State (Fig. 1). In the second application, eSTOMP was used to evaluate the long-term dissolution of low-level radioactive glass emplaced within a near-surface repository as part of the 2005 Integrated Disposal Facility (IDF) calculations at Hanford, a facility to be sited just south of the 200 East Area (Fig. 1).

The applications presented in this paper are used to support evaluation of the potential impact of future releases and remedy decisions. Within this context, the applications demonstrate that the eSTOMP simulator can provide more detailed modeling for understanding the impact of important coupled processes and model conceptualizations in dynamic environments. Moreover, recent qualification of eSTOMP as nuclear safety software means that it can be used to support major regulatory decisions such as those related to disposal system performance assessments (PAs) and remedy evaluation and selection at DOE-EM sites.

eSTOMP SIMULATOR

The eSTOMP simulator [3-5] is the highly scalable (parallel) version of STOMP [4-5]. Parallelization of the STOMP code is achieved through domain decomposition using the Global Arrays toolkit (GA) [6]. A key feature of this conversion is the definition of a data model to describe a grid that is distributed over multiple processors, and using the shared memory offered through GA. eSTOMP uses the Portable, Extensible Toolkit for Scientific Computation (PETSc) library as its parallel solver. The primary design guides for the eSTOMP simulator have been computational efficiency and alignment with the serial STOMP code. This means that whenever possible, input files, output files, and capabilities are the same between the serial and parallel codes.

Like STOMP, eSTOMP contains the batch geochemistry solution module ECKEChem [7], which provides a systematic procedure for converting geochemical systems for mixed equilibrium and kinetic reactions into a system of nonlinear equations. This objective was realized through a preprocessor developed for BIOGEOCHEM [8]. ECKEChem uses an operator split solution scheme that solves the transport equations and reaction equations sequentially.

The eSTOMP simulator can address the required process model complexity and spatially variable property detail via massively parallel processing. The code has also been qualified as Level C Safety and Hazard Analysis and Design Software under DOE Order 414.1C, making it applicable to PAs and other applications requiring the use of safety software. eSTOMP's ability to simulate coupled mechanistically detailed processes enables more realistic representations of the subsurface without compromising dimensionality, resolution, process model detail, or property variations to make the run times tractable. If simple models are to be used, simulation results obtained using more detailed and highly resolved models can be used to provide the technical basis for model abstraction.

HANFORD 300 AREA

The 300 Area, located in the southeast corner of the Hanford Site (Fig. 1), has been the subject of a great deal of field characterization and scientific inquiry for more than two decades due to a persistent groundwater uranium plume [9-12]. This plume is the result of past disposal practices in which liquid wastes from reactor fuel fabrication processes (an estimated 47,306 kg of uranium) were disposed of

directly to unlined ponds and trenches located immediately adjacent to the Columbia River.
The earliest modeling of the 300 Area uranium plume projected that natural flushing of the uranium from the aquifer would occur within a relatively short time frame (e.g., 20 years), and that concentrations would fall below the maximum contaminant level [13-14]. However, the plume has remained largely unchanged in mass and volume over the past 15 years. Research has attributed this to uranium in the vadose zone [12]. Residual uranium left in the vadose zone and capillary fringe region is periodically accessed by the rising water table during high river stage. Uranium in this region is then desorbed, resulting in increased uranium concentrations in the aquifer. Interpretations of uranium mass transfer behavior are confounded by complex geochemical processes, with dilute river water favoring stronger sorption of uranium to the sediments relative to groundwater [15], and by wellbore flow effects [16].

In this paper, a multi-component reactive transport modeling approach is used in conjunction with field data for sediment-associated uranium in the 300 Area. Details of this modeling work are not presented here, but can be found in Rockhold et al. [17].

300 AREA SIMULATION DESCRIPTION

The regional-scale flow and reactive transport model of the 300 Area represents an update to the groundwater model of the 300 Area developed previously by Williams et al. [18]. Modifications included updates to the domain and the geology, as well as the addition of reaction networks for uranium surface complexation, aqueous speciation, and mineral reactions associated with the addition of polyphosphate amendments for remediation were included in the updated model.

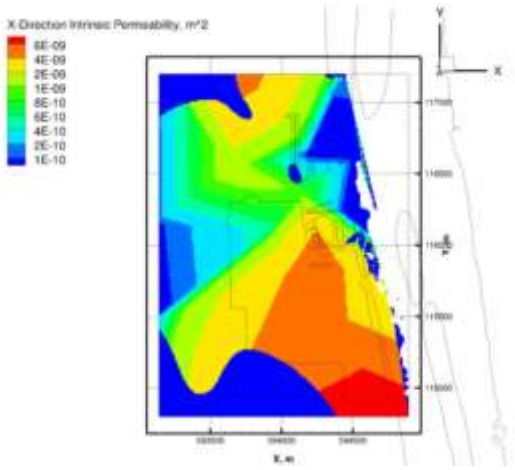

Fig. 2. Example of spatially variable permeability distributions at elevation 104 m.

The 300 Area model was grouped into two hydrogeologic units, with the Hanford formation described with spatially variable properties (Fig. 2), and an underlying, undifferentiated Ringold Formation, with uniform properties. Although there are

some differences in density, porosity, and other properties for the Ringold subunits [18], the reduced hydraulic conductivity of the overall Ringold relative to the Hanford is the dominant feature of importance to this system. Hence, the properties of the Ringold were assumed known, while spatially variable hydraulic conductivities for the Hanford were estimated by inverse modeling.

Model Calibration

Spatially variable depth-averaged hydraulic conductivities for the region representing the Hanford formation were estimated using a pilot point methodology with regularization constraints using parallel PEST [19]. A plan view of the model domain as a red box is shown in Fig. 3. Both monitoring well locations, as well as the pilot point locations used to perform model location, are shown in Fig. 3. The Columbia River is shown as the blue line and represents the model eastern boundary. Hourly water level data in 2011 from 24 wells in the 300 Area monitoring network, and quarterly measurements of chloride data from 21 wells were used for model calibration. In addition, daily measurements of chloride data obtained from one well during a tracer test performed at the DOE-Office of Science-supported Integrated Field Research Challenge (IFRC) Site well field in spring 2011 were used for model calibration. Although specific conductance data are more prevalent from the network of automated sensors and data loggers in the 300 Area well monitoring network, chloride data were used here to capitalize on a tracer test performed at the IFRC site (shown as a triangle in Fig. 3).

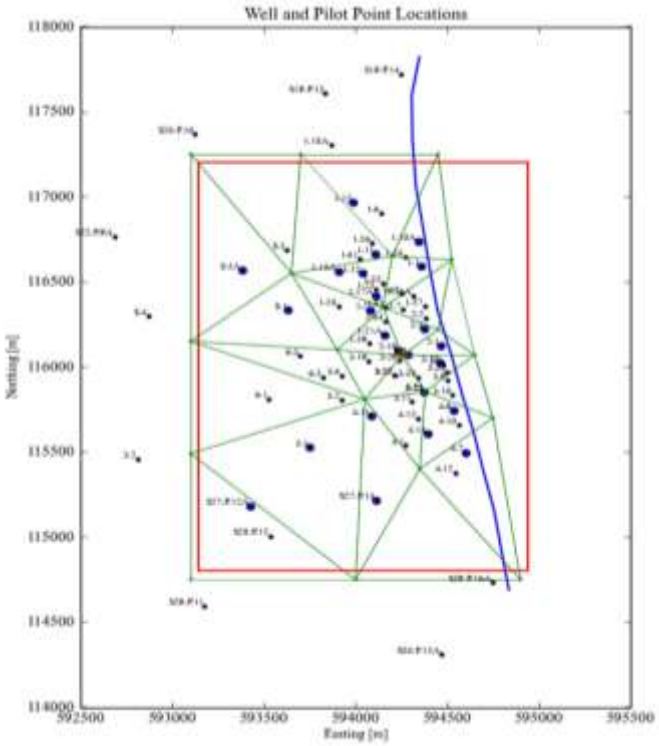

Fig. 3. Map showing plan view of model domain and well and pilot point locations. The red rectangle is the outline of the model domain, the blue line is the river, the

connected green points are pilot point locations, and the labeled points are monitoring wells. The larger blue points are wells used for water level observation data in inverse modeling. The small red triangle in the middle of the figure is the IFRC site (from Rockhold et al. [17]). The model domain spans 2400 m in the x- (N-S) direction, 1750 m in the y- (E-W) direction, and 28 m in the z- (vertical) direction. Uniform 10-m grid spacing was used for both the x- and y-directions, and uniform 1-m grid spacing was used in the vertical direction, for a total of 175, 240, and 28 grid cells in the x-, y-, and z-directions, respectively. This resulted in 1,176,000 model grid blocks. Cells lying above the ground surface or east of the main river channel were defined as inactive.

Boundary Conditions

The lower boundary of the model domain was specified as a zero flux or no-flow boundary condition for water, solutes, and reactive species. The upper boundary was assigned a Neumann or constant flux condition of 0.06 m/yr for water, based on the long-term average recharge rate for a 300 Area lysimeter [20], and fixed concentrations corresponding to average groundwater concentrations for solute or reactive species. All lateral boundary conditions were specified as linked-list seepage face boundaries for water flow, and inflow-outflow boundaries for solutes or aqueous species. Solute or aqueous species concentrations on the lateral boundaries were specified as the average groundwater concentrations for the northern, southern, and western boundaries, and as the average river water concentrations for the eastern boundary bordering the Columbia River. For the reactive transport simulations involving polyphosphate injection, a constant infiltration rate of 10 cm/hr was applied for 4 days during a period of low river stage. This water flux contained 4.74e-2 mol/L PO_4--- and 1.75e-3 mol/L $Na_5P_3O_{10}$(aq).

Geochemical System

Aqueous speciation reactions, as well as multi-rate surface complexation reactions, were used to simulate the system geochemistry. Details on the reaction network can be found in Rockhold et al. [17]. In general, surface complexation is a more rigorous approach because of the highly variable aqueous chemical conditions that result from cyclic incursion of river water of different chemical composition into the unconfined aquifer. In contrast, the standard *Kd*-based model is strictly applicable to the typically small range of variability of the single aqueous species [e.g., U(VI)] for which the *Kd* values were estimated. The *Kd* approach does not account for kinetic behavior, and it does not consider the finite sorption capacity of the sediment.

Model Output

Model calibration was first performed using only flow and chloride concentration data (i.e., no uranium reaction network). Fig. 4 at left shows observed water levels versus time and simulation results from the calibrated model for selected wells. Overall, the correspondence between simulated and observed water levels for these

and other wells (not shown here) is good. Fig. 4 at right shows observed and simulated chloride concentrations for the tracer test used in the IFRC well field experiment. The results indicated very good correspondence between simulated and observed results. Not all wells yielded the same fit.

Once the model was calibrated, simulations of the reactive transport of uranium for a hypothetical remediation scenario were executed. These simulations involved infiltration of a polyphosphate solution over a uranium hot spot.

Fig. 5 shows the total aqueous uranium concentrations at the 107.5 m elevation after 4 days of infiltration. The wetting front of the infiltrating polyphosphate solution appears to be displacing a fraction of the mobile uranium from the vadose zone and upper capillary fringe region in what essentially amounts to soil flushing, with calculated total aqueous uranium concentrations at the displayed elevation exceeding 400 µg/L. These results suggest that groundwater treatment may be required.

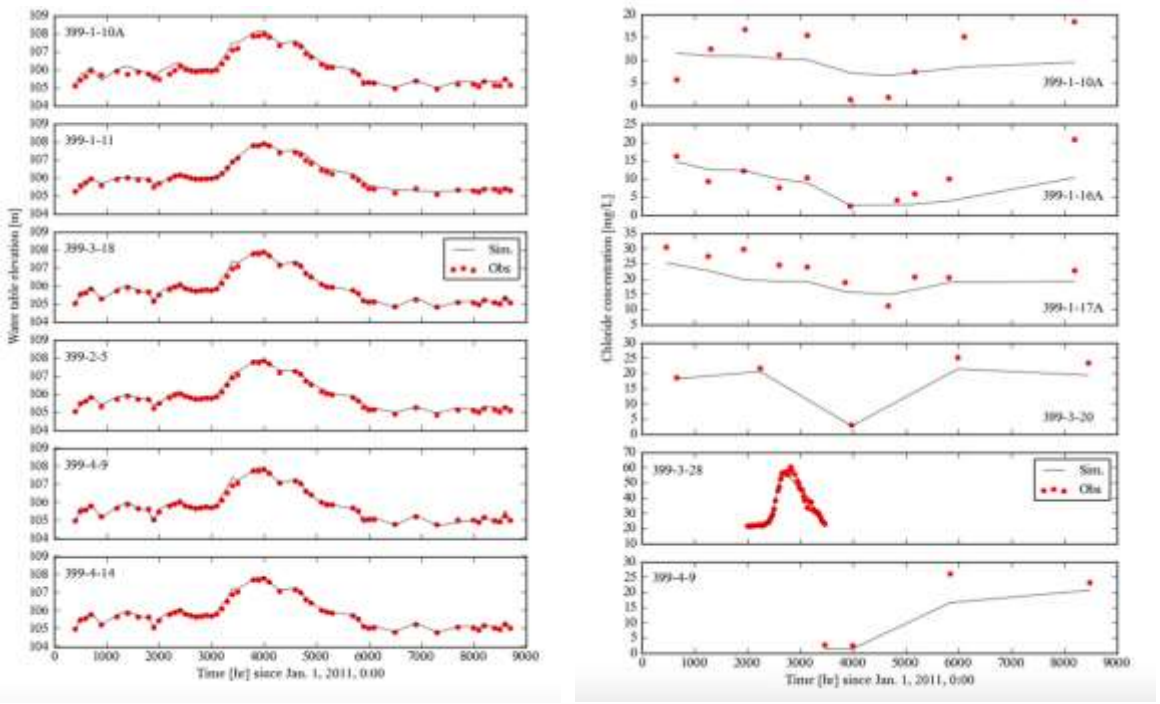

Fig. 4. Observed and simulated water levels for selected wells after pilot point optimization (left); observed and simulated chloride concentrations. Data for well 399-3-28 represent a tracer test at the IFRC well field.

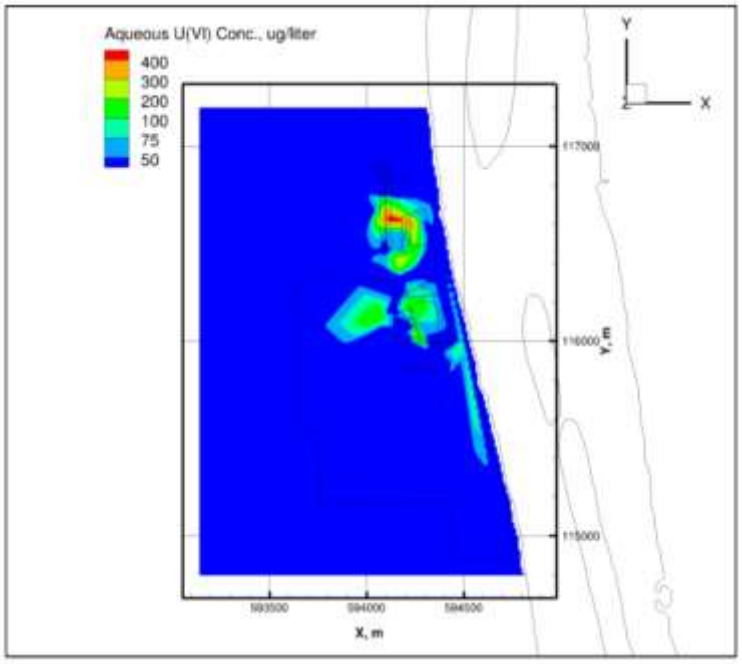

Fig. 5. Simulated aqueous uranium concentrations at the 107.5 m elevation after four days of polyphosphate infiltration.

Parallel Performance

Both the size of the 300 Area regional model and the complexity of representing the heterogeneous sediments and the Columbia River boundary warranted the use of parallel computing. Model calibration was executed using 3584 cores, utilizing 128 cores per task using the Olympus computing cluster located at Pacific Northwest National Laboratory. Olympus has 694 compute nodes (dual socket, 2.1 GHz, 16 core AMD Interlagos, with 64 GB, 1600 MHz memory), for a total of 22,208 processors, and is capable of ~185 Teraflops peak performance.

Total simulation time for the calibration was 1 week, whereas the equivalent simulation time without parallel processing would have been ~2.8 years. Model calibration would have been intractable without the use of a parallel simulator and a supercomputing environment. The strong scaling results for the uranium reactive transport simulation is shown in Fig. 6. This simulation contained 12,936,000 degrees of freedom, with 11 unknowns at each of 1,176,000 nodes in the domain. When the number of cores was increased eight-fold to 1024, the simulation time was five times faster. Large file reads to set up the boundary and initial conditions created a bottle-neck that impacted a one-to-one correspondence of the number of processor cores to the execution time.

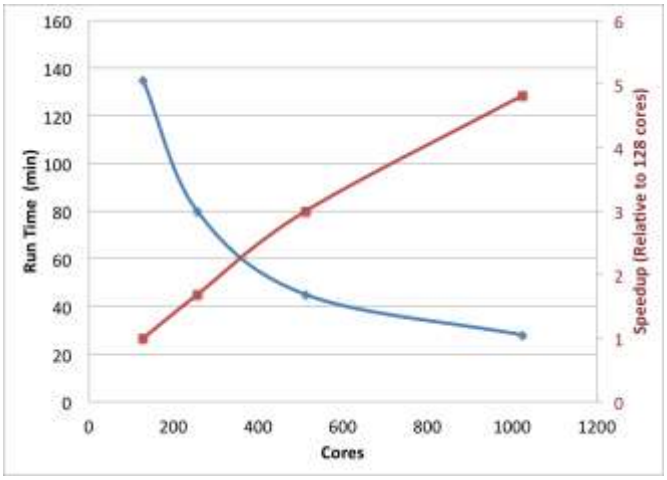

Fig. 6. Strong scaling for 300 Area simulation showing simulation times decreasing as the number of cores increases (~5 times faster on 1024 cores than on 128 cores.)

HANFORD INTEGRATED DISPOSAL FACILITY (IDF)

Low-level radioactive wastes will be retrieved from underground tanks at the Hanford Site and will be treated and vitrified at the Hanford Tank Waste Treatment and Immobilization Plant (WTP). The glass will be placed in steel containers and disposed of in a shallow trench. The trench will then be backfilled and covered with an infiltration barrier to limit percolation of meteoric water through the facility. However, before the glass can be placed in the facility, DOE must approve a PA that describes the long-term impacts of the disposal facility on public health and environmental resources. A sound scientific basis for determining the long-term release rates of radionuclides from low-activity waste (LAW) glasses is to be developed if the PA is to be accepted by regulatory agencies and stakeholders.

One input to the PA is an estimate of the radionuclide release rates from the engineered portion of the disposal facility. These estimates are based on chemical reactions in the near field and are controlled by the dissolution of the vitrified matrix. Therefore, to provide credible estimates, a mechanistic understanding of the basic physical and geochemical processes that control glass dissolution, and hence radionuclide release, must be understood and incorporated into models to effectively simulate the glass-water reaction over a 10,000 year period.

Apart from glass composition, the dissolution rate is a function of temperature, pH, and solution composition of the liquid contacting the glass. The temperature of the IDF is a known constant, 15°C. However, both the pH and the composition of the liquid contacting the glass are variables that are affected by flow rate, reactions with other engineered materials, gas-water equilibria, secondary-phase precipitation, alkali-ion exchange, and dissolution of the glass itself. Consequently, glass dissolution rates vary both in time and as a function of position in the disposal system. There is no physical constant such as a "leach rate" or radionuclide release rate parameter that can be assigned to the glass waste form because the glass will

interact with near-field materials. However, once that interaction has been quantified, a steady-state, or average release rate could be identified.

GLASS SIMULATION DESCRIPTION

The glass simulations presented in this paper are based on early simulations that were performed in 2005 to support the IDF PA [21]. Historically, glass simulations were performed using the STORM reactive transport simulator [22], which included a robust glass release algorithm and LAW glass formulations. The 2005 contaminant release calculations were performed in two dimensions, such that most of the infiltrating water travelled around the vitrified waste packages. For radionuclides, the key groundwater risk driver was ^{99}Tc.

To demonstrate eSTOMP capabilities, and to transition the use of the legacy STORM simulator to eSTOMP (NQA-1 qualified) for simulating glass dissolution, the 2005 simulation was re-executed for the LAWA44 glass. One of the goals of the eSTOMP simulations was to benchmark the results against the STORM results obtained in 2005. Details of the reactive transport simulation setup are not presented here, but can be found in Bacon and McGrail [21]. Detailed results of the comparison between eSTOMP and STORM simulations can be found in Pierce et al. [23-24].

The glass simulation domain was set up as a 2-D vertical stack of four waste packages near the center of a single trench (Fig. 7). The WTP glass waste packages are 2.3 m tall, 1.22 m wide, and filled with glass to a height of 1.96 m. The layers in the IDF trench were assumed to be 1 m apart vertically, while waste packages were spaced 30 cm apart horizontally. Since the waste packages will not likely be perfectly aligned horizontally, waste packages were offset horizontally 10 cm relative to the waste package above or below. The computational grid was set at 2 cm in vertical resolution, resulting in 67,640 nodes. With a total of 15 conservation equations, this model setup resulted in 1,014,600 total unknowns at each time step during the simulation.

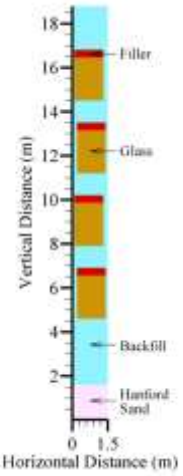

Fig. 7. Lithographic units for the glass waste form release simulation.

For each lithographic unit, a list of the solid species that make up the unit were required, as well as the relative volume and specific surface area for these variables for each solid within the lithographic unit. For Hanford sands and backfill soil, petrologic and particle-size data were obtained from the near-field hydrology data package [25]. The specific surface area was inferred from the particle-size data. The hydraulic properties for each lithographic unit in the simulation were determined in the near-field hydraulics data package [25] or the far-field hydraulic properties data package [26]. A summary of these values can be found in Bacon and McGrail [21].

Boundary Conditions

The upper boundary is located just beneath the engineered barrier system and was assigned a specified flux. A range of water flux rates, 0.1 to 4.2 mm/yr, was used at the top boundary to represent the upper bound of the recharge rate anticipated at the facility [27]. The location of the lower model boundary was selected so that horizontal gradients would be small. The lower boundary was a free drainage boundary 4.5 m below the lowest layer of backfill. For hydraulic boundary conditions at this lower boundary, free drainage under gravity was also assumed. Also, the side boundaries are placed at axes of symmetry so that no-flow boundaries could be assumed. A constant subsurface temperature, equal to the average ambient temperature of 15^{o}C, was applied. The dissolved gas content of the aqueous phase was assumed to be negligible with respect to flow. The relative humidity of the gas phase was assumed to be 100%.

Geochemical System

The eSTOMP simulation incorporated the geochemical reaction network needed to model the weathering of the LAWA44 glass. The reaction network included the kinetic reactions, equilibrium reactions, mineral species, and aqueous species used previously in the STORM simulations (see Bacon and McGrail [21]). A total of 36 aqueous (and gas) species were included in the simulation, as well as 13 solid-aqueous phase reactions. An alkali ion-exchange reaction was also included for the glass. For the dissolution reaction involving glass, a forward rate law was used based on a TST formulation. This reaction is an approximation for glass because glass is metastable, and the reaction proceeds one way (i.e., glass dissolves). Parameters for the rate law have been determined for ILAW glasses [28] and their values can be found in Bacon and McGrail [21].

Model Output

The goal of the reactive transport modeling was to obtain the flux of technetium-99 (^{99}Tc) to the vadose zone from the glass waste packages. Once this flux rate was obtained, it could be used in more simplified simulations that determine the far-field transport of the conservatively transported ^{99}Tc. Fig. 8 shows the estimated flux rates for a range of the simulated recharge rates, as well as the pH distribution throughout the domain.

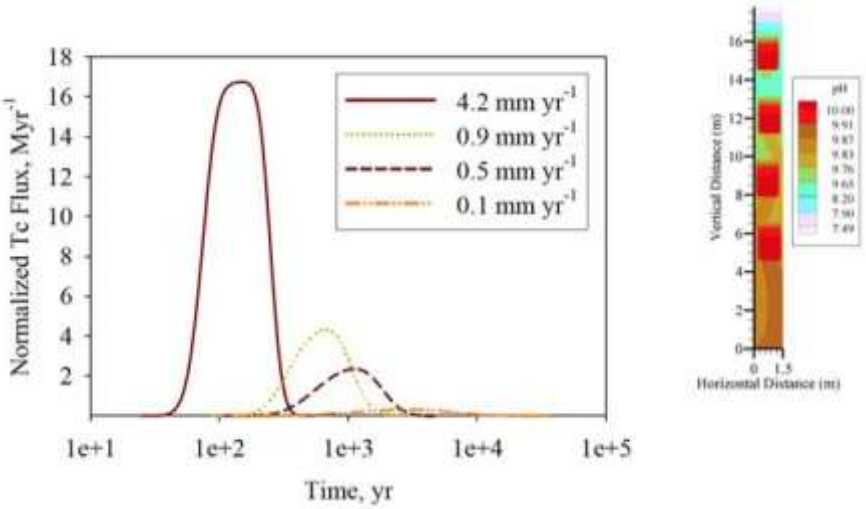

Fig. 8. Estimated ^{99}Tc flux rates and pH distribution.

Parallel Performance

This section presents the parallel performance of the eSTOMP simulator for the 2D glass simulation. Fig. 9 shows the strong scaling behavior of the coupled reactive transport simulation containing over a million degrees of freedom executed on the Olympus supercomputer. To test scaling, the glass dissolution was simulated for a period of 1 year, which involved 2145 time steps. When executed on a single core, the simulation completed in 53 hours. On 384 cores, the simulation completed in less than 30 minutes, nearly 150 times faster than the serial execution.

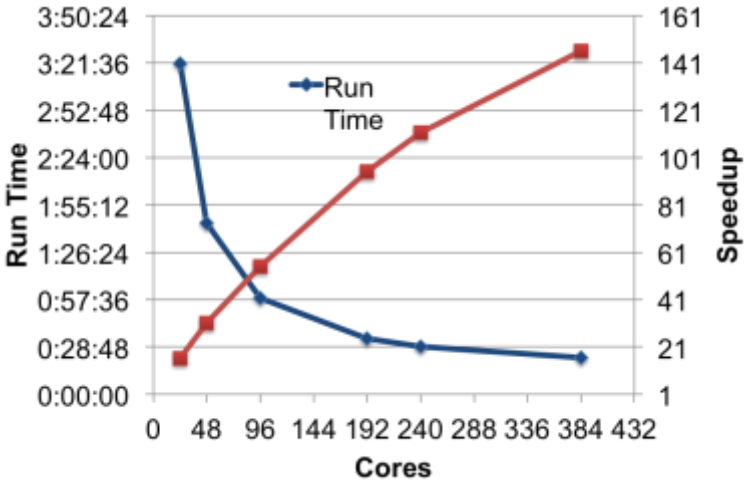

Fig. 9. Strong scaling for glass simulation showing simulation times decreasing as the number of cores increases (~150 times faster on 384 cores than on single core)

Because eSTOMP has been qualified as safety software under DOE Order 414.1C, both application models can also be used to make site management decisions within a regulatory framework. These types of models can also be used to address "what if" questions regarding different remediation endpoints, and to assist in both facility design and evaluation of field remediation efforts.

CONCLUSIONS

eSTOMP is the parallel version of the STOMP simulator, and can be executed on any Linux-based computing system. Both the Global Arrays and PETSc libraries are required for code compilation. Because STOMP and eSTOMP input files are identical, many of the details of the parallel implementation are hidden from the user. Two applications using the eSTOMP simulator have been presented and demonstrate that parallel execution was critical to simulation execution. The regional-scale model of the 300 Area was developed to be a decision-support tool to evaluate processes of the total system affecting the groundwater uranium plume. The sheer size of the domain and memory requirements warrants the use of a parallel simulator. Because the glass simulation had smaller domain and could be executed on a single processor, the long simulation times also warranted the use of parallel processing. Faster execution times not only translate to an ability to capture needed complexity, but also make quantifying uncertainty (e.g., multiple simulations, alternative conceptual models) and performing model calibration obtainable. For example, the glass simulation presented in this paper was accelerated 150-fold by taking advantage of parallel computing. If similar increases in speed can be obtained for even small, less complex simulations, the amount of time saved in simulation execution can significantly change the modeling approach and analysis.

REFERENCES

1. G. H. DE MARSILY, F. DELAY, J. GONCALVES, P. H. RENARD, V. TELES, and S. VIOLETTE, "Dealing with spatial heterogeneity," *Hydrogeology Journal*, 13, 161-183 (2005).
2. T.D. SCHEIBE, E. M. MURPHY, X. CHEN, A. K. RICE, K. C. CARROLL, B. J. PALMER, A. M. TARTAKOVSKY, I. BATTIATO, and B. D. WOOD, "An Analysis Platform for Multiscale Hydrogeologic Modeling with Emphasis on Hybrid Multiscale Methods," *Groundwater* 53, 38-56 (2015).
3. S. B. YABUSAKI, Y. FANG, K. H. WILLIAMS, C. J. MURRAY, A. L. WARD, R. DAYVAULT, S. R. WAICHLER, D. R. NEWCOMER, F. A. SPANE, and P. E. LONG, "Variably Saturated Flow and Multicomponent Biogeochemical Reactive Transport Modeling of a Uranium Bioremediation Field Experiment," *Journal of Contaminant Hydrology,* 126, 3-4, 271-290 (2011). doi:10.1016/j.jconhyd.2011.09.002
4. M.D. WHITE and M. OOSTROM. *STOMP Subsurface Transport Over Multiple Phases Version 2.0 Theory Guide,* PNNL-12030 UC-2010, Pacific Northwest National Laboratory, Richland, WA (2000).
5. M. D. WHITE, D. APPRIOU, D. H. BACON, Y. FANG, V. FREEDMAN, M. L. ROCKHOLD, C. RUPRECHT, G. TARTAKOVSKY, S. K. WHITE, and F. ZHANG,

2015, *eSTOMP Online User Guide* (2015). Available at: http://stomp.pnnl.gov/estomp_guide/eSTOMP_guide.stm.
6. J. NIEPLOCHA, B. PALMER, V. TIPPARAJU, M. KRISHNAN, H. TREASE and E. APRA. "Advances, Applications and Performance of the Global Arrays Shared Memory Programming Toolkit." International Journal of High Performance Computing and Applications, 20,2 (2006).
7. M. D. WHITE and B. P. MCGRAIL, *STOMP Subsurface Transport Over Multiple Phases Version 1.0 Addendum: ECKEChem Equilibrium-Conservation-Kinetic Equation Chemistry and Reactive Transport*, PNNL-15482, Pacific Northwest National Laboratory, Richland, WA (2005).
8. Y. L. FANG, G. T. YEH, and W. D. BURGOS, "A General Paradigm to Model Reaction-based Biogeochemical Processes in Batch Systems," *Water Resources Research* 39, 4, Art. No. 1083.c (2003).
9. R. E. PETERSON (ed.), *Uranium Contamination in the Subsurface Beneath the 300 Area, Hanford Site, Washington*, PNNL-17034. Pacific Northwest National Laboratory, Richland, WA (Contributors: R. E. Peterson, M. L. Rockhold, R. J. Serne, P. D. Thorne, and M. D. Williams) (2008).
10. J. M. ZACHARA (ed.), *Uranium Geochemistry in Vadose Zone and Aquifer Sediments from the 300 Area Uranium Plume*, PNNL-15121, Pacific Northwest National Laboratory, Richland, WA (Contributors: J. A. Davis, C. Liu, J. P. McKinley, N. Qafoku, D. M. Wellman, and S. B. Yabusaki) (2005).
11. J. M. ZACHARA, C. F. BROWN, J. CHRISTENSEN, P. E. DRESEL, S. KELLY, J. P. MCKINLEY, R. J. SERNE, and W. UM, *A Site-Wide Perspective on Uranium Geochemistry at the Hanford Site*, PNNL-17031, Pacific Northwest National Laboratory, Richland, WA (2007).
12. J. M. ZACHARA, M. D. FRESHLEY, G. V. LAST, R. E. PETERSON, and B. N. BJORNSTAD, *Updated Conceptual Model for the 300Area Uranium Groundwater Plume*, PNNL-22048, RPT-DVZ-AFRI-007, Pacific Northwest National Laboratory, Richland, WA (2012).
13. DOE-RL, *Phase 1 Remedial Investigation Report for the 300-FF-5 Operable Unit,* DOE/RL-93- 21, Rev. 0, Vols. 1 (information) and 2 (data listings), U.S. Department of Energy, Richland Operations Office, Richland, WA (1994).
14. DOE-RL, *Remedial Investigation/Feasibility Study Report for the 300-FF-5 Operable Unit*, DOE/RL-94-85, U.S. Department of Energy, Richland Operations Office, Richland, WA (1994).
15. D. L. STOLIKER, D. B. KENT, and J. M. ZACHARA, "Quantifying differences in the impact of variable chemistry on equilibrium uranium(VI) adsorption properties of aquifer sediments," *Environmental Science & Technology* 45, 8733-8740 (2011).
16. V. R. VERMEUL, J. P. MCKINLEY, D. R. NEWCOMER, R. D. MACKLEY, and J. M. ZACHARA, "River-induced flow dynamics in long-screen wells and impact on aqueous samples," *Groundwater* 49, 515-524 (2011).
17. M. L. ROCKHOLD, D. H. BACON, V. L. FREEDMAN, K. R. PARKER, S. R. WAICHLER, and M. D. WILLIAMS, *System-Scale Model of Aquifer, Vadose Zone, and River Interactions for the Hanford 300 Area - Application to Uranium Reactive Transport*, PNNL-22886, RPT-DVZ-AFRI-019, Pacific Northwest National Laboratory, Richland, WA (2013).

18. M. D. WILLIAMS, M. L. ROCKHOLD, P. D. THORNE, and Y. CHEN, *Three-dimensional groundwater models of the 300 Area at the Hanford Site, Washington State*, PNNL-17708, Pacific Northwest National Laboratory, Richland, WA (2008).
19. J. E. DOHERTY and R. J. HUNT, *Approaches to highly parameterized inversion – A guide to using PEST for groundwater-model calibration*, U.S. Geological Survey Scientific Investigations Report 2010-5169 (2010).
20. M. L. ROCKHOLD, D. L. SAUNDERS, C. E. STRICKLAND, S. R. WAICHLER, and R. E. CLAYTON, *Soil Water Balance and Recharge Monitoring at the Hanford Site – FY09 Status Report*, PNNL-18807, Pacific Northwest National Laboratory, Richland, WA (2009).
21. D. H. BACON and B. P. MCGRAIL, *Waste Form Release Calculations for the Integrated Disposal Facility,* PNNL-15198, Pacific Northwest National Laboratory, Richland, WA (2005).
22. D. H. BACON, M. D. WHITE, and B. P. MCGRAIL, *Subsurface Transport Over Reactive Multiphases (STORM): A Parallel, Coupled, Nonisothermal Multiphase Flow, Reactive Transport, and Porous Medium Alteration Simulator, Version 3.0*, PNNL-14783, Pacific Northwest National Laboratory, Richland, WA (2004).
23. E. M. PIERCE, D. H. BACON, S. N. KERISIT, C. F. WINDISCH, Jr, K. J. CANTRELL, M. M. VALENTA, S. D. BURTON, and J. H. WESTSIK, Jr, *Integrated Disposal Facility FY2011 Glass Testing Summary Report*, PNNL-20781, Pacific Northwest National Laboratory, Richland, WA (2011).
24. E. M. PIERCE, S. N. KERISIT, E. J. KROGSTAD, S. D. BURTON, B. N. BJORNSTAD, V. L. FREEDMAN, K. J. CANTRELL, M. M. V. SNYDER, J. V. CRUM, and J. H. WESTSIK, Jr, *Integrated Disposal Facility FY 2012 Glass Testing Summary Report*, PNNL-21812 Rev. 1, Pacific Northwest National Laboratory, Richland, WA (2013).
25. P. D. MEYER, K. P. SARIPALLI, and V. L. FREEDMAN, *Near-Field Hydrology Data Package for the Integrated Disposal Facility 2005 Performance Assessment*, PNNL-14700, Pacific Northwest National Laboratory, Richland, WA (2004).
26. R. KHALEEL, *Far-Field Hydrology Data Package for the Integrated Disposal Facility Performance Assessment*, RPP-20621, Rev. 0, CH2M Hill Hanford Group, Richland, WA (2004).
27. M.J. FAYER and SZECSODY, *Recharge Data Package for the 2005 Integrated Disposal Facility Performance Assessment*, PNNL-14744, Pacific Northwest National Laboratory, Richland, WA (2004).
28. E. M. PIERCE, B. P. MCGRAIL, E. A. RODRIGUEZ, H. T. SCHAEF, K. SARIPALLI, R. J. SERNE, P. F. MARTIN, S. R. BAUM, K. N. GEISZLER, L. R. REED, and W. J. SHAW, *Waste Form Release Data Package for the 2005 Integrated Disposal Facility Performance Assessment*, PNNL-14805, Pacific Northwest National Laboratory, Richland, WA (2004).