Source Sampling in Complex 3-D Geometries

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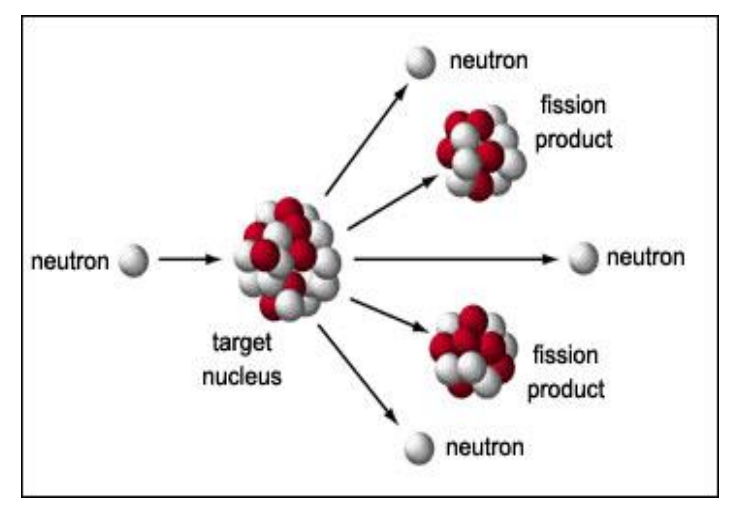
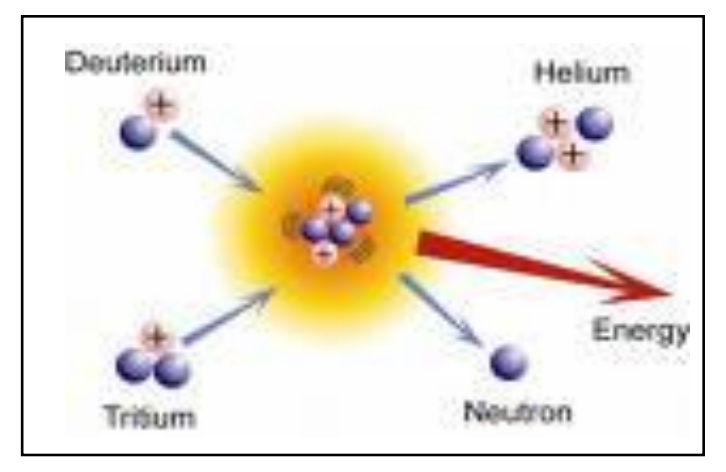
Nuclear Processes

Fission:

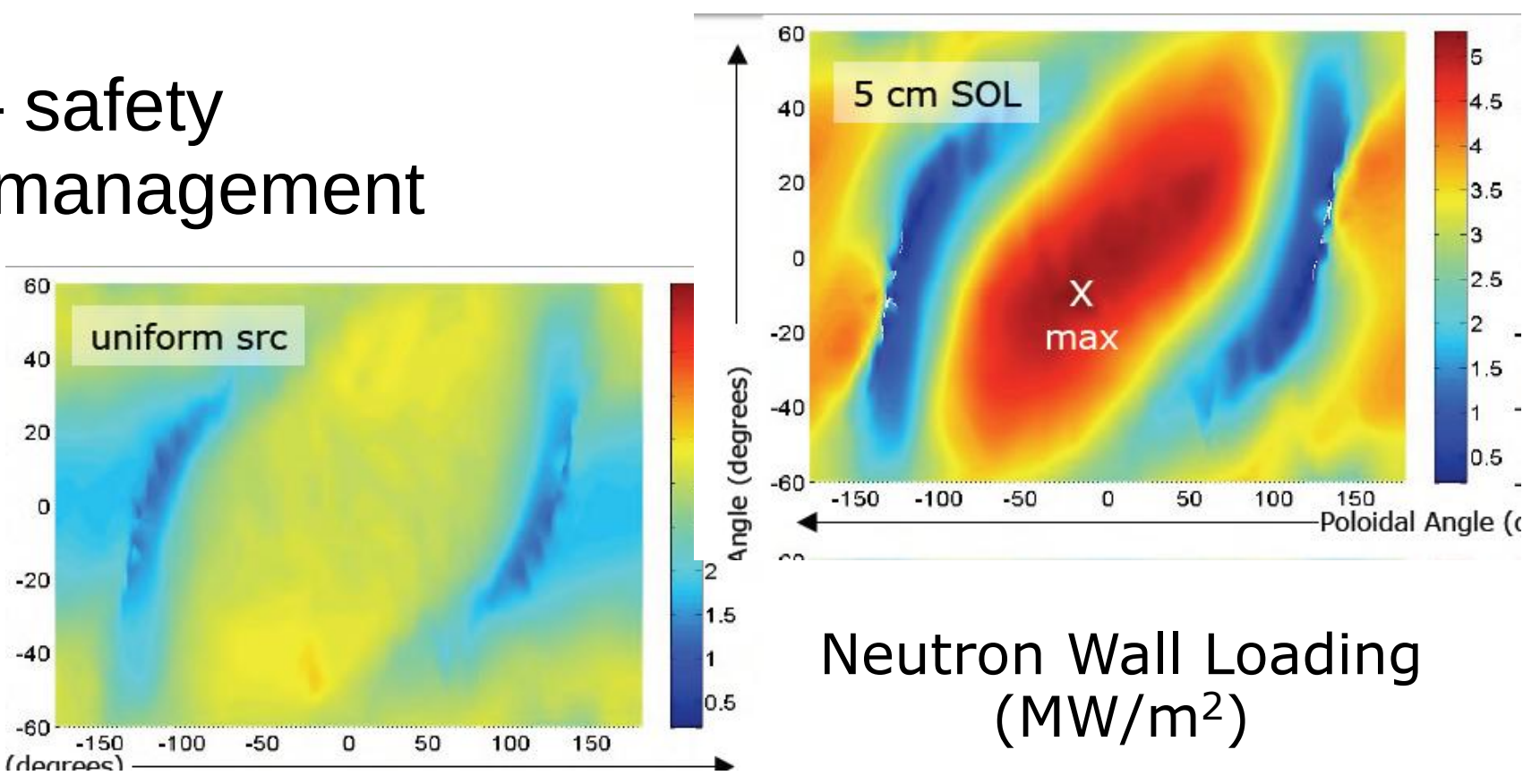


Fusion:



Fission neutrons average ~2 MeV and fusion neutrons are 14.1 MeV. These neutrons interact with structural materials and can cause:

- Activation of materials – safety assessment and waste management
- Radiation damage – structural integrity
- Heating of materials (energy deposition) – thermal analysis



Neutron Wall Loading (MW/m²)

Monte Carlo Basics

Method

- Uses probabilistic and statistical approach to solving the Boltzmann Equation
- The particle travel distance and interaction physics are converted to probabilistic and cumulative distributions (PDF and CDF) that are sampled using a random number.

Advantages

- Exact geometrical representation
- Exact treatment of the transport process
- Exact source modeling capability

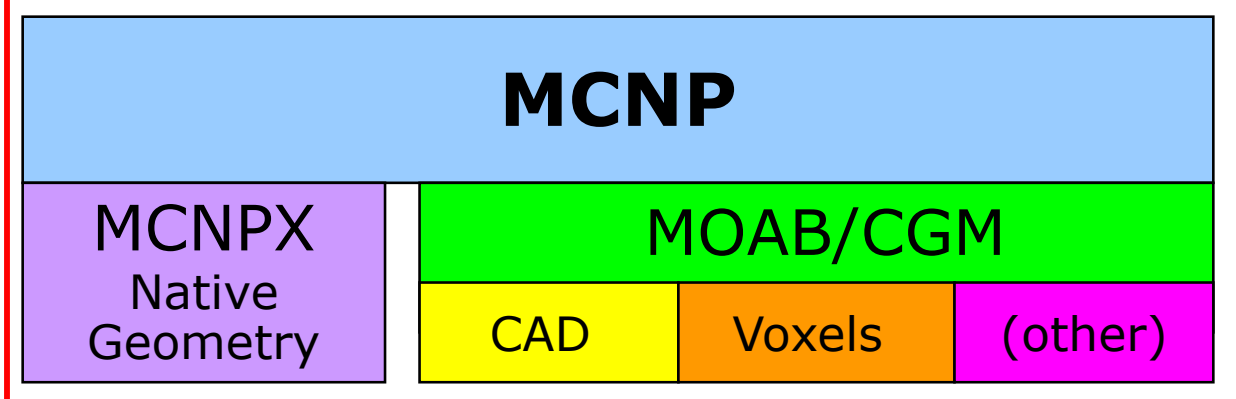
Disadvantages

- Difficult to generate accurate results in all locations
- Can require variance reduction techniques to improve accuracy
- Many particle histories and much CPU time may be required for accuracy

DAGMC

Direct Accelerated Geometry Monte Carlo (DAGMC)

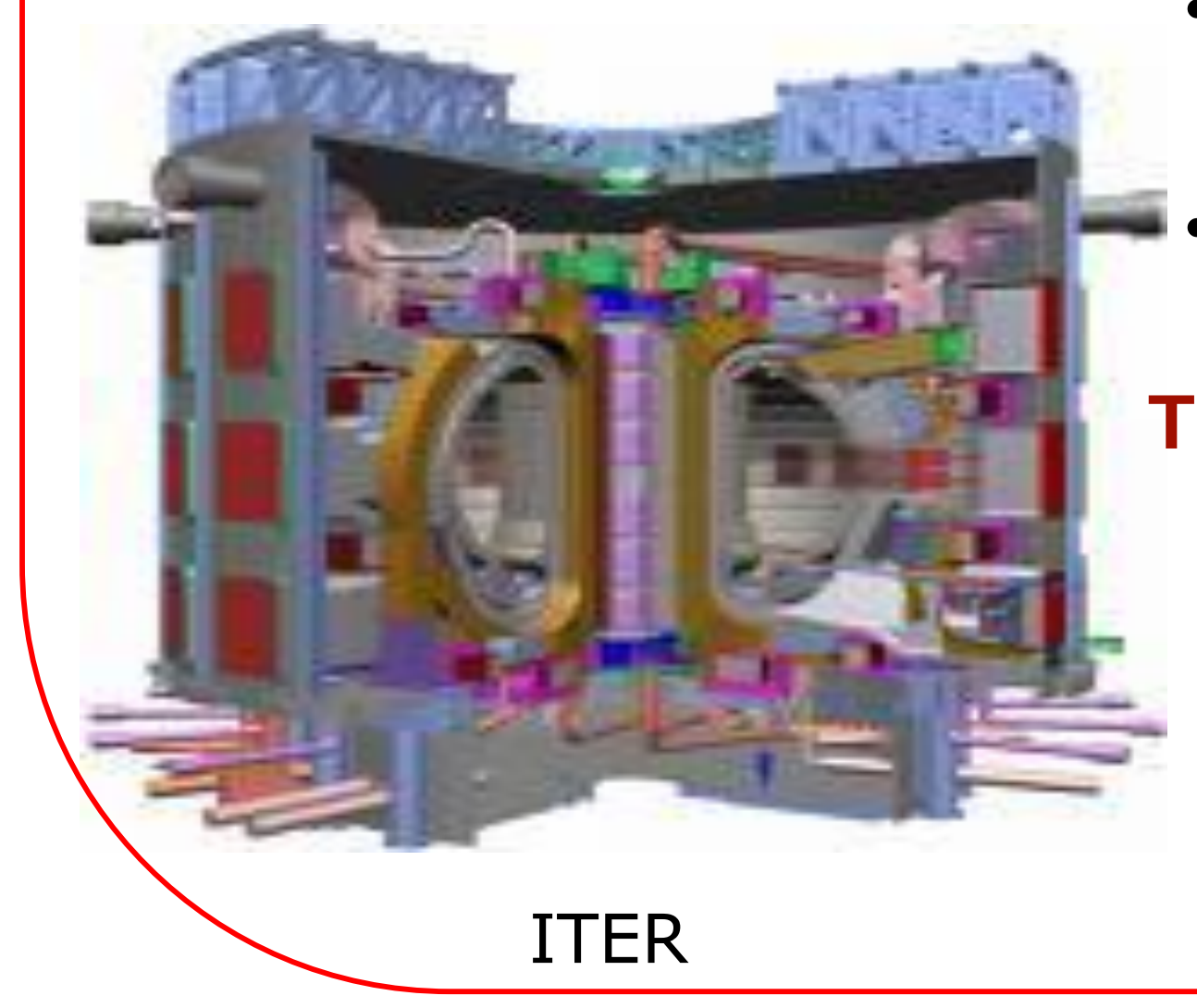
- Modified the Monte Carlo code MCNPX to *directly* use solid model geometry, i.e. CAD-Based.
- Engineering models made in a CAD program interface with MCNP



- Enables transport directly on complex 3-D systems
- Utilizes accelerations derived from computer graphics

Sources

- Fusion machines generally have complex shapes
- Activation can create sources in awkward shapes



ITER

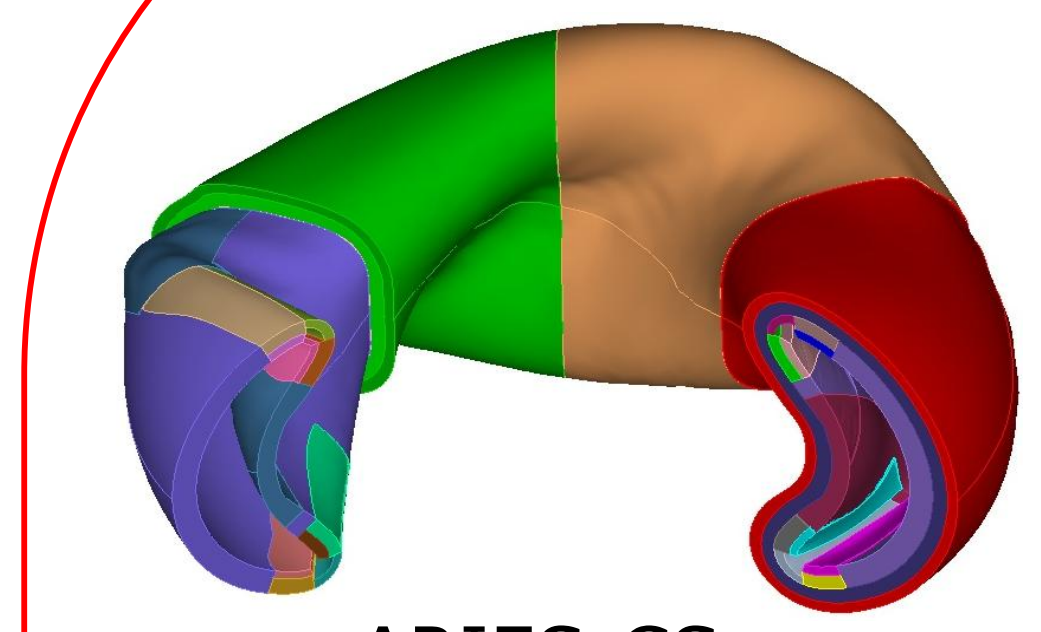
- Development of efficient 3-D source sampling techniques are required
- DAGMC capabilities facilitate this development

This is the motivation for this work:

1) Source generation and sampling for a complex plasma source

2) Source sampling of a volumetric source from activation

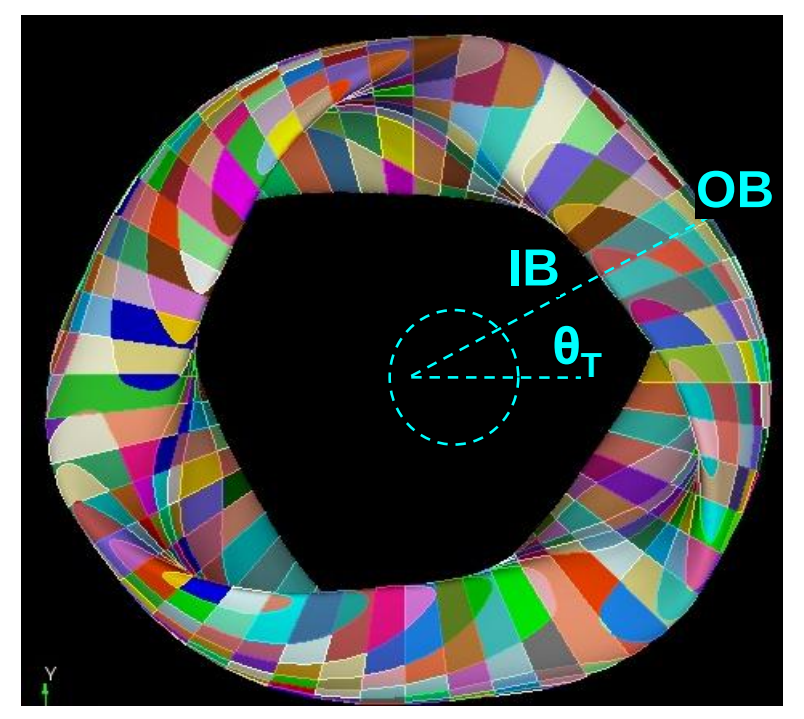
Source Defined By Fourier Coefficients



ARIES-CS

Problem

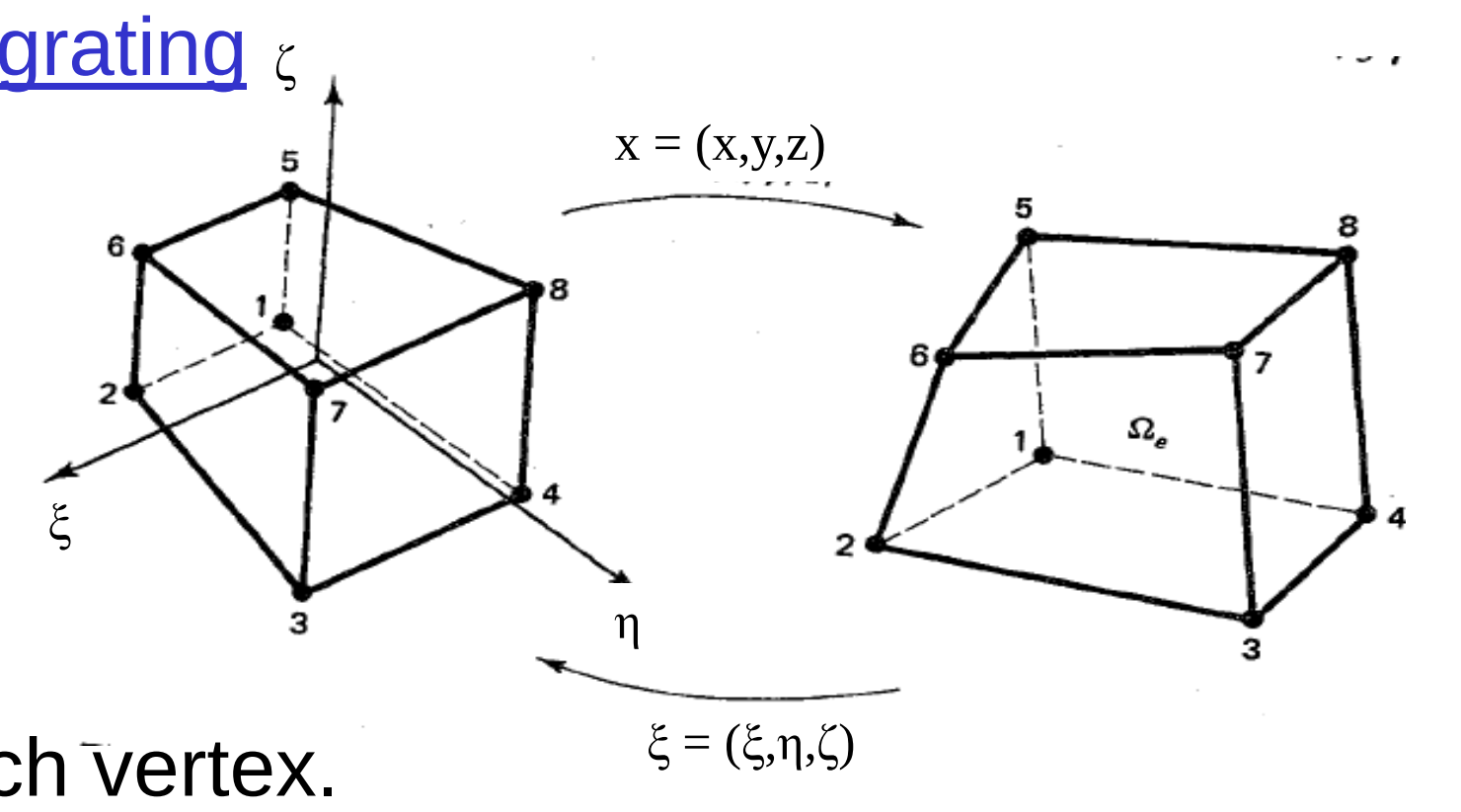
- Plasma power density is defined in a "plasma" coordinate system
- Related to real space through Fourier coefficients
- Defines the source on a set of known flux surfaces

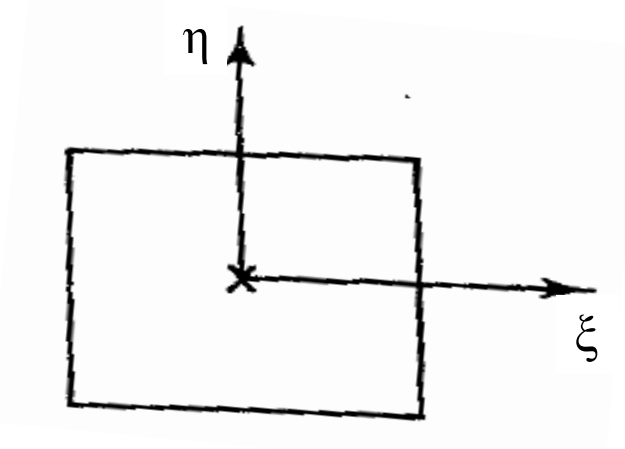


Plasma Source

Meshing, Transforming, Integrating

- A regular hexahedral mesh is created in the toroidal coordinate system – (φ,θ,s).
- The coordinates are transformed to cylindrical (r,z,φ) then to Cartesian (x,y,z) coordinates.
- Finally they are mapped to natural coordinates





Quadrature Points

- A source strength is attributed to each vertex.
- The average source at each vertex can be found by numerical integration with a Gaussian quadrature.
- The average source values are used to compute the source PDF and the source CDF

1) Convert a value from real space to natural space:

$$x(\vec{\xi}) = \sum_{a=1}^{8} N_a(\vec{\xi}) x_a^e$$

$$x_a^e = x(\vec{\xi}_a)$$

$$N_a(\vec{\xi}) = \frac{1}{8}(1+\xi_a\xi)(1+\eta_a\eta)(1+\zeta_a\zeta)$$

ξ η ζ : Any point

ξ_a η_a ζ_a: Vertices

2) Get the source values at integration points:

$$Src(\vec{\xi}_l) = \sum_{a=1}^{8} N_a(\vec{\xi}_l) Src_a^e$$

ξ_l η_l ζ_l: Integration points

$$N_a(\vec{\xi}_l) = \frac{1}{8}(1+\xi_a\xi_l)(1+\eta_a\eta_l)(1+\zeta_a\zeta_l)$$

3) Numerically integrate to get the average source for each vertex in real space:

$$\int_{\Omega^e} Src(\vec{x})d\Omega = \int_{-1}^{1}\int_{-1}^{1}\int_{-1}^{1} Src(x(\xi,\eta,\zeta), y(\xi,\eta,\zeta), z(\xi,\eta,\zeta))\, j(\xi,\eta,\zeta)\, d\xi d\eta d\zeta$$

Define:

$$j(\vec{\xi}) = \begin{vmatrix} x_\xi x_\eta x_\zeta \\ y_\xi y_\eta y_\zeta \\ z_\xi z_\eta z_\zeta \end{vmatrix} \quad \longrightarrow x_\xi(\vec{\xi}) = \sum_{a=1}^{8} N_{a,\xi}(\vec{\xi}) x_a^e \quad \longrightarrow N_{a,\xi}(\vec{\xi}) = \sum_{a=1}^{8} N_a(\eta) N_a(\zeta)\xi_a$$

$$g(\vec{\xi}) = Src(\vec{\xi})\, j(\vec{\xi}) \rightarrow \boxed{\int_{-1}^{1} g(\vec{\xi})d\vec{\xi} = \sum_{l=1}^{n_{\text{int}}} g(\tilde{\xi}_l, \tilde{\eta}_l, \tilde{\zeta}_l) W_l}$$

4) Use average source to get PDF and CDF.

$$CDF(\vec{x}) = \frac{\sum_{m=1}^{M} g(\vec{x}_m)}{\sum_{n=1}^{N} g(\vec{x}_n)} \qquad PDF(\vec{x}) = g(\vec{x})$$

N = total number of hexes
M = number of current hex

Sampling

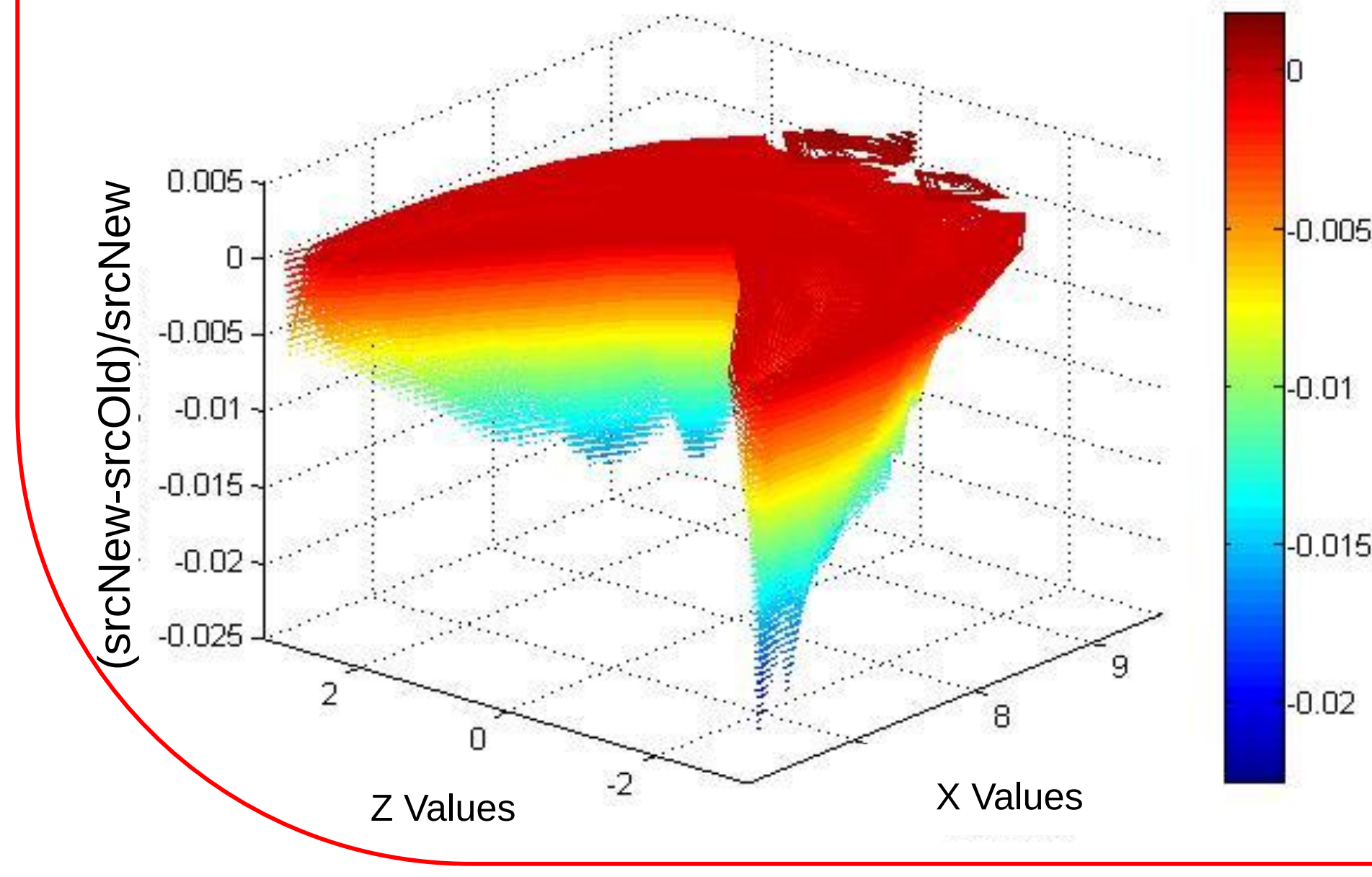
- The cell to be sampled is determined using a hierarchical (linear) search; a random number is compared against the CDF value.
- The location of the particle within the hex is found by: $[(Src)(j)](\vec{x}) \le Src_{\max} j_{\max}$

Previous vs. New Implementation

- Neutron source strength
  - previous: volume averaged
  - new: *numerically integrated average*
- Neutron source sampling
  - previous: uniform in volume
  - new: *rejection based on source variation*

Results

Relative difference in source from original



Discussion

- The relative difference between the methods for both source and volume (not shown) was generally less that 2%, i.e. small.
- For this case the new method will likely not give results significantly different from the previous method.
- New method resolves 1st order source variations which allows for a coarser mesh than the previous method.

Secondary Source from Activation

Problem

- Neutron activation generates a secondary photon source
- This source contributes to radiation dose
- Sampling source efficiently useful for dose analysis is desirable

ALARA

- Activation code used with DAGMC:
  1) Compute neutron flux in DAGMC
  2) Use ALARA to get activation source density from neutron flux
  3) Perform photon transport in DAGMC

Algorithm

For the first particle:

- Read from file:
  - -Volume numbers of source locations
  - -Energy group boundaries
  - -Group source density in each source volume
- Generate a PDF/CDF for total source in each cell: used for finding source location
- Generate a PDF/CDF for group sources in each cell: used for finding source energy

For all particles:

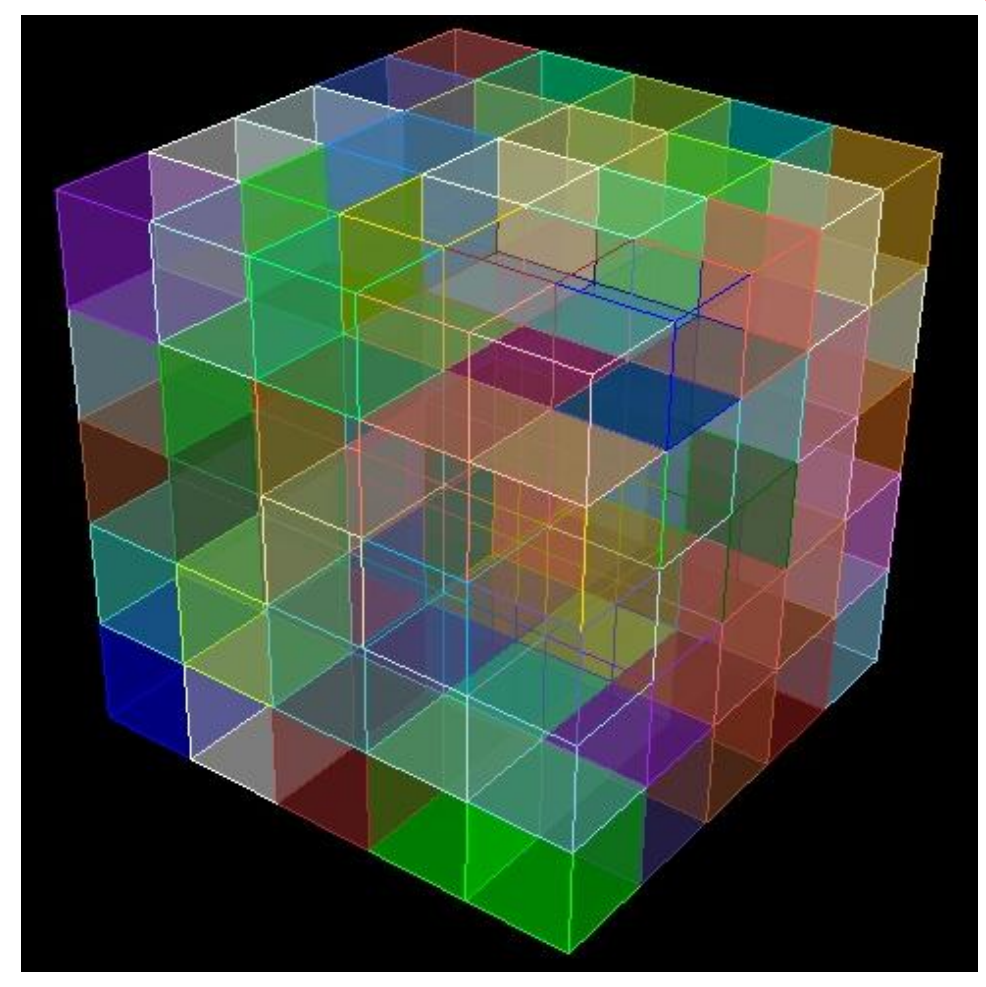
- Sample to find source cell (direct discrete sampling)
- Sample to find source location (linear)
- Check if location is in cell (rejection)
- Sample to find energy bin (direct discrete sampling)
- Sample in energy bin to find source energy (linear sampling)

Test Cases

Point Source: point source is just outside cube

Cube divided into equal squares

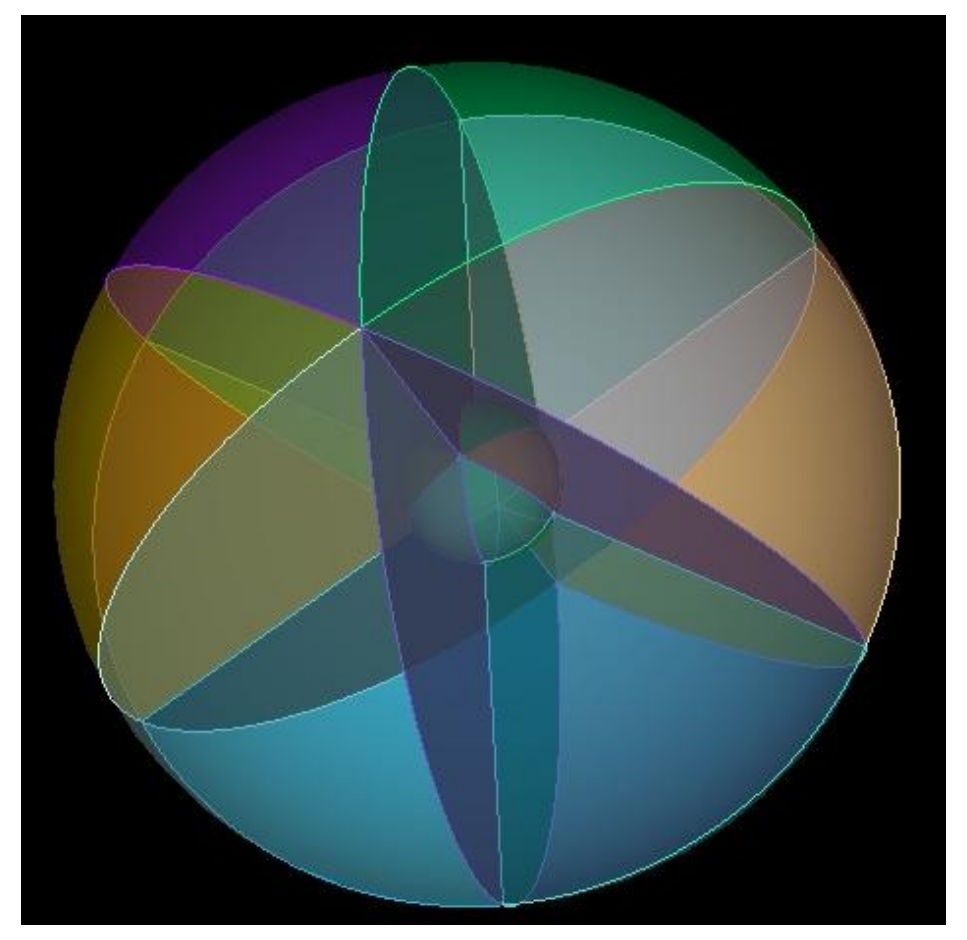
Proof of Principle



Sphere Source: contains small volumetric source

Outer sphere divided evenly

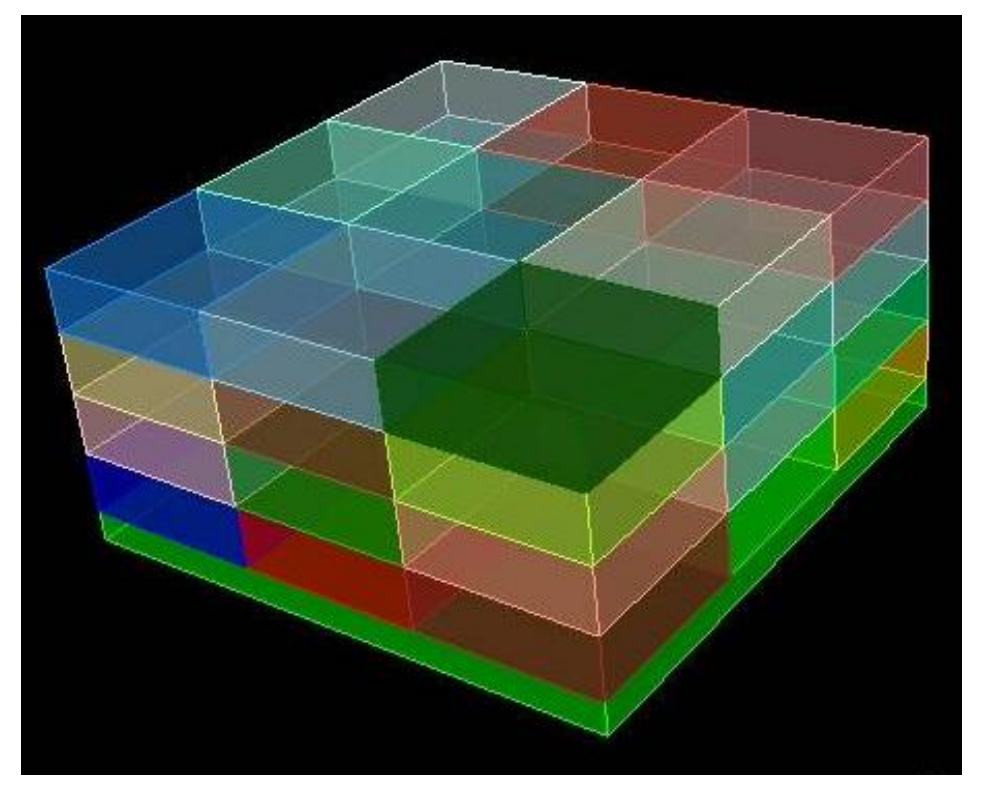
Tests uniformity in sampling method



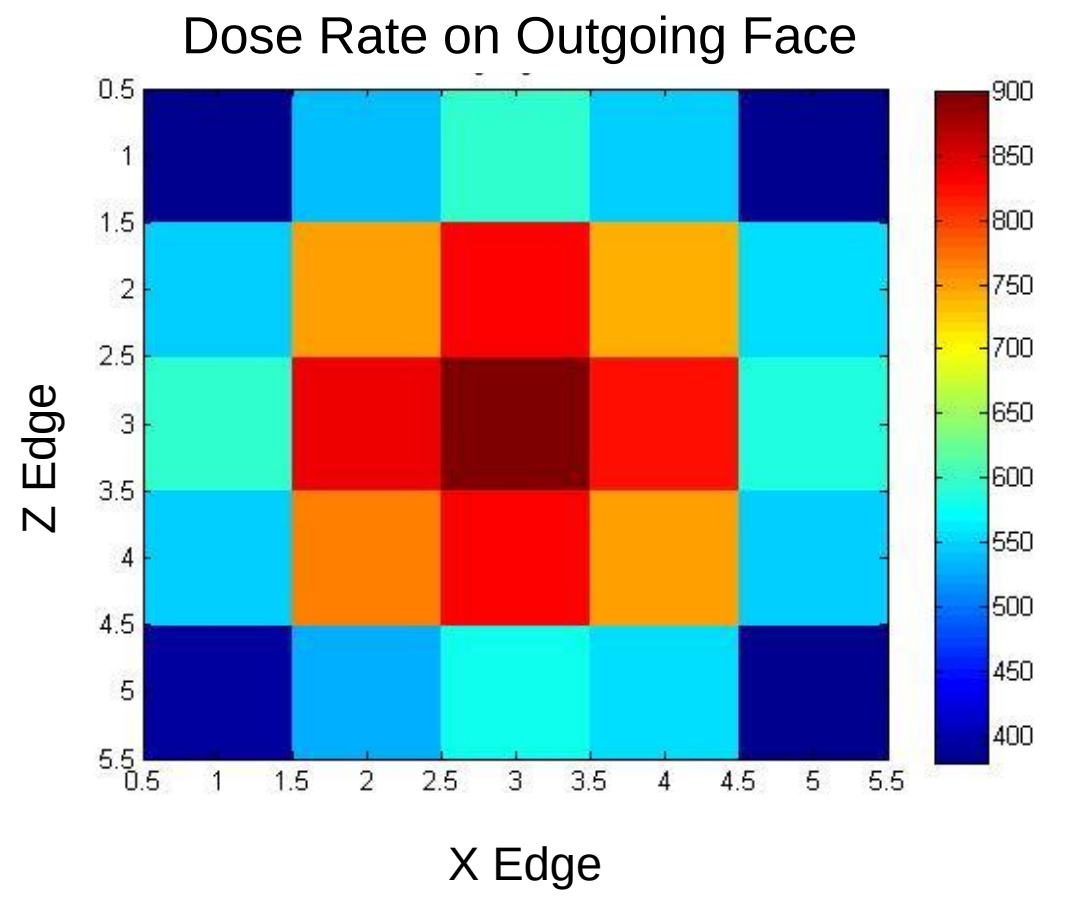
Plane Source: bottom plane contains source.

Cube divided into equal sections

Tests 1/R behavior



Results



Point Source

Point source was symmetric as expected

Sphere and Plane tests exposed bugs in the DAGMC software outside the source function

Discussion

- DAGMC stores geometry information in an oriented bounding box (OBB) structure.
- The sampling method takes advantage of the OBB structure to improve sampling efficiency over native MCNPX.
- The method uniformly samples sources in volumes defined by the CAD-geometry.
- The initial results from the test problems are encouraging.

Future Work

Source Defined by Fourier Coefficients:

- More extensive testing is required
- Test by comparing F1 tallies from new source method with native source definition
  1) Volumetrically uniform toroidal source
  2) Toroidal source with a power law distribution
- Test by generating source mesh tallies with a complex source distribution (ARIES-CS)
- Develop adaptively selected mesh

Secondary Source from Activation:

- Update source sampling code to make consistent with updates in DAGMC.
- The previously discussed tests must be repeated with the new version of DAGMC.
- More extensive testing is required.
- Automate the DAGMC → ALARA → DAGMC process.

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