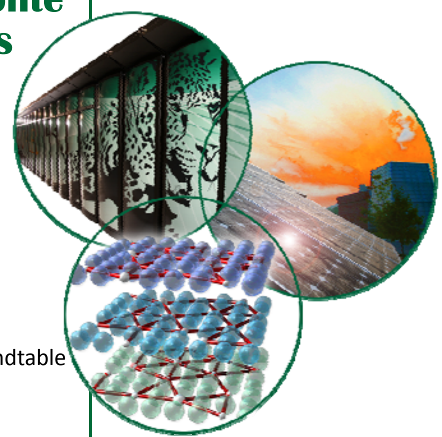
Hybrid and Parallel Domain-Decomposition Methods Development to Enable Monte Carlo for Reactor Analyses



Presenter: John Wagner

Contributors: Scott Mosher, Tom Evans, Douglas Peplow, Brenden Mervin, Nicholas Sly, Ahmad Ibrahim

Current Issues in Computational Methods – Roundtable
Monte Carlo Methods in Reactor Physics: Current Status and Future Prospects

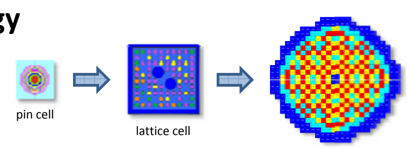
ANS Annual Meeting, June 27, 2011

U.S. DEPARTMENT OF ENERGY

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

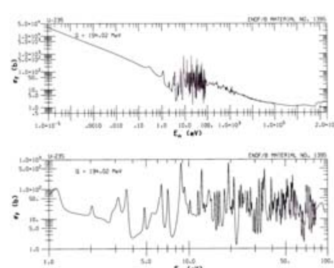
Our goal is to enable efficient full-core Monte Carlo reactor simulations on HPC platforms

- **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



pin cell
lattice cell
nodal core model

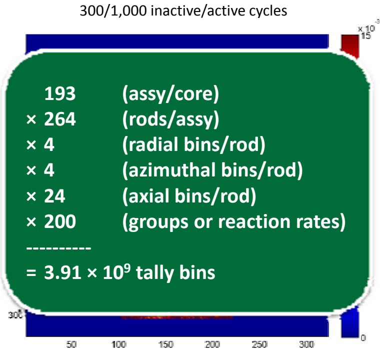
- **Continuous-energy Monte Carlo (MC)**
  - Explicit geometric, angular and nuclear data representation – **highly accurate**
  - Avoids problem-dependent multigroup xs processing – **easy to use**
  - Computationally intensive – **considered prohibitive for "real" reactor analyses**



U-235 fission cross section

We have to find solutions to several significant technical challenges

PWR Core Problem*
100k particles/cycle
300/1,000 inactive/active cycles

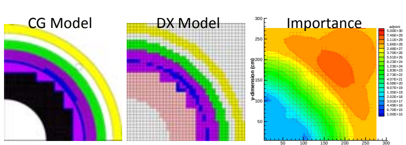


"Real" Std. Dev.

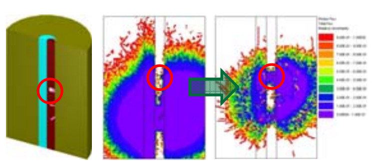
* from M.J. Lee, H.J. Joo, and D. Lee, "Multigroup Monte Carlo Reactor Calculation with Coarse Mesh Finite Difference Formulation for Real Variance Reduction" (2010).

- **Prohibitive computational time**
  - Tally convergence
    - Non-uniform: uncertainty increases with distance from core center
    - Must run batch of simulations to estimate true uncertainties (cycle-to-cycle correlation)
  - Source convergence
    - Slow in large systems and w/ high dominance ratio
    - Can be difficult to identify/confirm
- **Prohibitive memory requirements**
  - High fidelity → high information density
    - *O*(10^9) tally bins in fuel is not unreasonable
    - Too much tally information to store on every processor

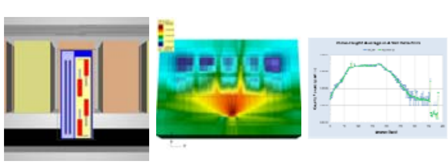
ORNL's hybrid methods have been successfully applied to many real-world fixed-source problems



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



Gamma response of litho-density tool



Pulse-height spectrum in portal NaI detectors

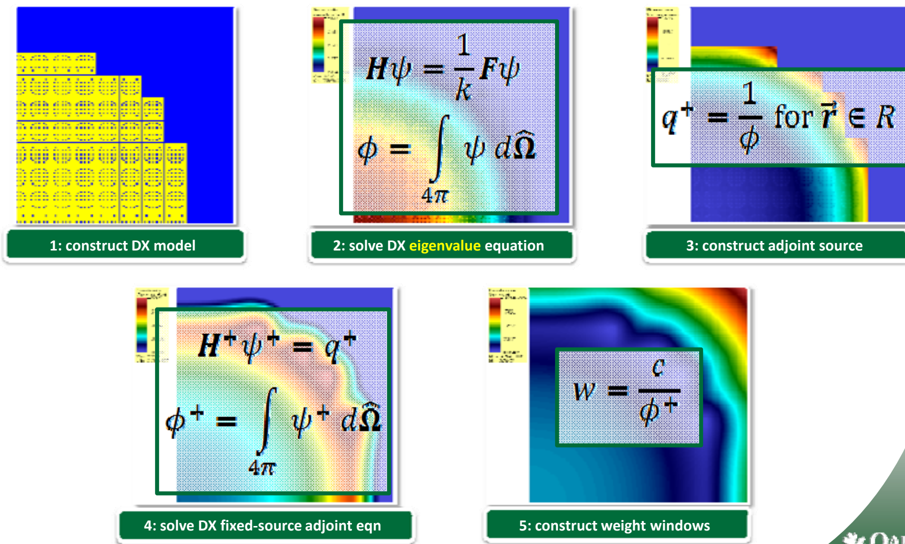
CADIS

Consistent Adjoint Driven Importance Sampling

goal: accelerate localized tallies

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

We extended the FW-CADIS method to reactor eigenvalue problems



The FW-CADIS method is flexible

- **The adjoint source can be defined to "optimize" MC for distributions or multiple individual quantities, for example:**

- For space- and energy-dependent flux: $$q^+(\vec{r},E) = \frac{1}{\phi(\vec{r},E)}$$

- For total flux: $$q^+(\vec{r},E) = \frac{1}{\int \phi(\vec{r},E')\,dE'}$$

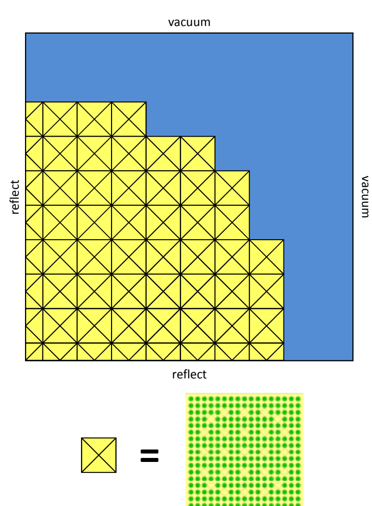
- For response, e.g., dose: $$q^+(\vec{r},E) = \frac{\sigma_d(\vec{r},E)}{\int \sigma_d(\vec{r},E')\phi(\vec{r},E')\,dE'}$$

For details, see: J. WAGNER, E. D. BLAKEMAN, and D. E. PEPLOW, "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.

Summary of the FW-CADIS method

- **The method weights the adjoint source with the inverse of the forward flux/response**
  - Where the forward flux/response is low, the adjoint importance will be high, and vise versa
- **Once the importance function is determined, the CADIS equations for calculating weight targets**
  - Hence, we refer to the method as ***Forward-Weighted CADIS***
- **The method requires:**
  - A forward solution (for adjoint source weighting)
  - An adjoint solution (for determining biasing parameters)
  - Both can be automated

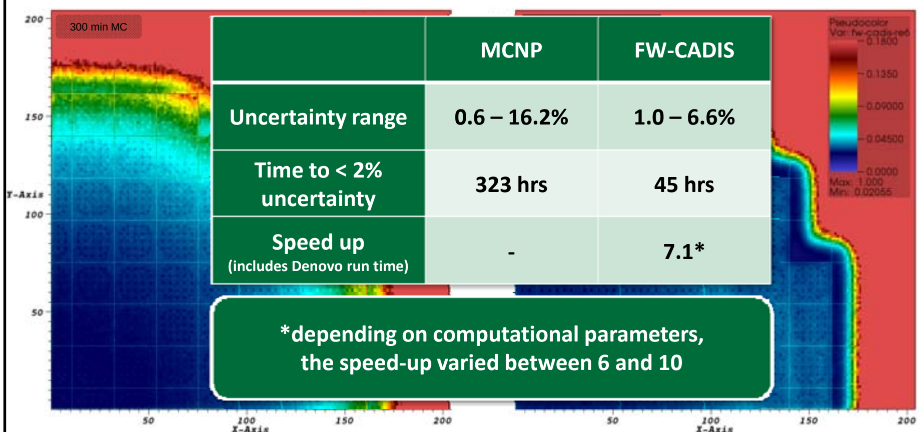
We conducted preliminary tests of the new hybrid method on a relevant model



- **Generic 2-D PWR Quarter Core**
  - 48¼ 17 × 17 fuel assemblies
  - 264 fuel rods per assembly
  - 3% fuel enrichment (uniform)
- **Denovo Model**
  - pin-cell-sized mesh (181 × 181 × 1)
  - cells are nominally 1.25 × 1.25cm
  - 8-group cross sections from CSAS-I
  - self-shielded, homogenized pin cells
- **Denovo Calculations**
  - S_4 quadrature; P_1 scattering expansion
  - step characteristic differencing
  - Krylov upscatter iterations
  - 50 min runtime (46 / 4)

FW-CADIS yields more uniform uncertainties throughout the core

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

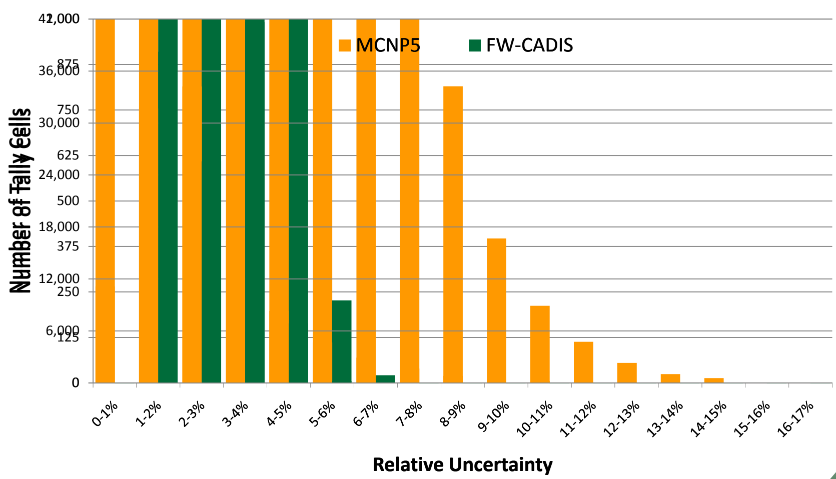


	MCNP	FW-CADIS
Uncertainty range	0.6 – 16.2%	1.0 – 6.6%
Time to < 2% uncertainty	323 hrs	45 hrs
Speed up (includes Denovo run time)	-	7.1*

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

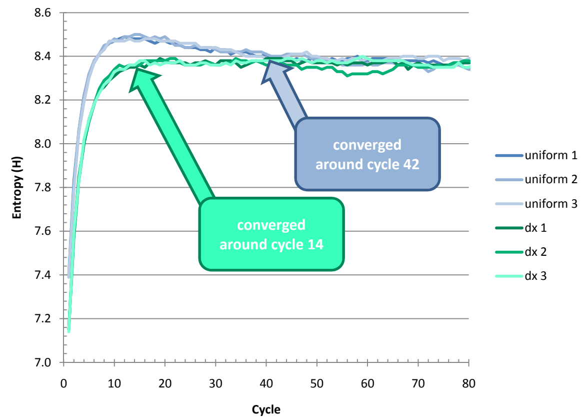
Conventional MC simulation | MC with FW-CADIS

The FW-CADIS method reduces the range of uncertainties



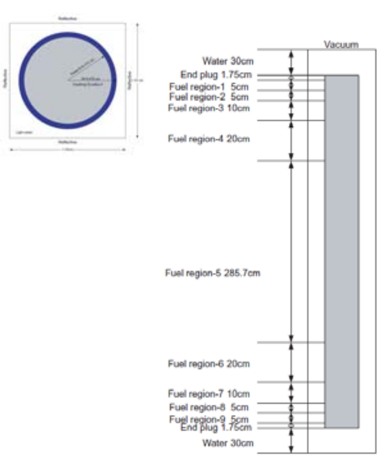
The FW-CADIS method DX solution can be exploited in additional ways

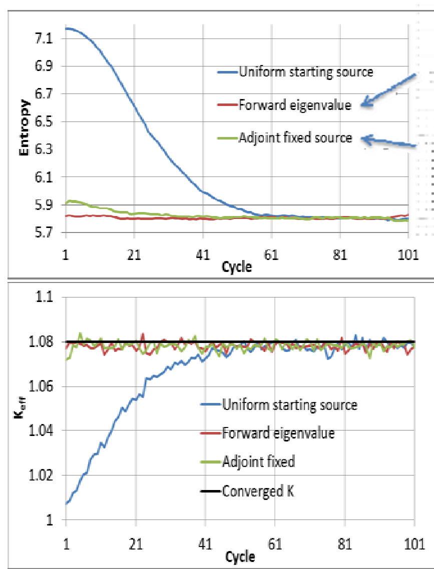
- **Generate initial fission source and *k***
  - accelerate source convergence
  - support more reliable convergence
- **Select domain boundaries**
  - improve load balancing
  - reduce Monte Carlo run time



Pin-Cell Array with irradiated fuel <u>symmetric</u> axial composition

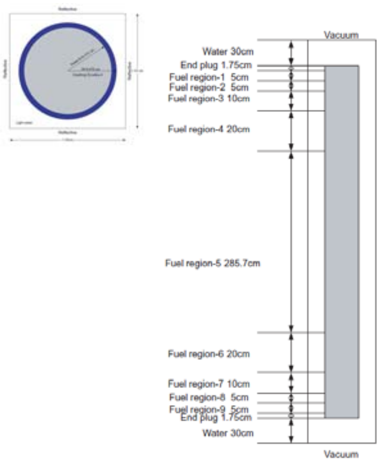
- **OECD/NEA Source Convergence Test Problem #2**

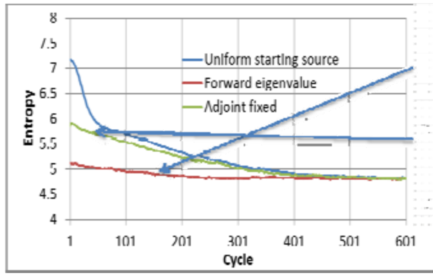


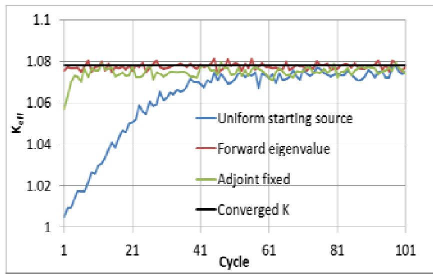


Pin-Cell Array with irradiated fuel asymmetric axial composition

- **OECD/NEA Source Convergence Test Problem #2**

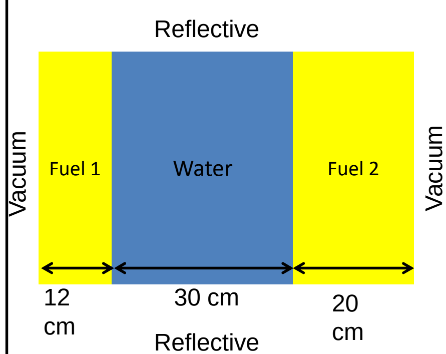


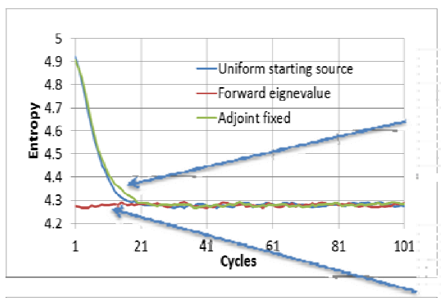


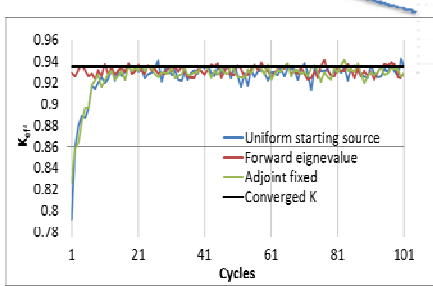


Loosely coupled uranyl nitrate solution slabs

- **OECD/NEA Source Convergence Test Problem #3**

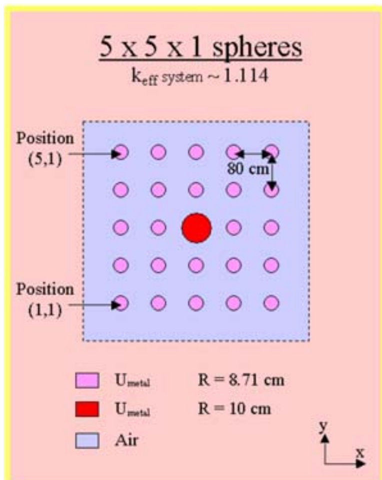


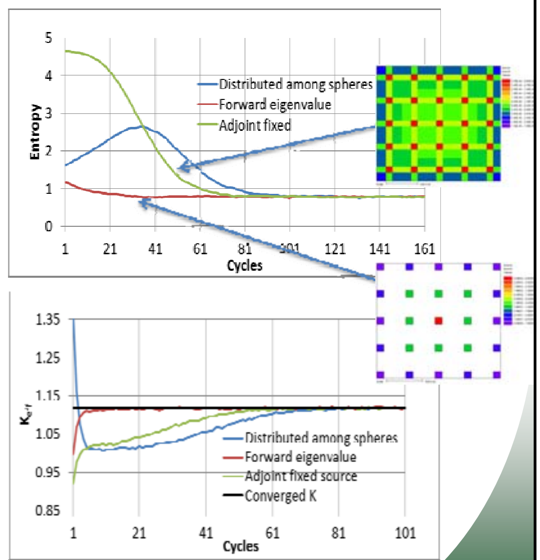




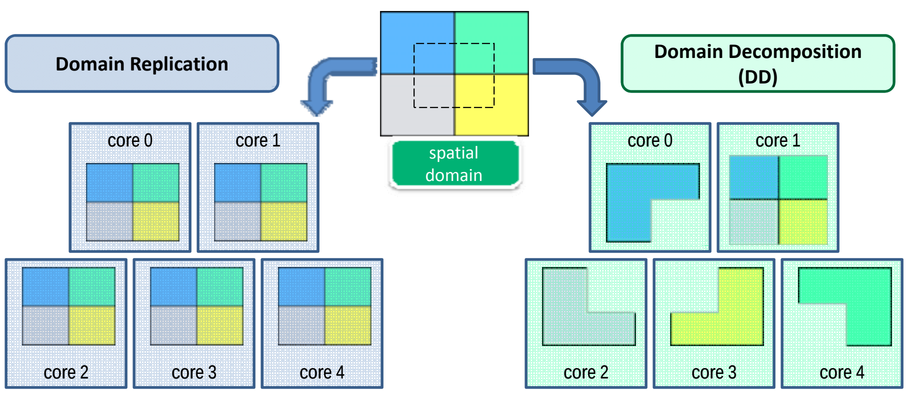
Array of interacting spheres

- **OECD/NEA Source Convergence Test Problem #4**





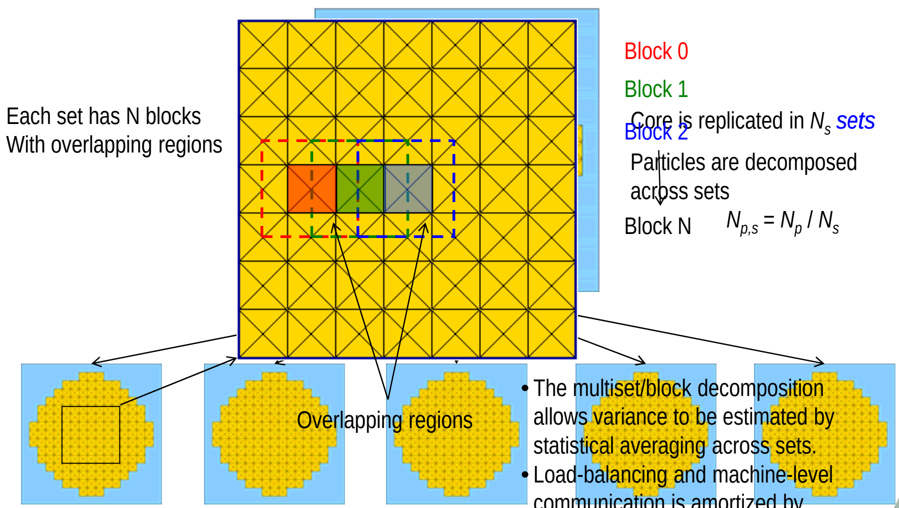
Domain Decomposition vs. Replication



- each core has a full copy of global data
- cores simulate one particle at time
- **no** within-cycle communication

- each core has a subset of global data
- cores simulate particles from the source and **entering from neighboring domains**
- within-cycle communication

A novel MSOD domain-decomposition algorithm



- The multiset/block decomposition allows variance to be estimated by statistical averaging across sets.
- Load-balancing and machine-level communication is amortized by reducing communication across entire geometry.

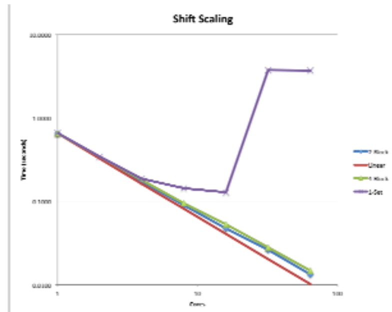
Initial studies indicate communication costs can be reduced with overlapping regions…

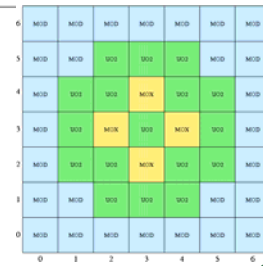
Width of over-lapping region (assemblies)	Total size of domain (assemblies)	Source particles in the central domain region that leave the domain (percentage)
No overlap	1	76.12
0.5	2 × 2	21.03
1.0	3 × 3	4.54
1.5	4 × 4	1.05
2	5 × 5	0.27
2.5	6 × 6	0.07
3.0	7 × 7	0.02

… while leaving source regions fixed

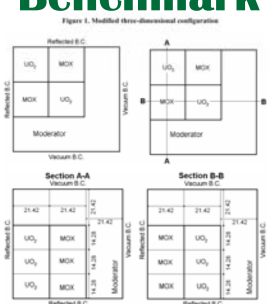
New DD MC code, *Shift*, under development

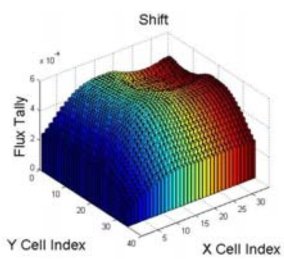
- **Designed from the outset for use on massively parallel platforms**
  - Domain replication and domain decomposition (MSOD); in Denovo code base
  - Performing parallel scaling studies
- **SCALE geometry**
- **Evaluating/testing strategies for variance estimation with DD**
  - **Batches**
  - **Ignoring variance contributions from particles that leave domains**
- **Implementing CE physics**
- **Verification and validation**

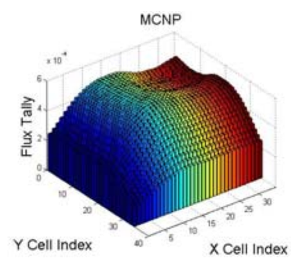




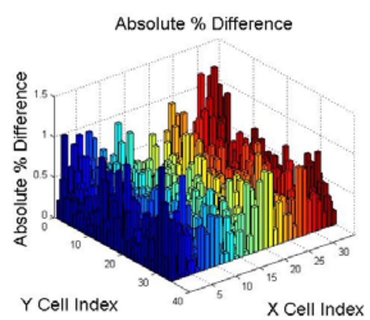
Example of Shift testing – 3-D C5G7 Benchmark







- Compared k_{eff} values and flux tallies between Shift and MCNP using domain replication
  - Results agree within statistical uncertainties
  - 30,000 particles, 1200 cycles, 500 skipped
  - Center control rods fully inserted
  - Tally over the 4 fuel assemblies; 1 tally per pin cell
- Upcoming: Variance calculation and continued benchmarking.



Summary

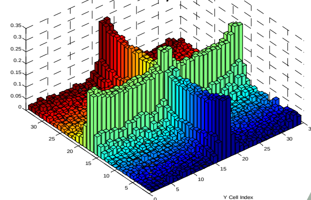
- **Hybrid FW-CADIS method has been extended/demonstrated for improving computational efficiency of MC eigenvalue problems**
  - Produces **relatively uniform statistical uncertainties**
  - Achieves **speed-ups of 6 – 10** in 2-D PWR quarter core test problem; larger speed-ups expected for more realistic 3-D problems
  - Additional opportunities to exploit DX solution being tested and evaluated
- **MC DD algorithm has been developed for addressing prohibitive memory requirements**
  - Uses multi-set/block decomposition for load-balancing and to reduce communication time/cost
  - Uses over-lapping regions to reduce communications
  - Expected benefits include:
    - no communication (message passing) between sets within a transport cycle
    - within-cycle communication that does occur takes advantage of the lower latency of within-cabinet communications (versus inter-cabinet communications)
    - ability to estimate statistical uncertainties based on the variance of the independent batches. This will eliminate the under-prediction of statistical uncertainties due to cycle-to-cycle correlations between fission generations.

Still in implementation and testing phase

Current activities

- **Hybrid methods development and testing**
  - **Acceleration of group-wise flux values for depletion and sensitivity calculations; evaluate lower-order deterministic methods for FW-CADIS**
  - **Source convergence assurance and acceleration**
  - Investigation of metrics for comparing performance of hybrid methods
- **DD testing and scaling studies**
  - **Particularly for overlapping regions**
- **Approaches for efficient variance estimation for MC DD**
- **Testing and V&V of Shift**
- **Integration of continuous-energy physics into Shift**

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



Examples of technical issues on our radar screen

- Statistical uncertainty propagation for MC depletion
- Metrics/diagnostics related to statistical uncertainties in MC calculations for depletion
- Impact of statistical uncertainties on coupling to other physics
- Efficient tallying for physics coupling, e.g., mesh coupling
- Efficiently handling of temperature-dependent continuous-energy cross sections
- Use of deterministic information to improve load balancing
- …

Closure – Questions & Discussion

- **Acknowledgements:**
  - Research sponsored by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory, managed by UT-Battelle, LLC, for the U.S. Department of Energy.
  - Research sponsored by the Joint Directed Research and Development (JDRD) program of the University of Tennessee (UT)
  - Parts of this research are supported by the Consortium for Advanced Simulation of Light Water Reactors (www.casl.gov), an Energy Innovation Hub (http://www.energy.gov/hubs) for Modeling and Simulation of Nuclear Reactors under U.S. Department of Energy Contract No. DE-AC05-00OR22725.

- **Contact Info:**
  - John Wagner, wagnerjc@ornl.gov