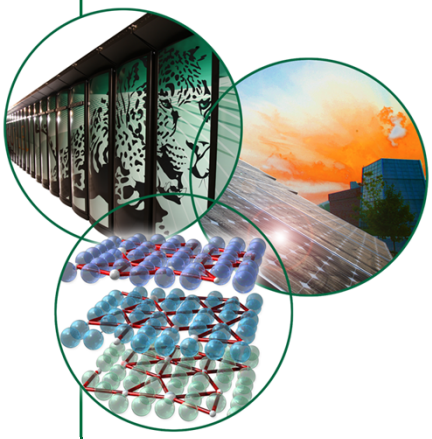
Enabling Capability Developments in Radiation Transport

Briefing for Nuclear Science & Engineering Directorate Advisory Committee



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U.S. DEPARTMENT OF ENERGY

OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

Overview

- Brief background on RT Methods
  - Deterministic methods
  - Stochastic methods
  - Hybrid methods
- Advanced RT Methods & Codes at ORNL
  - Deterministic – Denovo
  - Hybrid methods/codes
  - Monte Carlo – Shift
- Summary Remarks
- Contributors and Acknowledgments

Deterministic methods produce system-wide solutions and are computationally efficient, but require discretization approximations

- Deterministic methods (e.g., discrete ordinates, S_N)
  - Solve the Boltzmann transport equation for the average particle behavior
  - Produce detailed information throughout the problem space
  - Computational inexpensive (relatively)
  - Accuracy limited by required approximations
    - space/energy/angle discretization → more resolution provides higher accuracy
  - Examples of codes:
    - ORNL – ANISN, DOT, DORT, TORT, XSPRNPM, NEWT, Denovo
    - LANL – DTF, ONEDANT, TWODANT, THREEDANT, PARTISN

Stochastic methods are considered the most accurate, but are computationally intensive

- Stochastic methods (Monte Carlo, MC)
  - Simulates individual particles and infers the average behavior from the average behavior of the simulated particles
  - Highly accurate
    - Explicit geometric, angular and nuclear data representation
    - Avoids geometric meshing and problem-dependent multi-group cross-section processing – easy to use
  - Computationally expensive; results have associated statistical uncertainties

$$RE \propto 1/\sqrt{N}$$

  - Examples of codes:
    - ORNL – MORSE, KENO, Monaco
    - LANL – MCNP, MCNPX

Hybrid methods use the best attributes of different methods in a complementary manner

- In this discussion, the Hybrid Methods *use fast, approximate (deterministic) calculations to speed-up highly accurate (MC) simulations*
  - Best of both worlds…
    - Calculate 3-D adjoint (importance) function with a deterministic code
    - Calculate variance reduction (VR) parameters based on adjoint function
    - Utilize the VR parameters in the MC simulation
    - Automate above steps (key to usefulness)
  - Examples of codes:
    - ORNL – ADVANTG (MCNP/X), SCALE

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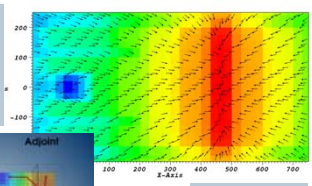
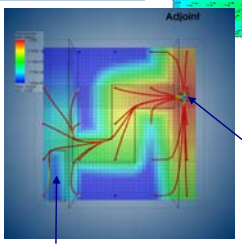
Denovo is a new, modern S_N RT code that takes advantage of decades of research/experience

- **Originally developed to support hybrid methods, but has expanded well beyond that**

Denovo provides adjoint data used to generate consistent mesh-based weight windows & source biasing parameters for accelerating MC calculations.



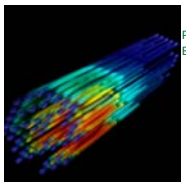


adjoint currents show preference from source to tally region

Tally region in forward problem

forward source region

- **State of the art transport methods**
  - 3D/2D, non-uniform, regular grid S_N
  - 2D MoC Solver
  - Multi-group energy, anisotropic P_N scattering
  - Forward/Adjoint
  - Fixed-source/*k*-eigenvalue
  - 6 spatial discretization algorithms
  - Parallel first-collision
  - Multiple quadratures
- **Modern, Innovative, High-Performance Solvers**



Power distribution in a BWR assembly0

Denovo was developed to use parallel computing to enable solutions to very large problems

- **Parallel Algorithms**
  - Koch-Baker-Alcouffe (KBA) wavefront decomposition
  - Domain-replicated (DR) and domain-decomposed first-collision solvers
  - Multilevel energy decomposition in development
  - Parallel I/O built on SILO/HDF5

Core Neutronics Package in VERA Toolset
2012-13 INCITE Award
The Solution of 3D PWR Neutronics Benchmark Problems for CASL, 19 MCPU-HOURS
2010-11 INCITE Award
Uncertainty Quantification for Three Dimensional Reactor Assembly Simulations, 26 MCPU-HOURS
2010 ASCR Joule Code
2009-2011 2 ORNL LDRDs

- **Advanced visualization, run-time, and development environment**
  - 3 front-ends (HPC, SCALE, Python-bindings)
  - Automated mesh generation
  - Direct connection to SCALE geometry and data (MG cross section processing)
  - Direct connection to MCNP input through ADVANTG
  - HDF5 output directly interfaced with VisIt
  - Built-in unit-testing and regression harness with DBC
  - Emacs-based code-development environment

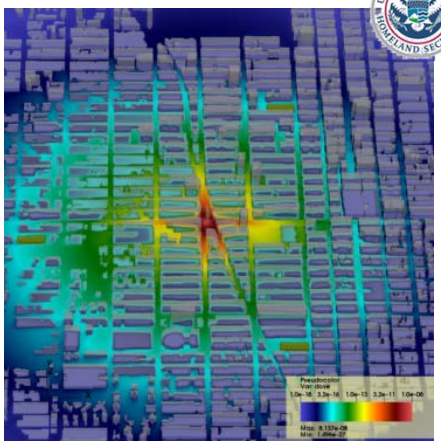
Denovo is being used to solve enormous problems of national interest

Postulated nuclear detonation in Manhattan, NY

- Num cells: 224,438,368
- Num angles: 288
- Num groups: 46
- Num moments: 16

- Num Unknowns in State: 1.36459e+11
- Memory of State (GB): 1.27087e+02
- Solved unknowns: 3.93001e+13
- Cores: 10080
- Wall-clock time (min): 1.79583e+01
- CPU-HOURS: 3.01700e+03

- Setup time (min): 1.15526e+00
- Ray-tracing (min): 4.08660e-02
- Solver time (min): 1.38992e+01
- Output time (min): 2.90386e+00



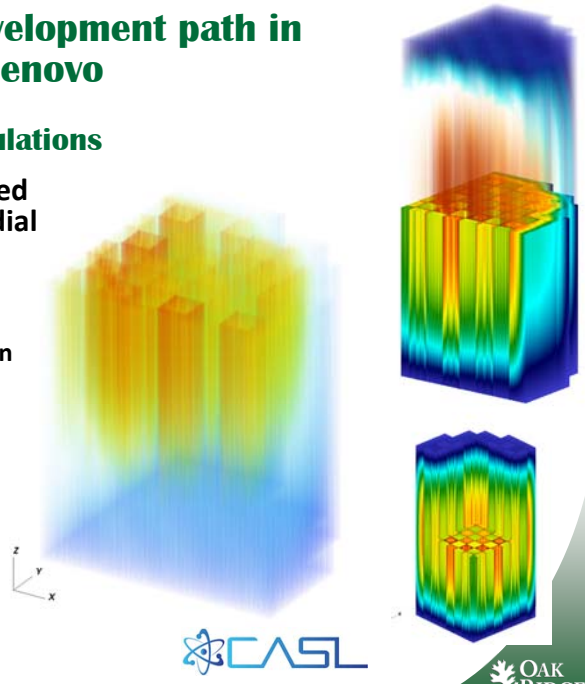
Prompt neutron dose per neutron

> 224M spatial cells, 46 neutron groups, P_3 Scattering, S_{16} angular quadrature, full-field solution in < 18 minutes with 10,080 cores on JAGUAR (3,017 CPU-Hrs)

The primary RT development path in CASL is based on Denovo

CASL Quarter Core Simulations

- Good results are achieved (< 40 pcm) using 4x4 radial zoning, 15.24 cm axial zoning, and QR 2/4 quadrature
  - Results attained in 42 min runtime using 960 cores
- Running a 1.6G-cell problem is feasible (190KCPU-hours)
- Current focus is on developing capabilities to enable 3D full-core pin-resolved transport with fewer meshes



Denovo is the centerpiece of ORNL's deterministic HPC transport

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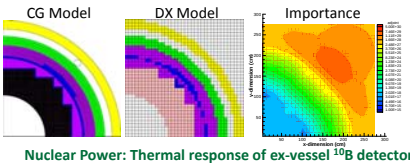
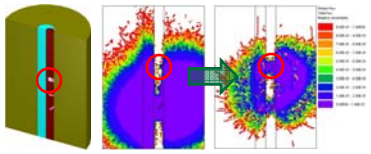
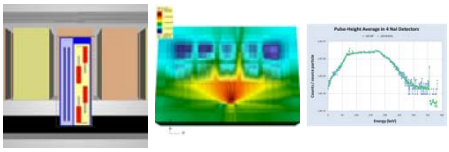
ORNL's hybrid methods have accelerated and/or enabled MC solutions for many real-world problems



Nuclear Power: Thermal response of ex-vessel ^{10}B detector



Oil/Gas Exploration: Gamma response of litho-density tool



National Security: Pulse-height spectrum in portal NaI detectors

CADIS

Consistent Adjoint Driven Importance Sampling

goal: accelerate localized tallies

1: construct deterministic (DX) model
2: solve DX importance equation
3: compute weight targets & biased source
4: accelerate Monte Carlo

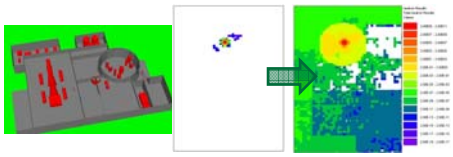
FW-CADIS method is transformational in that it enables high-fidelity MC results for distributions

FW-CADIS

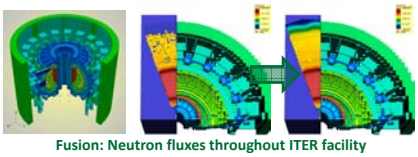
Forward Weighted Consistent Adjoint Driven Importance Sampling

goal: obtain uniform uncertainties

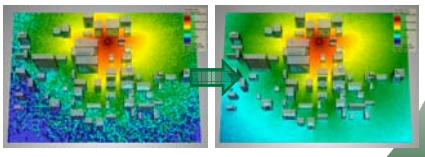
1: construct deterministic (DX) model
2: solve DX transport equation
3: construct importance source
4: solve DX importance equation
5: compute weight targets & biased source
6: accelerate Monte Carlo



Radiation Protection: Dose rates throughout PWR facility



Fusion: Neutron fluxes throughout ITER facility

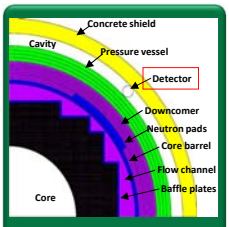


National Security: Prompt dose rates throughout Times Square

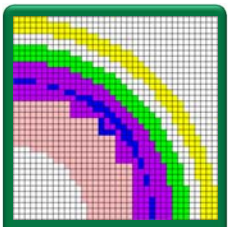
CADIS Example: PWR ex-vessel thermal detector response

Duke Energy

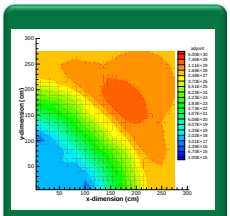
Goal: estimate the response of a ^{10}B ex-core detector to thermal neutrons



Monte Carlo model



deterministic model



importance estimate

$$w(\mathbf{P}) = \frac{R}{\phi^{+}(\mathbf{P})}$$

$$\hat{q}(\mathbf{P}) = \frac{\phi^{+}(\mathbf{P})\, q(\mathbf{P})}{R}$$

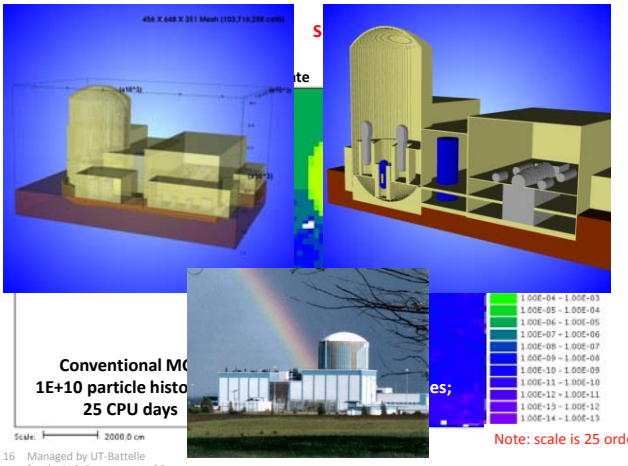
variance reduction parameters

Case	CPU Time (h) to 1% Relative Error	Speed-up
no VR	88,600 (10.1 y)	
manual VR	13.6	6,500*
CADIS	1.02	87,000

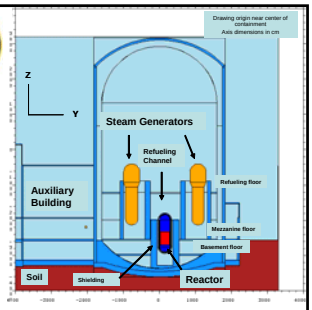
*Required 3 weeks by an experienced Monte Carlo practitioner (H.P. Smith and J.C. Wagner, *Nucl. Sci. Eng.* **149**, 2005)

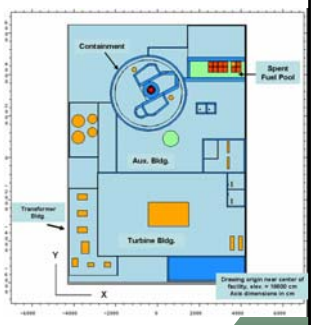
FW-CADIS example: dose throughout a PWR facility

- Full-scale PWR facility, including containment, auxiliary, turbine, and transformer buildings
  - Extent: 85 × 125 × 70 m
  - Sources modeled: reactor core, spent fuel pool, coolant activation



Conventional MC
1E+10 particle histo
25 CPU days

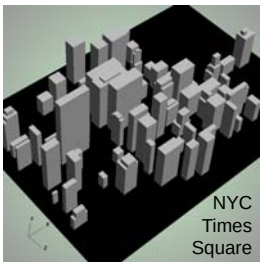




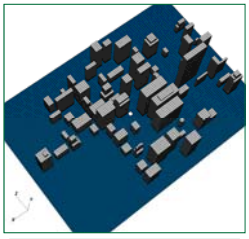
Note: scale is 25 orders of magnitude

The FW-CADIS method illustrated

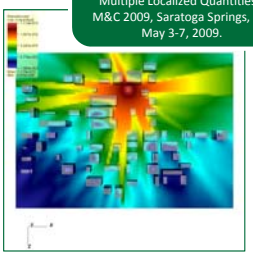
For details, see: "Forward-Weighted CADIS Method for Variance Reduction of Monte Carlo Calculations of Distributions and Multiple Localized Quantities," M&C 2009, Saratoga Springs, NY, May 3-7, 2009.



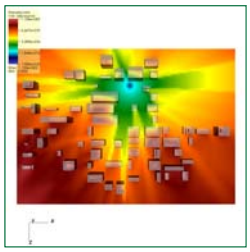
0: MC model



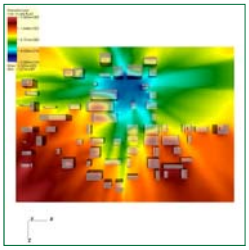
1: construct DX model



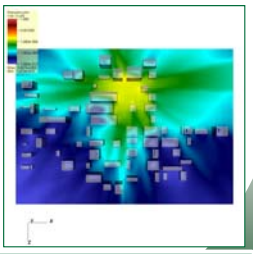
2: solve DX transport equation



3: construct importance source



4: solve DX importance equation

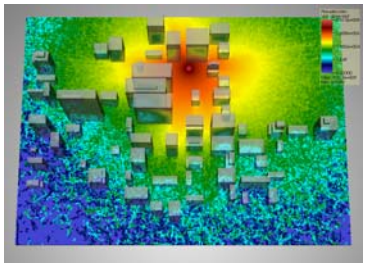


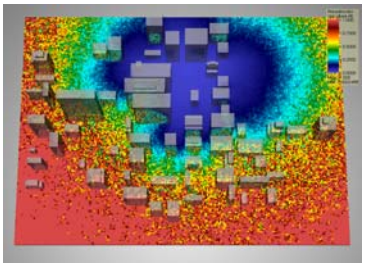
5: construct weight windows

ADVANTG FW-CADIS hybrid results

24-hr Monte Carlo simulation of a 20kT Hiroshima-like weapon

Conventional MC

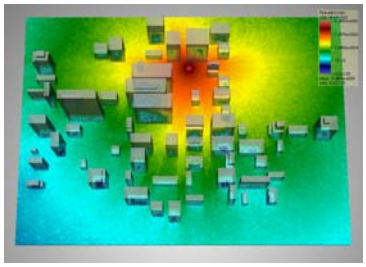


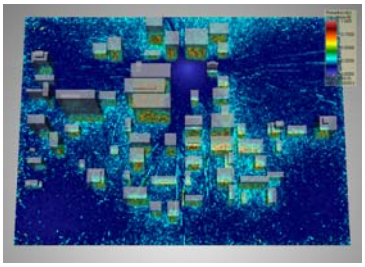


25% of cells have RE < 20%

48% of cells have RE < 50%

Hybrid





77% of cells have RE < 20%

97% of cells have RE < 50%

neutron dose (rad)

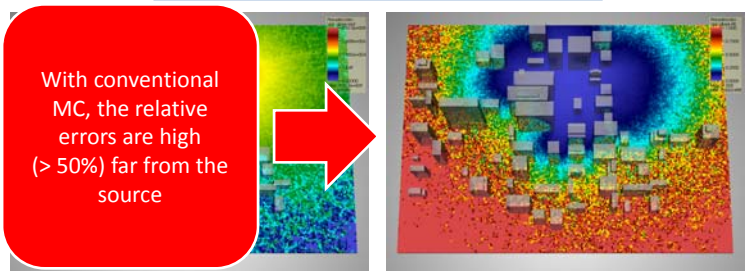
relative uncertainty

ADVANTG FW-CADIS hybrid results

24-hr Monte Carlo simulation of a 20kT Hiroshima-like weapon

Conventional MC

With conventional MC, the relative errors are high (> 50%) far from the source

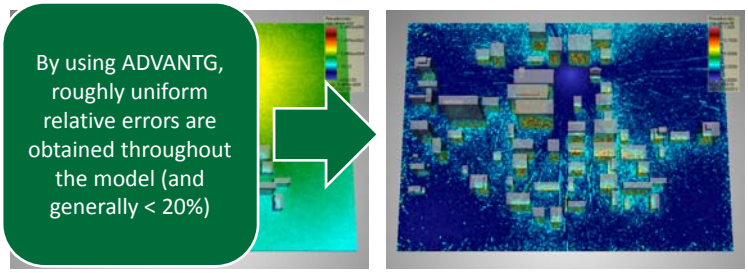


25% of cells have RE < 20%

48% of cells have RE < 50%

Hybrid

By using ADVANTG, roughly uniform relative errors are obtained throughout the model (and generally < 20%)



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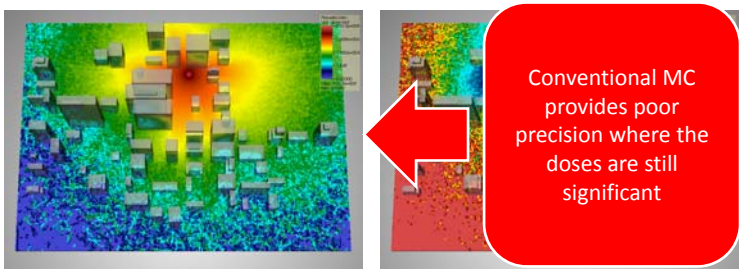
Conventional MC

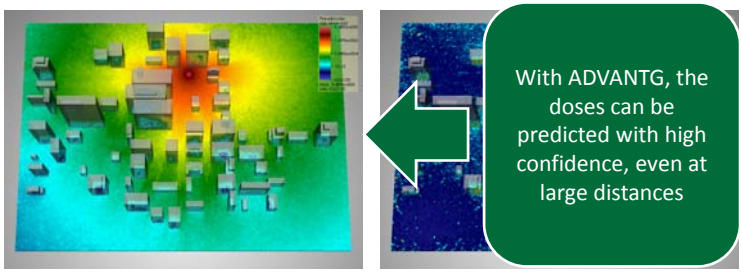


Conventional MC provides poor precision where the doses are still significant

25% of cells have RE < 20%

48% of cells have RE < 50%

Hybrid



With ADVANTG, the doses can be predicted with high confidence, even at large distances

77% of cells have RE < 20%

97% of cells have RE < 50%

neutron dose (rad)

relative uncertainty

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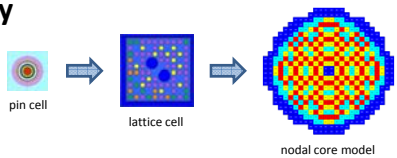
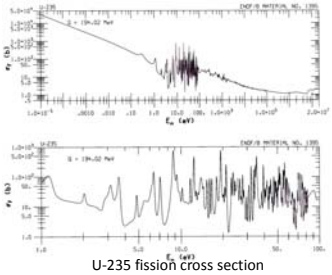
Shift Goal: Enable efficient full-core Monte Carlo reactor simulations on HPC platforms

- **Current state-of-the-art methodology**
  - Based on nodal framework (late 1970's)
  - High-order transport at small scale, diffusion at large scale
  - Single workstation paradigm



- **Continuous-energy Monte Carlo (MC)**
  - Explicit geometric, angular and nuclear data representation – **highly accurate**
  - Avoids problem-dependent multigroup xs processing – **easy to use**
  - Computationally intensive – **considered prohibitive for "real" reactor analyses**

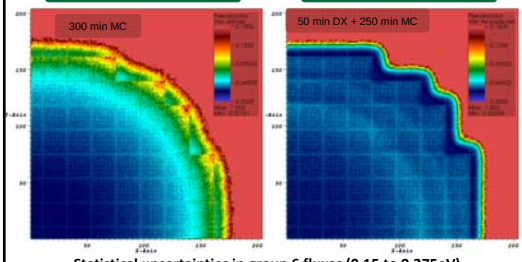


U-235 fission cross section

CHALLENGE: Prohibitive computational TIME and MEMORY requirements

FW-CADIS method helps to overcome prohibitive computational TIME requirements

Conventional MC | **MC w/FW-CADIS**



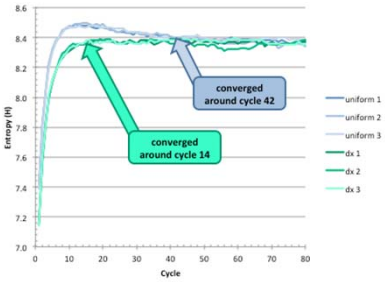
Statistical uncertainties in group 6 fluxes (0.15 to 0.275eV)

	MCNP	FW-CADIS
Uncertainty range	0.6 – 16.2%	1.0 – 6.6%
Time to < 2% uncertainty	323 hrs	45 hrs
Speed up (includes Denovo run time)	-	7.1*

*depending on computational parameters, the speed-up varied between 6 and 10

FW-CADIS deterministic solution can be exploited in other ways:

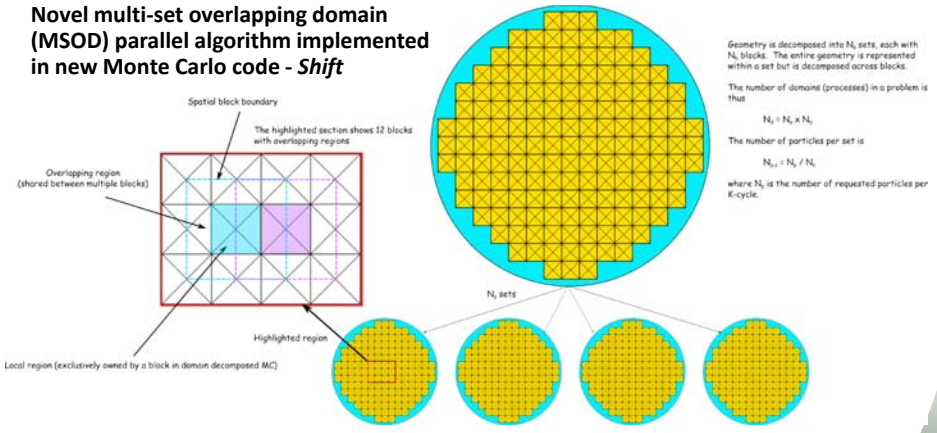
- **Generate initial fission source and *k* for MC**
  - accelerate source convergence
  - Improve convergence reliability



- **Select domain boundaries**
  - improve parallel load balancing
  - reduce Monte Carlo run time

Domain decomposition parallelism overcomes prohibitive computational MEMORY requirements

Novel multi-set overlapping domain (MSOD) parallel algorithm implemented in new Monte Carlo code - *Shift*

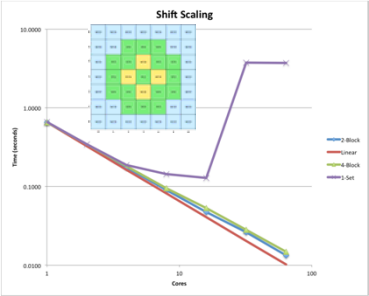


Pictorial representation of MSOD parallel decomposition. Here the core geometry is decomposed into N_s = 4 sets. Each set has N_b blocks with overlapping regions such that the total number of parallel domains is $N_b \times N_s$. Particles are decomposed across sets where the number of particles per set is $N_{p,s} = N_p / N_s$. Each block can define an overlapping domain (shown in inset) to reduce block-to-block communication for particles that scatter at the interfaces between blocks.

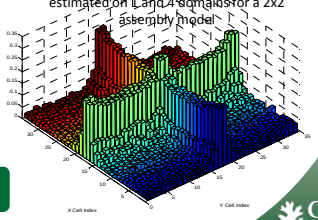
J.C. WAGNER, S.W. MOSHER, T.M. EVANS, D.E. PEPLOW, and J.A. TURNER, "Hybrid and Parallel Domain-Decomposition Methods Development to Enable Monte Carlo for Reactor Analyses," accepted for publication in Progress Nucl. Sci. Technol.

New DD MC code, *Shift*, under development

- **Designed from outset for use on massively parallel platforms**
  - Domain replication and domain decomposition
  - Parallel scaling studies on-going
- ***SCALE* geometry**
- **Implementing hybrid methods**
  (Shift + Denovo in common code base)
- **Approaches for efficient variance estimation**
  - Evaluating batches vs. neglecting variance contributions from particles that leave domains
- **Implementing continuous energy physics**
- **Implemented Shannon Entropy**
- **Testing, verification and validation**



Relative difference between variances estimated on 1 and 4 domains for a 2x2 assembly model



Shift has been selected as the MC code for CASL

Summary Remarks

- **Denovo provides an enabling deterministic RT capability**
  - **modern solvers → far more robust than legacy codes**
  - **parallel implementation → power to solve enormous problems**
  - **working toward enabling 3D full-core pin-resolved transport**
- **Hybrid methods/codes developed at ORNL are making the impossible/impractical possible/practical**
  - **techniques are flexible and robust**
  - **optimize local, semi-global, or global tallies**
  - **methods are being implemented and used around the world**
- **Shift being developed with goal of enabling Monte Carlo for reactor analysis and design in the future**
  - **unique Domain Decomposition strategy to utilize HPC**
  - **hybrid methods for improving computational efficiency**

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