Hybrid Transport Methods for Shielding Challenges

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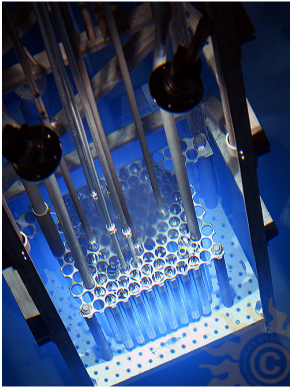
OUTLINE

- Hybrid methods overview
  - Motivation
  - CADIS and FW-CADIS
  - Challenges
- MC importances with space and energy self-shielding
  - Cross section processing
  - Problem investigation
  - Resonance factor method
  - Results and wrap-up
- MC importances with strong anisotropies
- Other Projects



PROJECT MOTIVATION

- Need to accurately model radiation for shielding
- Challenging: dense shields; streaming paths; multigroup x-secs
- Current methods are insufficient
- Goal: accurate solutions in reasonable time

Figure: Used fuel storage pad

SOLVING THE TE

Monte Carlo

- Solution has statistical error
- *Continuous* phase space: "gold standard answers"
- *Long* compute times
- Optically thick = *slow*

Deterministic

- Solution equally valid everywhere
- *Discretized* phase space: drives solution quality
- *Short* compute times
- Streaming = *ray effects*

$$\hat{\Omega} \cdot \nabla \psi(\vec{r}, E, \hat{\Omega}) + \Sigma_t \psi(\vec{r}, E, \hat{\Omega}) = S(\vec{r}, E, \hat{\Omega}) + \int_{4\pi} d\hat{\Omega}' \int_0^\infty dE' \, \Sigma_s(E', \hat{\Omega}' \to E, \hat{\Omega}) \psi(\vec{r}, E', \hat{\Omega}')$$

SPEEDING UP MC

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

$$\mathrm{FOM} = \frac{1}{\mathrm{R}^2 \mathrm{t}} , \qquad \mathrm{R} = \text{relative error}$$

$$\mathrm{t} = \text{time}$$

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

→ **Hybrid Methods**

FORWARD-ADJOINT RELATIONSHIP

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

$$R = \int_E \int_{V_r} f(\mathbf{r}, E)\phi(\mathbf{r}, E) dV dE \tag{1}$$

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

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.

CADIS [1]

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

$$
\begin{aligned}
imp(\mathbf{r}, E) &= \frac{\phi^\dagger(\mathbf{r}, E)}{\langle q(\mathbf{r}, E), \phi^\dagger(\mathbf{r}, E)\rangle} = \frac{\phi^\dagger(\mathbf{r}, E)}{R} \\
\hat{q}(\mathbf{r}, E) &= \frac{\phi^\dagger(\mathbf{r}, E) q(\mathbf{r}, E)}{R} \\
w_0(\mathbf{r}, E) &= \frac{q(\mathbf{r}, E)}{\hat{q}(\mathbf{r}, E)} = \frac{R}{\phi^\dagger(\mathbf{r}, E)}
\end{aligned}
$$

Birth weights match weight targets: <u>C</u>onsistent <u>A</u>djoint <u>D</u>riven <u>I</u>mportance <u>S</u>ampling <u>M</u>ethod

FW-CADIS [1]

- We often want to optimize solutions in **all** of phase space
- Then, the adjoint source needs to be a global forward solution: Forward Weighted-CADIS

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

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** shielding problems...

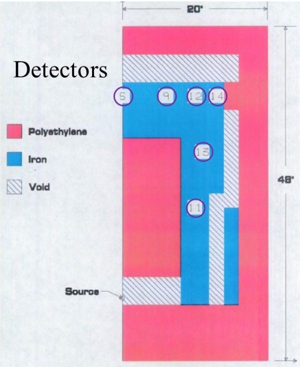


Figure: Dog Legged Void Neutron shielding benchmark

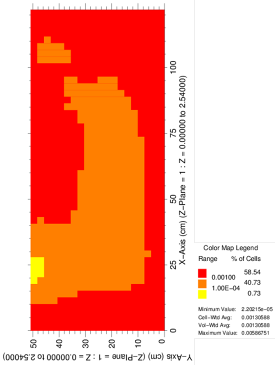


Figure: MC 95% CI RE using FW-CADIS, DLVN [2]

CHALLENGES

...but not **all** of them

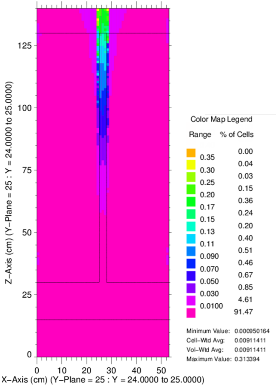


Figure: MC 95% CI RE using FW-CADIS, plate [3]

- An example case:
  - Energy self-shielding +
  - Spatial self-shielding +
  - Angular collimation
- FW-CADIS only includes space and energy, *not angle*
- We're also using multigroup x-secs
- Result: high relative error through location of interest

Cross section processing [4]

- General Case

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

- Bondarenko method uses a background cross section

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

- W(u) changed to include the spectral difference assumption ($1/\sigma_t$) and effect of other isotopes (adding σ_0)

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

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

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

PROBLEM INVESTIGATION

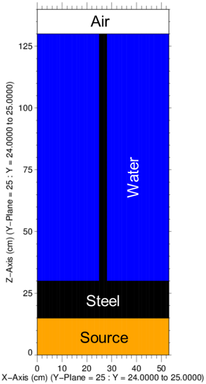


Figure: Shielding Stack Up

- 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 H_2O

- 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 / cont.
Angular quad	QR-18-252	QR-8-36
Scattering order	P_3	P_3
Convergence	0.01	0.05
TRANSX settings	$\bar{l}$ = 10,000	$\bar{l}$ = 10,000
Dose Conv. Facs.	58 grps	27 grps

ERRORS IN PLATE

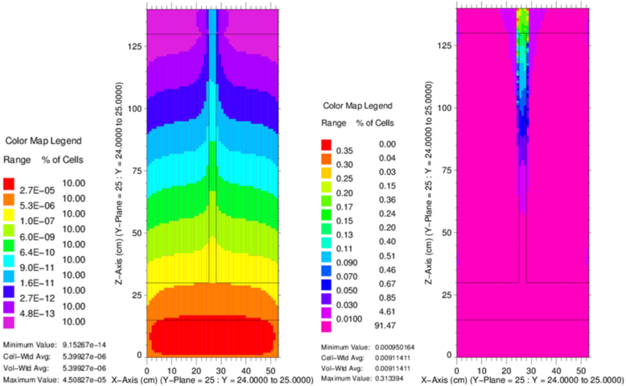


Figure: Base-case FW-CADIS MC21 dose rate (left) and 95CI RE (right) (xz-slice through y=25 cm)

DETERMINISTIC MC MISMATCH: FLUX

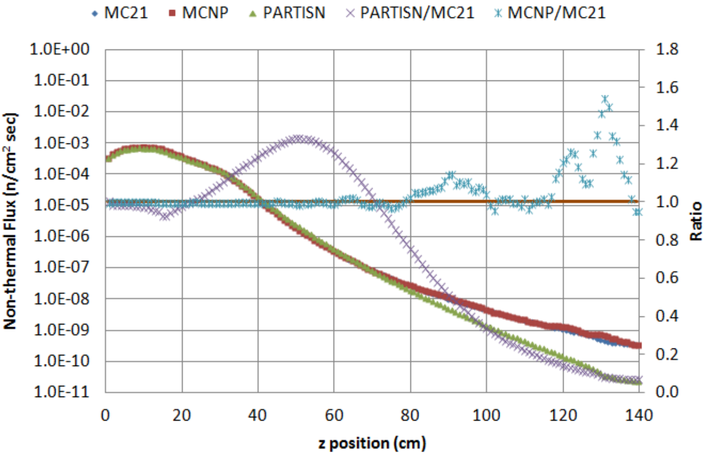


Figure: Plate non-thermal flux (left axis) and method ratios (right axis) down the x-y centerline

CORRECT WITHOUT PLATE

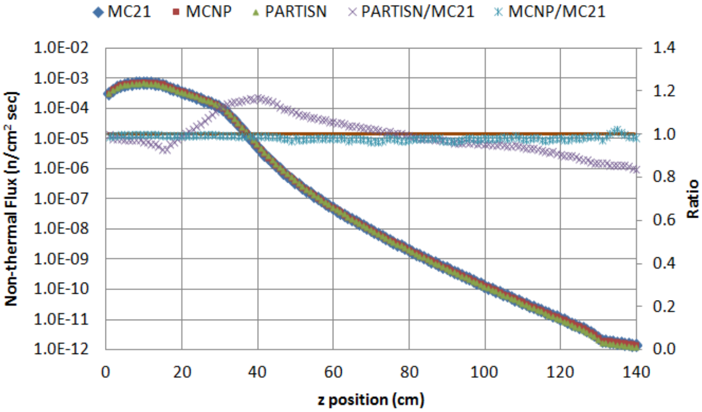


Figure: Plate non-thermal flux (left axis) and method ratios (right axis) down the x-y centerline

Deterministic MC mismatch: spectra

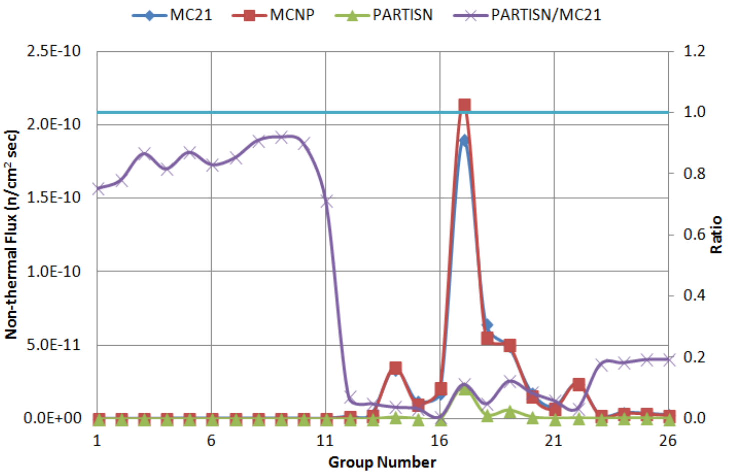


Figure: Plate flux spectra (left axis) and PARTSN/MC21 (right axis) at start of air region (z = 130.5 cm)

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

- Physics
  - Cr plate (diff. res. mat.)
  - Air in plate (no res. mat.)

PARAMETERS RESULTS

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

Case	N	CPU-hrs	Max RE	Avg RE	Min F	Avg F
Base	1e10	849.77	0.810	1.02e-2	1.79e-3	11.3
1e11	1e11	8,543.47	0.164	3.28e-3	4.33e-3	10.9
58 g	1e10	954.89	0.522	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	0.343	4.00e-3	4.62e-4	3.40

RESONANCE STREAMING

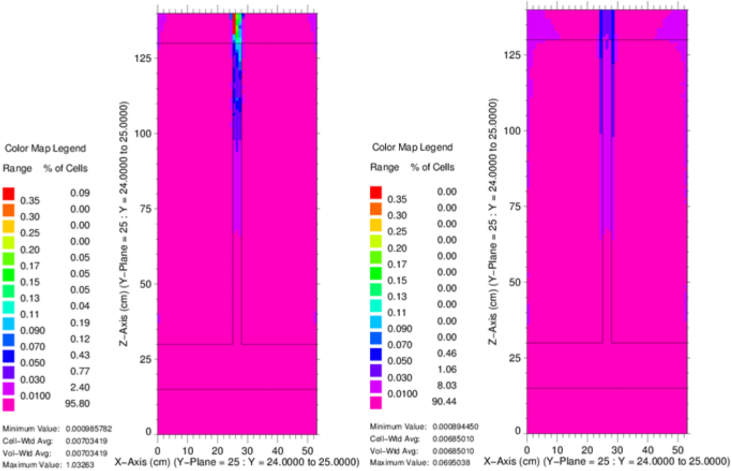


Figure: Cr plate (left) and air plate (right) FW-CADIS MC21 dose rate 95CI RE (xz-slice through y=25 cm)

INVESTIGATION SUMMARY

- These items did not improve PARTISN:
  - finer quadrature
  - higher scattering order
  - more theoretically-accurate mean chord length
- These items in imp. map creation did not reduce REs:
  - finer spatial mesh in plate
  - finer energy group structure
- Behavior is related to space and energy self-shielding

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

So, we had to come up with something else...

Resonance factor method [3]

New Method developed to deal with this.

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

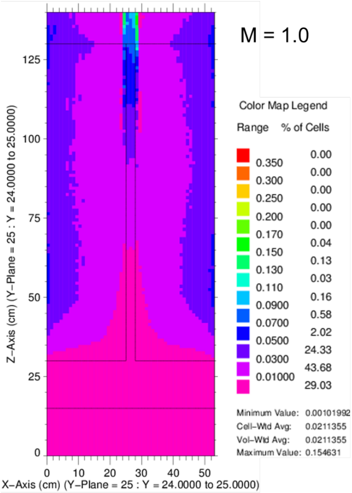
$$q^{\dagger}(\mathbf{r}, E) = \left(\frac{\phi_{res(\sigma_0)}(\mathbf{r}, E)}{\phi_{dilute(\sigma_0)}(\mathbf{r}, E)} \right)^{M} q^{\dagger}_{FWC}$$

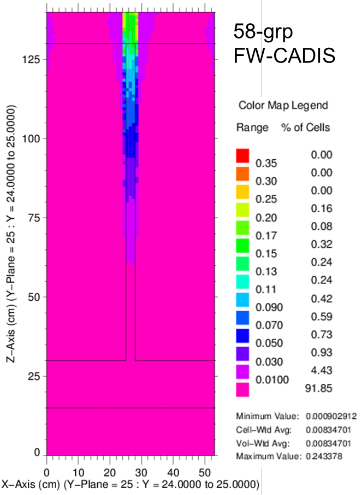
where

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

The resulting adjoint flux is used to make importances

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	0.810	1.02e-2	1.79e-3	11.3
58 g	954.89	0.522	9.33e-3	3.85e-3	12.0
M = 1	534.80	0.269	2.44e-2	2.58e-2	3.13

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

RESONANCE FACTOR WRAP-UP

- Space and energy self-shielding make VR difficult
- Caused by multigroup x-secs 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
  - Raises $\mathrm{FOM}_{\mathrm{min}}$ and brings $\mathrm{FOM}_{\mathrm{min}}$ closer to $\mathrm{FOM}_{\mathrm{avg}}$
  - 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
- Difficult to capture with current tools:
  - Ray effects with deterministic
  - Too slow with analog MC
  - Insufficient acceleration of MC with current hybrid

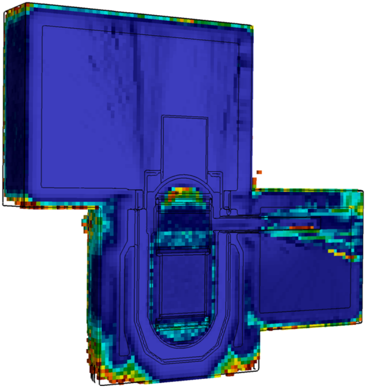


Figure: PWR relative error [5]

CURRENT HYBRID METHODS ARE INSUFFICIENT

- MC VR parameters created from adjoint deterministic scalar 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 MC 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

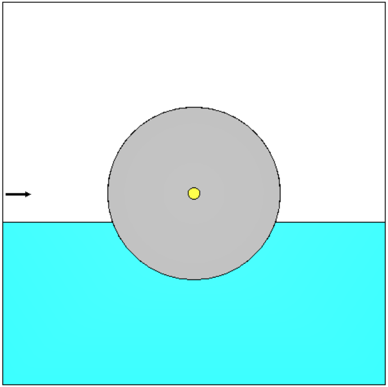


Figure: Spherical boat model with source on left and fissionable material at center

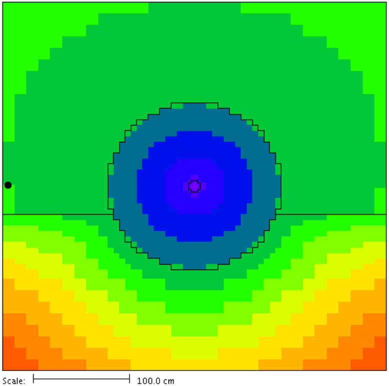


Figure: CADIS target weight window values for 14.1 MeV neutrons

MANY ATTEMPTS AT RESOLUTION → LIMITED SUCCESS

- Automatic WW generator in MCNP [6]
- AVATAR [7]
- LIFT [8]
- Cooper and Larsen's global weight windows [9]
- FW/CADIS
- Resonance Factor method

All of these have worked in *some* situations
They often require *significant* user expertise

Better hybrid methods are needed: two ideas.

Integration weighting (MMM)

Different integration plan captures angles in scalar flux creation

$$\phi^{\dagger}(\mathbf{r}, E) = \int \psi^{\dagger}(\hat{\Omega}, \mathbf{r}, E) d\hat{\Omega} \qquad \text{original}$$

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

Major challenges and areas of investigation:

1. Data storage and handling (many GBs)
2. More, less, or differently sensitive to
   - quality of the discrete ordinates calculation?
   - ray effects?

Lagrange discrete ordinate equations

Use a formulation that is more flexible in the ways it handles quadrature: new LDO equations [10]

- Re-derivation of S_N with an interpolatory quadrature framework
- Allows evaluation at directions not on quadrature set
- Can use asymmetric angles
- No need to store spherical harmonic moments
- May be useful for more accurately capturing strong anisotropies

METHOD IMPLEMENTATION

- The space- and energy-dependent importance map will be normalized and source biasing parameters will be generated in the same ways as the current implementation of FW/CADIS
- Immediately useful; widely applicable
- We will study both strategies and characterize the impact
- Will be available in SCALE [11] and ADVANTG [5]

OTHER PROJECTS: MC

Monte Carlo on advanced architectures

- WARP, developed at Berkeley, for GPGPUs
- Investigating delta-tracking vs. ray tracing
- Up next: MC on MICs

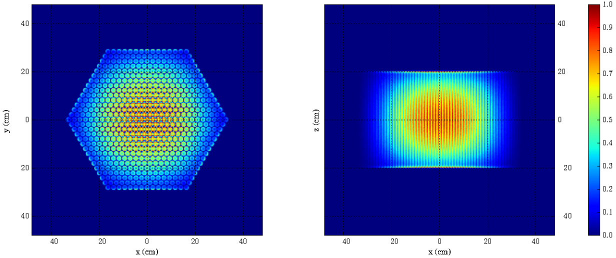


Figure: WARP fission source locations, hex assembly

Other projects: ETA

Energy Tuning Assembly design, optimization, and use

- Developing meta-heuristic optimization techniques to automate the design process for ETAs
- Optimizing for spectra with forensics applications
- To be fielded on 88″ cyclotron and/or NIF

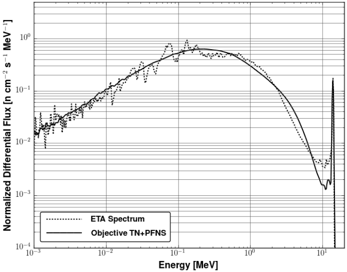
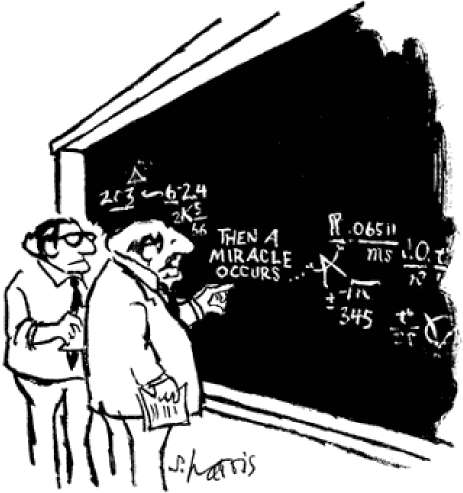


Figure: ETA-produced spectrum (MCNP) and the objective

OTHER PROJECTS: JUST STARTING

- α-eigenvalue acceleration methods
- Nuclear data processing and multigroup cross section generation
- Non-classical Botlzmann transport equation applied to BWRs
- PyNE development: nuclear data processing, better burnup methods
- Multiphysics in collaboration with CIET?

QUESTIONS?



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

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