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

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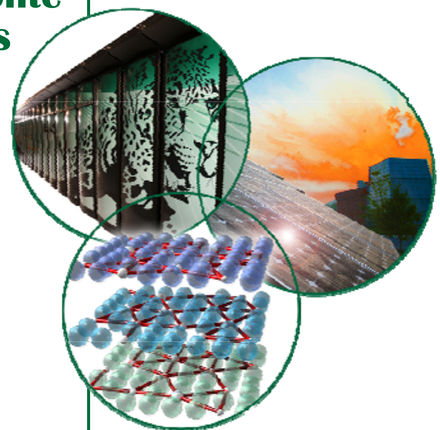

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U.S. DEPARTMENT OF ENERGY

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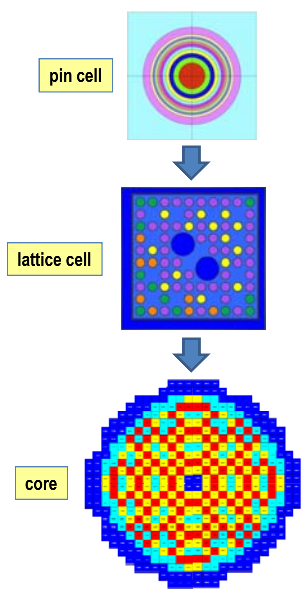
Current State-of-the-Art in Reactor Analysis

General Electric ESBWR



- 1-D transport (high-order)
- High energy fidelity (> 200 groups)
- Approximate state and BCs

- 2-D transport
- Moderate energy fidelity (30-50 groups)
- Approximate state and BCs
- Depletion with spectral corrections
- Spatial homogenization

- 3-D diffusion (low-order)
- Low energy fidelity (2-4 groups)
- Homogeneous lattice cells
- Heterogeneous flux reconstruction
- Coupled physics

Current state-of-the-art has significant deficiencies and will be problematic for design and licensing of advanced nuclear systems

- **Spatial decomposition is not rigorous**
  - Lattice cell model is not valid for highly heterogeneous cores & new reactor designs
  - Nodal diffusion solution poorly suited for providing localized power densities, which are needed to ensure fuel integrity and related principle core safety limits
- **Decades of research were required to correct, validate, and subsequently enable the current methodology to work reasonably well for conventional LWR designs**
- **For new systems, years of effort and expense will be required to correct and validate this approach**
  - Cost & availability of experimental facilities will limit role of testing/measured data
  - Monte Carlo will be used as a benchmarking and validation tool in a limited manner, but to the extent possible
  - Protracted licensing review period will likely follow

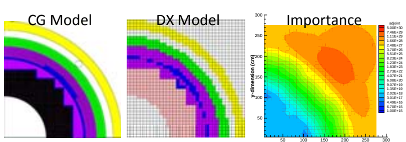
Conventional Monte Carlo (MC) offers desired accuracy, but is computationally prohibitive

- **MC is considered the "gold standard" in radiation transport**
  - Explicit geometric, angular and nuclear data representation – highly accurate
  - Computationally intensive – prohibitive for "real" reactor analyses
  - Does not exhibit non-physical behavior like deterministic methods can – reliable
- **Industry and others use MC to the extent they can**
  - Restricted to benchmarking deterministic results at a limited number of state-points and for a limited number of relevant quantities
- **Perceived advantages associated with MC will continue to motivate the community to use it in an increasing manner**, with limited extent
- However, the prevailing view in the community is that **MC is not computationally viable for "real" reactor analyses, and it will not become so for many decades, if ever**
  - Prevailing views are based on knowledge and experience with conventional MC, and in that context are accurate

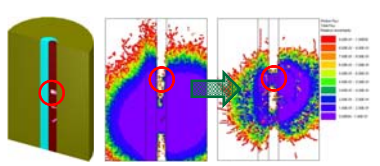
Our goal is to enable MC for "real" reactor analyses

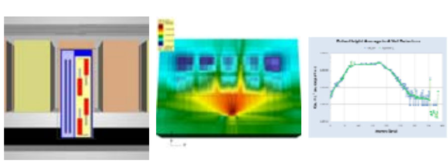
- *Instead of using MC to correct a fundamentally flawed approach, we envision solving the multi-level problem directly with the "gold standard" MC method*
- **Two of the most significant technical challenges are:**
  - Prohibitive computational time
    - Slow, non-uniform tally convergence of system-wide MC estimates
  - Prohibitive memory requirements
    - High fidelity → high information density
      - $O(10^9)$ tally bins in fuel is not unreasonable
      - Too much tally and material information to store on every processor
- **Our approach:**
  - Hybrid (MC/deterministic) transport methods
  - Effective use of high-performance computing

ORNL's hybrid methods for real-world, fixed-source applications



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

$$\hat{q}(\vec{r},E) = \frac{\phi^{+}(\vec{r},E)\,q(\vec{r},E)}{R} \qquad w(\vec{r},E) = \frac{R}{\phi^{+}(\vec{r},E)}$$

A few more words on the FW-CADIS method (1/2)

- Physically, 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 consistent source biasing & WWs are used
  - 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

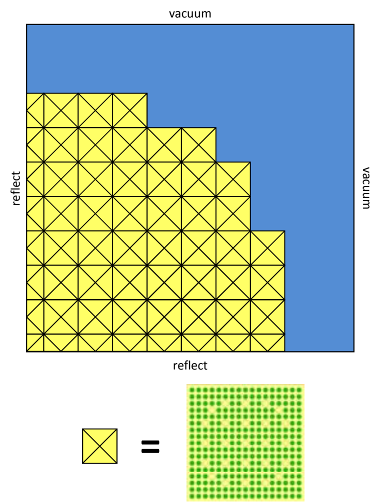
A few more words on the FW-CADIS method (2/2)

- The adjoint source can be defined to optimize MC for distributions or multiple individual quantities, e.g.,

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

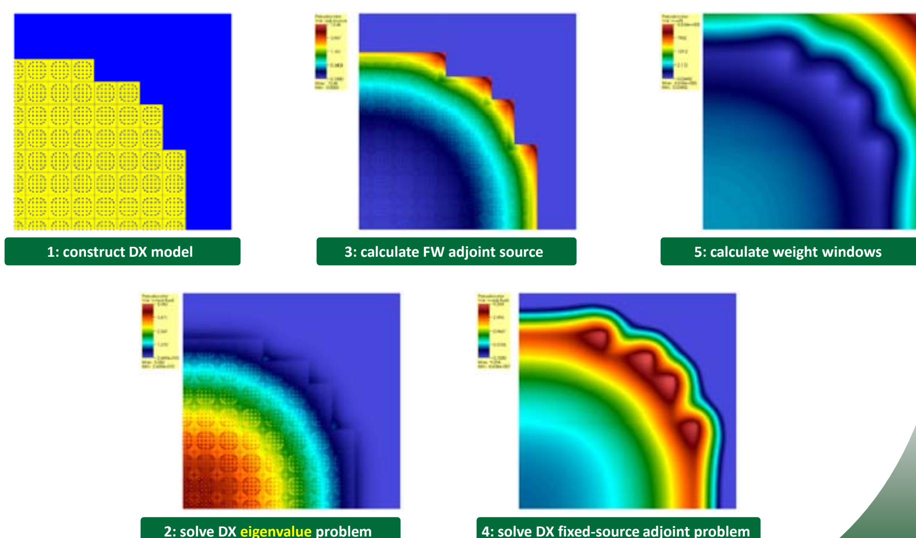
For details, see: J. WAGNER, E. D. BLAKEMAN, and D. E. PEPLOW, "Forward-Weighted CADIS Method for Variance Reduction of Monte Carlo Calculations of Distributions and Multiple Localized Quantities," M&C 2009, Saratoga Springs, NY, May 3-7, 2009.

Test problem



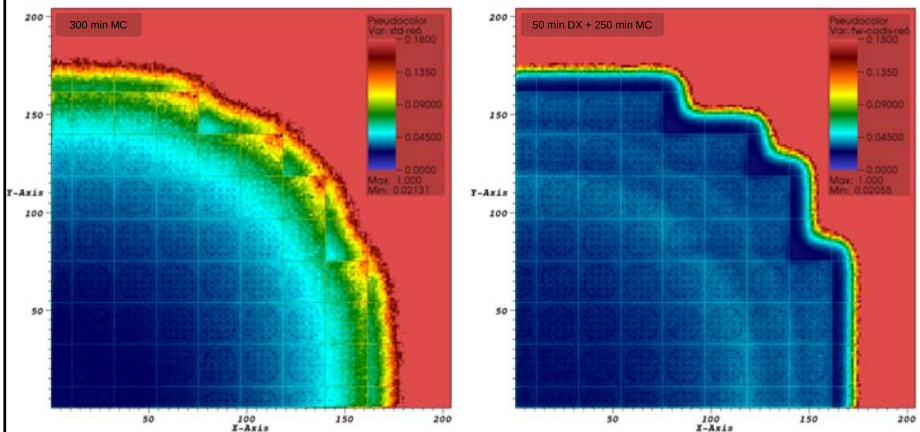
- **Generic 2-D PWR Quarter Core**
  - 48¼ 17 × 17 fuel assemblies
  - 264 fuel rods per assembly
  - 3% fuel enrichment (uniform)
- **Denovo Model**
  - pin-cell-sized mesh (181 × 181 × 1)
  - cells are nominally 1.25 × 1.25cm
  - 8-group cross sections from SCALE
  - self-shielded, homogenized pin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

FW-CADIS method for reactor eigenvalue problems



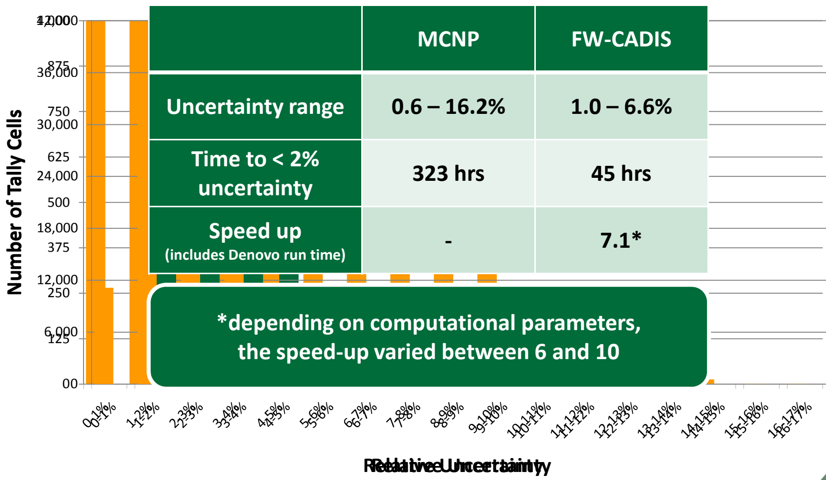
FW-CADIS yields more uniform uncertainties throughout the core

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



Conventional MC simulation | **MC with new hybrid method**

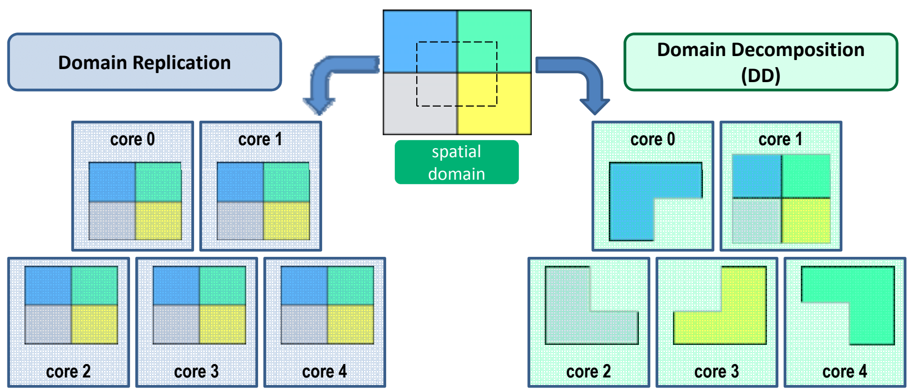
FW-CADIS method reduces the range of uncertainties



	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

Domain Decomposition vs. Replication

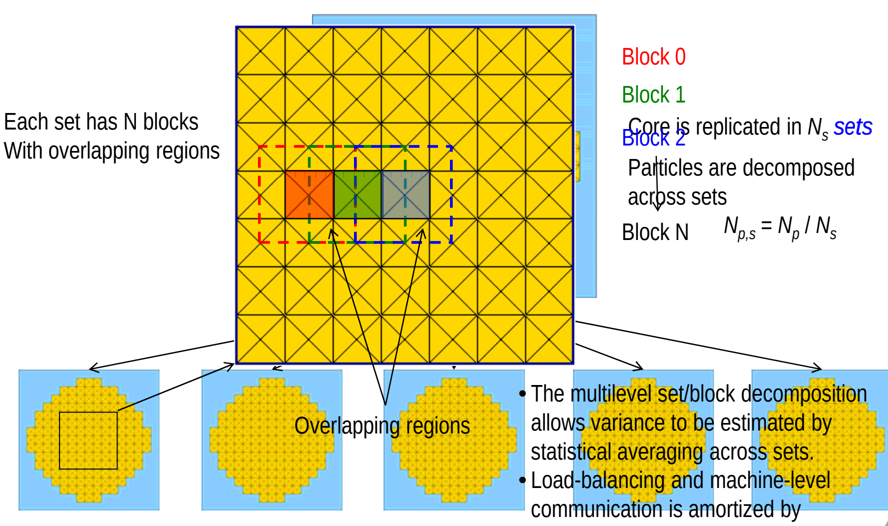


- each core has a full copy of global data
- cores simulate one particle at time
- **no** within-cycle communication

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

A novel MLOR domain-decomposition algorithm

Each set has N blocks
With overlapping regions



Core is replicated in N_s *sets*
Particles are decomposed across sets
$N_{p,s} = N_p / N_s$

- The multilevel set/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 via overlapping regions…

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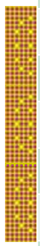
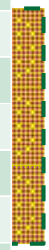


Width of over-lapping region (assemblies)	Total size of domain (assemblies)	Source particles in the central domain region that leave the domain (percentage)
No overlap	1	76.12
0.5	2 × 2	21.03
1.0	3 × 3	4.54
1.5	4 × 4	1.05
2	5 × 5	0.27
2.5	6 × 6	0.07
3.0	7 × 7	0.02



… while leaving source regions fixed

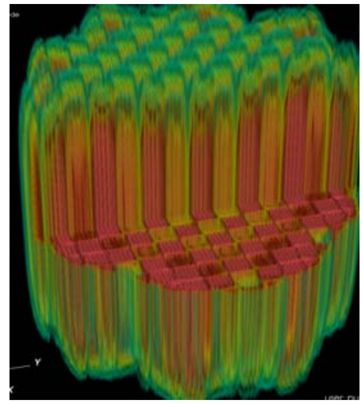
Summary

- **FW-CADIS method has been extended/demonstrated for 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 have yet to be realized
- **A novel DD algorithm has been conceived/developed**
  - Uses multi-level 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, a requirement not handled by existing domain decomposition schemes. This will eliminate the under-prediction of statistical uncertainties due to cycle-to-cycle correlations between fission generations.

Still in implementation phase

Planned Work

- **Complete prototypic hybrid method implementation & testing**
  - Apply to 3-D core benchmark problem(s) (e.g., Hoogenboom and Martin)
  - Investigate impact on source convergence and "real" vs. apparent variance
- **Complete implementation, test, and refine the new DD algorithm**
  - Use distributed memory to enable solving full core problems
  - Demonstrate scalability on Jaguar (Cray XT5)
- **Integrate DD and hybrid capabilities**



TOP500 #1 Nov. 2009

Peak performance	2.332 PF
System memory	300 TB
Disk space	10 PB
Disk bandwidth	240+ GB/s
Interconnect bandwidth	374 TB/s

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.

- **Contact Info:**

  - John Wagner, wagnerjc@ornl.gov

- Another related paper at this conference:
  - *Review of Hybrid (Deterministic/Monte Carlo) Radiation Transport Methods, Codes, and Applications at Oak Ridge National Laboratory, 9:30-11:40, Session H9: Variance Reduction Techniques in Monte Carlo Calculation, Conference Room 3*