Sandia National Laboratories

Newton Trust-Region Applied to Porous Media Flow and Transport

Heeho Park[1], Glenn Hammond[2], Albert Valocchi[3]

[1]Sandia National Laboratories, [2]Pacific Northwest National Laboratory, [3]University of Illinois at Urbana-Champaign

Introduction

Numerical simulation of non-isothermal multiphase porous flow combined with reactive transport is used in a wide range of applications, which include *nuclear waste repositories*, enhanced recovery of petroleum reservoirs, contaminant remediation, geothermal engineering, carbon sequestration, and hydrogen storage. The simulation is well known to be computationally demanding especially for field-scale simulations. These challenges arise from: (1) presence of small scale engineered features like shafts, tunnels, and barriers; (2) heterogeneity in the domain and strong contrast in material properties such as permeability, porosity; (3) the nonlinear constitutive relations; (4) any perturbation in the domain caused by human activity like boiling caused by heat source of nuclear waste, dry-out condition by injection of gas, or precipitation and dissolution by injection of chemicals. For these large-scale practical problems, we observed that many Newton-Raphson (NR) iterations failed to converge due to oscillatory behavior. This problem is causing unacceptably large computational time due to lack of growth in time step sizes in the simulator. Newton trust-region (NTR) method largely reduces the oscillatory behavior by truncating the NR update within the quadratic model trust-region of the objective function. The demonstration of the effectiveness of NTR is done by PFLOTRAN, an open-source massively parallel porous media reactive flow code and the implementation of NTR is done in PETSc, portable, extensible toolkit for scientific computation.

Newton Trust-Region Dogleg Cauchy

Newton Trust-Region Dogleg Cauchy (NTRDC) works in a way that first defines a region around the current best solution in which a quadratic model can, to some extent, approximate the original objective function (Park et al., 2021)

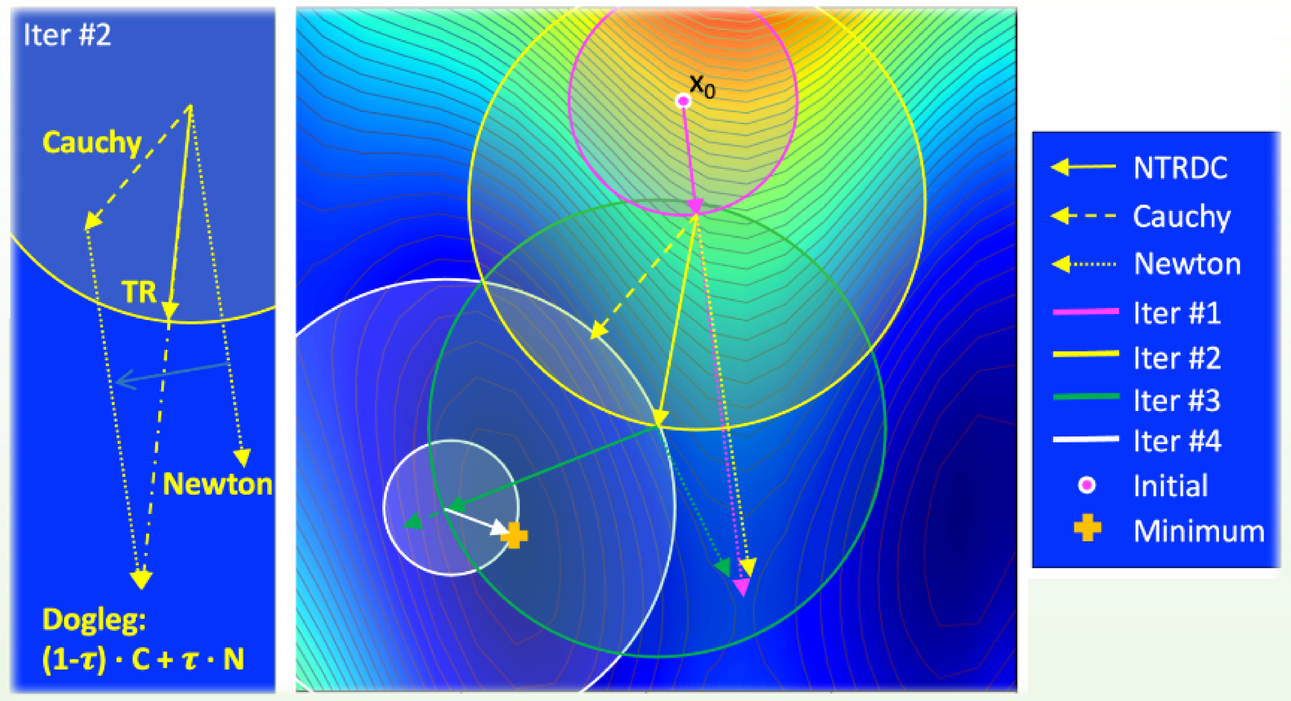
$$f(u) := \frac{1}{2}||F(u)||_2^2 : \mathbb{R}^n \to \mathbb{R}.$$

$F(u)$: original objective function

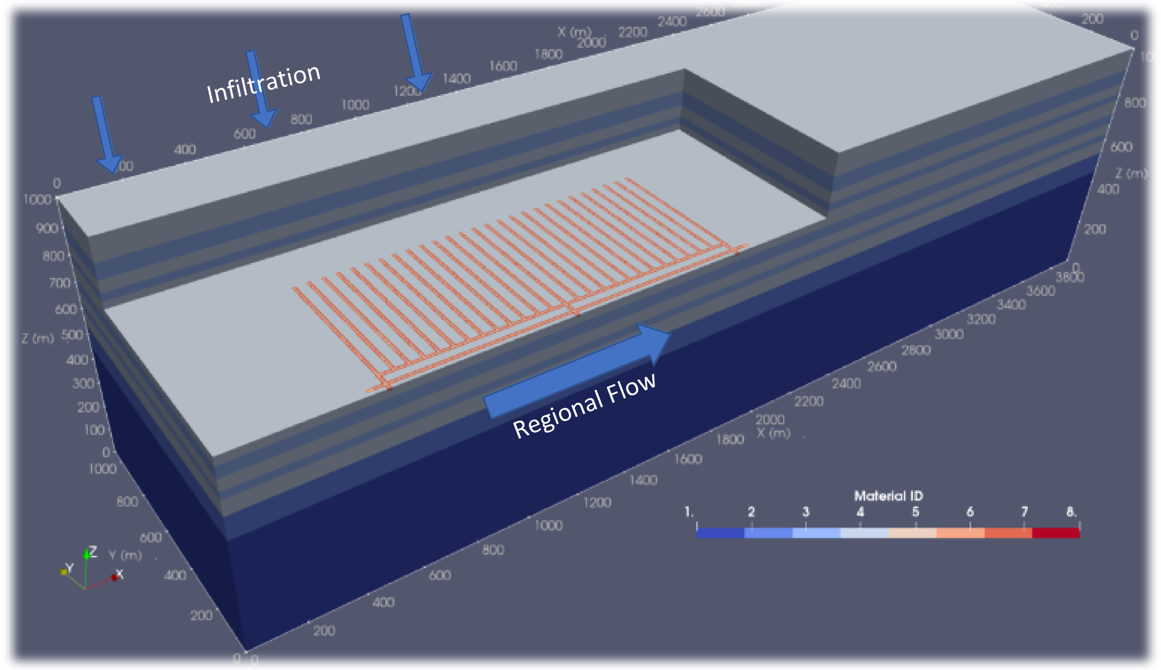
$f(u)$: 2-norm

We want to find a solution $\vec{p}$ that is within the step size of Δ that minimizes the quadratic model m.

$$m_k(\vec{p}) = f_k + g_k^T \vec{p} + \frac{1}{2}\vec{p}^T B_k \vec{p} \;\; s.t. \;\; ||\vec{p}|| <= \Delta_k$$



Challenges

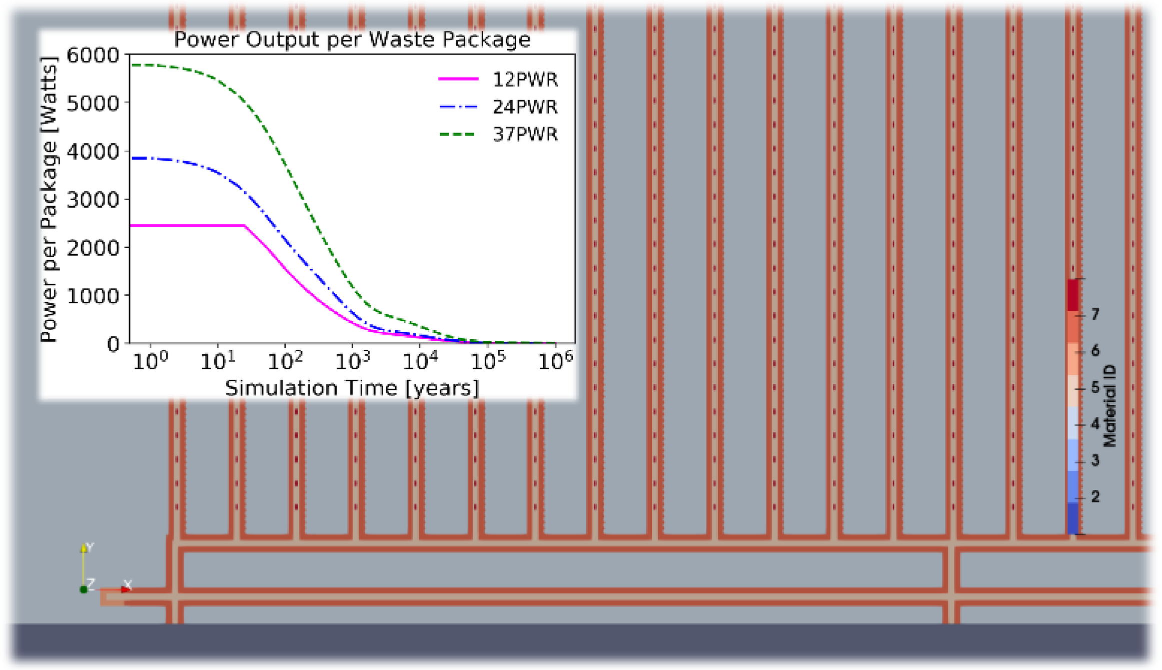


Cropped view of the symmetric simulation domain of hypothetical Alluvial unsaturated zone radioactive waste repository.

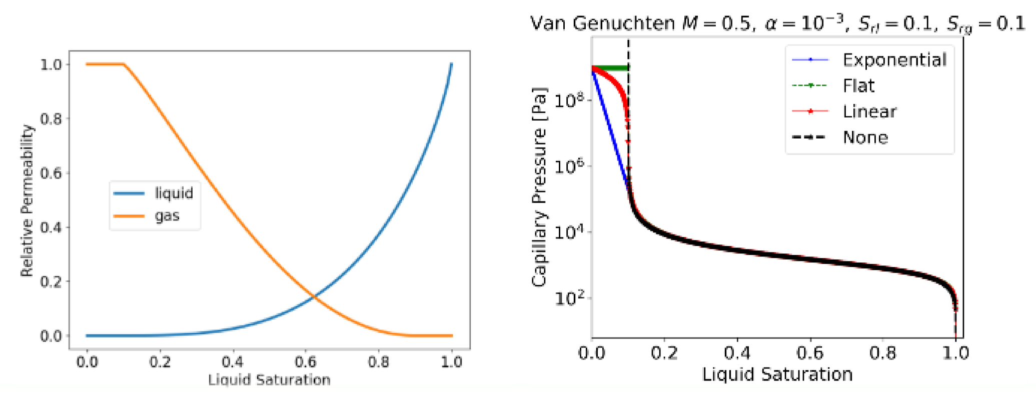
2.4M grid cells
7.2M unknowns

Meshed by: Emily Stein (Park et al., 2022)

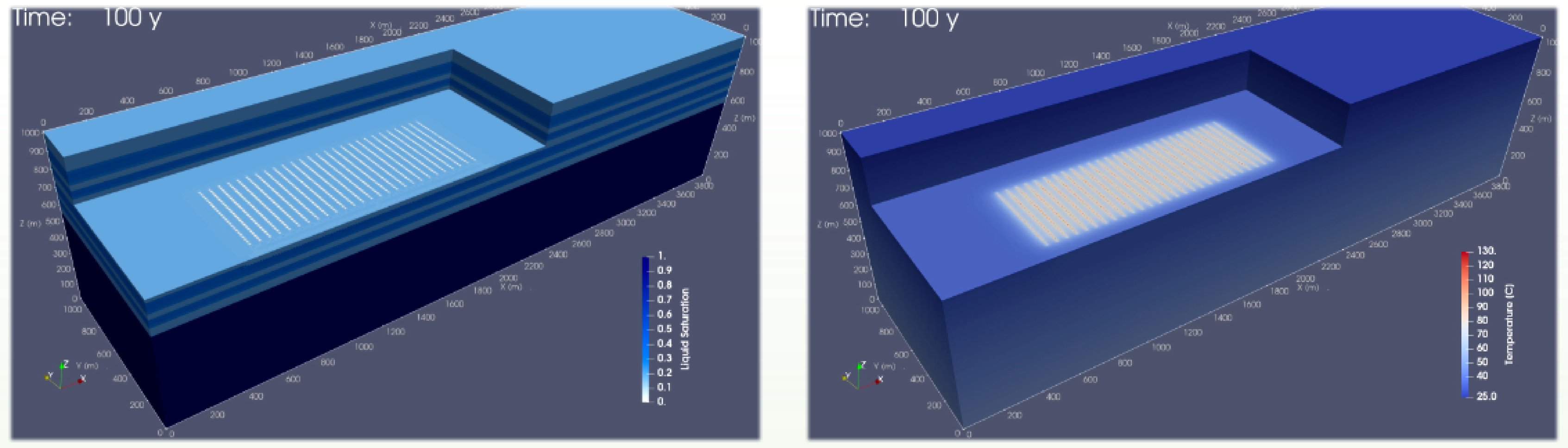
Material ID
1: Lower basin
2: Aquifer
3: Upper basin (UB, low perm.)
4: Upper basin (high permeability)
5: Backfill
6: UB DRZ (low permeability)
7: UB disturbed rock zone (DRZ)
8: Waste package



- Radioactive waste geologic disposal system
- Heterogeneous geologic features, infiltration, and regional flow
- Small discrete features like shafts, tunnels, waste packages, and backfills
- Discrete and large contrasts in porosity and permeability



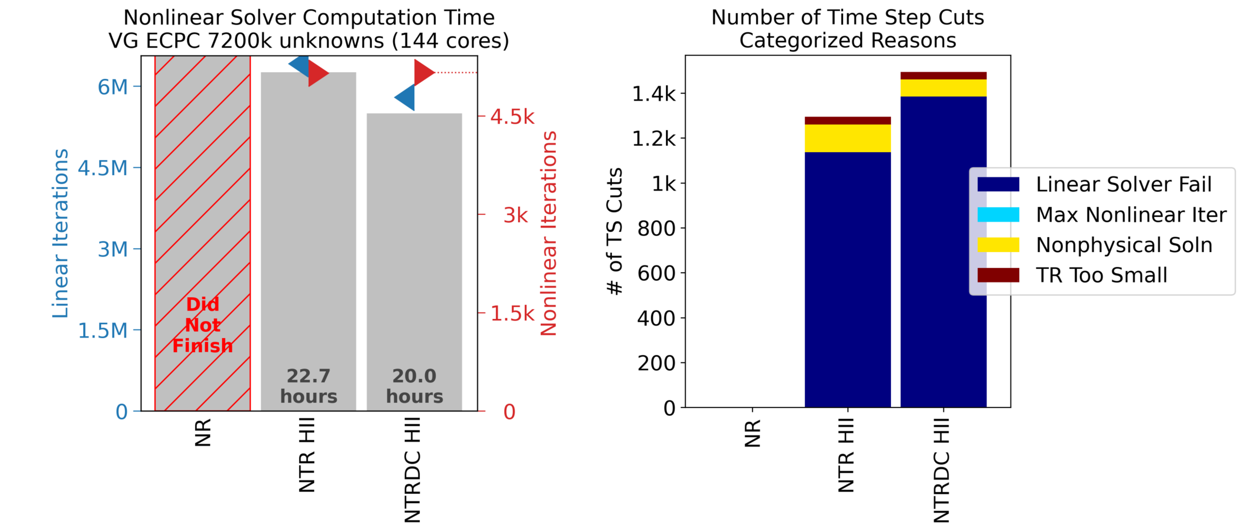
- High decay temperatures from radioactive wastes
- Heat-forced dry-out and re-saturation by natural forces
- Testing extreme nonlinearities on both ends of the capillary pressure and relative permeability curve



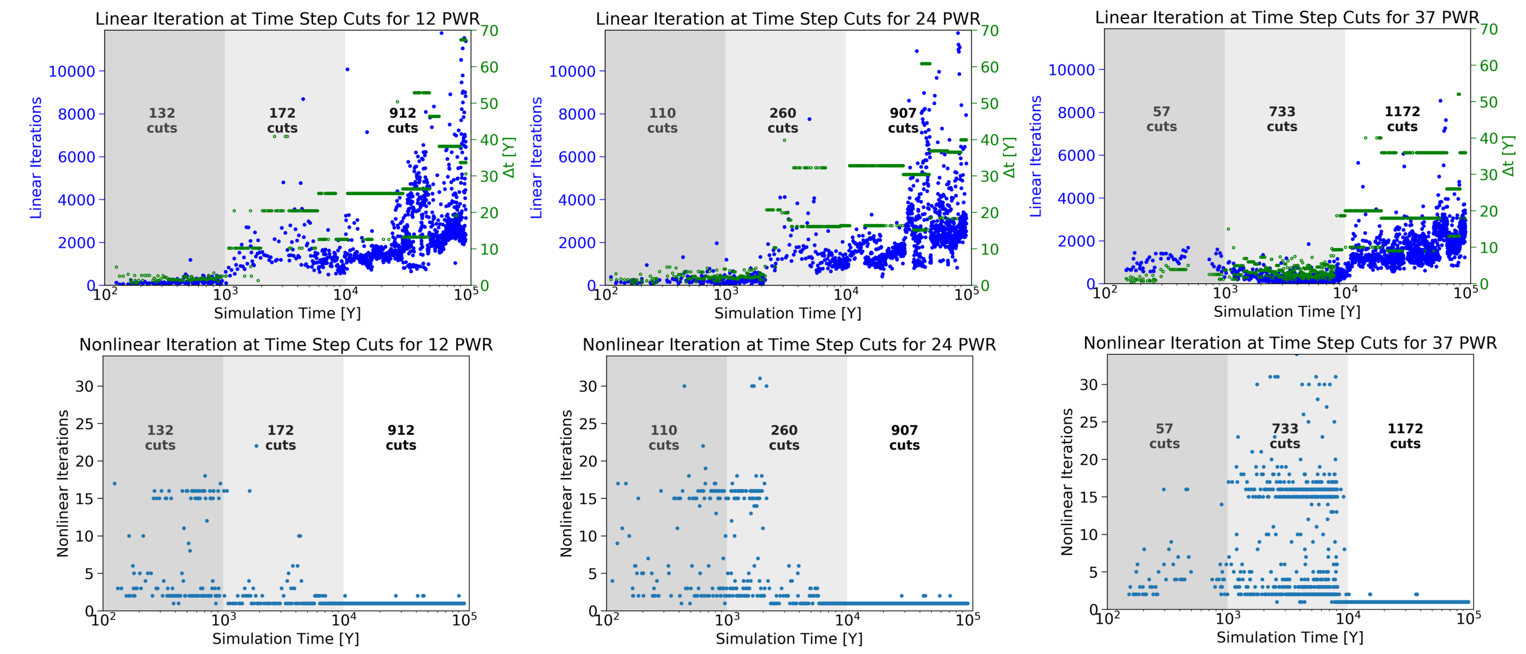
References

- Park H., et al. (2021), Linear and nonlinear solvers for simulating multiphase flow within large-scale engineered subsurface systems, Advances in Water Resources, DOI: 10.1016/j.advwatres.2021.104029
- Park H., et al. (2022), Newton trust-region methods with primary variable switching for simulating high temperature multiphase porous media flow, Advances in Water Resources, DOI: 10.1016/j.advwatres.2022.104285

Full-scale Flow Model and Solver Behavior

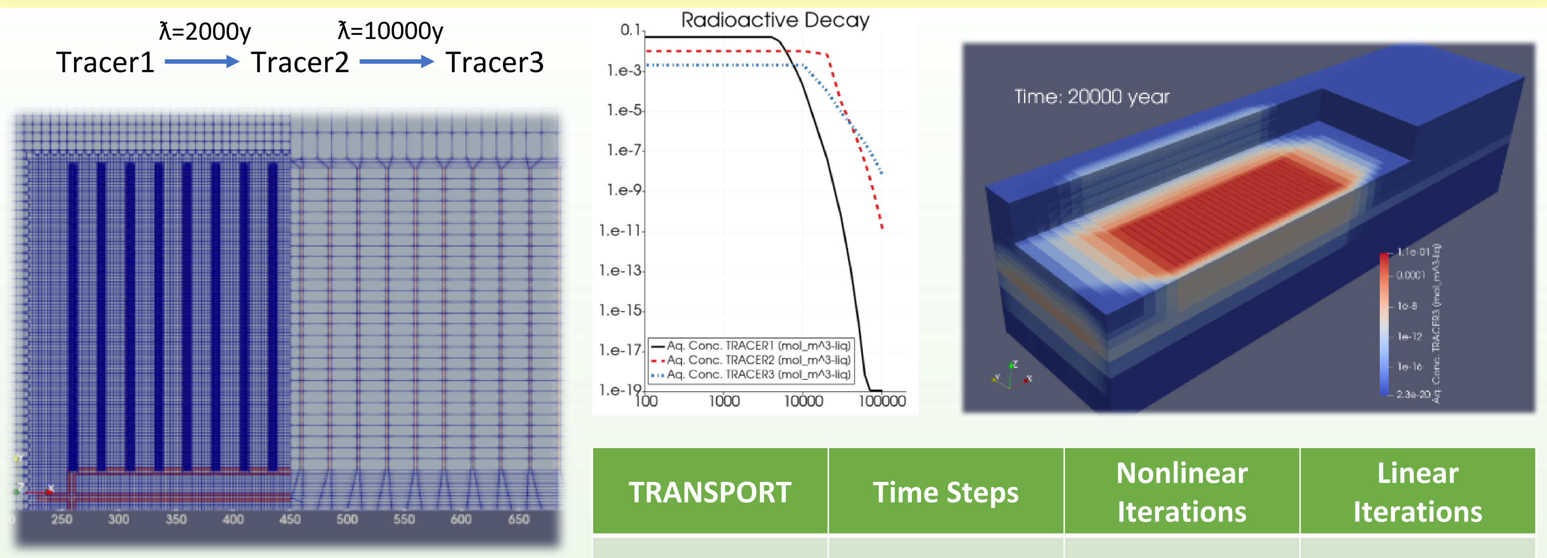


The fully-refined 12 PWR model computational wall clock time with 144 cores. Newton solver was not able to complete this simulation with 144 cores in 96 h because it could not resolve all the state changes that occur near the peak temperature in the simulation. 40,000 non-physical solution time step cuts were recorded for Newton in 96 h of the incomplete simulation. (Park et al., 2022)



The time history of nonlinear iterations after time step cuts, linear iterations and time step size for the fully-refined model run with NTR. The top figures show the number of linear iterations and the time step size after the time cuts, Δt [Y]. The bottom figures show the time history of time step cuts and the number of nonlinear iterations needed to complete the time step after one or more time step cuts for the three different power levels of the radioactive wastes. The 37 PWR (highest power output) had the greatest number of cuts, but had the shortest overall computation time because the average number of linear iterations required to complete the time step was the lowest. Resaturation of the repository area was easiest to resolve nonlinear constitutive relations for the 37 PWR case because it generated the largest pressure and saturation gradient among the three cases.

Coarse Flow and Transport Model



The coarse model was used for this study to better understand transport behavior of the model.

TRANSPORT	Time Steps	Nonlinear Iterations	Linear Iterations
Newton	20966	130742	130742
NTRDC	21293	65882	72955

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology &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.
SAND No. ____________

Sandia National Laboratories