Recent Past and Planned Research

Reactor Design and Neutronics Group

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OUTLINE

- Hybrid methods overview
  - Motivation
  - CADIS
  - FW-CADIS
  - Challenges
- MC importances in the presence of space and energy self-shielding
  - Cross Section Processing
  - Problem Investigation
  - Resonance Factor Method
  - Results
  - Summary and Conclusions
- MC importances for problems with strong anisotropies
- Other potential projects

SOLVING THE TE

<u>Monte Carlo</u>

- Solution has associated statistical error
- Continuous phase space: "gold standard answers"
- Can take a long time
- Good for streaming
- Optically thick = slow

<u>Deterministic</u>

- Solution equally valid everywhere
- Discretized phase space: drives solution quality
- Can be fast
- Streaming = ray effects
- Good for optically thick

ACCELERATION

- To use MC in many applications, we need to *accelerate* it
- Variance reduction is designed to improve the FOM:

$$\text{FOM} = \frac{1}{R^2 t}$$

R = relative error

t = time

- Idea: can we use deterministic and Monte Carlo methods together to lessen the weaknesses of each?

$\rightarrow$ **Hybrid Methods**

FORWARD-ADJOINT RELATIONSHIP

Define response with function $f(\mathbf{r}, E)$ in volume V_d as

$$R = \int_E \int_{V_f} f(\mathbf{r}, E)\phi(\mathbf{r}, E)dVdE \tag{1}$$

$$H\phi = q \quad \text{(forward)} \qquad \langle H\phi, \phi^\dagger \rangle = \langle H^\dagger \phi^\dagger, \phi \rangle \text{, and therefore}$$
$$H^\dagger \phi^\dagger = q^\dagger \quad \text{(adjoint)} \qquad \langle q, \phi^\dagger \rangle = \langle q^\dagger, \phi \rangle$$

If we let $q^\dagger = f(\mathbf{r}, E)$ then

$$\langle q^\dagger, \phi \rangle = \langle f, \phi \rangle = R = \langle q, \phi^\dagger \rangle \tag{2}$$

Eq. (2) expresses that $\phi^\dagger$ represents the expected contribution of a source particle to the response given the source, q.

CADIS

1. Define $q^\dagger$ as the local response of interest
2. Coarse deterministic calculation to get $\phi^\dagger$ and R

$$imp(\mathbf{r},E) = \frac{\phi^\dagger(\mathbf{r},E)}{\langle q(\mathbf{r},E), \phi^\dagger(\mathbf{r},E)\rangle} = \frac{\phi^\dagger(\mathbf{r},E)}{R} \tag{3}$$

$$\hat{q}(\mathbf{r},E) = \frac{\phi^\dagger(\mathbf{r},E) q(\mathbf{r},E)}{R} \tag{4}$$

$$w_0(\mathbf{r},E) = \frac{q(\mathbf{r},E)}{\hat{q}(\mathbf{r},E)} = \frac{R}{\phi^\dagger(\mathbf{r},E)} \tag{5}$$

Birth weights match weight targets, making this the Consistent Adjoint Driven Importance Sampling Method

FW-CADIS

- We often what to optimize solutions in all of phase space
- In this case the adjoint source needs to be a global forward solution: Forward Weighted-CADIS

To Optimize	Adjoint Source
$\phi(\mathbf{r}, E)$	$f(\mathbf{r}, E) = \dfrac{1}{\phi(\mathbf{r}, E)}$
$\int \phi(\mathbf{r}, E)\sigma_d(\mathbf{r}, E)$	$f(\mathbf{r}, E) = \dfrac{\sigma_d(\mathbf{r}, E)}{\int \phi(\mathbf{r}, E)\sigma_d(\mathbf{r}, E)}$

For example

$$R = \int_E \int_{V_f} f(\mathbf{r}, E)\phi(\mathbf{r}, E) dV dE = \int_E \int_V \frac{1}{\phi(\mathbf{r}, E)} \phi(\mathbf{r}, E) dV dE \approx 1$$

CHALLENGES

FW-CADIS works well for **most** deep penetration shielding problems...

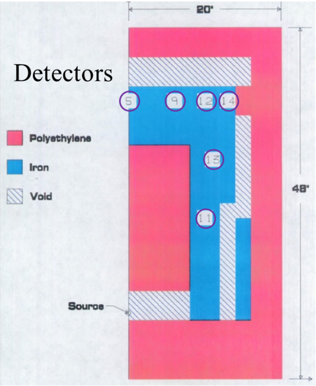


Figure: Dog Legged Void Neutron Shielding Benchmark

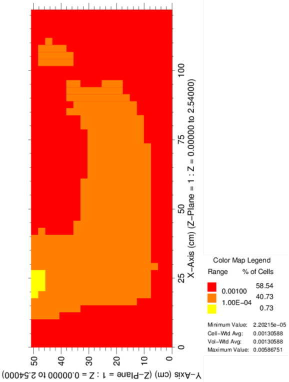


Figure: MC 95% CI RE using FW-CADIS, DLVN

CHALLENGES

...but not all of them

- FW-CADIS only includes space and energy, *not angle*
- One pathological case:
  - Energy self-shielding +
  - Spatial self-shielding
- High relative error through location of Interest
- **Need** new methods based on FW-CADIS
- E.g., Resonance Factor method (uses different cross section processing)

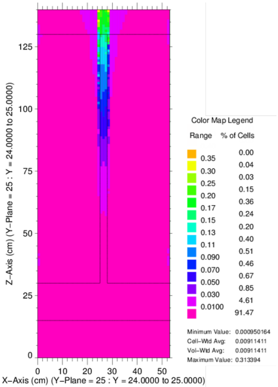


Figure: MC 95% CI RE using FW-CADIS, Plate

CROSS SECTION PROCESSING

- General Case

$$\sigma_{x,g}^{(j)} = \frac{\langle \sigma_x^{(j)}(u) W(u) \rangle}{\langle W(u) \rangle}, \quad W(u) = \phi_\infty(u) \tag{6}$$

- Bondarenko method uses a background cross section

$$\sigma_0^{(j)} = \frac{1}{N_j} \sum_{m \neq j} \sigma_t^{(m)} N_m, \quad \sigma_{x,g}^{(j)}(\sigma_0^{(j)}) = \frac{\langle \sigma_x^{(j)}(u) \frac{\phi_\infty(u)}{\sigma_t^{(j)}(u) + \sigma_0^{(j)}} \rangle}{\langle \frac{\phi_\infty(u)}{\sigma_t^{(j)}(u) + \sigma_0^{(j)}} \rangle} \tag{7}$$

- W(u) changed to include the spectral difference assumption and effect of other isotopes

CROSS SECTION PROCESSING

- When a nuclide is dilute, $\sigma_0^{(j)} >> \sigma_t^{(j)}$, $W(u) \rightarrow$ uncorrected
  - Large σ_0 = infinitely dilute case
- When a nuclide is concentrated, $\sigma_0^{(j)} << \sigma_t^{(j)}$, resonances have a larger impact
  - Small σ_0 = resonance case

- Add correction for 'thin slab' of resonance material in 'thick slab' of moderator

$$\sigma_0^{*,(j)} = \frac{1}{N_j} \sum_{m \neq j} \sigma_t^{(m)} N_m + \frac{1}{N_j \bar{l}} \tag{8}$$

thin slab: $\bar{l} \approx \frac{4V}{S}$ no effect: $\bar{l} \approx$ large

PROBLEM INVESTIGATION

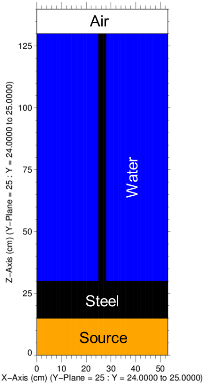


Figure: Shielding Stack Up

- 53 cm × 50 cm × 140 cm
- Uniform in x except plate (25-28 cm in x; 30-130 cm in z)
- Uniform in y
- U-235 fission spectrum; homogenized U, Zr, and H2O

- MC21, MCNP, and PARTISN
- ENDF/B-VII data (all codes)
- Processed by TRANSX (multigroup)

BASE CALCULATION PARAMETERS

Variable	PARTISN	MC21
Deterministic Mesh	0.5 cm unif; 0.25 cm in x over 24 to 29 cm	1 cm uniform
Tally mesh	N/A	1 cm uniform
N particles	N/A	1×10^{10}
Energy structure	58 grps	27 grps / continuous
Angular quad	QR-18-252	QR-8-36
Scattering order	P_3	P_3
Convergence	0.01	0.05
TRANSX settings	default	default
DCFs	58 grps	27 grps

ERRORS IN PLATE

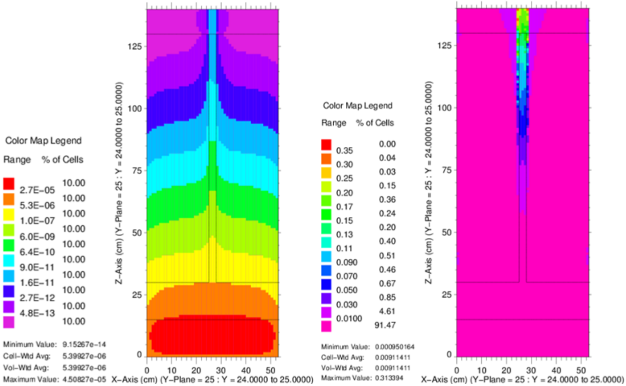


Figure: Plate base FW-CADIS MC21 dose rate (left) and 95CI RE (right) (xz-slice through y=25 cm)

CORRECT WITHOUT PLATE

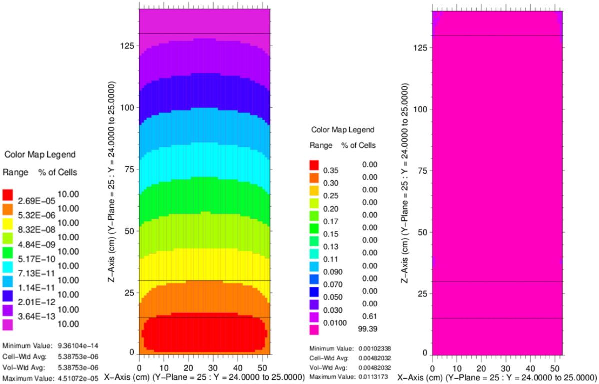


Figure: No-Plate MC21 dose rate (left) and 95CI RE (right) (xz-slice through y=25 cm)

DETERMINISTIC MC MISMATCH

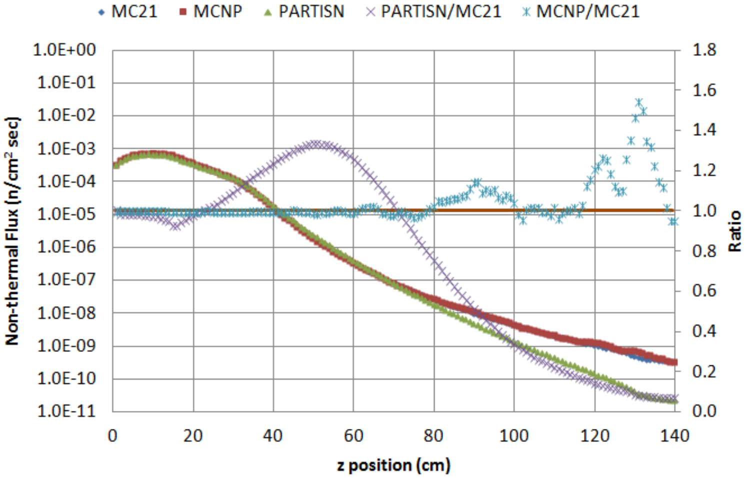


Figure: Plate non-thermal flux (left axis) and method ratios (right axis) down the x-y centerline

DETERMINISTIC MC MISMATCH

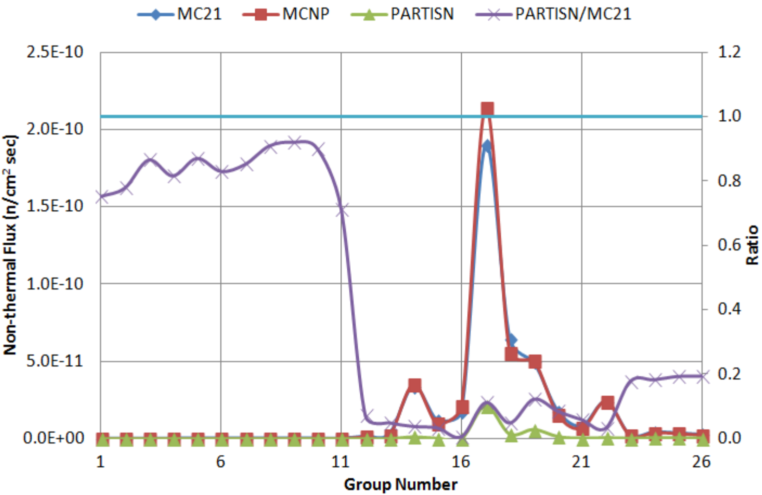


Figure: Plate flux spectra (left axis) and PARTSN/MC21 (right axis) at start of air region (z = 130.5 cm)

CORRECT WITHOUT PLATE

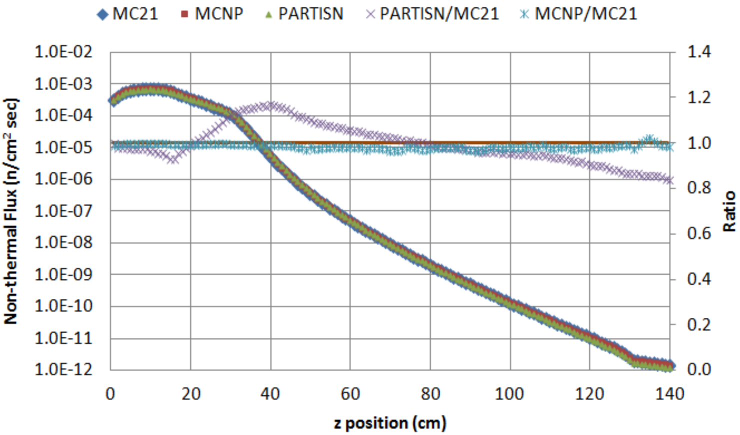


Figure: Plate non-thermal flux (left axis) and method ratios (right axis) down the x-y centerline

INVESTIGATION

- Parameters
  * Mean chord length: $\bar{l} = \frac{4V}{S}$ vs. $\bar{l} = 10,000$
  * Angular quadrature: CMG-591 vs. QR-18-252
  * Scattering expansion: P_5 vs. P_3
  * Importance mesh: 0.25 cm (x), 0.5 cm (y,z) in plate vs. 1 cm
  * Energy Structure: 58 vs. 27 groups
- CADIS in 2 cm area following plate

- Physics
  - Polyethylene follow-on
  - Cr plate (different resonance material)
  - Air in plate (no resonance material)

$$\mathrm{FOM}_{\mathrm{min}} = \frac{1}{R_{\mathrm{max}}^2 t}$$

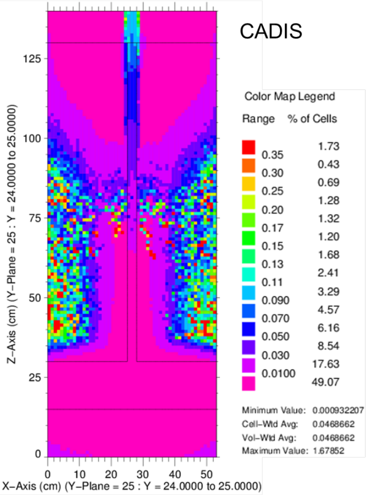
$$\mathrm{FOM}_{\mathrm{max}} = \frac{1}{R_{\mathrm{min}}^2 t}$$

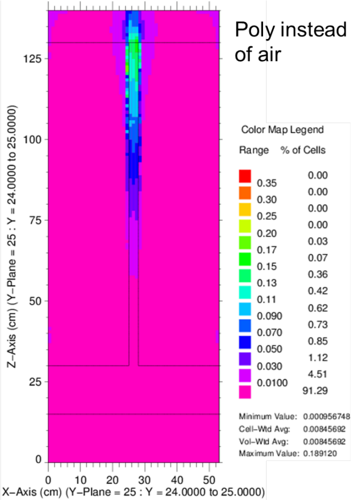
PARAMETERS RESULTS

- Geometric chord length → PARTISN flux even farther from correct, especially in plate
- Angular quadrature → no differences with impact
- Scattering order → (nearly) no change

Case	NPS	CPU-hrs	Max RE	Avg RE	Min F	Avg F
Base	1e10	849.77	8.10e-1	1.02e-2	1.79e-3	11.3
1e11	1e11	8,543.47	1.64e-1	3.28e-3	4.33e-3	10.9
58 g	1e10	954.89	5.22e-1	9.33e-3	3.85e-3	12.0
Fine	1e10	905.34	1.55	1.71e-2	4.63e-4	3.78
F2e11	2e11	18,367.67	3.43e-1	4.00e-3	4.62e-4	3.40

CADIS, POLY FOLLOW





RESONANCE STREAMING

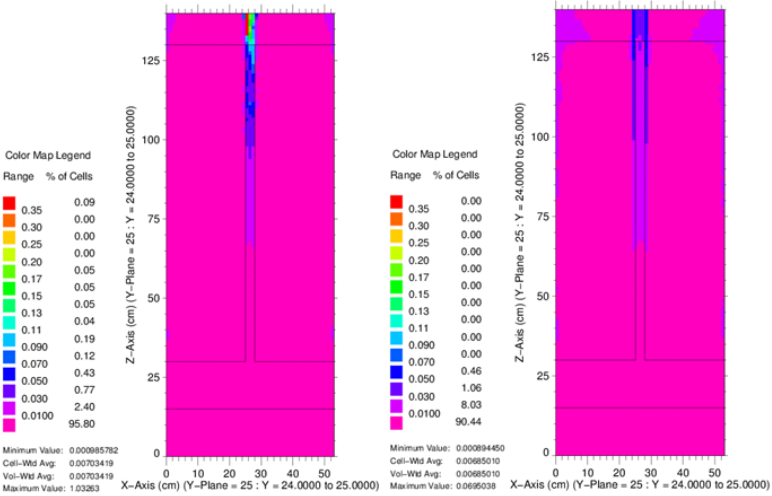


Figure: Cr plate (left) and air plate (right) FW-CADIS MC21 dose rate 95CI RE (xz-slice through y=25 cm)

MAVRIC

- We also ran this problem with and without the plate in MAVRIC (a multigroup MC code in SCALE)
- MAVRIC has more advanced cross section processing options
- Used 27 g and 200 g
- One 200 g case the plate was broken into 9 separate 10-cm segments each with different xsecs
- Without plate case was correct
- 27 g $\rightarrow$ completely missed the behavior
- Both 200 g cases $\rightarrow$ exhibited the same streaming and high relative error behavior

INVESTIGATION SUMMARY

- Behavior is related to space and energy self-shielding
- Using these items did not improve PARTISN
  - finer quadrature
  - higher scattering order
  - more theoretically-accurate mean chord length
- Using these items in imp map creation did not reduce REs
  - finer spatial mesh in the problem area
  - finer energy group structure to create the importance map
- The high RE in and following the plate is present when using different codes and different methods to produce VR parameters, and exists when a different resonance material is used.

A sufficiently accurate PARTISN solution would be better (probably), but prohibitively expensive.

RESONANCE FACTOR METHOD

Apply renormalization factor to FW-CADIS source $q^{\dagger}_{FWC}$:

$$q^{\dagger}(\mathbf{r}, E) = \left(\frac{\phi_{res(\sigma_0)}(\mathbf{r}, E)}{\phi_{dilute(\sigma_0)}(\mathbf{r}, E)}\right)^{M} q^{\dagger}_{FWC} \tag{9}$$

where

- M is problem-dependent constant
- $\phi_{res(\sigma_0)}(\mathbf{r}, E)$ is forward flux using a small background xsec
- $\phi_{dilute(\sigma_0)}(\mathbf{r}, E)$ is forward flux using a large background xsec

The resulting adjoint flux is used to make importances

Implementation: use $\phi_{res(\sigma_0)}(\mathbf{r}, E)$ in all locations where ϕ would be used in the FW-CADIS method

RESONANCE FACTOR METHOD

Example: optimize the space- and energy-dependent flux

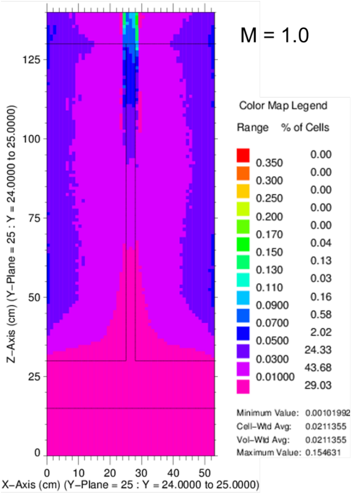
$q^{\dagger}_{FWC} = 1/\phi$ and results in this corrected response:

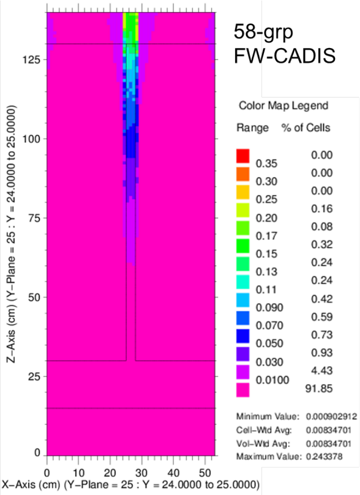
$$R = \int_E \int_V \left(\frac{\phi_{res(\sigma_0)}(\mathbf{r}, E)}{\phi_{dilute(\sigma_0)}(\mathbf{r}, E)} \right)^M \frac{1}{\phi_{res(\sigma_0)}(\mathbf{r}, E)} \phi_{res(\sigma_0)}(\mathbf{r}, E) dV dE$$
$$\approx \int_E \int_V \left(\frac{\phi_{res(\sigma_0)}(\mathbf{r}, E)}{\phi_{dilute(\sigma_0)}(\mathbf{r}, E)} \right)^M dV dE \,.$$

The expanded version of importance map in plate becomes:

$$imp(\mathbf{r}, E) = \frac{\phi^{\dagger}_{res(\sigma_0)}(\mathbf{r}, E)}{\int_E \int_V \left(\frac{\phi_{res(\sigma_0)}(\mathbf{r},E)}{\phi_{dilute(\sigma_0)}(\mathbf{r},E)} \right)^M dV dE} \tag{10}$$

Results


M = 1.0
Color Map Legend
Range % of Cells
0.350 0.00
0.300 0.00
0.250 0.00
0.200 0.00
0.170 0.00
0.150 0.04
0.130 0.13
0.110 0.03
0.0900 0.16
0.0700 0.58
0.0500 2.02
0.0300 24.33
0.01000 43.68
29.03
Minimum Value: 0.00101992
Cell-Wtd Avg: 0.0211355
Vol-Wtd Avg: 0.0211355
Maximum Value: 0.154631
Z-Axis (cm) (Y-Plane = 25 : Y = 24.0000 to 25.0000)
X-Axis (cm) (Y-Plane = 25 : Y = 24.0000 to 25.0000)


58-grp
FW-CADIS
Color Map Legend
Range % of Cells
0.35 0.00
0.30 0.00
0.25 0.00
0.20 0.16
0.17 0.08
0.15 0.32
0.13 0.24
0.11 0.24
0.090 0.42
0.070 0.59
0.050 0.73
0.030 0.93
0.0100 4.43
91.85
Minimum Value: 0.000902912
Cell-Wtd Avg: 0.00834701
Vol-Wtd Avg: 0.00834701
Maximum Value: 0.243378
Z-Axis (cm) (Y-Plane = 25 : Y = 24.0000 to 25.0000)
X-Axis (cm) (Y-Plane = 25 : Y = 24.0000 to 25.0000)

RESULTS

Case	CPU-hrs	Max RE	Avg RE	Min FOM	Avg FOM
base	849.77	8.10e-1	1.02e-2	1.79e-3	11.3
58 g	954.89	5.22e-1	9.33e-3	3.85e-3	12.0
M = 1	534.80	2.69e-1	2.44e-2	2.58e-2	3.13

- M = 1.0 used the same deterministic parameters as the base case
- FOM_{min} $\sim$10x better than best FW-CADIS case
- FOM_{min} and FOM_{avg} are $\sim$100x closer together than best FW-CADIS case

SUMMARY AND CONCLUSIONS

- Space and energy self-shielding make variance reduction difficult
- Caused by multigroup cross sections in angle-independent implementation
- Not resolved by
  - Finer spatial mesh, energy group structure, or angular quadrature; higher order scattering expansion; or Bondarenko method
- New method
  - Adds a factor accounting for resonances to FW-CADIS adjoint source
  - Tunable based on degree of problem manifestation
  - Lowers FOM_{min} and brings FOM_{min} closer to FOM_{avg}
  - More work, but useful in these pathological cases

Anisotropy: a computational challenge

- Many important nuclear applications have strong anisotropies
  - Used fuel casks
  - Reprocessing facilities
  - Reactor facilities
  - Active interrogation
- These are difficult to capture with current tools:
  - Ray effects with deterministic
  - Too slow with analog MC
  - Insufficient acceleration of MC with hybrid

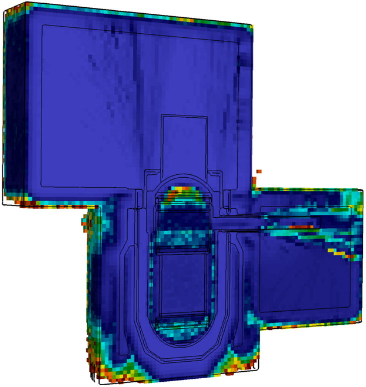


Figure: PWR, 1 CPU-month, FW-CADIS for mesh-tally (500K cells)

CURRENT HYBRID METHODS ARE INSUFFICIENT

- MC VR parameters created from adjoint deterministic flux that is a function of space and energy only
- Angular dependence of the importance function is not retained, otherwise the map would be very large (tens or hundreds of GB) and more costly and complex to use in the Monte Carlo simulation
- Drawback: within a given space/energy cell, the map provides the average importance of a particle moving in any direction through the cell – excluding information about how particles move toward the objective

CURRENT HYBRID METHODS ARE INSUFFICIENT

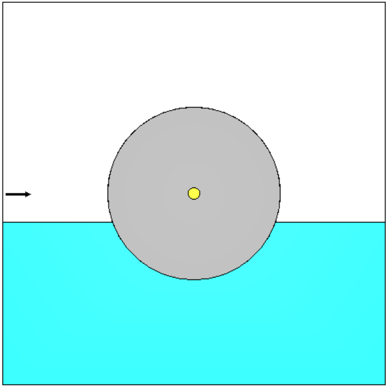


Figure: Spherical boat model with source on left and fissionable material at center

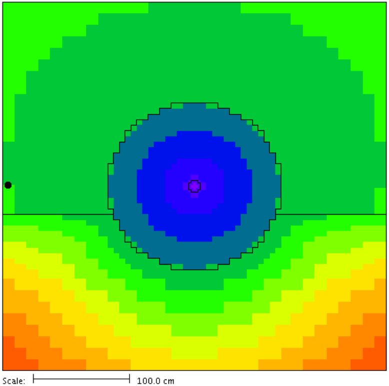


Figure: Target weight window values for 14.1 MeV neutrons

BETTER HYBRID METHODS ARE NEEDED

- We can use angular information to improve performance

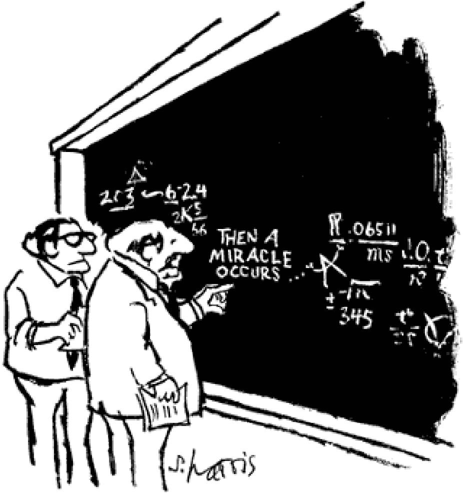
$$\phi^{\dagger}(\mathbf{r}, E) = \frac{\int \psi(\hat{\Omega}, \mathbf{r}, E)\psi^{\dagger}(\hat{\Omega}, \mathbf{r}, E)d\hat{\Omega}}{\int \psi(\hat{\Omega}, \mathbf{r}, E)d\hat{\Omega}} \tag{11}$$

- The space- and energy-dependent importance map will be normalized and source biasing parameters will be generated in a manner similar to the current implementation of hybrid methods
- Immediately useful; widely applicable

OTHER (POTENTIAL) PROJECTS

- Continuing development of MC on GPU
- 3D shielding optimization: applicable to SMRs
- Parallelization of open source deterministic code, Detran
- Investigating use of hybrid methods for interrogation of SNM with neutron time-correlations
- Using SP_N in multigrid preconditioner in Denovo
- Contributing methods to PyNE; investigating a long term research relationship

QUESTIONS?



"I think you should be more explicit here in step two."