An Overview of New Monte Carlo Capabilities in SCALE: The *Shift* Monte Carlo Code

Gregory Davidson

HPC Methods and Applications Team
Elliott Biondo
Thomas Evans (Team Lead)
Steven Hamilton
Seth Johnson
Tara Pandya

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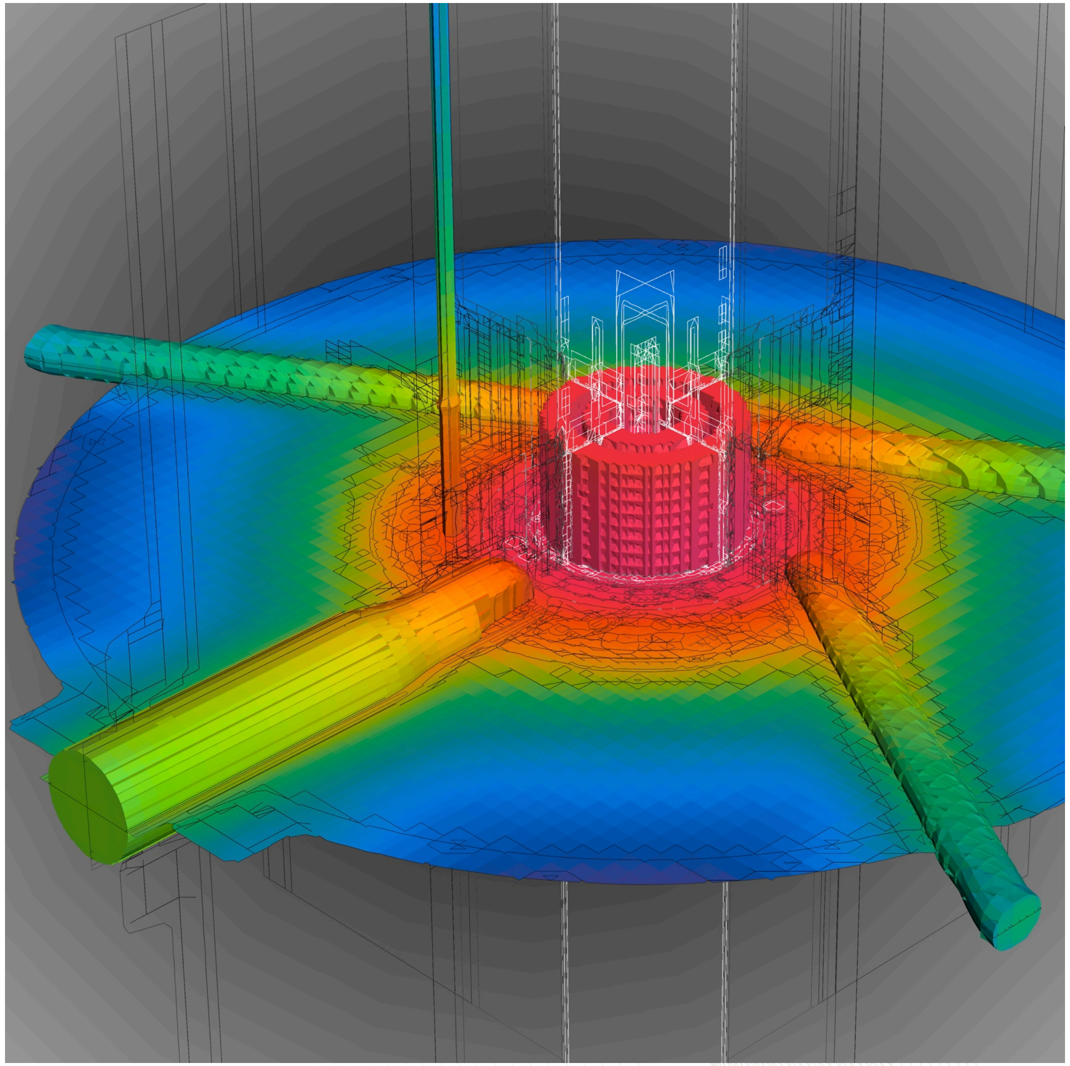
Outline

- Radiation transport development at ORNL
- Overall description of the Exnihilo code suite
- Ongoing development efforts in Shift
  - Scalable tallies
  - Hybrid methods
  - Sourcerer
  - Depletion
- Current ongoing work on Shift-SCALE integration
- Shift and CASL'S VERA core simulator



General computational transport methods

- **Deterministic methods**
  - Solve the Boltzmann transport equation for average particle behavior in a discretized system
  - Produce system-wide solutions with detailed information throughout problem space
  - Computationally inexpensive
  - Accuracy limited by discretization approximations
- **Stochastic or "Monte Carlo" methods**
  - Simulate individual particles and infer average particle behavior from the average behavior of the simulated particles
  - Tally results in pre-determined regions of problem space
  - Computationally expensive
  - Accuracy limited only by the physics, geometry and material approximations used in the simulations
- **Hybrid methods**
  - Use fast, approximate deterministic simulations to speed-up highly accurate Monte Carlo simulations
    - Calculate 3D adjoint (importance) and/or forward functions with deterministic simulations
    - Calculate variance reduction parameters based on deterministic solutions (source and weight window parameters)
    - Utilize the variance reduction parameters to focus the Monte Carlo simulation on "important" particles
    - Automate above steps (key to usefulness)
  - ***ORNL holds a strong leadership position in this area – signature capabilities***

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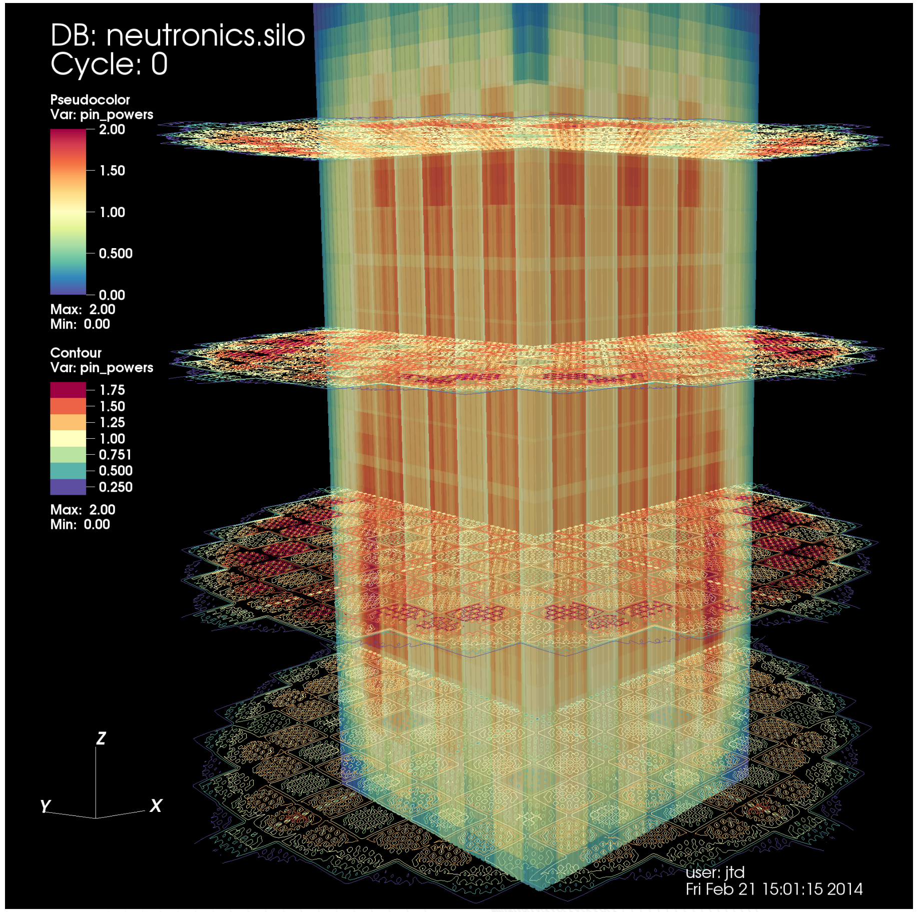
Application-Driven Methods Development

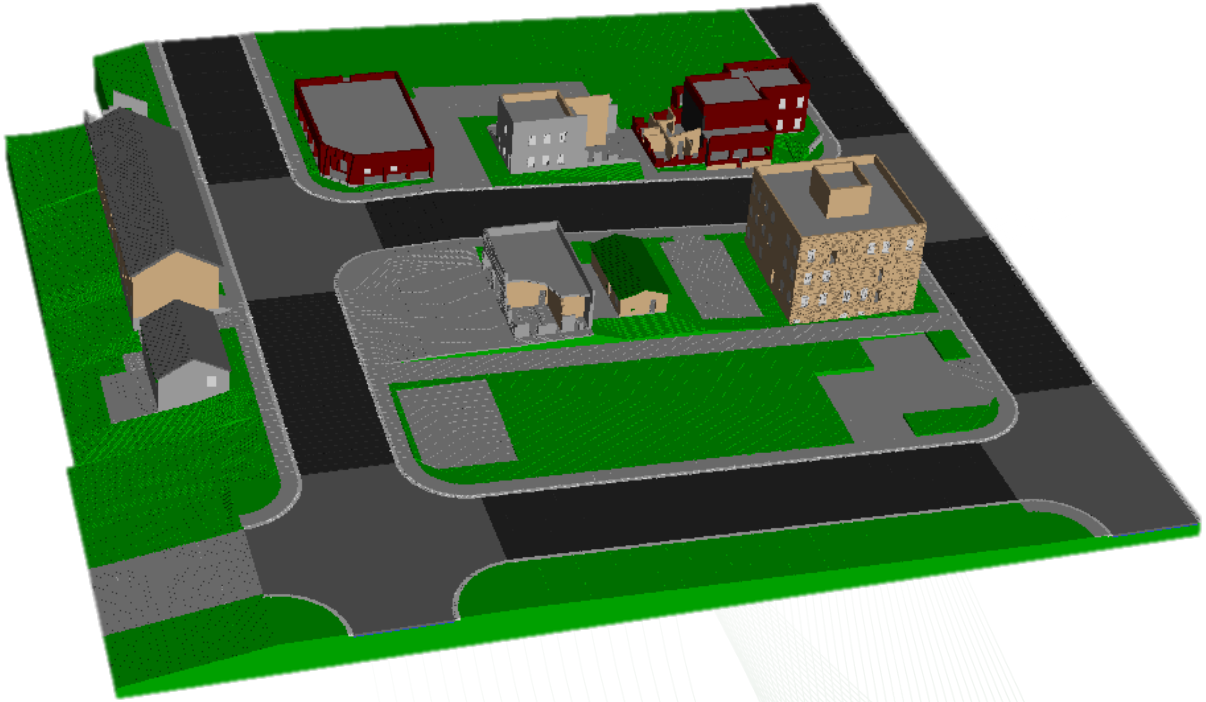
- Research and Development driven by application needs
- Requires close interaction/collaboration with users
  - We have a long history of tightly integrated application development teams
- Motivates the development of methods that enable the solution of problems previously thought impossible



User-developer interaction is an ORNL core strength

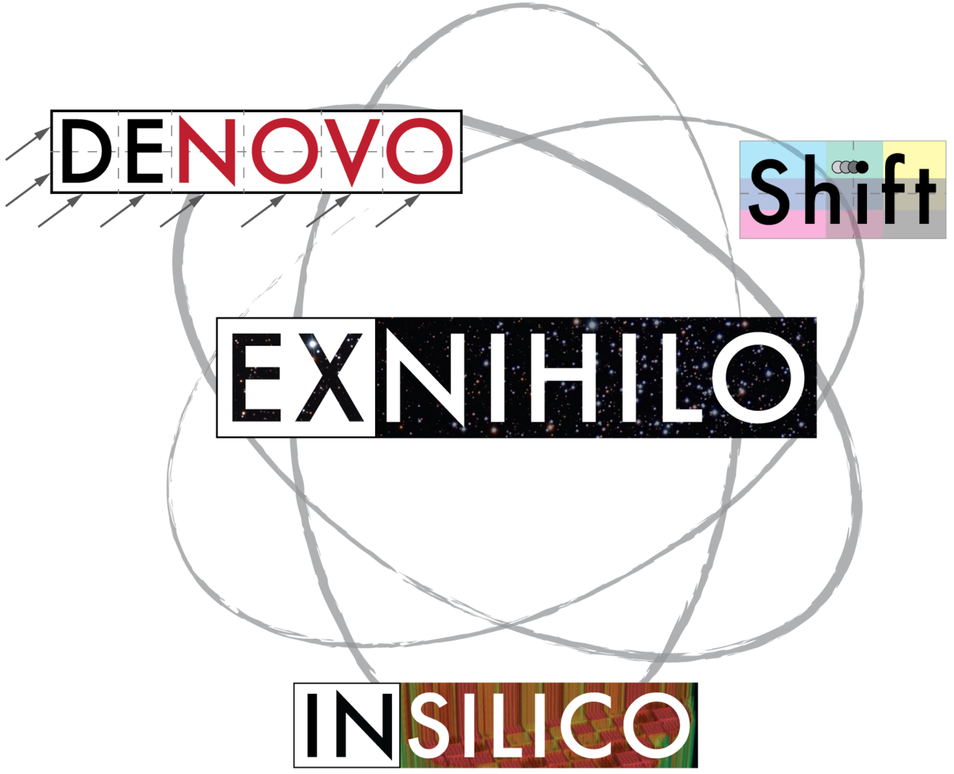
Drivers for transport methods development

- Difficult modeling problems in radiation transport generally feature the following:
  - Geometric complexity
  - Deep penetration (large flux gradients)
  - Spectral resolution
  - Global solutions
  - Large distributed sources
- Generally, no single method will provide high-fidelity solutions on problems with these requirements



The Exnihilo Code Suite

- Provide a parallel, component library for transport application development on HPC platforms
- Provide pre- and post-processing tools integrated with ***Jupyter notebook***
- Leverage existing functionality from other libraries: **SCALE**, **Trilinos, HDF5**
- Internal GitLab code repository and issue tracking: https://code-int.ornl.gov/exnihilo/Exnihilo



Language	Executable	Test
C++	247 969	250 840
Python	29 690	17 460
C	1 559	—
Fortran	936	55

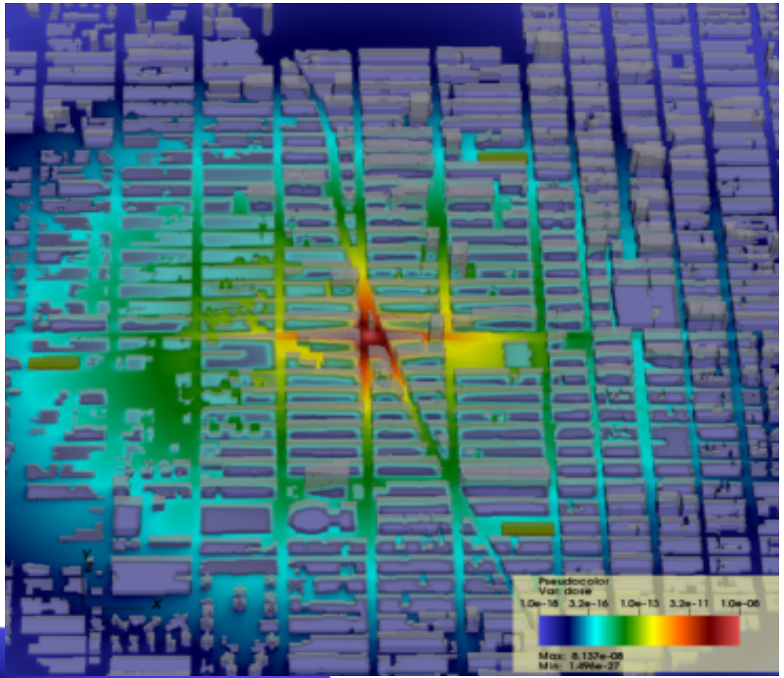
Denovo: deterministic solvers including S_N and SP_N

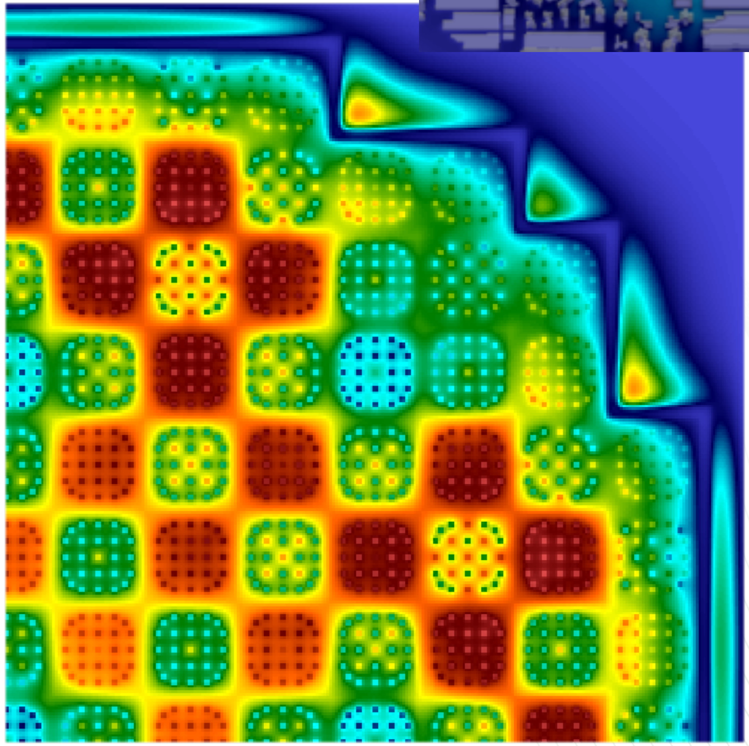
Shift: Monte Carlo solver (multiple physics and geometry options)

Insilico: Neutronics front-end for reactor physics (CASL) – employs Shift or Denovo solvers

Denovo Overview
(Deterministic solutions for MC acceleration)

- High-performance S_N, SP_N, and MOC solvers on a distributed Cartesian Mesh
  - Mesh is automatically generated on any geometry using Exnihilo's parallel ray tracer
  - Materials are volume-mixed in each Cartesian cell
  - Cross sections are generated using the SCALE XSProc sequence
- Fixed-source and eigenvalue solvers
- Multigroup energy, anisotropic P_N scattering
- Forward/Adjoint
- Features parallel decomposition over both spatial domains and energy groups, enabling scaling to *O(100k)* cores
- GPU-accelerated implementation of S_N (provides ~6x speedup)
- Denovo MOC solver currently used in Polaris





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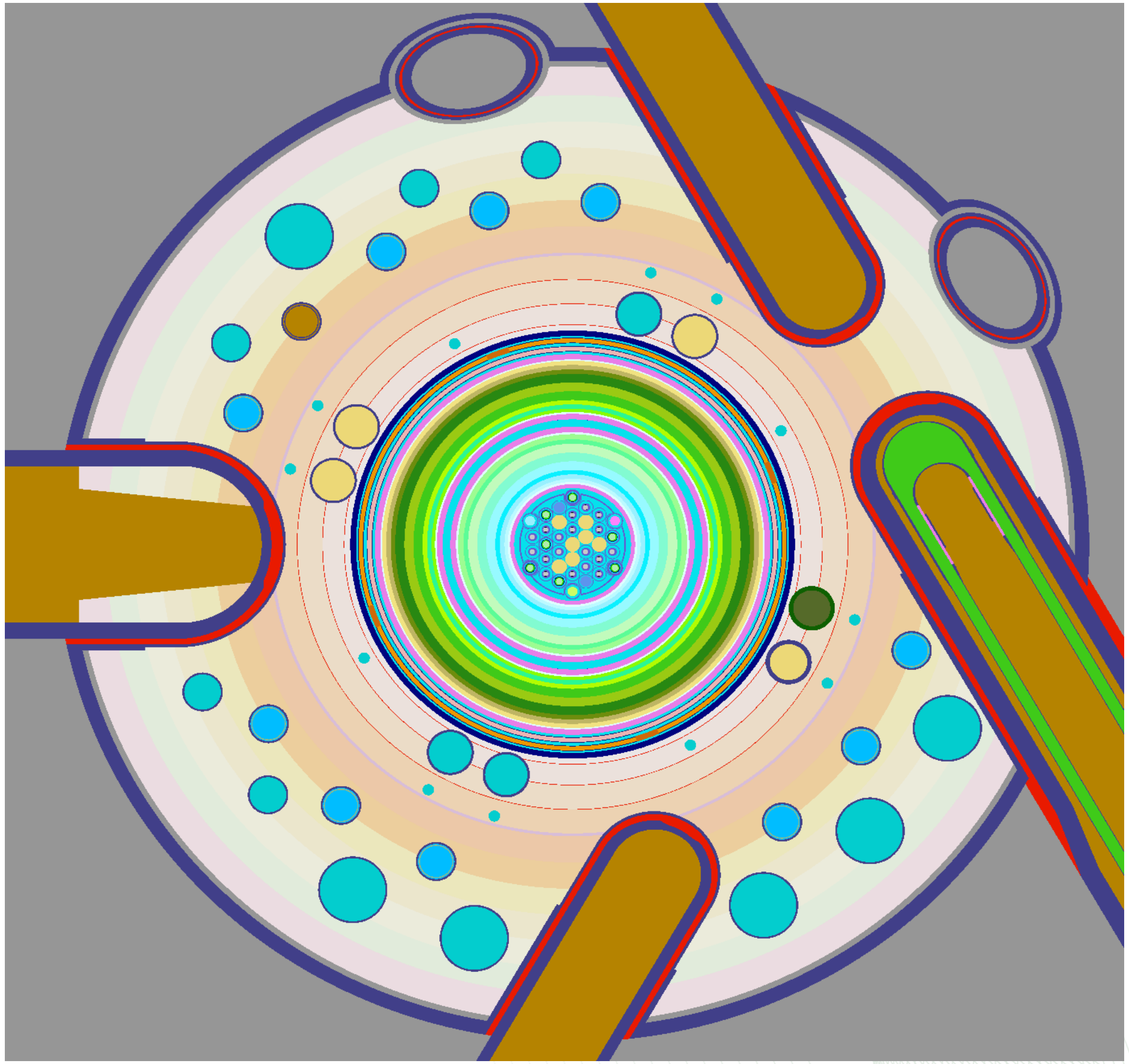
Shift Overview

- Flexible, high-performance Monte Carlo radiation transport *framework*
- Shift is physics agnostic
  - SCALE CE physics
  - SCALE MG physics
- Shift is geometry agnostic
  - SCALE geometry
  - Exnihilo RTK geometry
  - MCNP geometry
  - DagMC-CUBIT CAD geometry
- Fixed-source and eigenvalue solvers
- Integrated with Denovo for hybrid methods
- Multiple parallel decompositions and concurrency models
- Shift is designed to scale from supercomputers to laptops



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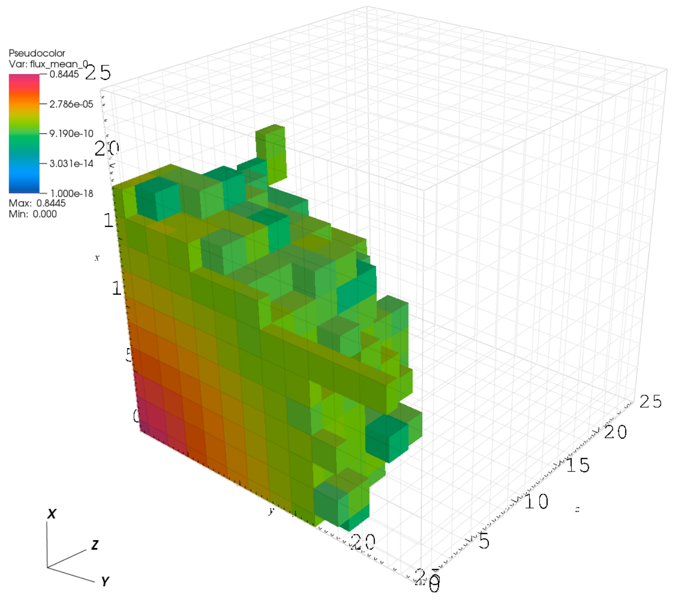
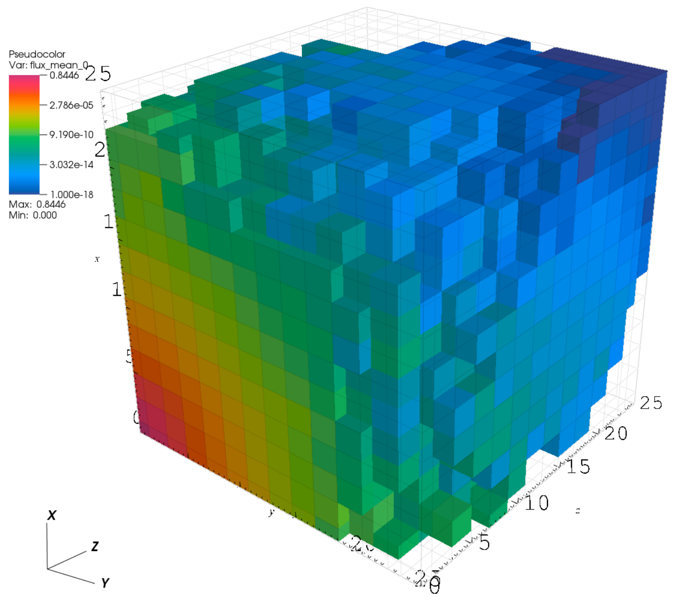
Shift's Scalable Tallies

- Shift features a high-performance, extensible tally system
  - Tallies are in an object-oriented hierarchy, enabling straightforward implementation of new tallies
- Shift supports a wide range of tallies
  - Reactions
  - Cells/mesh/unions
  - Energy
  - Diagnostic (e.g. source and Shannon entropy)
- The tally system is designed to scale ~*O(1)* with number of tally cells (as opposed to *O(N)*)
  - Tallies use hash table lookup instead of linear searches over number of tally cells/regions

Hybrid methods make Monte Carlo more efficient



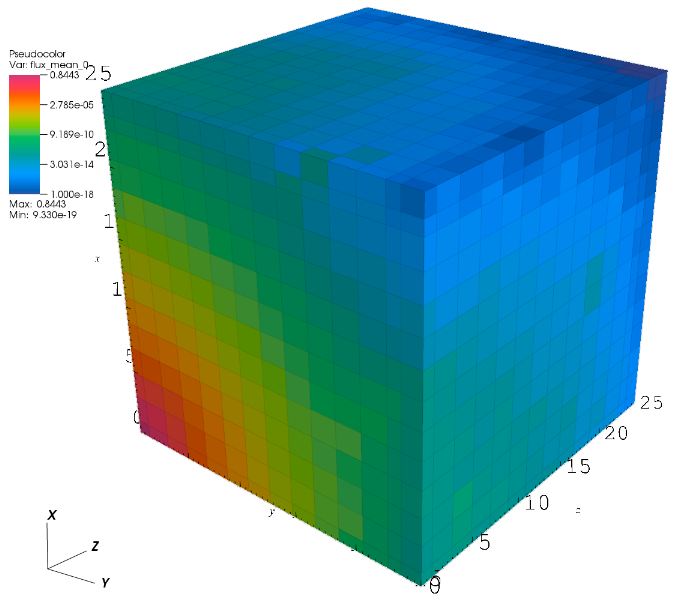
Analog MC



CADIS

Consistent Adjoint Driven Importance Sampling

Optimization of a single region



FW-CADIS

Forward-Weighted CADIS

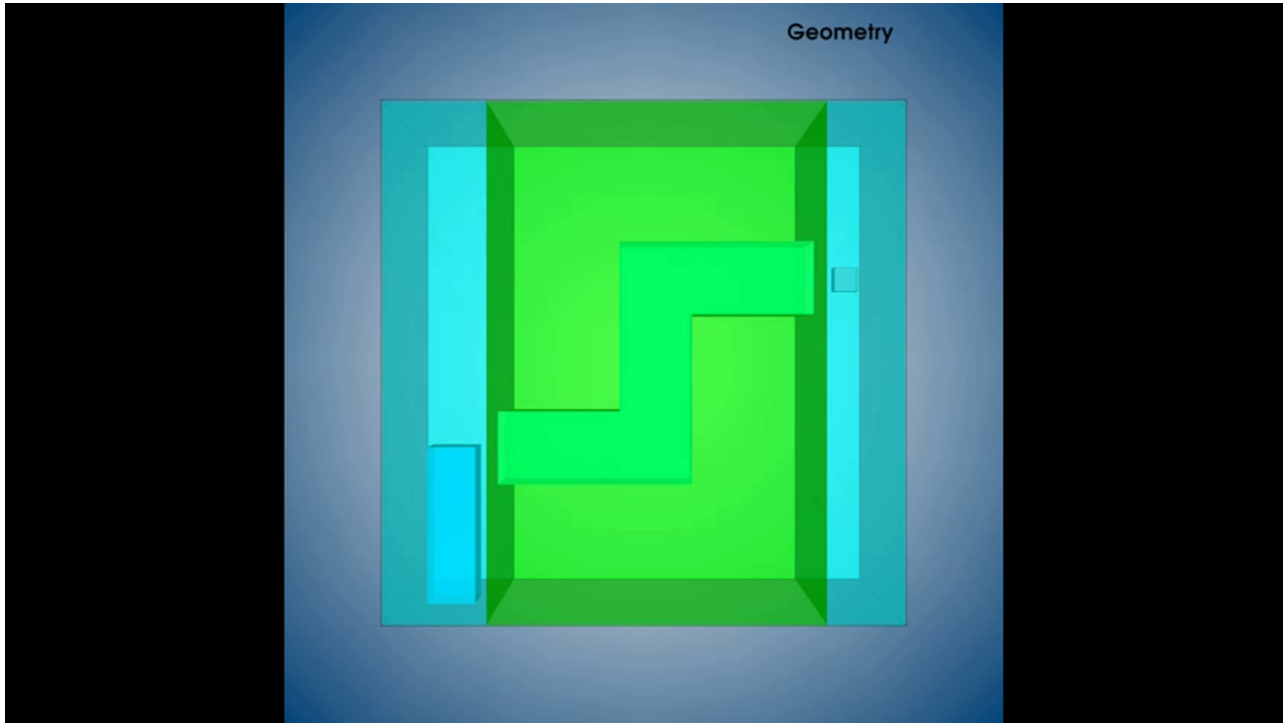
Optimization of distributions

FW-CADIS enables Monte Carlo solutions on problems that were previously considered impossible

How hybrid methods work

Monte Carlo accuracy at deterministic speeds

CADIS and FW-CADIS are 10 – 100,000 more efficient than analog Monte Carlo (measured by FOM)



CADIS

Detector response

$$\mathcal{R} = \iint q(\mathbf{r}, E)\phi^\dagger \, d\mathbf{r} dE$$

Biased source

$$\hat{q}(\mathbf{r}, E) = \frac{q(\mathbf{r}, E)\phi^\dagger(\mathbf{r}, E)}{\mathcal{R}}$$

Conservation of weight

$$w\hat{q} = w_o q$$

Particle weight

$$w = \frac{\mathcal{R}}{\phi^\dagger(\mathbf{r}, E)}$$

Weight window

$$w = \frac{1}{2}(w_L + w_U)$$

$$w_L = \frac{2\mathcal{R}}{(1+c)\phi^\dagger(\mathbf{r}, E)}$$

FW-CADIS

Forward weighting

$$q^\dagger(\mathbf{r}, E) = \frac{1}{\phi(\mathbf{r}, E)}$$

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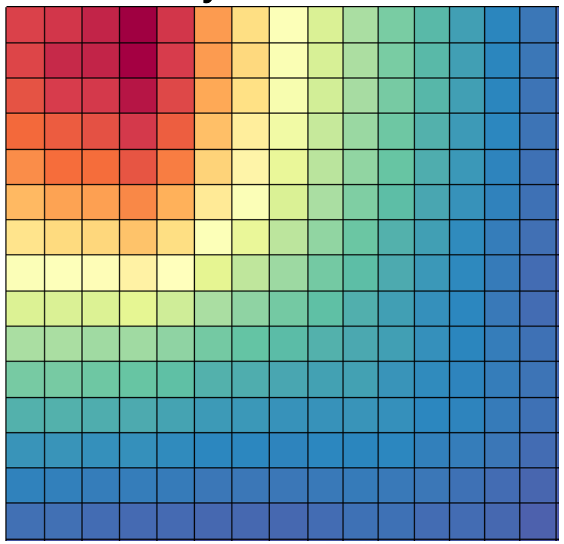
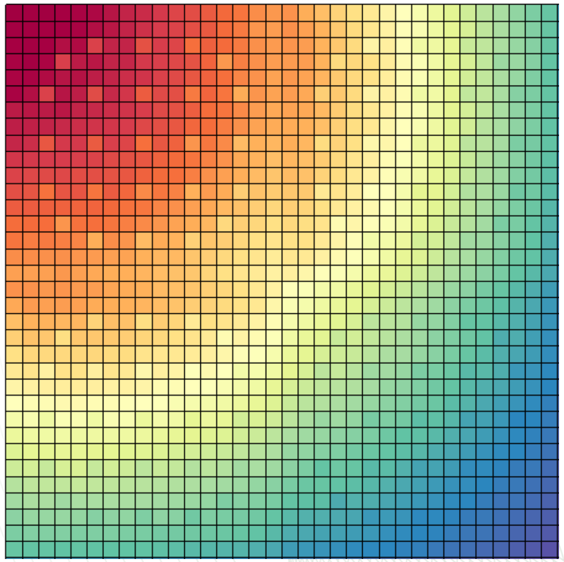
Sourcerer Method

- ***Concept:*** Estimate fission source using a low-order solver for an improved initial guess for fission source distribution (i.e., inactive cycles).
- Sourcerer method has been implemented in Exnihilo and is currently being tested.
- Not original to Exnihilo
  - Modeled on the SOURCERER sequence in SCALE
  - Infrequently used due to computational cost of S_N
- Exnihilo implementation is method-agnostic
  - Integrated into *all* Denovo deterministic methods
  - Only SP_N studied thus far
  - MG Monte Carlo could be used in the future
- ***Research Question:*** How does the fidelity of the deterministic solution affect performance?
  - SP_N order
  - Cross sections (assumptions for resonance self-shielding)
  - Energy resolution
  - Mesh resolution
  - χ-spectrum (Watt fission vs. material-specific)

Low-fidelity Denovo solution



Shift solution



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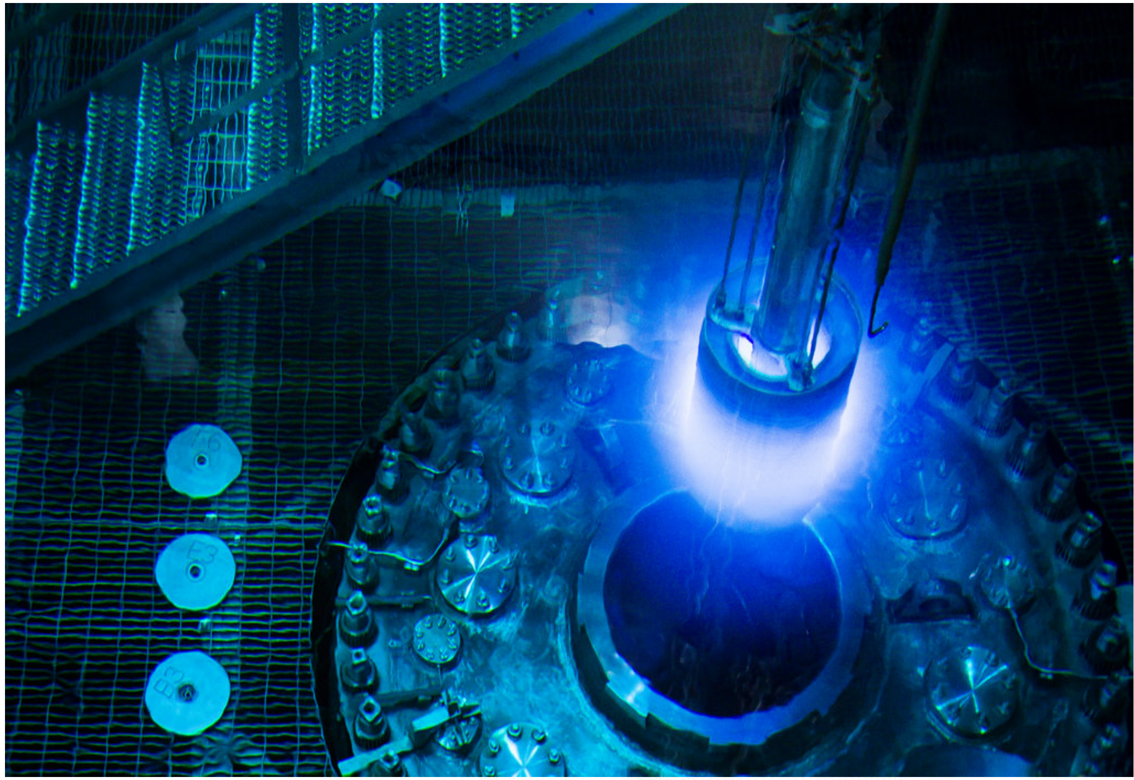
Shift Depletion Package

- In-memory coupling to ORIGEN-6.2
- Supports Shift's multilevel parallel decomposition
- Features multiple transport-depletion coupling methods:
  - Fully-explicit, middlestep, several predictor/corrector methods
  - Enables accurate solutions with longer timesteps
- Features advanced power normalization methods for accurate constant-power depletion
  - Optional substep-based predictor/corrector power normalization
  - Energy-integrated substep normalization



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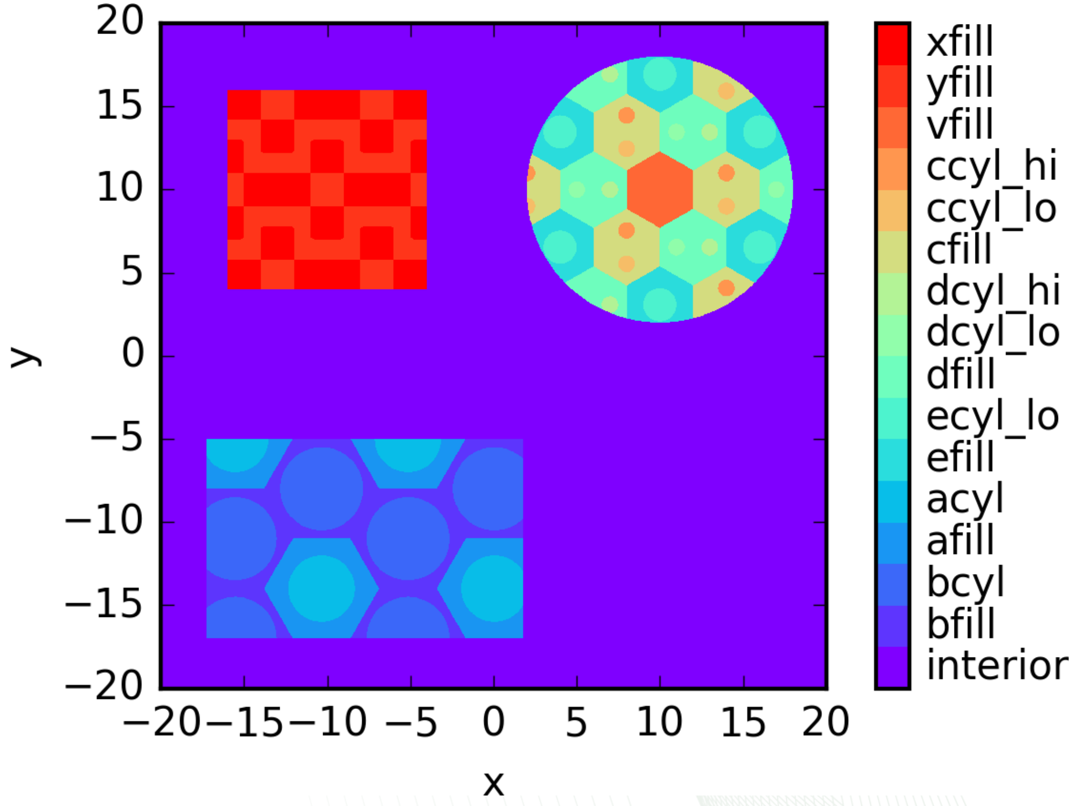
Exnihilo-Integration into SCALE

✓Integrated in CSAS sequence
- Eigenvalue mode for criticality safety
- Uses standard Scale geometry, material, and control specifications

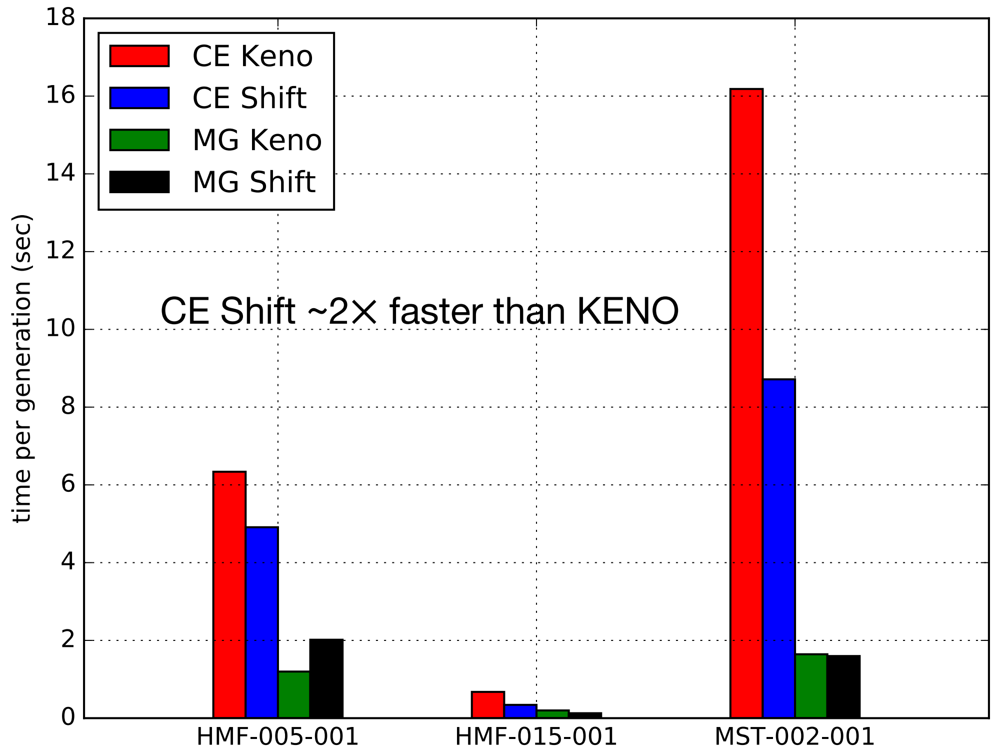
✓Integration in TRITON lattice-physics
- Used as the flux solver for depletion calculations
  - Both CE and MG physics supported
- Calculates nodal tallies for feeding to a nodal solver (PARCS)

❑Integration in MAVRIC
- Fixed-source shielding problems using hybrid methods
- Planned for FY18

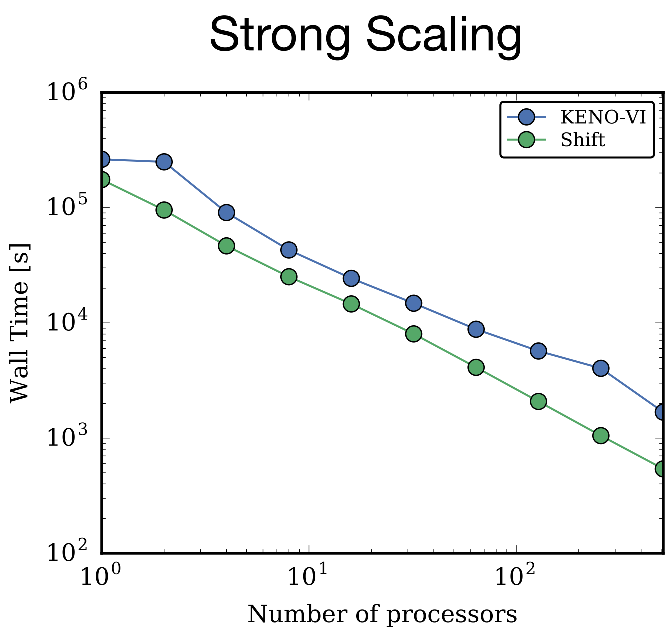
❑Integration in Polaris
- CE Flux solutions to Polaris solver
- Planned for FY18

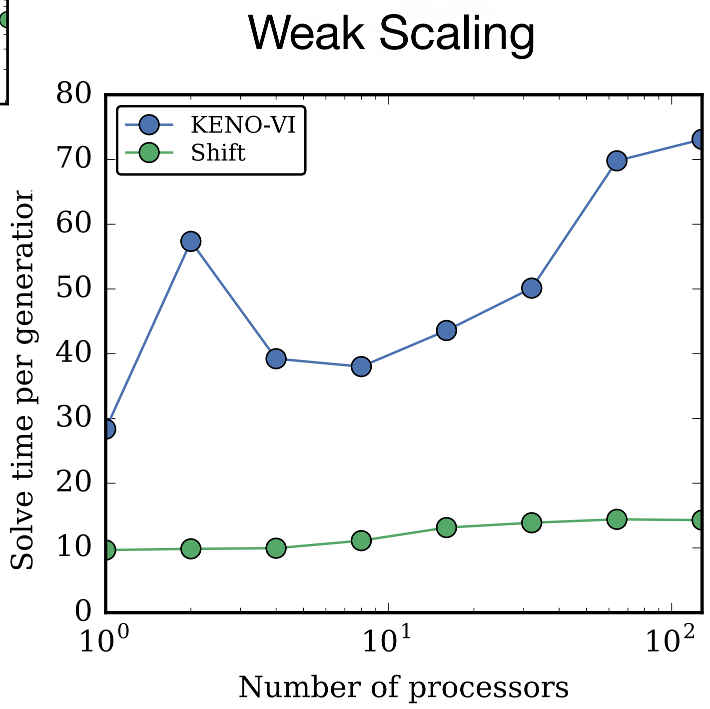


SCALE-Shift Performance



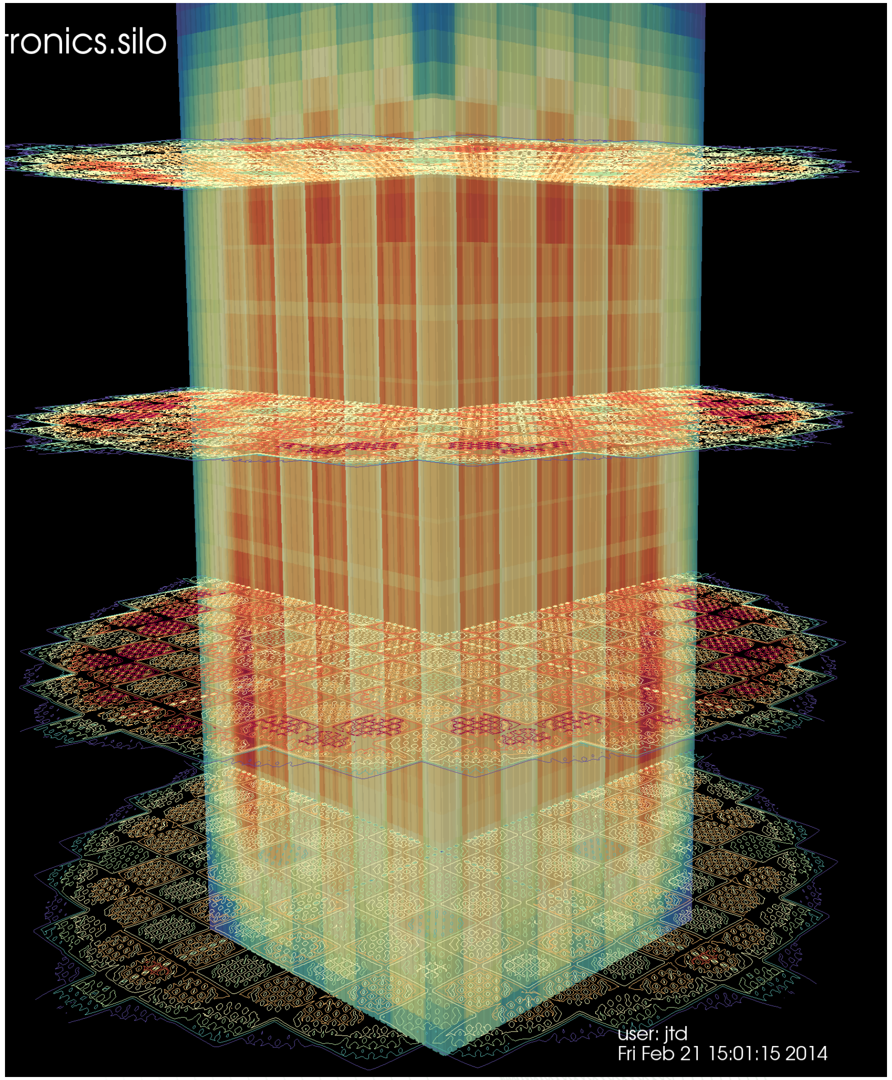
Serial Runtimes





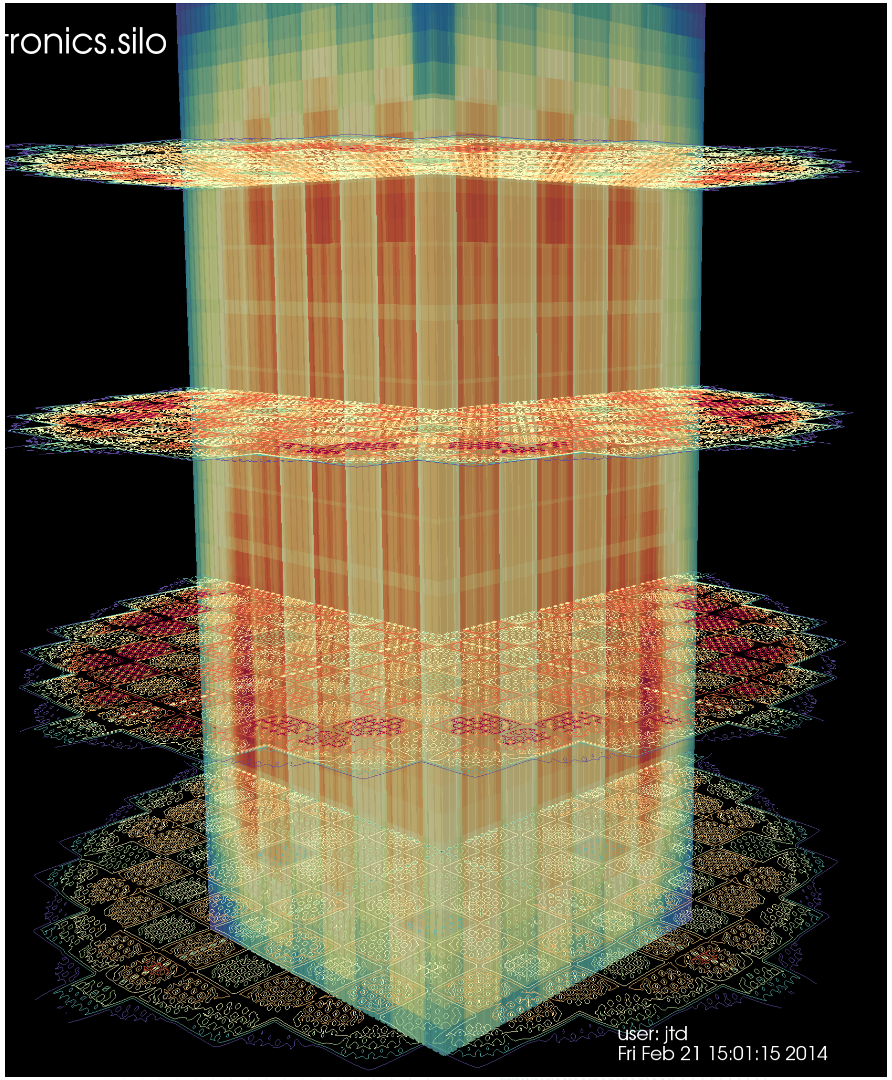
VERA – CASL'S Core Simulator

- **In-core analysis**
  - Standard VERA-CS analysis: MPACT, COBRA, ORIGEN
  - Validates MPACT neutronics results inline during simulations
  - Shift runs on its own MPI communicator
    - VERA-CS can be setup to run on nominal number of cores (*O(1000)*)
    - Shift can utilize remaining computing resource (*O(100K)* on Titan)
    - VERA-CS continues multicycle calculation while Shift executes at state points

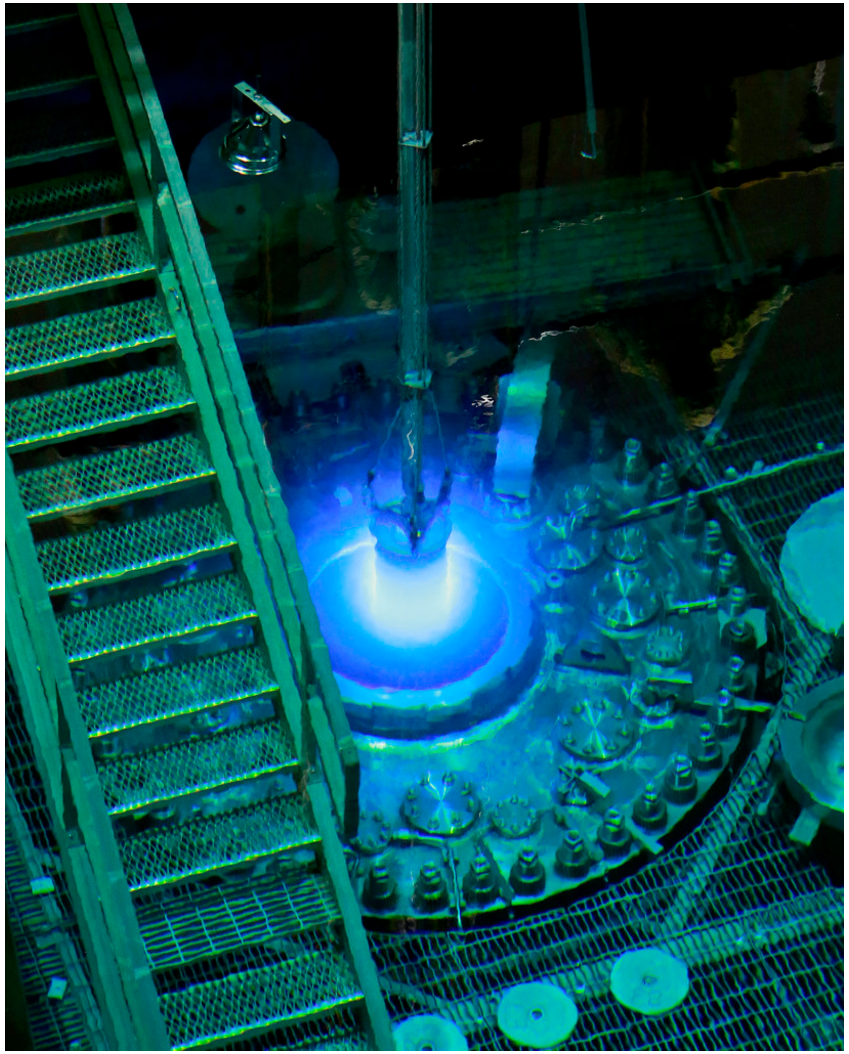


VERA – CASL'S Core Simulator

- **Ex-core analysis**
  - Fixed-source
    - Uses fission source from VERA-CS
    - Hybrid methods (optional)
  - Flux tally in core barrel, core pads, and vessel
  - Supplementary general model specification allows user description of more details outside core barrel with user-defined tallies



Questions?



Extra Slides

HPC ORNL radiation transport tools

ADVANTG
Fixed-source applications

- Hybrid Monte Carlo/deterministic using *CADIS* and *FW-CADIS*
- Uses **Denovo** to accelerate **MCNP** Transport application for DTRAs **SWORD** simulation system
- Distributed through RSICC

Exnihilo
HPC radiation transport

- Transport application framework
- **Denovo**, **Shift**, **Insilico** applications coupled through *Omnibus* frontend
- Provides the Monte Carlo neutronics in **VERA-CS**
- Distributed through RSICC as part of **SCALE** and CASL **VERA**

MPACT
Reactor Physics

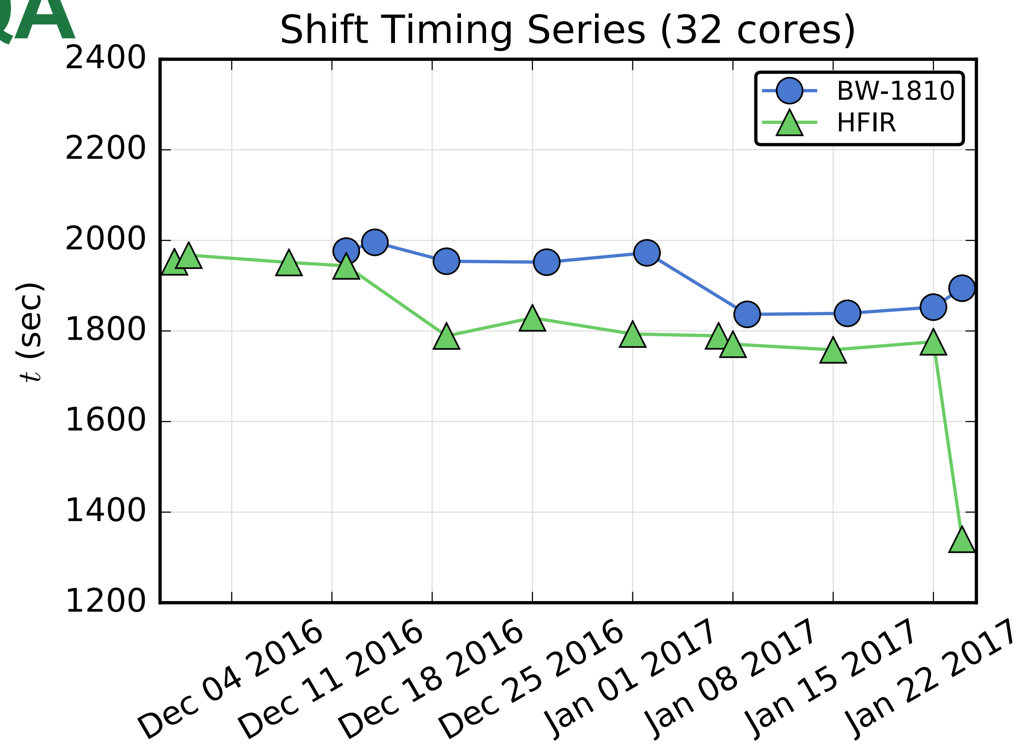
- Standard engine in CASL Core Simulator (**VERA-CS**)
- Co-owned by ORNL and UM
- Released through RSICC as part of CASL **VERA** toolset

VERA-CS

SCALE

The appropriate tool set is meeting programmatic requirements

Software Engineering Practices/QA



Development workflow

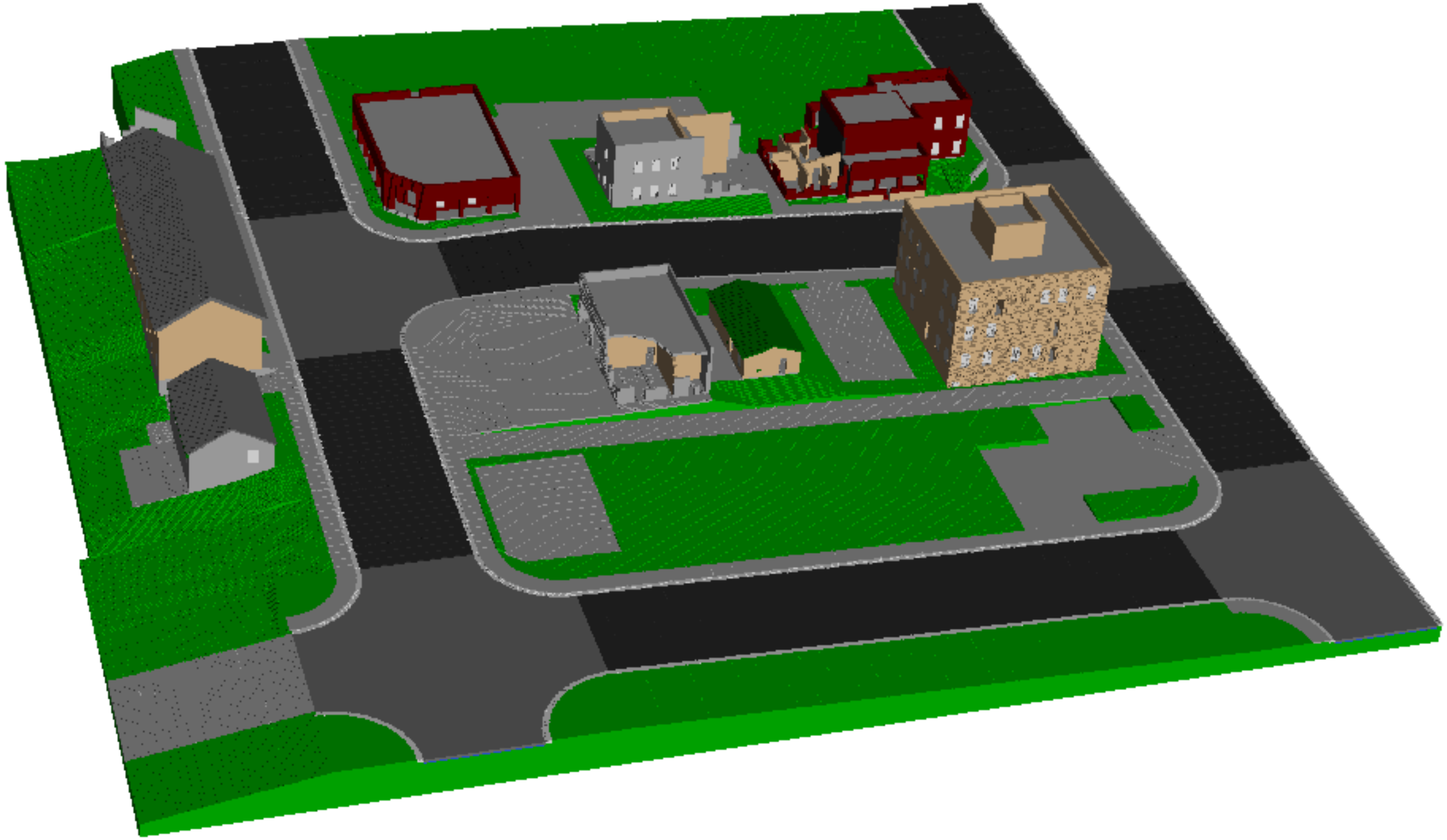
- Topic-branch configuration – workflow model
- Agile development model
- Continuous integration/testing
  - 782 individually compiled unit-tests run on branch merge
  - Daily regression
  - Weekly tests
    - Performance suite
    - Acceptance (verification) suite
- Master repository ***always*** works

Documentation

- Code in Doxygen
- Sphinx for user/developer manual
- LaTeX for methods manual
- Issue tracking in GitLab

Ongoing work in Hybrid Methods

- Using SVD to produce optimal separable adjoint fluxes
  - Reduces memory consumption by a factor of 27 for a 27 group library
- Optimized parallel load balancing
- Using GPUs for source discretization



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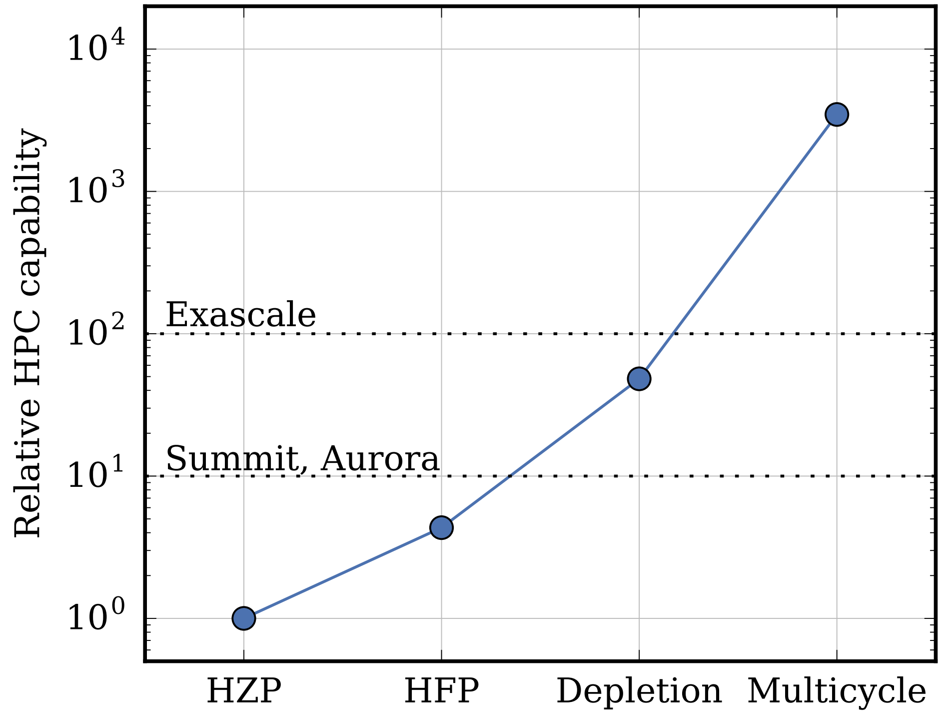
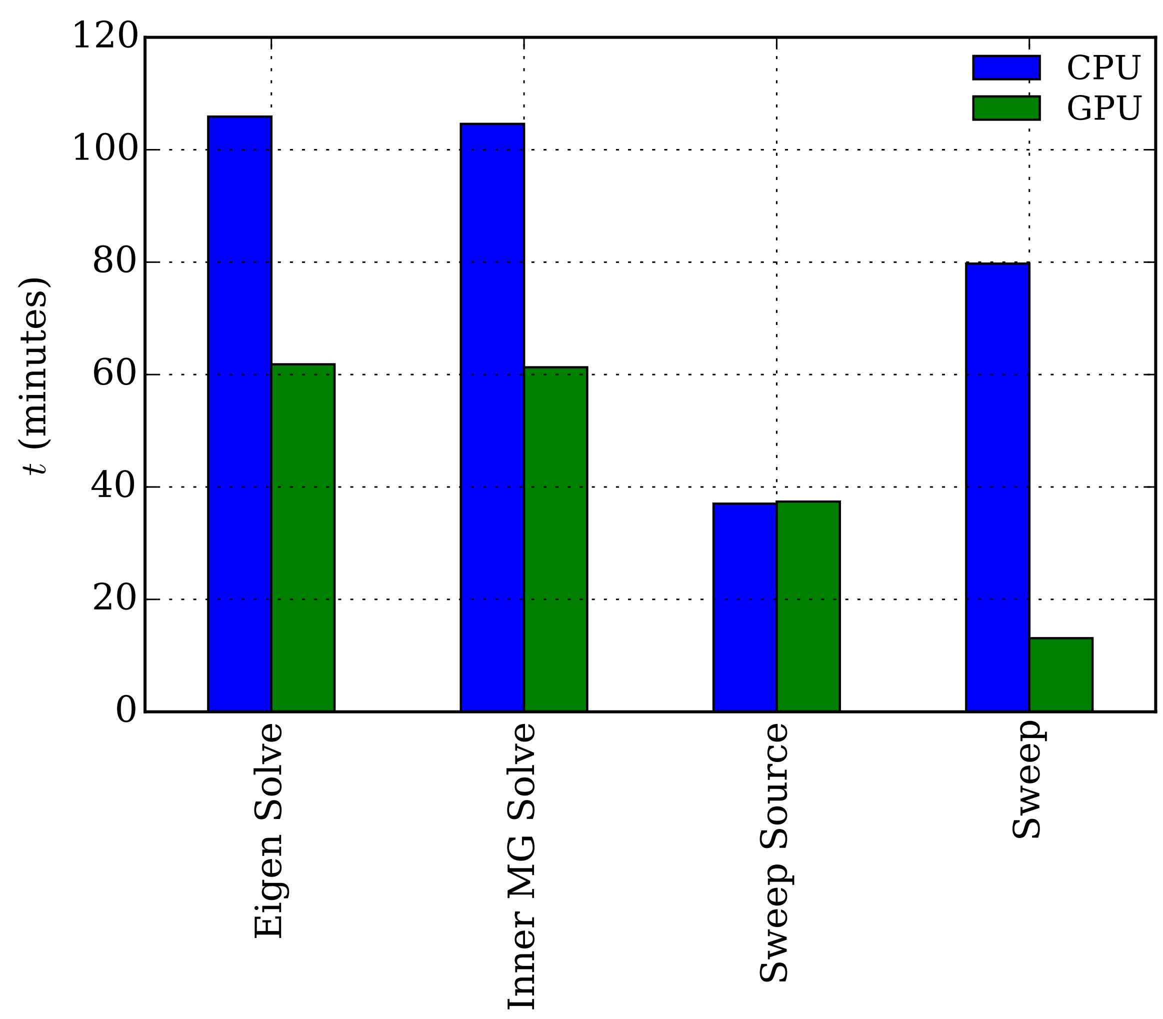
Shift is an application in DOE ASCR Exascale Computing Project

- Use highest resolution models to provide benchmark data sets for multi-cycle SMR operation
  - 10 year target: 2025 operational deployment
- Couple MC neutronics to multiphase CFD
  - Shift-MC (ORNL) + Nek5000 (ANL)
- Demonstrated results at Petascale
  - Coupled multi-cycle simulations are an exascale problem



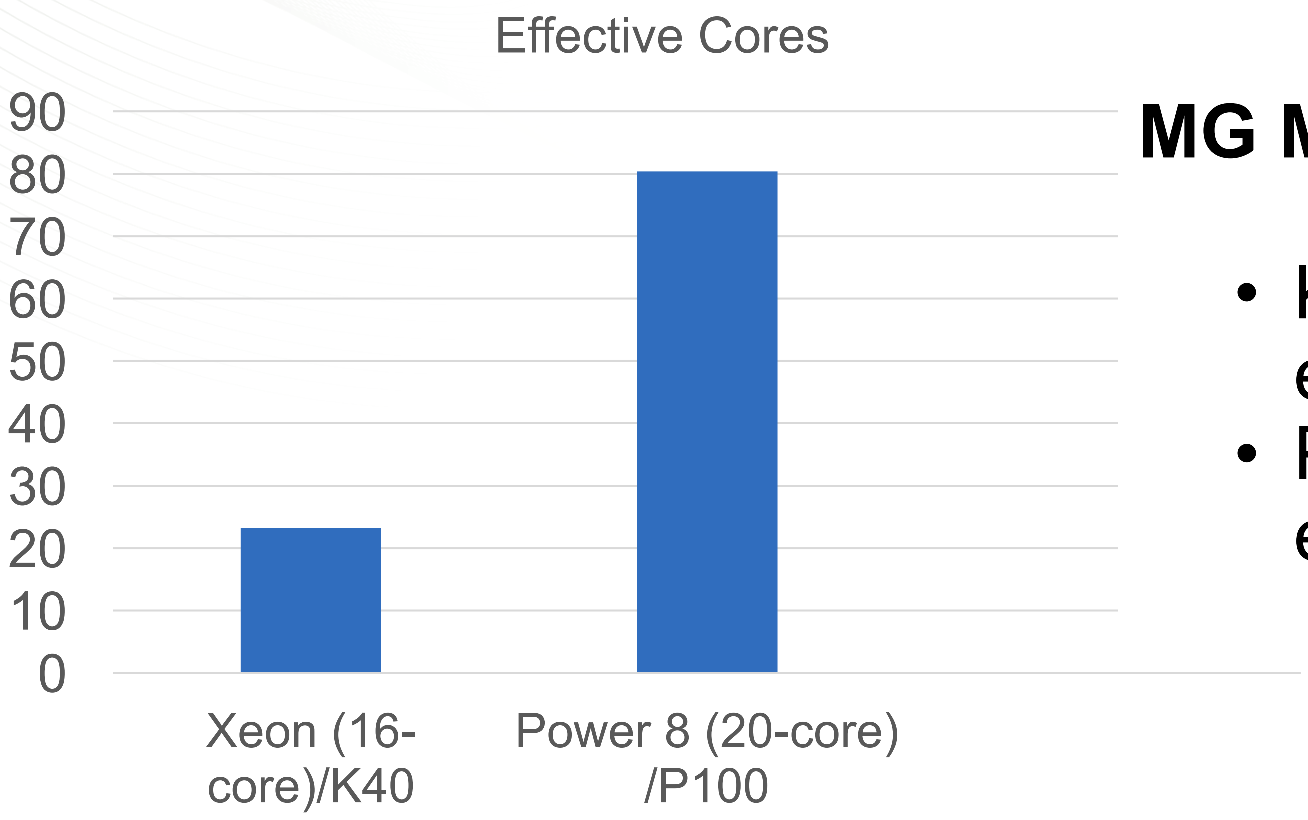
GPU-Enabled Denovo Sn solver



Denovo Sn solver performance

- GPU sweep is 6.1x faster than CPU sweep
- Total solution time 1.7x faster with GPU

GPU-Enabled Multigroup Monte Carlo (Profugus)



MG Monte Carlo performance:

- K40 GPU is 23.2 CPU-equivalent
- P100 GPU is 80.4 CPU-equivalent

VERA Execution Modes

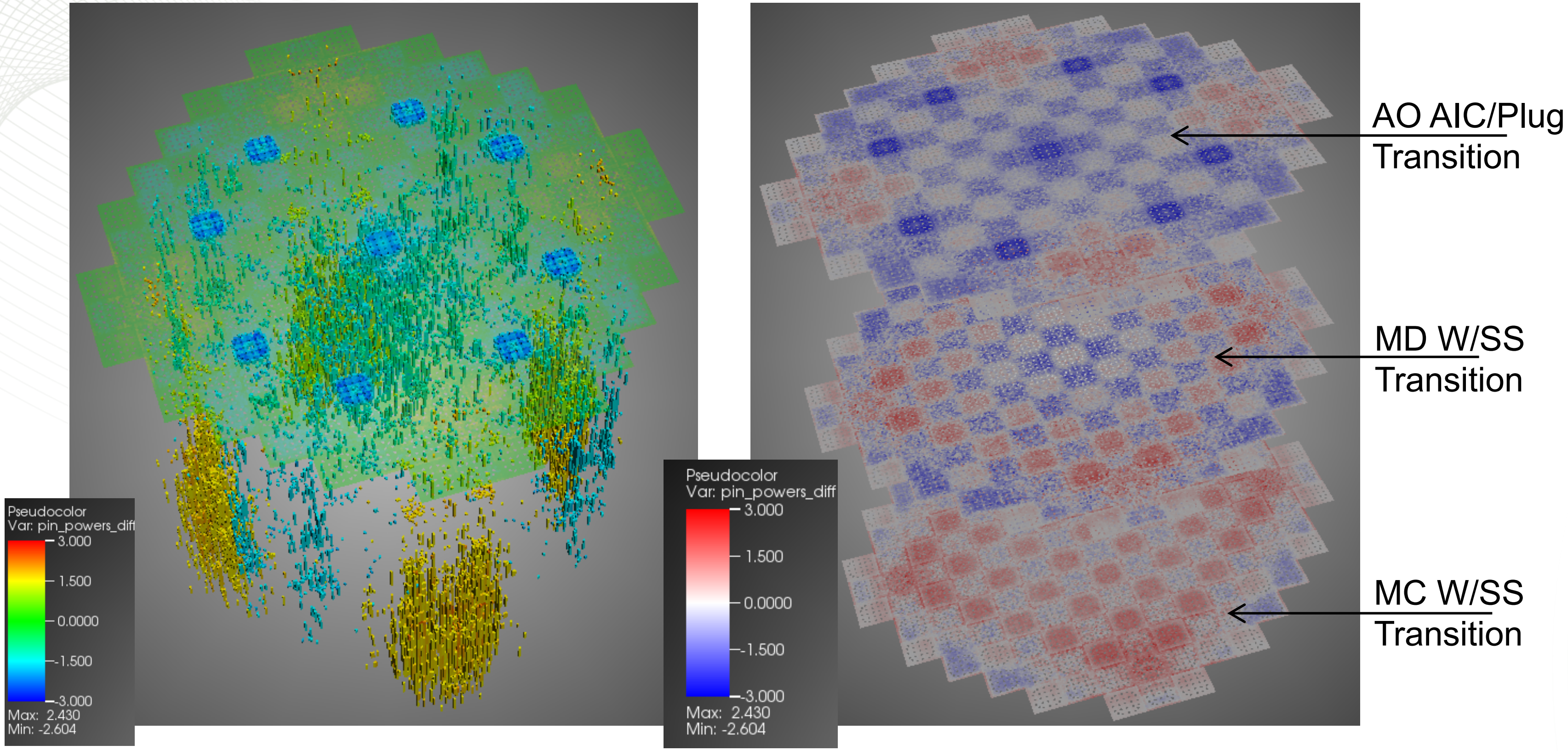
In-core analysis

- *k*-eigenvalue
- Reactor core model completely specified by VERA input
- Automated tallies:
  - Pin powers
  - Shannon entropy

Ex-core analysis

- Fixed-source
  - Uses fission source from VERA-CS
  - Hybrid methods (optional)
- In-core model generated from VERA input
- Supplementary general model specification allows user description of problem outside of core barrel
- User-defined tallies

Summary 3D power distributions



Case	Bank Position (% Inserted)	AO (%)	ΔAO (%) MPACT	RMS ΔP (%) MPACT	Max ΔP (%) MPACT
3x3 Reg. B and D	AO, 17% In	-7.5	-0.1	0.4	1.9
Quarter Core	AO, 17% In MD, 66% In MC, 100% In	-8.7	+0.2	0.6	2.6

- Shift – generated reference solutions provide benchmarks for VERA-CS
- HPC scalability of Shift enables the highest resolution possible solutions of 3D LWR cores using OLCF resources (Titan)
- Integration with VERA allows analysts to generate benchmarks from the same inputs and models as production runs