Nodal Data Generation

2018 SCALE Users' Group

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Project Goals

- Integrate SHIFT as a Monte Carlo transport method in 3D TRITON
- Enable Monte Carlo continuous energy reference for nodal data for PARCS
- Motivations
  - Before this work
    - TRITON had general 3D transport (KENO) + depletion (ORIGEN)
    - But no ability to generate nodal data (T16) file for PARCS
  - After this work: **reference nodal data for any reactor system!**

What is Nodal Data?

- diffusion coefficient
- macro total cross section
- macro absorption cross section
- macro nu-fission cross section
- macro scattering matrix
- Xe,Sm,I,Pm yields
- region power factors (e.g. pin power maps)
- detector response functions
- assembly discontinuity factors (ADFs)
- corner discontinuity factors (CDFs)
- line currents
- delayed neutron fractions
- delayed neutron precursors

Diffusion coefficient is hard (1/4)

- By definition $$D_g = \frac{1}{3\Sigma_{tr,g}}$$

- Start with transport corrected P0 scattering

$$\nabla \cdot \Omega\psi_g + \Sigma_{tr,g}\psi_g = \sum_{g'} \Sigma_{s,0}^{g' \to g} \phi_{g'} + Q_g$$

$$\Sigma_{tr,g} \equiv \sum_i N_i \sigma_{i,tr,g}$$

$$\sigma_{i,tr,g} = \begin{cases} \sigma_{i,t,g} - \sigma_{i,s,1}^{g}, & \text{outscatter approximation} \\ f_g * \sigma_{i,t,g}, & \text{H-1 factors using NLC method} \end{cases}$$

NEWT approach

Polaris approach to solve transport equation in TCP0 mode (default is P2)

Diffusion coefficient is hard (2/4)

- **Polaris** then performs a critical spectrum correction on a homogeneous problem with buckling such that k=1

$$B^2 \sum_{g'} \mathscr{D}^{g'\to g}\phi_{g'} + \Sigma_{t,g}\phi_g = \sum_{g'} \Sigma_{s,0}^{g'\to g}\phi_{g'} + \chi_g$$

$$\sum_g \nu\Sigma_{f,g}\phi_g = 1$$

alpha=1 for P1

$$\mathscr{D}^{g'\to g} \equiv [3\alpha_g \Sigma_{t,g} - \Sigma_{s,1}^{g'\to g}]^{-1}_{g'\to g}$$

$$\Rightarrow J_g = \mp iB \sum_{g'} \mathscr{D}^{g'\to g}\phi_{g'}$$

Polaris approach to generate nodal diffusion coefficient

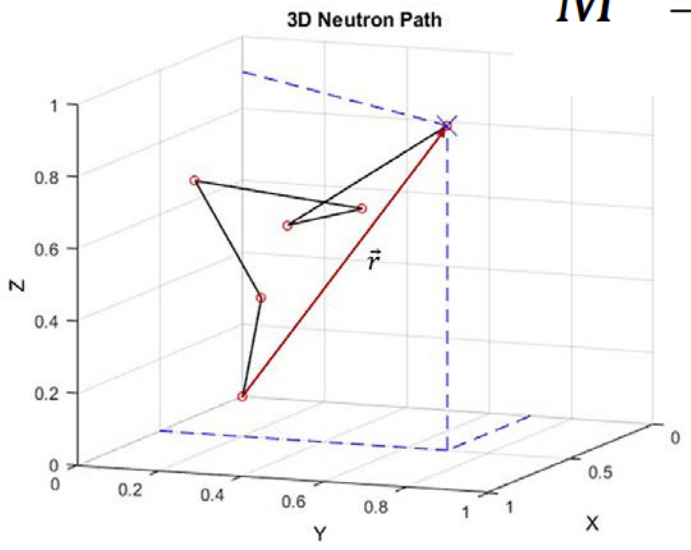
- Diffusion coefficient falls out as $D_g = \frac{\sum_{g'} \mathscr{D}^{g'\to g}\phi_{g'}}{\phi_g}$

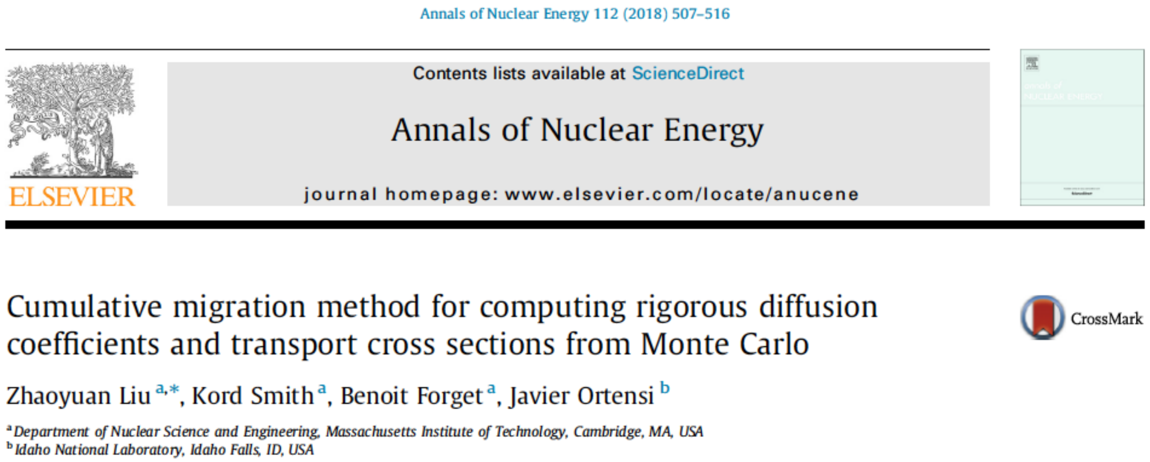
Diffusion coefficient is hard (3/4)

- **OpenMC** developed an ingeniously simple method using the migration area

$$M^2 = \frac{D}{\Sigma_a} = \frac{1}{6}\overline{r^2}$$

average square of crow flight length of the neutron from the position where it is born to the position absorbed

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Cumulative migration method for computing rigorous diffusion coefficients and transport cross sections from Monte Carlo

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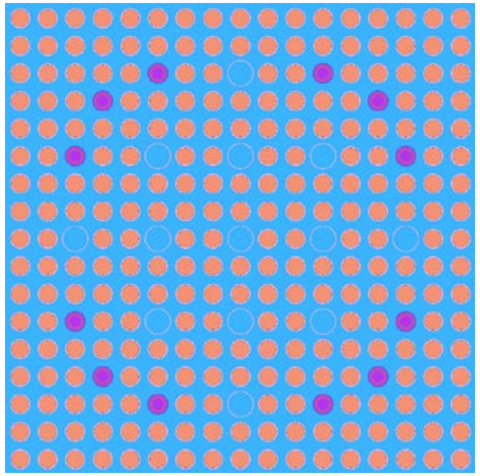
- Can get high-quality diffusion coefficient tally in any volume!

Diffusion coefficient is hard (4/4)

- Cumulative Migration Method (CMM) has been implemented in **Shift.**
- Compares very well for BEAVRS W17x17 with 12 BAs



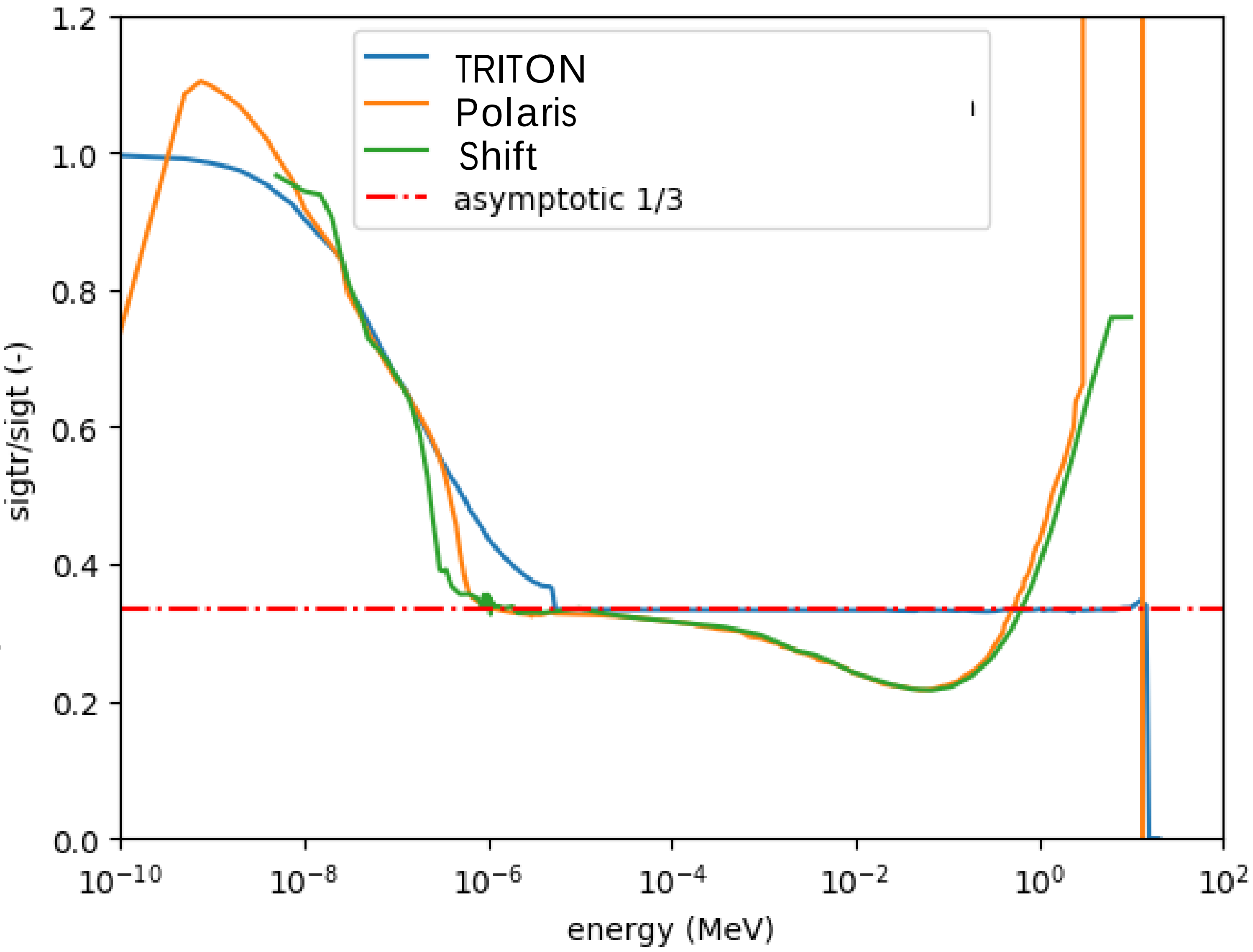
Fast diffusion coefficient

Method	Code	D1 (cm)	Rel Diff
P1	CASMO	1.430	-
Out-scatter	OpenMC	1.102	-22.94%
B1	Serpent	1.397	-2.31%
CMM	OpenMC	1.426	-0.28%
CMM	Shift	1.455	1.75%
Out-scatter	Shift	1.113	-22.15%

- P1 and B1 are considered "in-scatter" methods
- *P1 is thought to be correct due to consistency with CMM*

Comparison of 252-group transport cross section

- Infinite homogeneous media test
  (hydrogen+trace fissionable)
- Comparison
  - **Polaris** "in-scatter" looks good except for high-energy 0/0
  - **TRITON** has no mid/high-energy shape
  - **Shift** compares well with reference OpenMC



Generating few-group XS data with TRITON/Shift

- Arbitrary energy group structure
- Multiple tally regions in a single model
- Supports typical XS data, ADFs, scatting matrix, etc.
- Based on a rectangular mesh
- Working on hexagonal meshes…

Input Format

```
read fgxs
     shape cuboid id=NUM Xmax Xmin Ymax Ymin Zmax Zmin
     energy       id=NUM  E0 E1 E2 ... EN end
     tallytype    id=NUM [options]
end fgxs
```

3 Tally Region Example:

```
read fgxs
     shape cuboid id=10  5.0 -5.0  5.0 -5.0   40.0  0.0
     energy       id=10  0 0.625 20E6 end
     tallyset t16 id=10

     shape cuboid id=20  5.0 -5.0  5.0 -5.0   70.0 40.0
     energy       id=20  0 0.625 20E6 end
     tallyset t16 id=20

     shape cuboid id=30  5.0 -5.0  5.0 -5.0  100.0 70.0
     energy       id=30  0 0.625 20E6 end
     tallyset t16 id=30
end fgxs
```

Tally ID=0 Example:

```
read fgxs
     energy       id=0   0 0.625 20E6 end
     tallyset t16 id=0
     shape cuboid id=10  5.0 -5.0  5.0 -5.0   40.0  0.0
     shape cuboid id=20  5.0 -5.0  5.0 -5.0   70.0 40.0
     shape cuboid id=30  5.0 -5.0  5.0 -5.0  100.0 70.0
end fgxs
```

Comparison of TRITON/SHIFT to Serpent

TRITON with SHIFT in SCALE 6.3

- AMPX CE data verified and validated based on latest ENDF/B (ENDF/B-VIII)
- Full range temperature interpolation
- Much more scalable for many CPUs + GPUs / memory not as restrictive
  - Nuclide/reaction-specific energy grid represents nuclear data faithfully
  - Domain decomposition for scalability
- Nodal data tally (6.3-beta1)
  - Cumulative Migration Method (CMM) for diffusion coefficient
  - No leakage correction
- SQA-ed domestic code system

Serpent

- MCNP-interoperable ACE format CE data
- Incomplete range temperature interpolation
- Much faster for few CPUs / memory limits for large problems
  - Union energy grid for all nuclides/reactions for speed
  - Delta tracking for speed
- Nodal data tally (2.1.30)
  - CMM for diffusion coefficient option (most users do in-scatter option)
  - Global P1/B1 leakage correction
- R&D foreign code system

Summary

- New nodal data tally capability in TRITON/Shift
- Includes best-in-class CMM diffusion coefficient calculation

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- Will be released in 6.3-beta1 in Fall 2018

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