Shift – Hybrid Monte Carlo Particle Transport

Kat Royston, ORNL
Thomas Evans, ORNL
Eva Davidson, ORNL
Tara Pandya, ORNL

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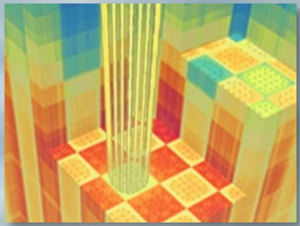
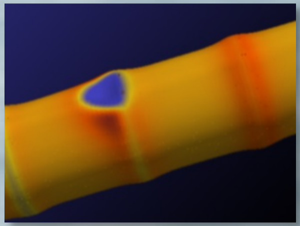
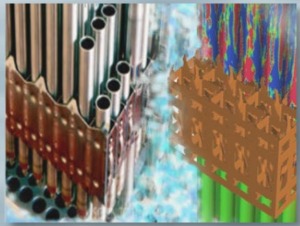
VERA Workshop







CASL The Consortium for Advanced Simulation of LWRs
A DOE Energy Innovation Hub

U.S. DEPARTMENT OF ENERGY

Overview

- Review of computational transport methods
- Shift Monte Carlo Code
- Hybrid transport methods
- Shift capabilities in VERA
- Conclusions and future development

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

Fixed source form of the transport equation:

$$\hat{\mathbf{\Omega}} \cdot \nabla \psi(\mathbf{r}, \hat{\Omega}, E) + \sigma(\mathbf{r}, E)\psi(\mathbf{r}, \hat{\Omega}, E) = \int dE' \int_{4\pi} d\hat{\Omega}' \ \sigma_{\mathrm{s}}(\mathbf{r}, \hat{\mathbf{\Omega}}' \cdot \mathbf{\Omega}, E' \rightarrow E)\psi(\mathbf{r}, \hat{\Omega}', E') + \frac{1}{4\pi} q_{\mathrm{e}}(\mathbf{r}, \hat{\Omega}, E)$$

Computational transport methods

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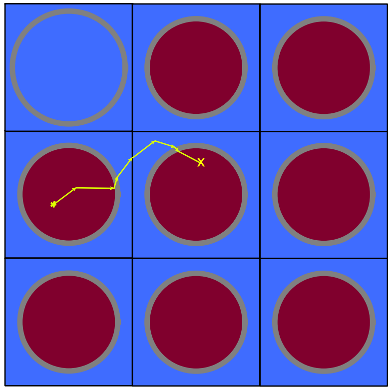
  - Accuracy limited by discretization approximations
- **Stochastic or “Monte Carlo” methods**
  - Simulate individual particles and infer average particle behavior from the average behavior of the simulated particles
  - Tally results in pre-determined regions of problem space
  - Computationally expensive
  - Accuracy limited only by the physics, geometry and material approximations used



1. Sample starting neutron
2. Sample distance to collision
3. Calculate distance to boundary
4. Move particle
5. Accumulate state data
6. Repeat 2 – 5

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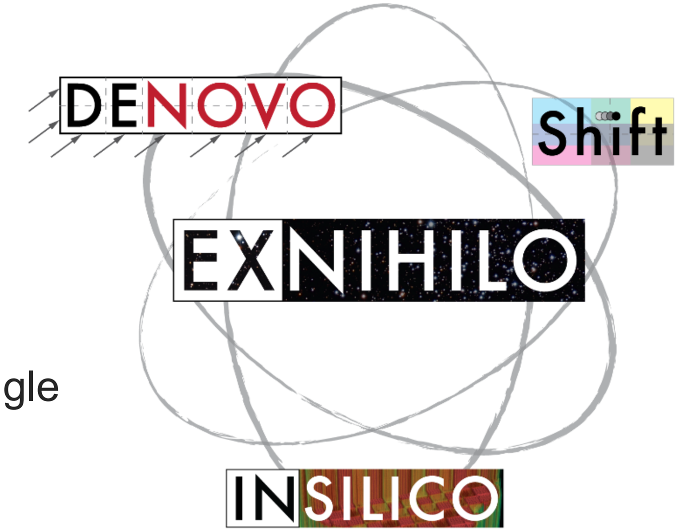
- **Hybrid methods**
  - Use fast, approximate deterministic simulations to speed-up highly accurate Monte Carlo simulations
    - Calculate 3D adjoint (importance) and/or forward functions with deterministic simulations
    - Calculate variance reduction (VR) parameters based on deterministic solutions
    - Utilize VR parameters to focus the Monte Carlo simulation on “important” particles
  - Automate above steps

Shift Monte Carlo Code

Shift is part of the Exnihilo code suite

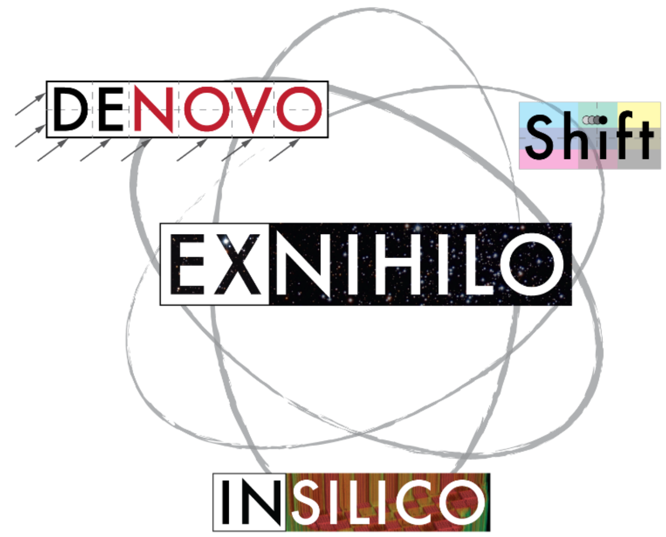
- Provide a parallel, component library for transport application development on HPC platforms
- Provide pre- and post-processing tools integrated with ***Jupyter notebook***
- Flexible & scalable by design; deployed for multiple applications
- Monte Carlo and deterministic transport solvers in a single code system
- Internal GitLab code repository and issue tracking: https://code-int.ornl.gov/exnihilo/Exnihilo



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
Omnibus	General front-end for solving radiation transport problems

The Exnihilo Code Suite

Exnihilo Team	
HPC Methods and Applications Team	Reactor and Nuclear Systems Division
Elliott Biondo Greg Davidson Tom Evans (lead) Steven Hamilton Seth Johnson Tara Pandya Kat Royston	Kursat Bekar Cihangir Celik Eva Davidson Rob Lefebvre



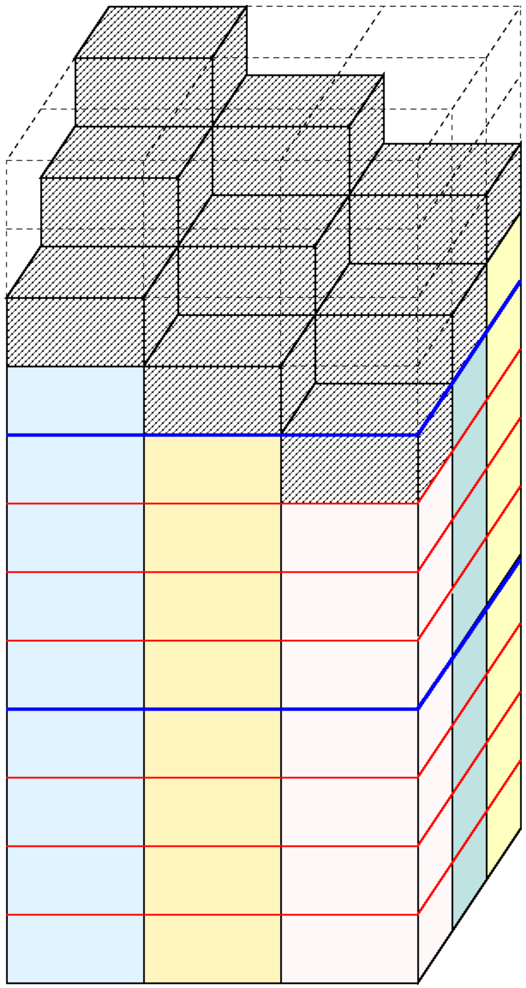
Developed using Agile, Continuous-Integration workflow

- 1,177 individual unit tests checked on merge
- Acceptance and runtime performance tests run weekly

Language	Executable	Test
C++	274,648	279,170
Python	30,543	19,569
CUDA	12,356	8,804
C	1,555	—
Fortran	934	55

Denovo Deterministic Transport Code

- 2- and 3-D Cartesian brick mesh with automatic discretization of Shift-compatible geometry inputs
- S_N and SP_N angular discretizations (Level symmetric, Gauss-Legendre Product, Quadruple Range quadratures)
- Spatial discretizations (weighted-diamond, theta-weighted diamond, step-characteristic, and more)
- KBA parallel decomposition, multi-set energy decomposition
  - Maximize parallelism on 100K CPUs
  - Parallel GPU implementation
- Advanced Krylov solvers
  - State-of-the-art numerical methods
  - Fast within-group, multigroup, and eigenvalue solutions
- Automatic multigroup cross section generation
  - Built-in SCALE cross section processing
  - Cross section mixing for discretized cells that contain multiple materials



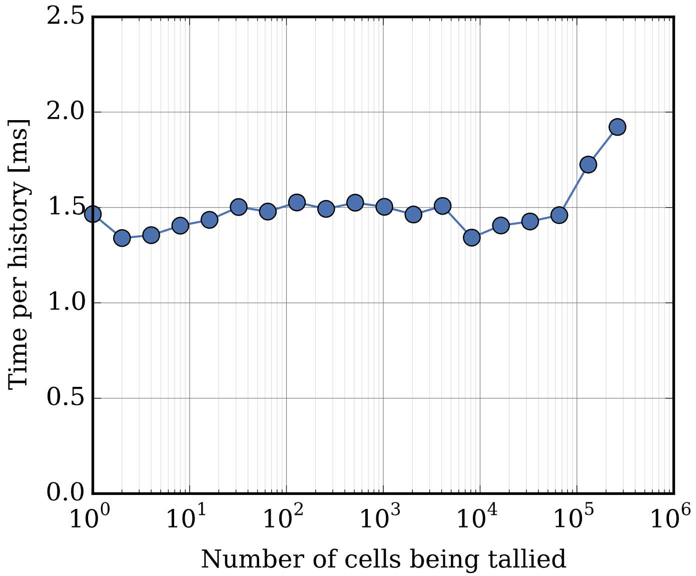
Shift Monte Carlo Transport Code

- Flexible, high-performance Monte Carlo radiation transport *framework*
- Multiple front-ends
  - Omnibus: Fully featured general front-end
  - SCALE: Integrated into CSAS, TRITON, and MAVRIC
  - Insilico: Integrated into VERA for in-core and ex-core analyses
- Shift is physics and geometry agnostic
  - Physics engines: SCALE CE and MG
  - Geometry engines: Exnihilo RTK, MCNP, GG (KENO/SCALE), DAGMC CAD
- Fixed-source and eigenvalue solvers
- State-of-the-art methods, algorithms, and implementations
  - GPU implementation for CE physics with reactor geometry
  - Hybrid MC/deterministic methods
- Shift is designed to scale from supercomputers to laptops

Tallies in Shift

- Shift supports a wide range of tallies, including reactions, cells/unions, meshes, energy, and diagnostic (e.g., source and Shannon entropy)

- Scalable tallies
  - Tally system 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

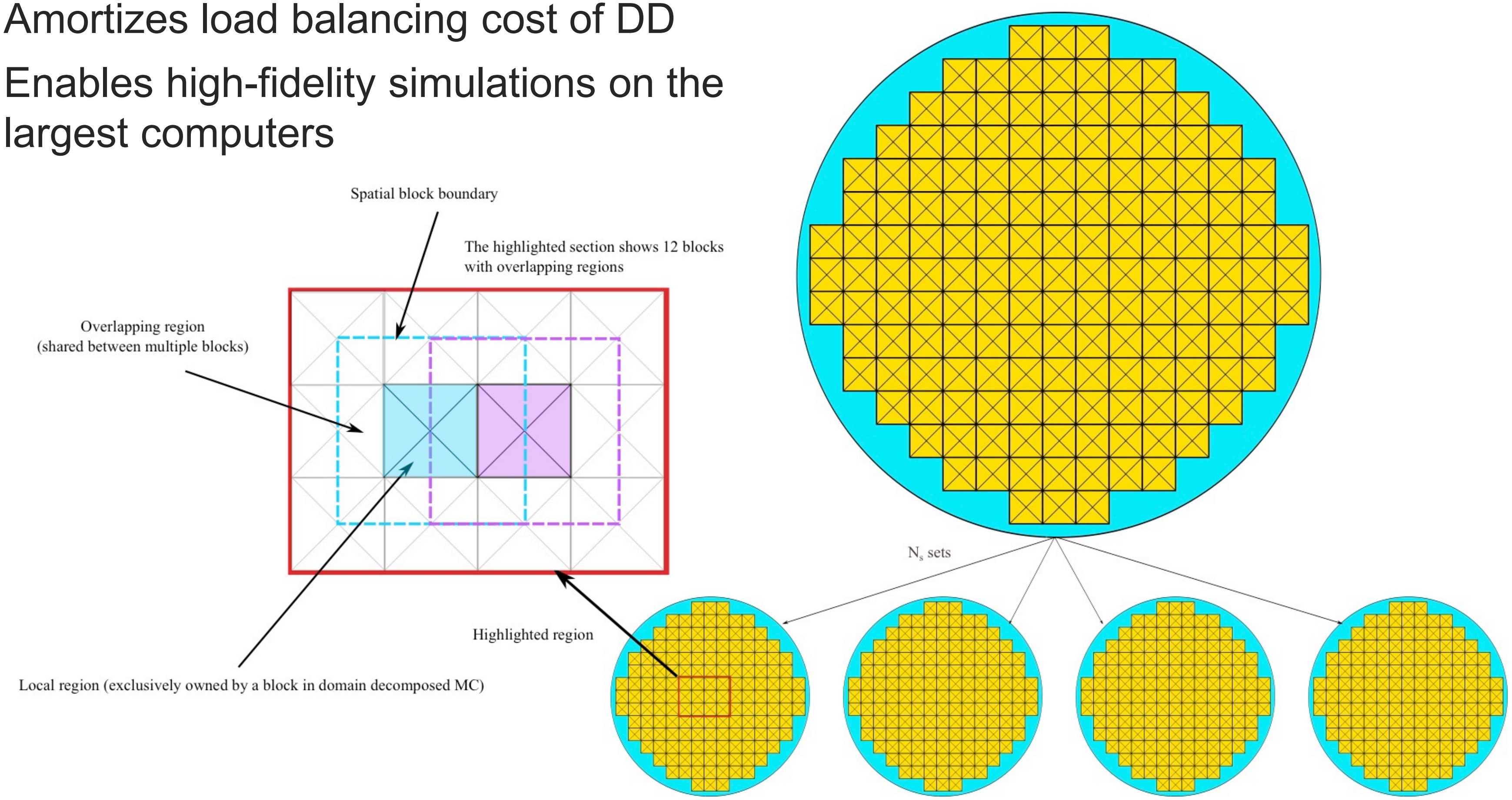


Time per history for a geometry containing 262,144 unique cells with energy-integrated flux tallies in randomly selected cells

Spatial domain decomposition

Multi-Set Overlapping Domain (MSOD)

- Spread the problem across multiple "blocks" if memory usage is too high for a single processor
- Amortizes load balancing cost of DD
- Enables high-fidelity simulations on the largest computers



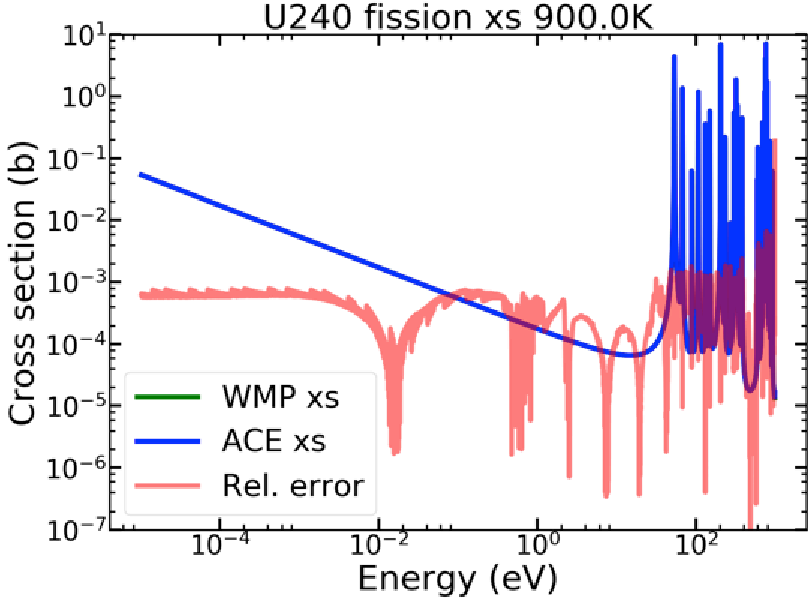
On-the-Fly Doppler Broadening

- Traditional method: obtain $\sigma(E,T)$ by interpolating between data on a temperature grid
  - Many grid points required, large memory requirements
  - Interpolated $\sigma(E,T)$ is approximate
- Pole Method:
  - Formulate cross section in terms of poles (p), residues (r), and temperature (T) for on-the-fly evaluation:

$$\sigma(E,T) = \frac{1}{E}\sum_j Re\left[\frac{1}{2\sqrt{E}}\sqrt{\pi}r_j W\left(\frac{\sqrt{E}-p_j}{2\sqrt{\frac{k_B T}{4A}}}\right)\right]$$

$W()$: Faddeeva function

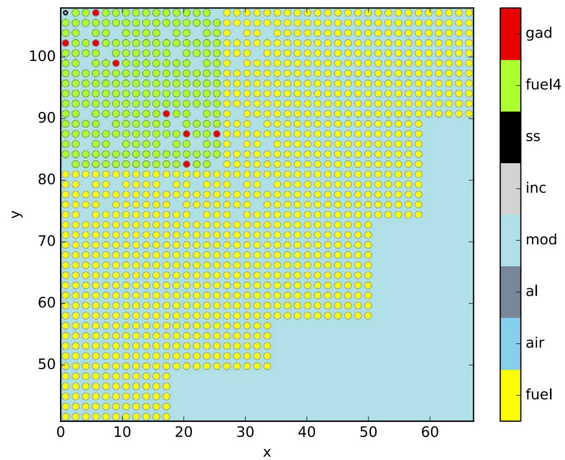
  - Windowed pole method only analytically calculates contributions from poles within a window of energies and fits a curve for contributions outside the window

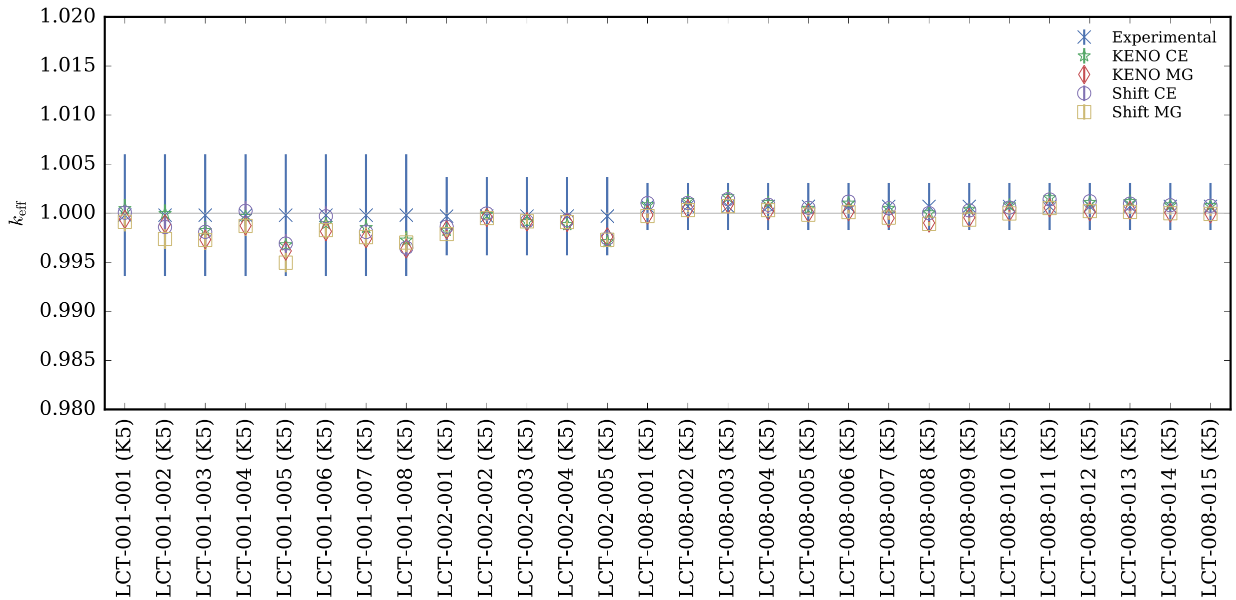


Accuracy of windowed multipole method relative to reference data.

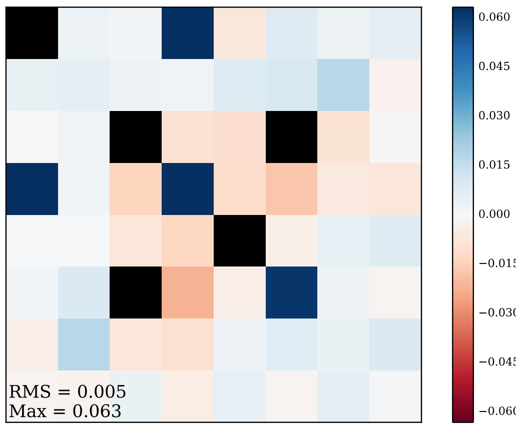
Shift V&V (CASL-U-2016-1186-000)

- Small critical problems (BW1484, BW1810)
- LWR full-core and pincell problems (WEC AP1000®, Watts Bar Unit 1 startup, KRSKO)
- Coupled (n, g) problems
- Fixed-source gamma transport problem (CACTF)
- Depletion/burnup problems (AP1000® lattices)
- Performance benchmarks (OECD NEA, WEC AP1000®)



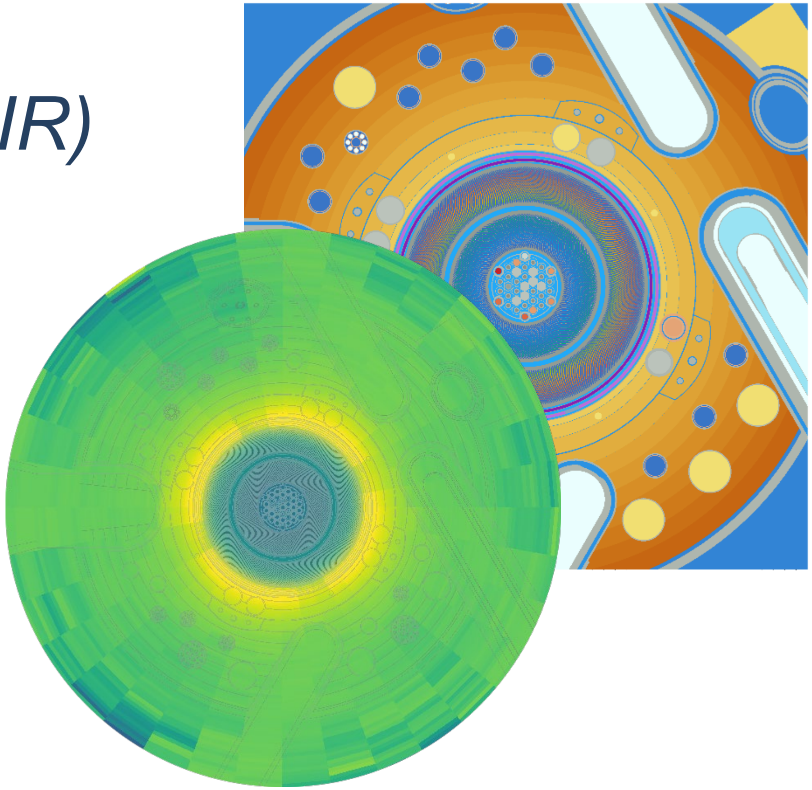


LEU-COMP-THERM VALID Benchmark Results

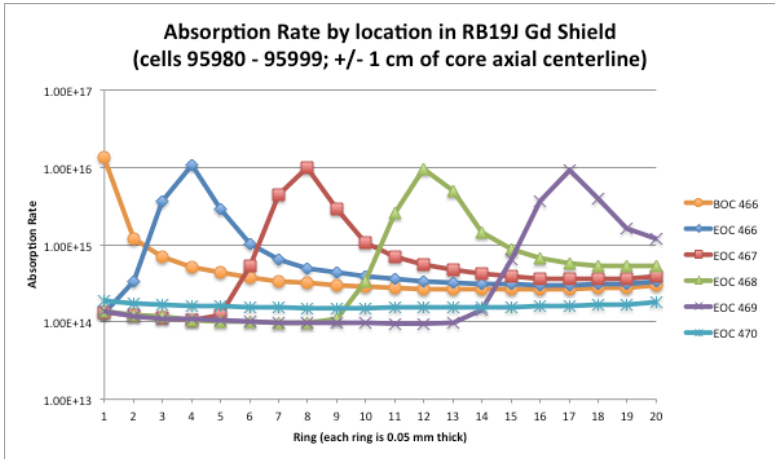


BW1810 Core XIV

Shift Applications:
High Flux Isotope Reactor (HFIR)

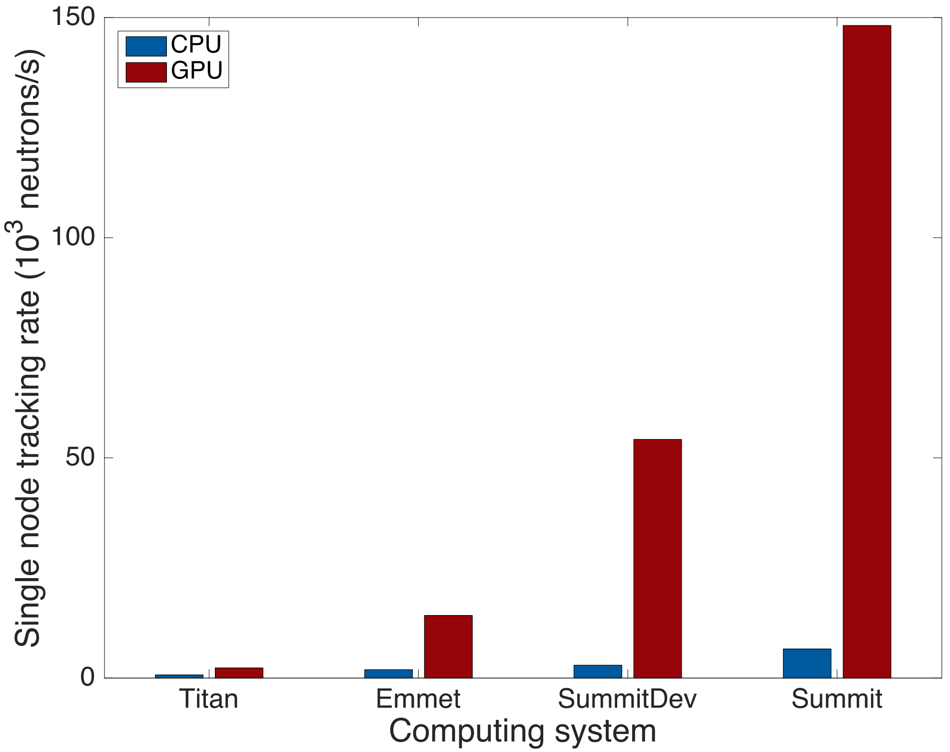


- ORNL Research Reactor Division
- Parallel depletion/activation
  - Full cycle analysis time reduced from ~8 days to ~8 hours
  - Uses MCNP geometry, supports in-memory geometry changes
  - Advanced diagnostic tools for geometry debugging
- RB19J Gd-shielded experiment shield lifetime analysis
  - ~3700 depletion zones
  - Calculations performed on ORNL's Panacea cluster
    - 56 or 64 nodes (20 cores/node)
    - 28 time steps
    - ~2.5 – 3.5 hrs per HFIR full-cycle calculation

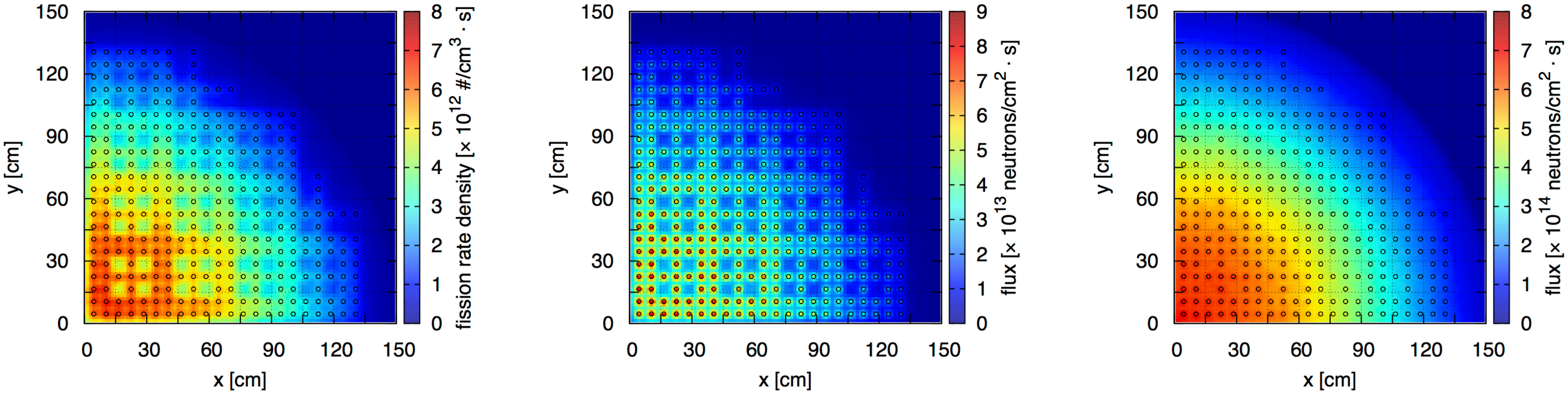


Shift Applications:
DOE Exascale Computing Project

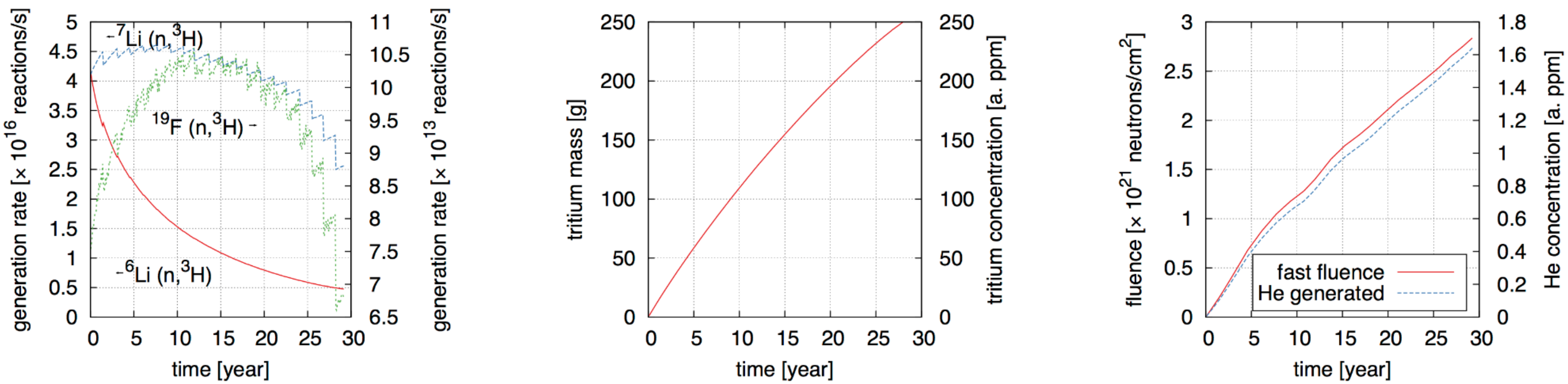
- Established to accelerate development of a capable exascale computing system
- Use highest resolution models to provide benchmark data sets for multi-cycle SMR operation
  - 10 year target: 2025 operational deployment
- Couple MC neutronics to multiphase CFD:
  - Shift-MC (ORNL) + Nek5000 (ANL
- Demonstrated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



Shift Applications:
Transatomic Power MSR Reactor Physics Calculations



Power and flux distributions obtained from Monte Carlo mesh tallies



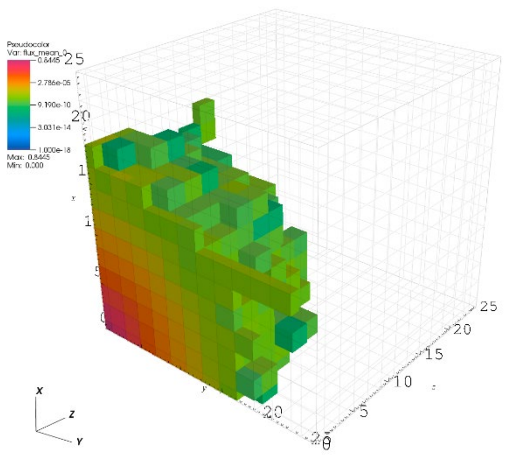
Tritium generation rates and core vessel metrics help identify potential operational issues

Figures provided by Ben Betzler

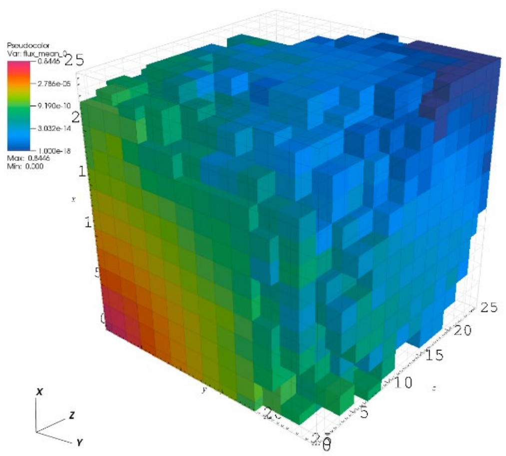
Hybrid Transport Methods

Hybrid methods make Monte Carlo more efficient

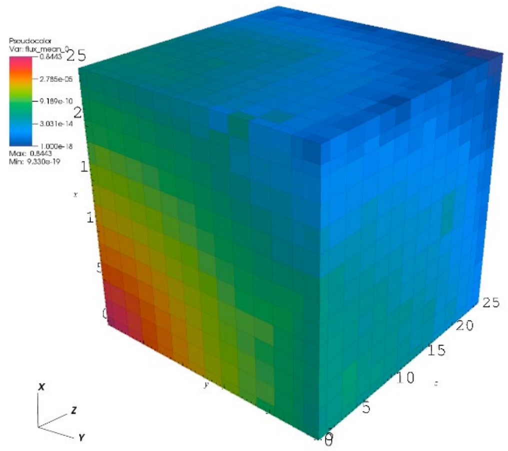
- Analog Monte Carlo convergence can be prohibitively slow, especially in large, shielded systems
- Advanced variance reduction techniques are necessary to generate Monte Carlo results with acceptable statistical errors
- These methods seek to increase the figure of merit: $\text{FOM} = \frac{1}{R^2 T}$



Analog MC



CADIS
Consistent Adjoint Driven Importance Sampling
Optimization of a single region



FW-CADIS
Forward-Weighted CADIS
Optimization of distributions

Hybrid methods enable Monte Carlo solutions on problems that were previously considered impossible

Hybrid Transport Methods

Consider a single response that we want to tally:

$$\underbrace{R}_{\substack{\text{scalar}\\\text{response}}} = \int_V \int_0^\infty \underbrace{\sigma_d(\vec{\mathbf{r}}, E)}_{\substack{\text{known response function}\\\text{(e.g., detector cross section)}}} \int_{4\pi} \psi(\vec{\mathbf{r}}, E, \widehat{\mathbf{\Omega}}) d\widehat{\mathbf{\Omega}}\, dE\, dV = \langle \psi, \sigma_d \rangle$$

where the angular flux ψ is the solution of the transport equation (subject to boundary condition on ∂V):

$$\boldsymbol{H}\psi(\vec{\mathbf{r}}, E, \widehat{\mathbf{\Omega}}) = \underbrace{q(\vec{\mathbf{r}}, E, \widehat{\mathbf{\Omega}})}_{\text{known, fixed source}}$$

$$\boldsymbol{H} = \widehat{\mathbf{\Omega}} \cdot \vec{\mathbf{\nabla}} + \sigma(\vec{\mathbf{r}}, E) - \iint d\widehat{\mathbf{\Omega}}' dE' \sigma_s(\vec{\mathbf{r}}, E', \widehat{\mathbf{\Omega}}' \rightarrow E, \widehat{\mathbf{\Omega}})$$

Slide from Scott Mosher, ADVANTG lead developer

Hybrid Transport Methods

The solution of the adjoint transport equation is an *importance function* or *map*:

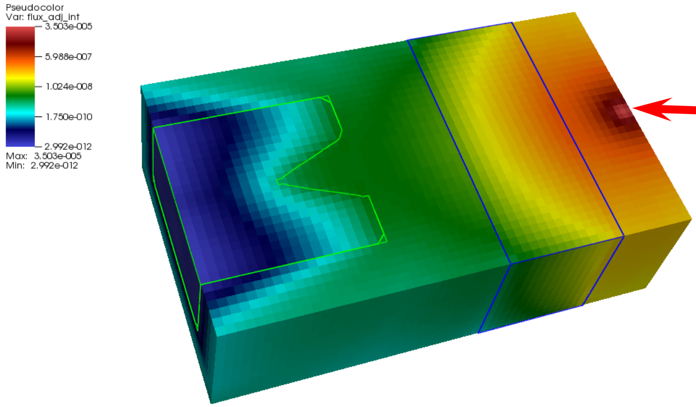
$$\underbrace{\boldsymbol{H}^{\dagger}\psi^{\dagger}\left(\vec{\mathbf{r}}, E, \widehat{\boldsymbol{\Omega}}\right)}_{\text{also subject to BCs on } \partial V} = \underbrace{\sigma_d\left(\vec{\mathbf{r}}, E\right)}_{\text{response function from previous slide}}$$

$$\underbrace{\boldsymbol{H}^{\dagger} = -\widehat{\boldsymbol{\Omega}} \cdot \vec{\boldsymbol{\nabla}} + \sigma\left(\vec{\mathbf{r}}, E\right) - \iint d\widehat{\boldsymbol{\Omega}} dE \, \sigma_s\left(\vec{\mathbf{r}}, E, \widehat{\boldsymbol{\Omega}} \to E', \widehat{\boldsymbol{\Omega}}'\right)}_{\text{adjoint transport operator}}$$

EXAMPLE

$$\iint \psi^{\dagger}\left(\vec{\mathbf{r}}, E, \widehat{\boldsymbol{\Omega}}\right) d\widehat{\boldsymbol{\Omega}} dE$$

(approximately)



$\sigma_d\left(\vec{\mathbf{r}}, E\right)$

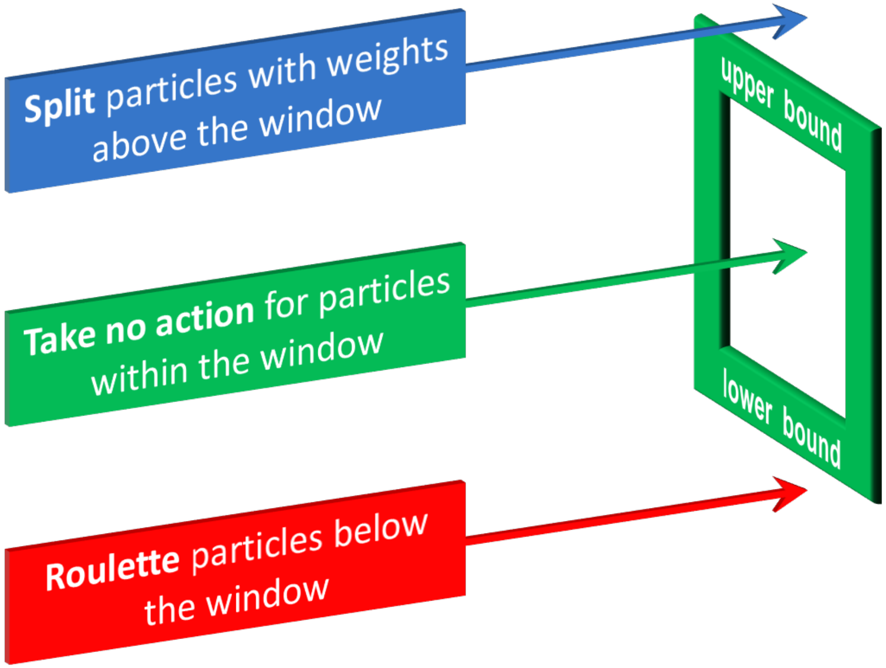
Flux-to-dose-rate conversion factor (E) localized at a point $(\vec{\mathbf{r}})$

Slide from Scott Mosher, ADVANTG lead developer

Hybrid Transport Methods

How can we use this *importance function* to accelerate a Monte Carlo simulation?

Weight Window Technique



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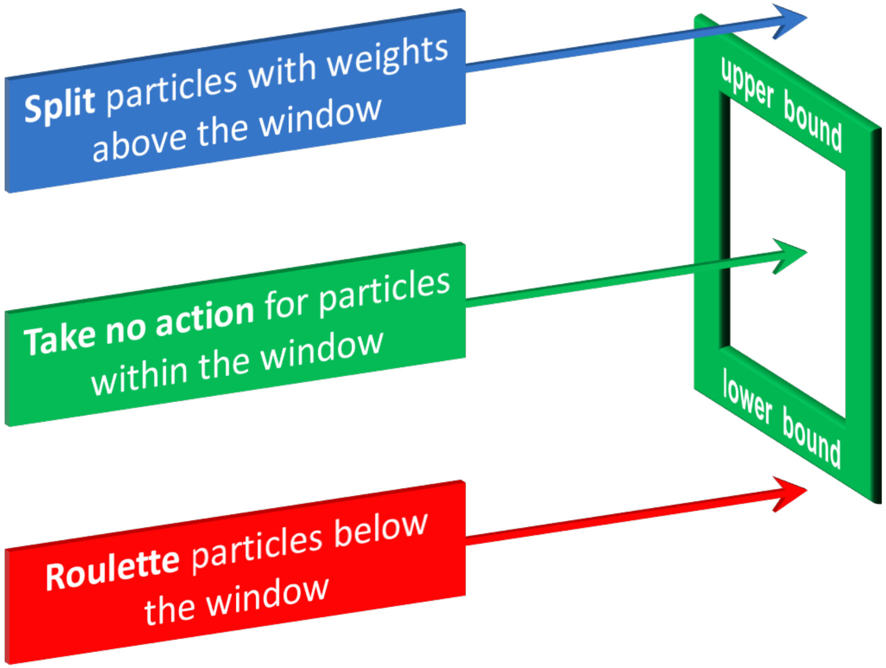
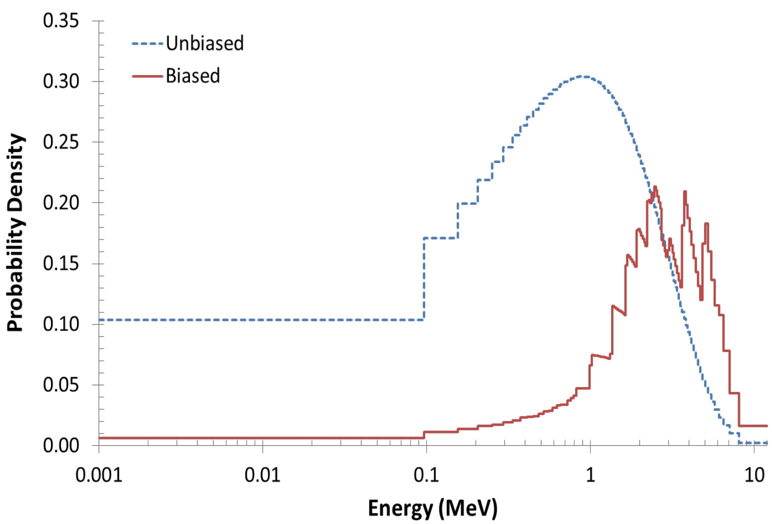


Source Biasing



Figures provided by Scott Mosher, ADVANTG lead developer

How hybrid variance reduction methods work

Monte Carlo accuracy at deterministic speeds

The CADIS Method

Consistent Adjoint-Driven Importance Sampling (CADIS)

- Solve the adjoint transport equation with a fast deterministic simulation, using the detector response as the adjoint source
- Estimate the detector response

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

- Calculate consistently biased source

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

- Conserve particle weights

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

- Calculate weight windows

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

J. C. Wagner and A. Haghighat, "Automated Variance Reduction of Monte Carlo Shielding Calculations Using the Discrete Ordinates Adjoint Function," *Nuclear Science and Engineering*, **128**, 186-208 (1998).

The FW-CADIS Method

Forward Weighted CADIS

- Optimize variance reduction parameters for multiple tallies or a mesh tally
- Solve the forward transport equation with a deterministic simulation to estimate the responses
- Construct an adjoint source at all detector locations and weight it with the response estimate

$$q_i^\dagger = \frac{\sigma_d^i}{R_i}$$

- Continue with the CADIS procedure

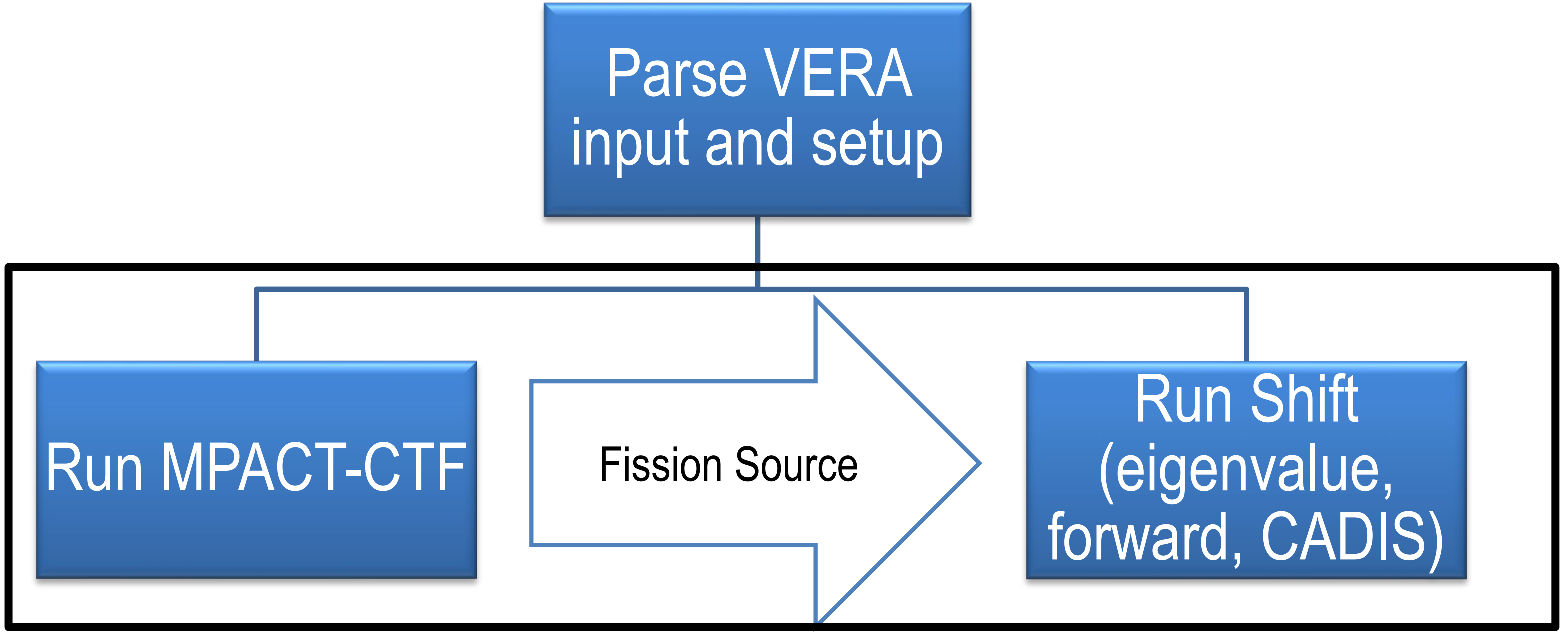
J.C. Wagner, D.E. Peplow, and S.W. Mosher, "FW-CADIS Method for Global and Regional Variance Reduction of Monte Carlo Radiation Transport Calculations," *Nuclear Science and Engineering*, **176**, 37-57 (2014).

Shift Capabilities in VERA

Shift Capabilities in VERA

- Shift is coupled to MPACT-CTF in VERA for validation and excore calculations
- Shift and MPACT-CTF run on their own separate sets of processors
- Shift capabilities through VERA include:
  - Automatically generating a detailed geometric core model
  - Running in eigenvalue, forward, and CADIS (using S_N adjoint) modes
  - Vessel fluence: tallying energy-binned flux in user-defined azimuthally divided rings and writing to HDF5 output at each state point through *standard* VERA input
  - Through a *supplemental* Omnibus input:
    - Inserting a detailed core model into a broader user-defined excore model
    - Obtaining excore tallies for any user-defined unknowns in the excore geometry with the requested tally output for each state point to HDF5

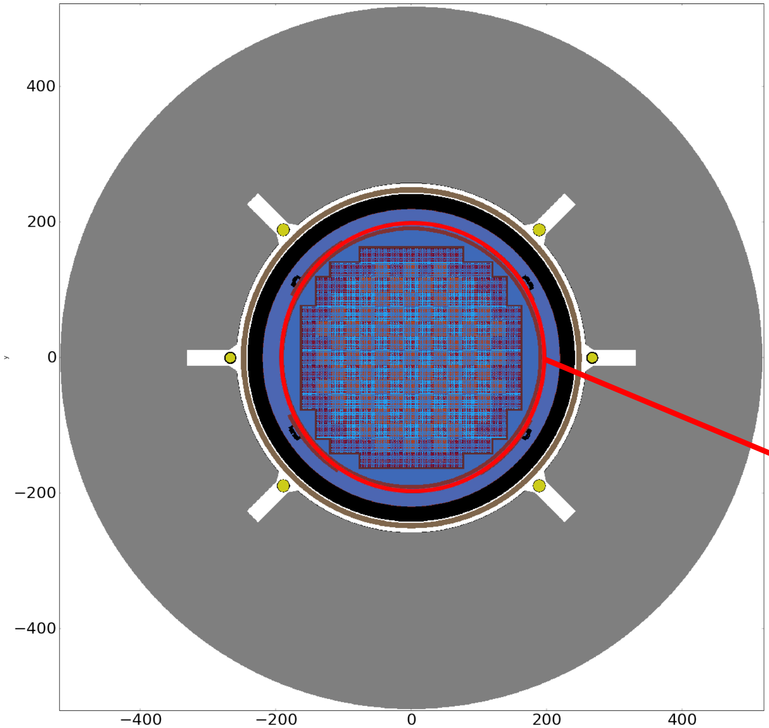
Shift coupling in VERA



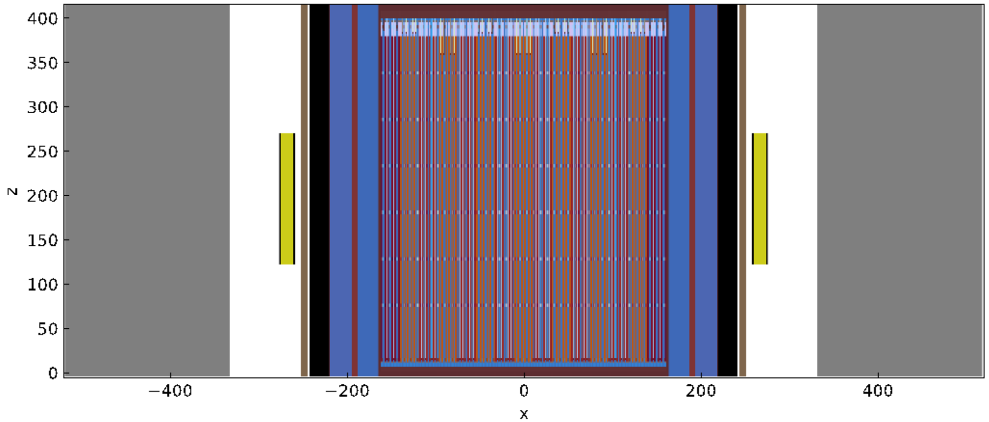
Receive in-core isotopics, temperatures, and densities at first state point

The user can define coupling to determine what Shift receives from MPACT-CTF. Currently, memory consumption limits the ability to couple at each state point for large problems.

VERA with Shift handles the intricate core details automatically



Full core Watts Bar model: (4x2) power range detectors, 2 source range detectors, 2 dual surveillance capsules and 2 single surveillance capsules



- The core model is defined in the VERA input
- The core and physics parameters can be inserted into a larger model that includes ex-core features
- VERA couples Shift with MPACT-CTF
  - Fission source, isotopics, densities, and temperatures can be automatically transferred from MPACT-CTF calculation
  - Coupling requires no direct user-intervention

Shift Execution Modes in VERA

In-core analysis

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

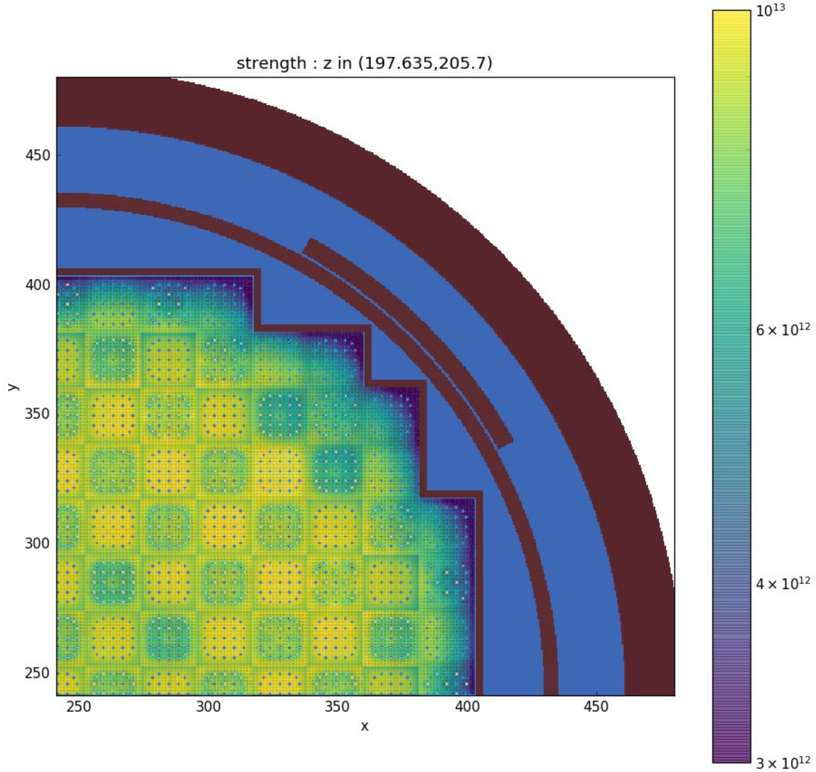
Ex-core analysis

- Fixed-source
  - Uses fission source from VERA-CS
  - Hybrid methods (optional)
- In-core model generated from VERA input
- Supplemental *Omnibus* input allows user description of geometry outside of core barrel and user-defined tallies

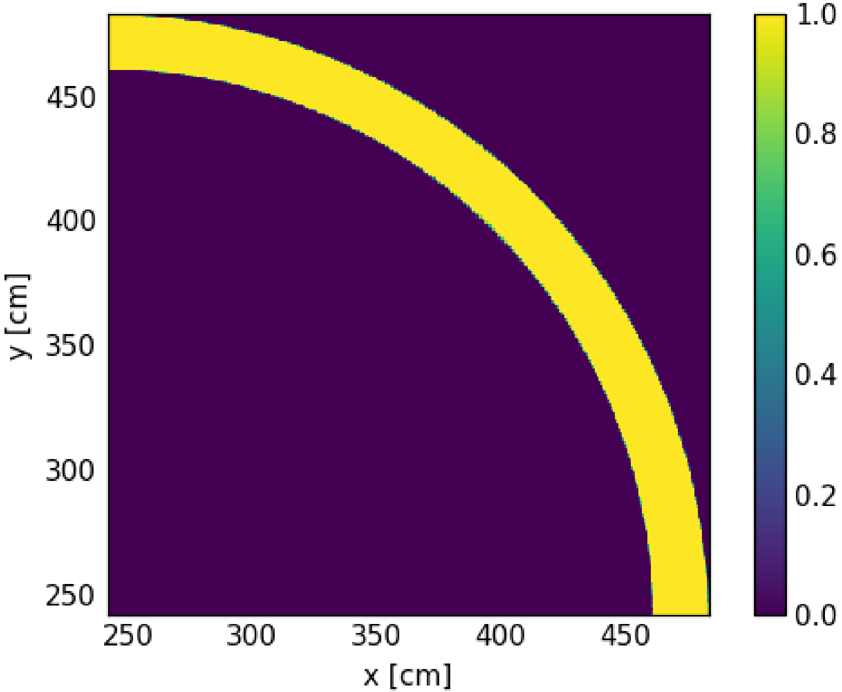
Shift Variance Reduction in VERA

- For excore calculations, Shift can perform the simulation in forward or CADIS (Consistent Adjoint-Driven Importance Sampling) mode
- CADIS mode:
  - Runs the Denovo deterministic transport code to solve for the adjoint across the problem space
  - Creates weight windows and consistently biased source
  - Optimizes for vessel fluence or a user-defined tally in the excore geometry specified via a separate *Omnibus* input
- Shift can output the adjoint flux, adjoint source, and weight windows for the first state point

Shift Variance Reduction in VERA



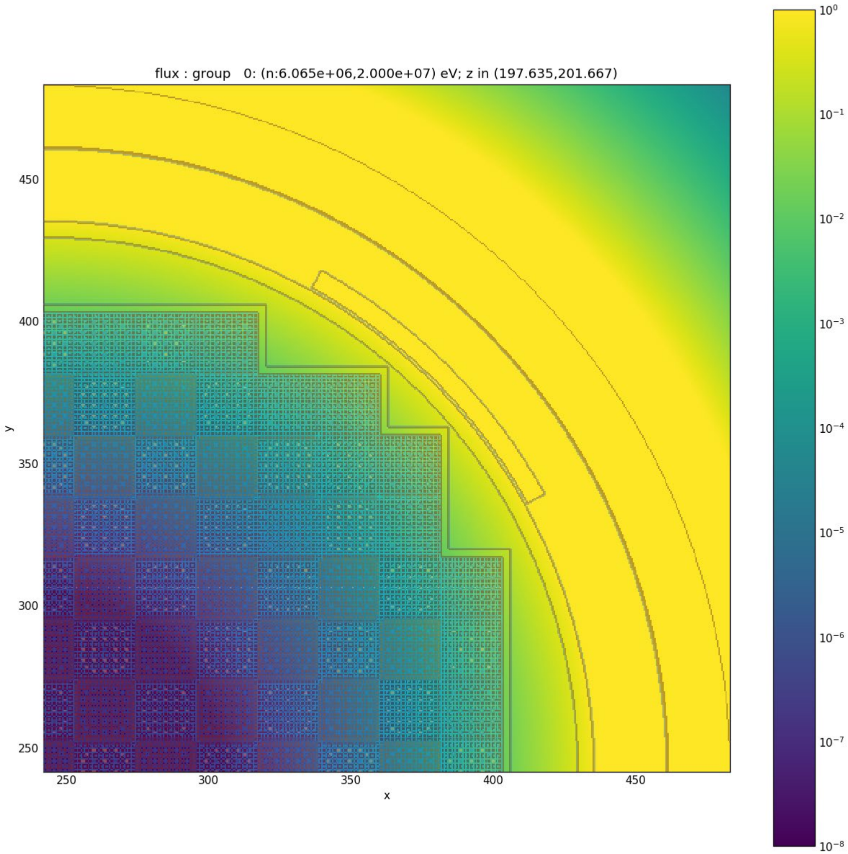
Fission source from MPACT for Watts Bar state 2 at the specified axial location in units of neutrons/cm^3-s



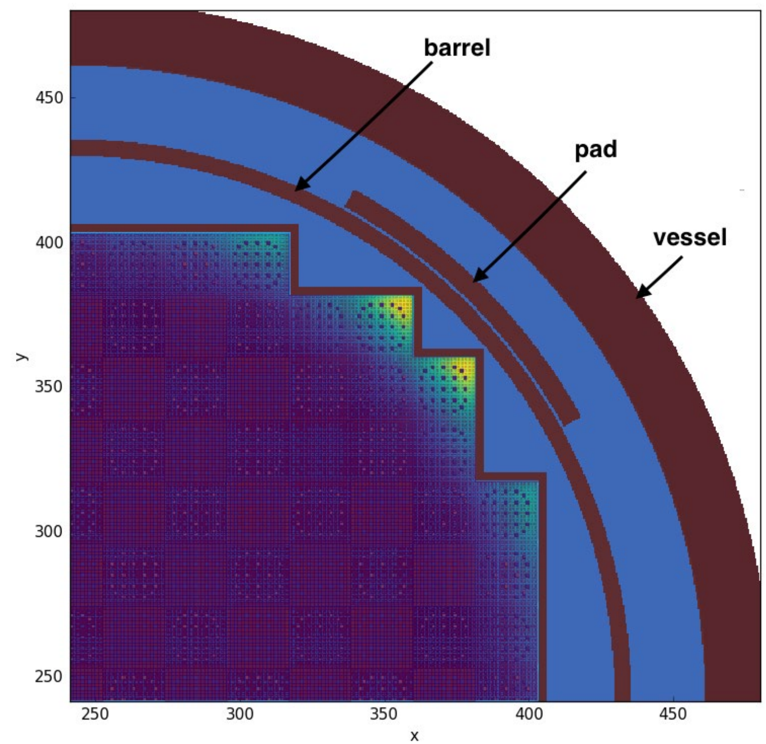
Adjoint source located in pressure vessel

Plots produced using Shift python post-processing tools

Shift Variance Reduction in VERA



Adjoint function for Watts Bar

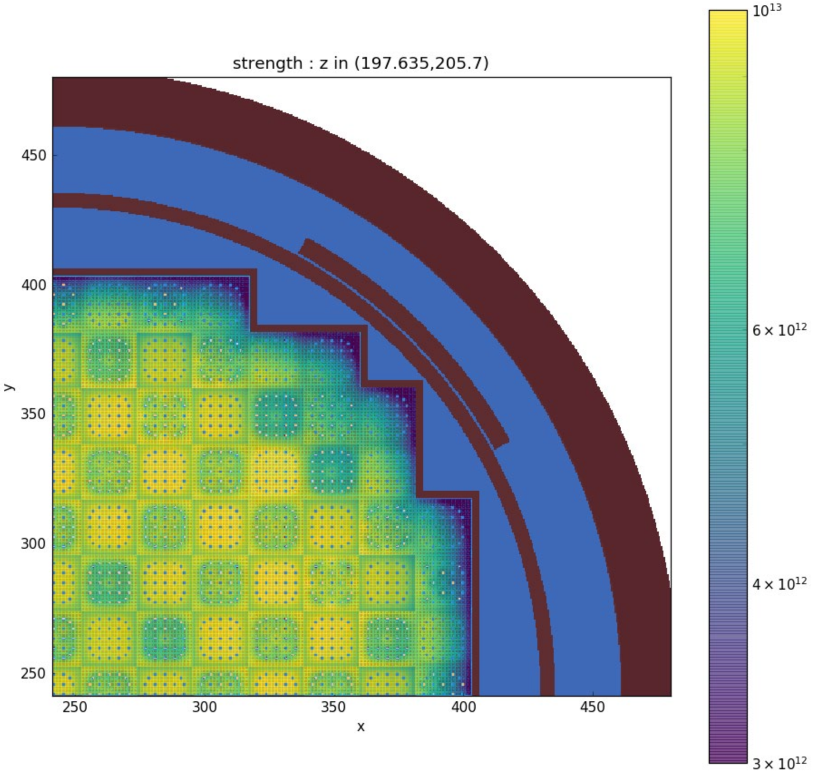


Source region importance for Watts Bar over all axial locations (adjoint flux folded with the fission source for first depletion state)

Plots produced using Shift python post-processing tools

Shift excore capabilities with VERA

- CADIS implementation
  - Consistent source biasing
  - Full or separable weight windows
  - Excore mesh size parameter selection
  - Optimize for user defined excore tallies
- Fission source spectrum used by Shift
  - ^{235}U Watt spectrum
  - MPACT 51-group fission spectrum



- Shift passes vessel flux for each state back to MPACT, which then accumulates vessel fluence and outputs it

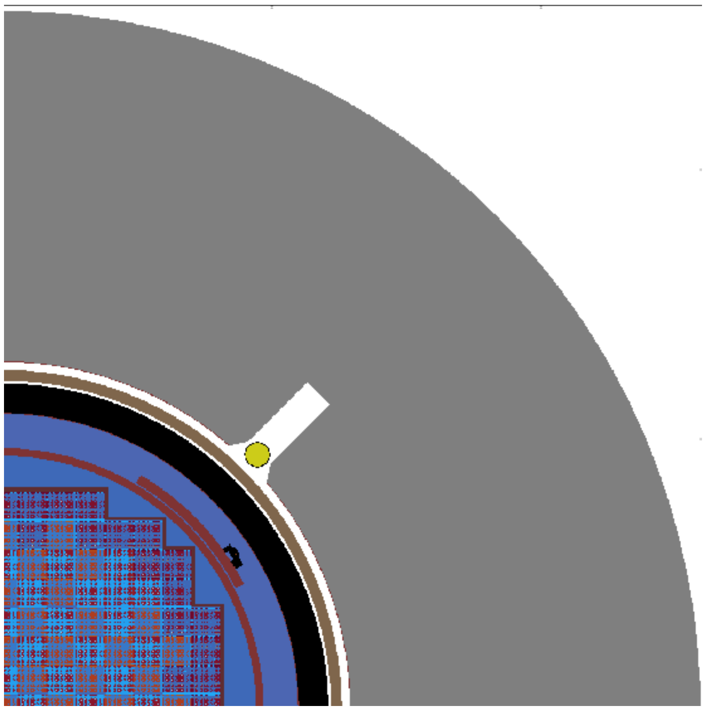
Shift excore capabilities with VERA

- Excore geometry options
  - Using the supplemental *Omnibus* input file, the user can define:
    - A detailed geometric model of features outside the core
    - Excore tallies
  - Always use core out to barrel from VERA input
  - Option to pull in up to outer vessel from VERA input

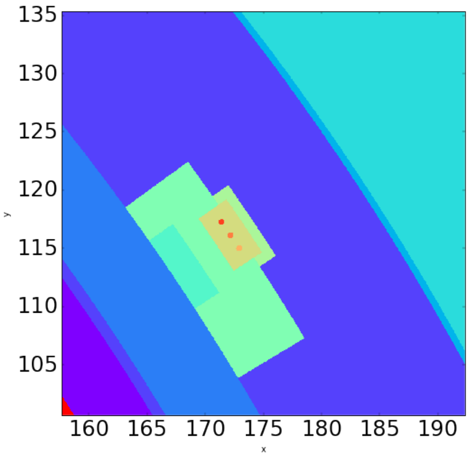
- Shift passes the results of tallies specified in the *Omnibus* excore input back to MPACT at each state point

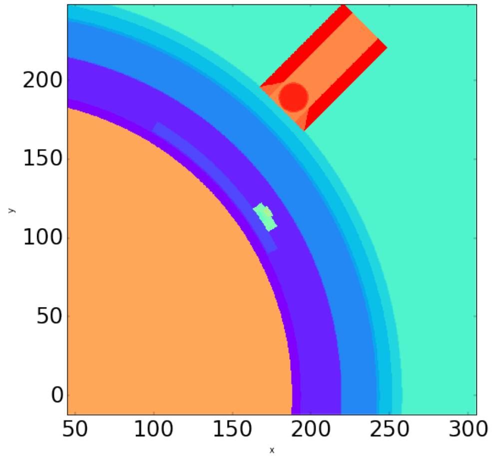
Excore modeling with VERA and Omnibus

Quarter core model: power range detector and coupons (Co, Cu, Fe) in the single surveillance capsule



Materials with Watts Bar Core (XY slice @ Z=200 cm)



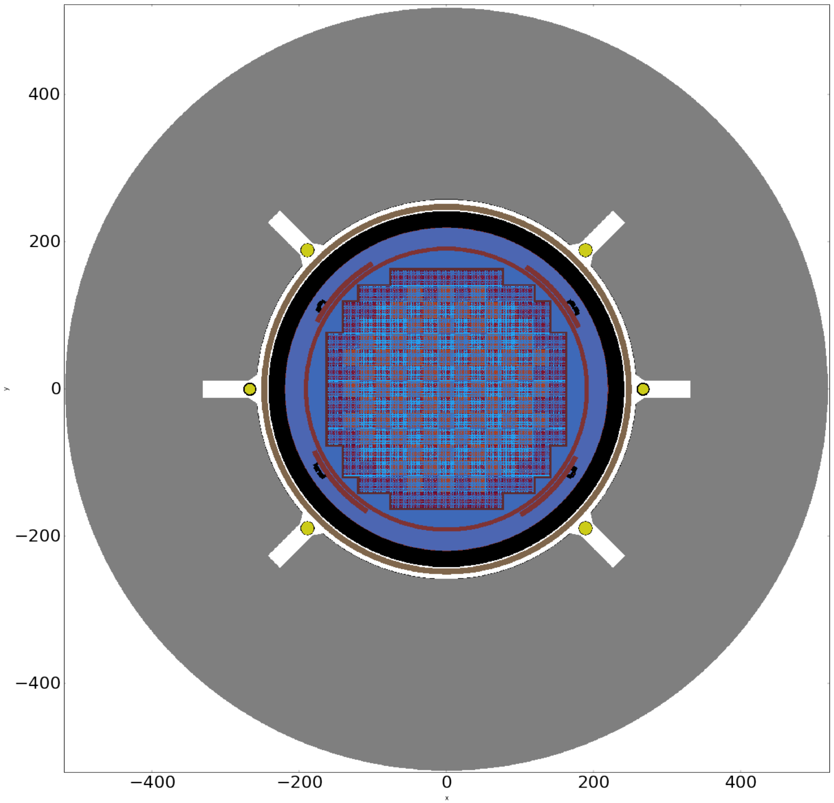


Different colors are different geometric cell definitions

Generated by Eva Davidson

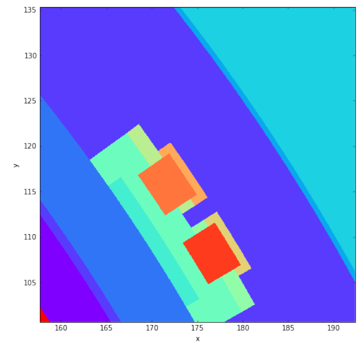
Excore modeling with VERA and Omnibus

Full core model: (4x2) power range detectors, 2 source range detectors, 2 dual surveillance capsules and 2 single surveillance capsules

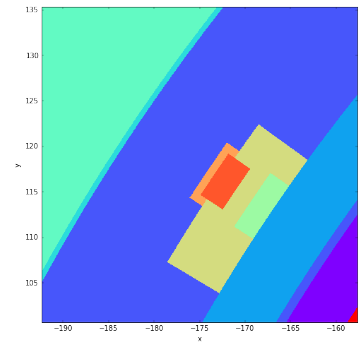


Materials with Watts Bar Core
(XY slice @ Z=200 cm)

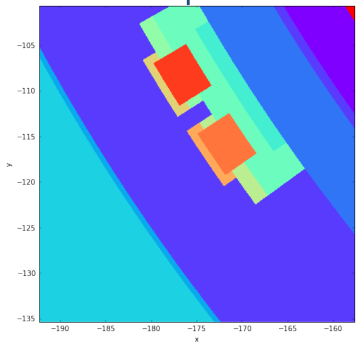
Double surveillance capsule
NE quadrant



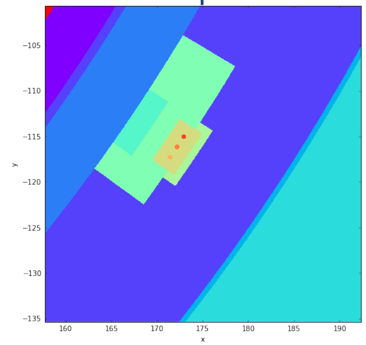
Single surveillance capsule
NW quadrant



Double surveillance capsule
SW quadrant



Single surveillance capsule
SE quadrant

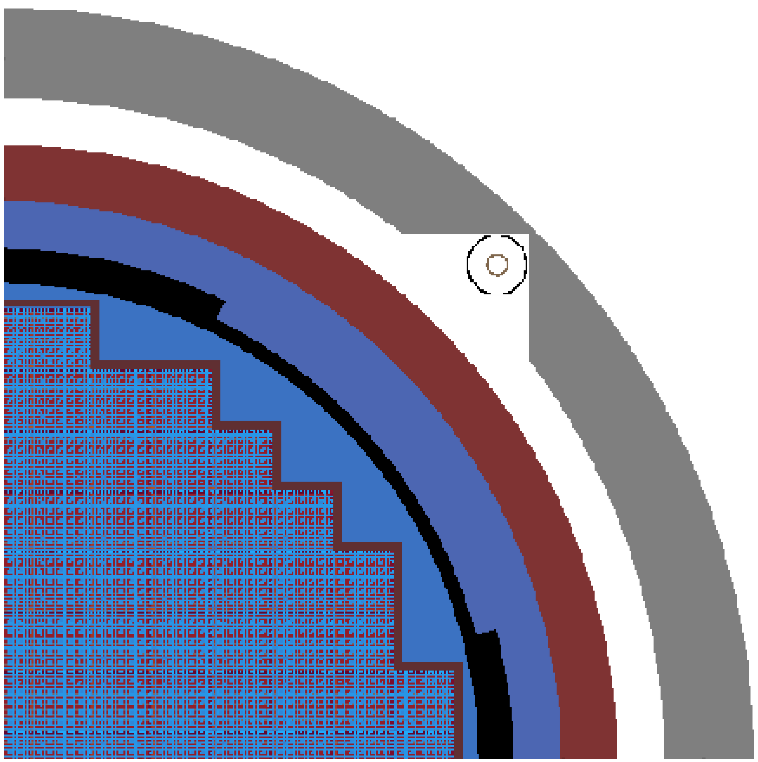


Different colors are different geometric cell definitions

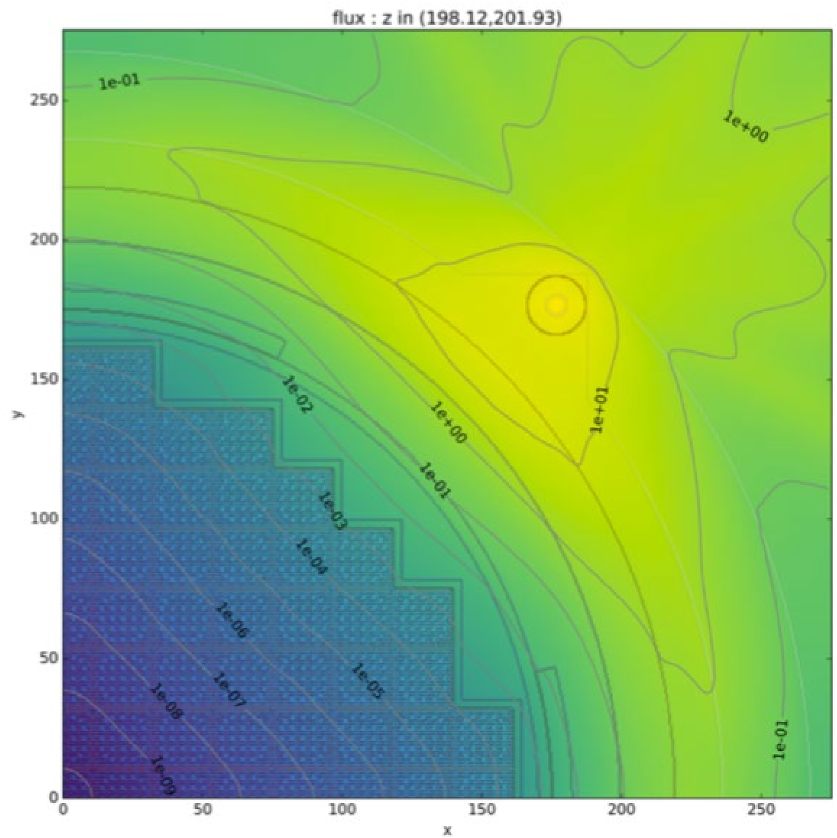
Generated by Eva Davidson

Excore Detector Response: Harris PWR

- Excore detector modeled with Omnibus
- Varied moderator and downcomer density and examined relative detector response



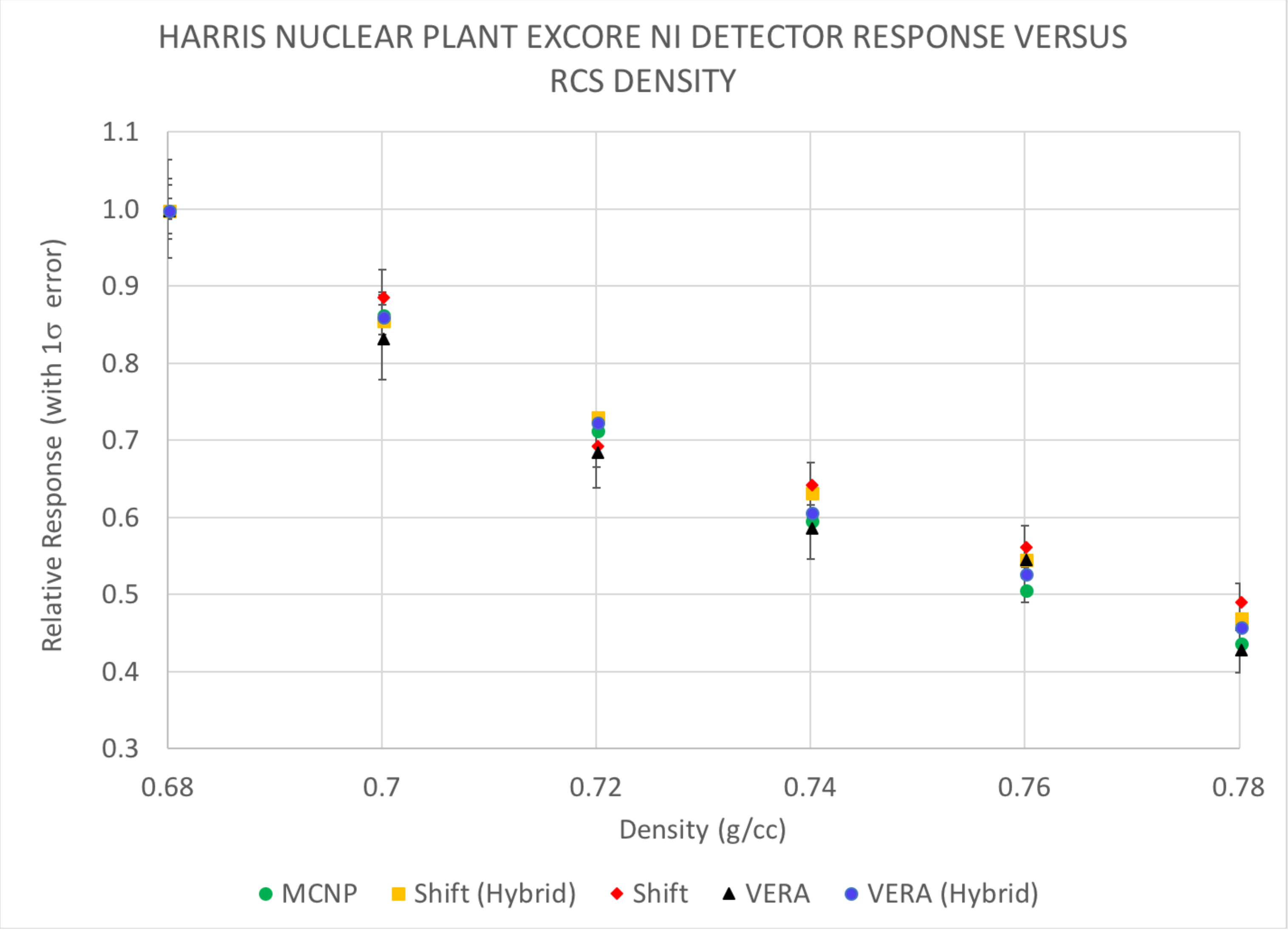
Integrated in-core and ex-core Harris Model



Adjoint function

Work done by Eva Davidson and Herschel Smith

Excore Detector Response: Harris PWR



Work done by Eva Davidson and Herschel Smith

Excore Detector Response: Harris PWR

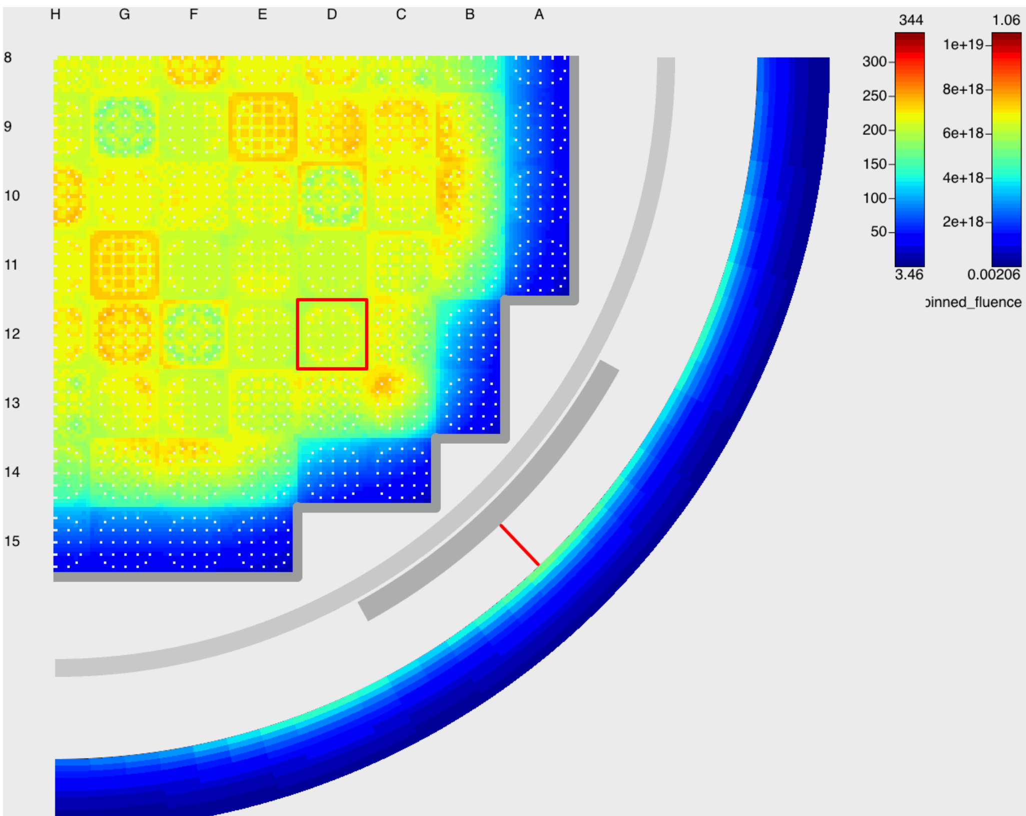
All calculations run on ORNL's Panacea cluster with 738 cores (338 MPACT, 400 Shift)

Case	Forward Mode			CADIS Mode			FOM Ratio
	Rel. Error	Time (min)	FOM	Rel. Error	Time (min)	FOM	
shqca1	4%	145.6	0.17	1%	4.5	35.7	216
shqca3	5%	143.8	0.14	1%	4.6	30.5	216
shqca5	5%	142.0	0.14	1%	3.8	47.4	337
shqca7	6%	140.5	0.12	1%	5.3	20.1	166
shqca9	12%	139.0	0.06	1%	3.9	42.2	708
shqca11	6%	137.9	0.11	1%	4.2	37.6	327

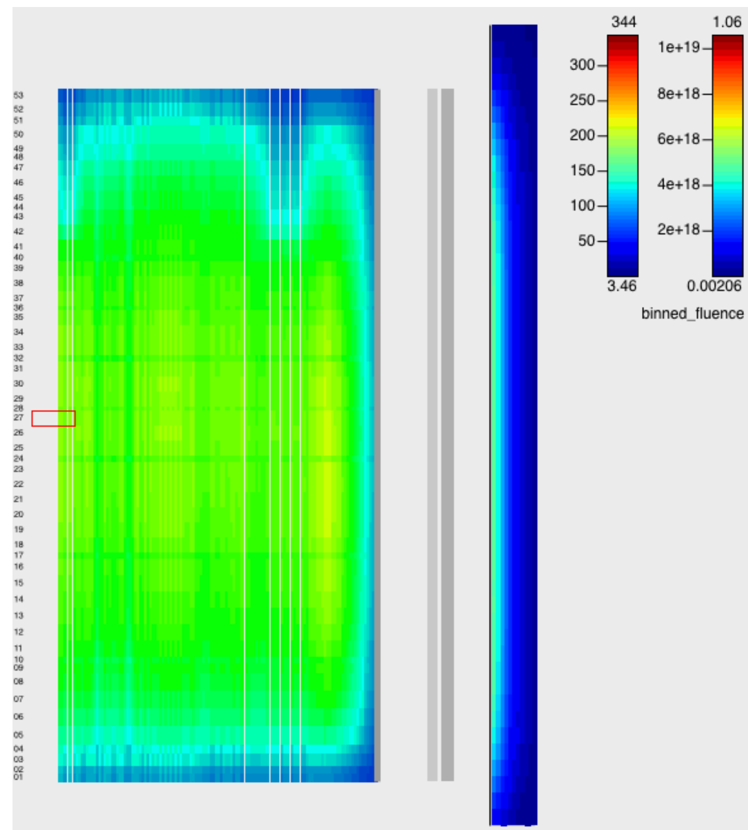
Work done by Eva Davidson and Herschel Smith

Vessel Fluence Calculation: *Watts Bar Unit 1*

- Simulated 15 cycles of Watts Bar Unit 1 using VERA
- Typical core follow simulations with BOC fuel shuffle, HFP cycle depletion using MPACT, CTF, and ORIGEN
- Vessel fluence calculated from Shift vessel flux (Neutron flux > 1 MeV)



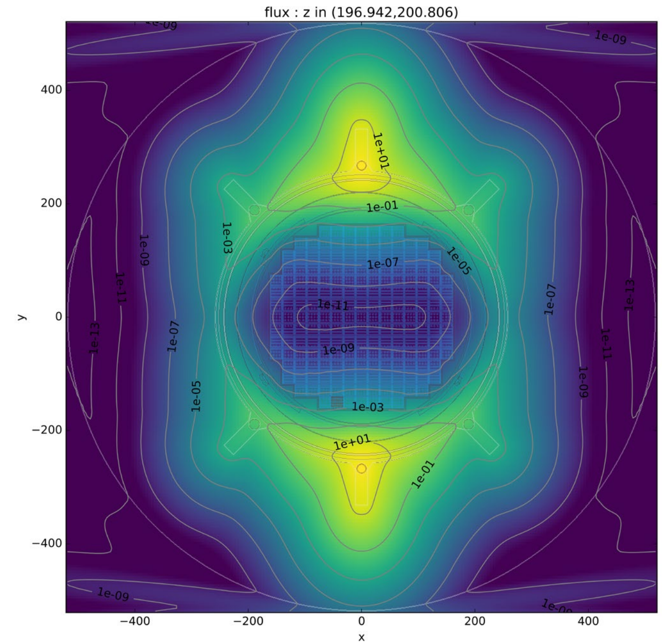
pin_lhr: Axial 200.806, vessel_tally/binned_fluence (flux/mean) at 203.550, exposure_efpy 9.309



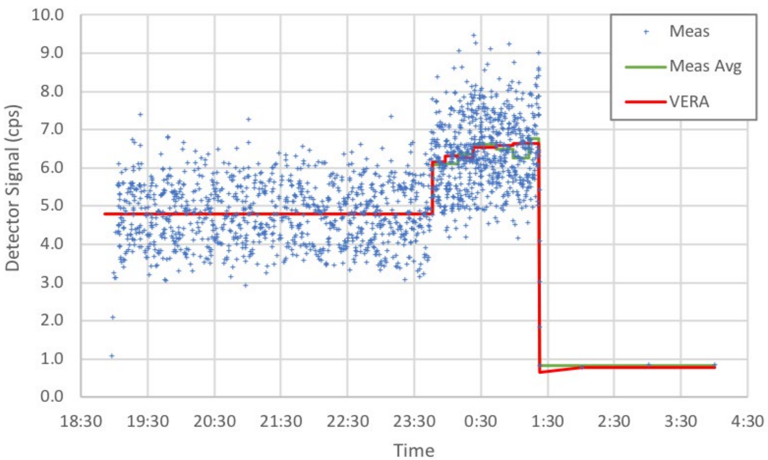
pin_lhr: vessel_tally/binned_fluence (flux/mean), th=43 deg, exposure_efpy 9.309

Source Range Detector Response Validation

- Latest VERA methods used to predict detector signals outside of the pressure vessel in Watts Bar Unit 1
- Conditions difficult to predict with industry codes: partially-loaded, subcritical cores with secondary neutron sources
- Excellent agreement between calculations and measurements: **-0.3±3.9%** over ~17,000 measured points averaged over 140 total intervals (8 fuel cycles)
- Publicly available report delivered to DOE headquarters on Dec. 31, 2018



Adjoint Flux Calculated by Shift for Source Range Detectors (Image by Eva Davidson)



Detector Response Results for Cycle 10 Refueling

RNSD Contributors:
Ben Collins, Eva Davidson, Cole Gentry, Andrew Godfrey, Germina Ilas, Tara Pandya, Katherine Royston, and many others

Conclusions

- Shift is a flexible, high-performance Monte Carlo radiation transport *framework*
  - Multiple front-ends
  - Physics and geometry agnostic
- Shift implements advance variance reduction techniques
  - Denovo deterministic transport code calculates adjoint and/or forward solution
  - Generates weight windows and a consistently biased source
  - Focuses the Monte Carlo simulation on “important” particles
- In VERA, Shift is coupled with MPACT-CTF for in-core and ex-core analyses
  - Detailed in-core model created from VERA input
  - Fission source, isotopics, densities, and temperatures automatically transferred
  - Optional *Omnibus* input allows for modeling ex-core details and tallies
  - CADIS mode allows for significant improvement in performance

Future development

- Performance optimization:
  - Full isotopic, temperature coupling in core (reduce CE data memory usage)
  - Multithreading to allow more efficient use of node-based shared memory
  - Method of Poles for on-the-fly Doppler broading (ECP)
    - Smaller memory footprint required for CE data (GB to MB)
    - More computational cost (1.2 – 2x)
  - Domain Decomposition to enable machine scaling to arbitrary-sized problems
- User interface updates
  - Add basic excore detector specification to VERA input
    - Simple detectors outside the vessel
    - Will not require user to create supplemental *Omnibus* file
  - Automate excore post-processing utilities
  - Allow weight windows and biased source to be calculated at user selected state points during multicycle calculations
- Visualization: extend VERAView capabilities to plot fission source and pin importances for vessel fluence calculations

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