Tutorial: Nodal Data with TRITON-Shift

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SCALE Users Group Workshop

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Oak Ridge National Laboratory

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Introduction

- Nodal data generation for use in nodal diffusion codes was so far enabled in SCALE through 2D multigroup calculations with Polaris or TRITON-NEWT
- New in SCALE 6.3: Capability to generate nodal data based on continuous-energy calculations of 3D geometries with the Monte Carlo code Shift
- Capability available with TRITON-Shift (T6-DEPL-Shift) using regular TRITON-KENO input with a new nodal data block (fgxs)
- Nodal data
  - Include few-group cross sections, scattering matrix, betas, lambdas, ADFs, etc.
  - Provided in arbitrary energy group structure
  - Enabled for individual cells and global meshes
  - Provided in SCALE's standard t16 text files

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Tutorial Goals and Structure

- Structure:
  - Background on nodal data
  - Methodology for nodal data in TRITON-Shift
  - Input format
  - Hands-on examples
  - Summary and outlook
- Goals:
  - Learn how to set up fgxs input
  - Understand output in out-file and t16-files
  - Understand limitations of current capability

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Background

Nodal Data Basics: Lattice Physics and Nodal Simulator

Lattice Physics

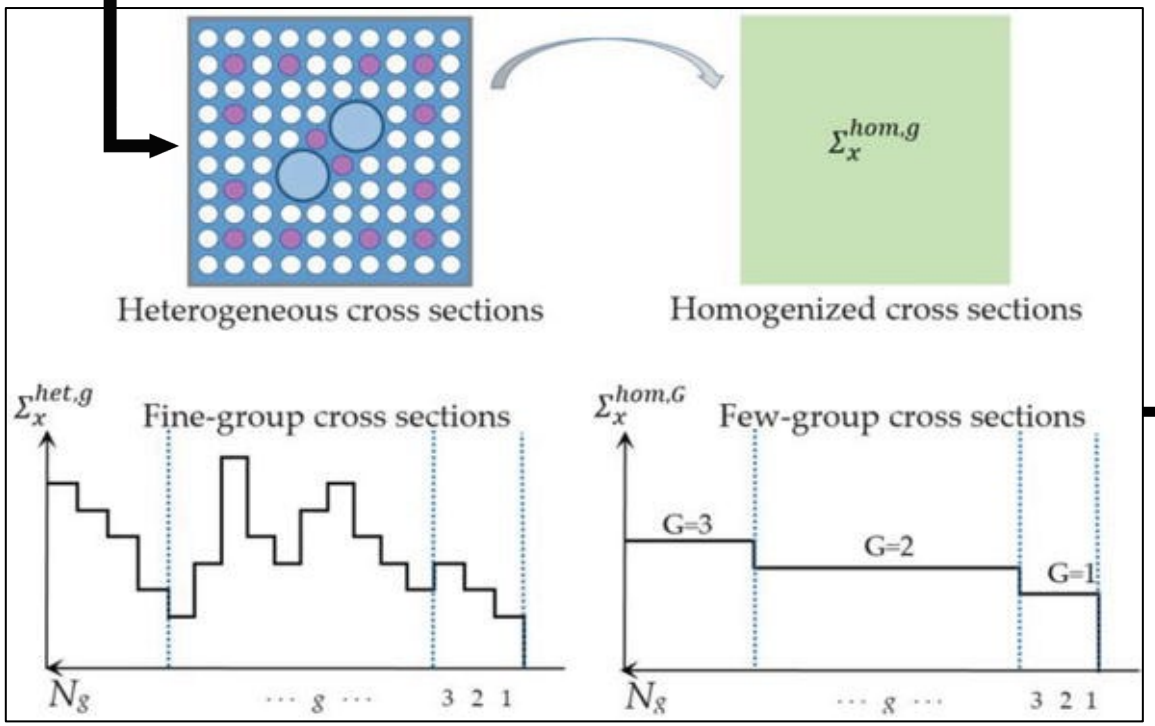
- Fine-group pin-resolved simulations
- Isotopic depletion
- Pin power data

Nodal Simulator

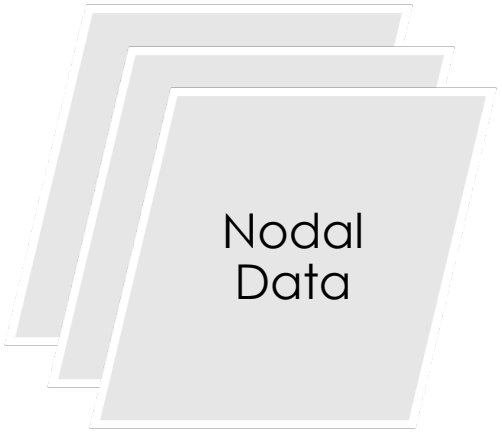
- Full core simulation
- Pin power reconstruction
- Thermal feedback
- Steady-state and transient simulation

ENDF data

Point data
10,000s of energy groups

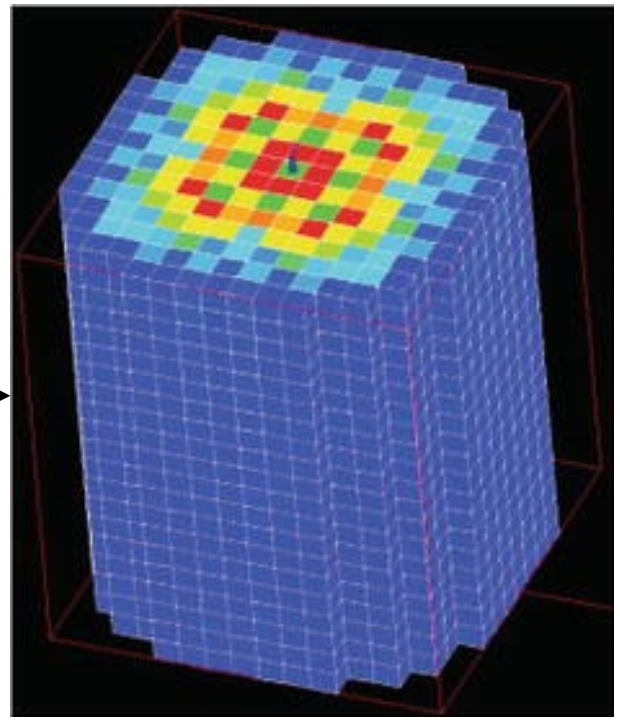


DOI: 10.5772/intechopen.79723



Functionalized over:

- Depletion states
- Temperatures
- Densities
- Control states
- Additional variables based on reactor being modeled



DOI: 10.5772/intechopen.79723

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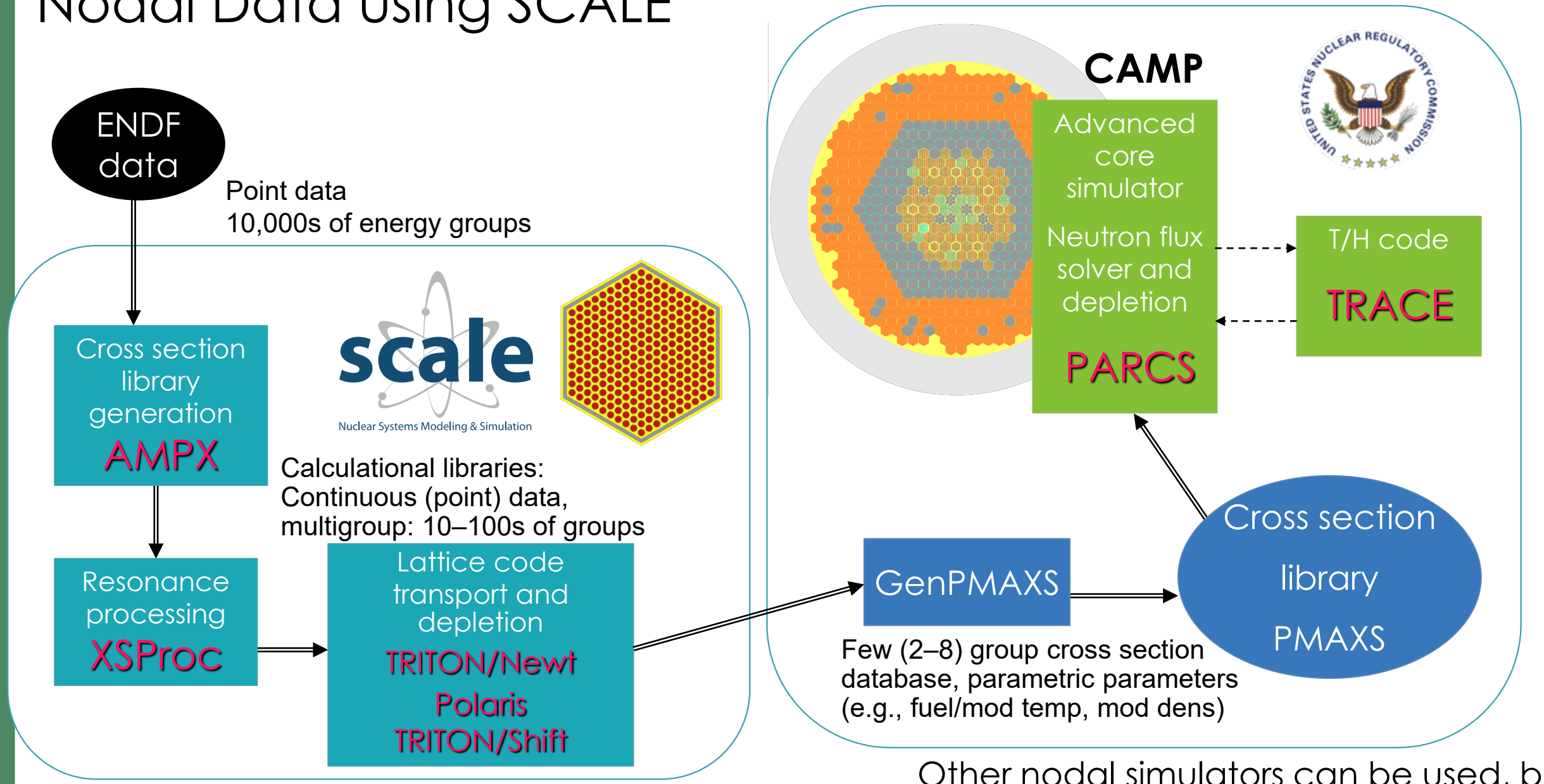
Nodal Data using SCALE



Other nodal simulators can be used, but formatting the nodal data is up to the user

Monte Carlo in Reactor Physics

- Compared to criticality safety and radiation shielding, Monte Carlo methods in reactor physics have special challenges
- Need lots of tallies
  - Reaction rates for many isotopes, many regions
  - Scalar flux and power everywhere
  - Uncertainty in transport solutions propagates into isotopes
  - Additional tally types and tally methods are still being developed (such as nodal data)
- Time-dependent calculation with branches (many state points) so potentially very expensive
- Users need to ensure calculation convergence
  - Sufficient number of active, inactive generations, total number of particles
  - Vary random seed to initialize random number generator
  - Analyze all outputs of interest for convergence

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Nodal Tally Methodology

Path-length-based Nodal Tallies

- Shift path-length tallies are used to compute the following reaction rates in the user-energy grid and spatial regions
  - non-fission absorption, i.e. capture
  - fission, nu-fission
  - non-fission transfer_1n, _2n, _3n, _4n
  - kappa-fission
  - flux

$$RR_x^g = \int_D dV \int_{4\pi} d\Omega \int_{E^g}^{E^{g-1}} dE\, \psi(E,\vec{\Omega})\, \Sigma_x(E)$$

$$(\phi^g\, V) = \int_D dV \int_{4\pi} d\Omega \int_{E^g}^{E^{g-1}} dE\, \psi(E,\vec{\Omega})$$

- TRITON converts the reaction rates to cross sections: $\Sigma_x^g = \dfrac{RR_x^g}{\phi^g\, V}$
- TRITON computes total, transfer, and total-transfer:

$$\Sigma_t^g = \Sigma_c^g + \Sigma_f^g + \Sigma_{*1n,0}^g + \Sigma_{*2n,0}^g + \Sigma_{*3n,0}^g + \Sigma_{*4n,0}^g$$

$$\Sigma_{X,0}^g = \Sigma_{*1n,0}^g + 2\Sigma_{*2n,0}^g + 3\Sigma_{*3n,0}^g + 4\Sigma_{*4n,0}^g$$

$$\Sigma_t^g - \Sigma_{X,0}^g = \Sigma_c^g + \Sigma_f^g - \Sigma_{*2n,0}^g - 2\Sigma_{*3n,0}^g - 3\Sigma_{*4n,0}^g$$

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T16 file

- Path length tallies in red box

```
Record 1: nblk, lblk, record sizes.
  13  1000  5120    14     4     0     0     0     3   115     0     0     0
Record 2: dimensioning data.
        1         0         1         2         1         6         6         0
        0         6         1         0
Record 6 not currently used.
Record 7: Energy group boundaries.
Energy bounds
92.000000E+07 1.005180E+05 1.000000E-05
Remaining records are written in sets of 4 for each branch calculation
Depletion pass no.    0, branch no.    0
Cross sections
k-eff
1.28564453E+00
Betas
3.04900E-02  2.51151E-01  1.93986E-01  3.23142E-01  1.12965E-01  3.93232E-02
Lambdas
1.28799E-02  3.08094E-02  1.31119E-01  3.32884E-01  1.26662E+00  3.27481E+00
Yields: I,Xe,Pm
6.61114E-02  8.96877E-03  2.11437E-02
Identifier,Number Density,Atom Density
500000000  1.00000E+00  1.00000E+00
 Energy group    1
  total          total-transfer   xe macro         sm macro         capture
2.08166778E-01  3.60213337E-03  0.00000000E+00  0.00000000E+00  1.37940445E-03
 fission          n-2n            transport       nu*fission       kappa*fission
2.22272892E-03 -1.00000000E+00  1.60414025E-01  6.57716626E-03  7.18424547E-14
   nu             chi            diff coeff        flux          elastic scat
2.95905018E+00  9.87645209E-01  2.07795644E+00  5.88952415E-02 -1.00000000E+00
 micro xe abs    micro sm abs   detector xsec   detector flux   inverse vel
0.00000000E+00  0.00000000E+00 -1.00000000E+00 -1.00000000E+00  1.30709965E-09
 sigtr (insc)    sigtr (ousc)
1.60414025E-01  1.60414025E-01
ADFs
0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
LineCurrents
0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
Scattering cross sections
2.00852841E-01  3.71181429E-03
 Energy group    2
  total          total-transfer   xe macro         sm macro         capture
3.06866288E-01  6.74236938E-03  0.00000000E+00  0.00000000E+00  4.94147092E-03
 fission          n-2n            transport       nu*fission       kappa*fission
1.80089858E-03 -1.00000000E+00  2.70781666E-01  5.23435092E-03  6.12847989E-14
   nu             chi            diff coeff        flux          elastic scat
2.90652180E+00  1.23547921E-02  1.23100400E+00  3.34382169E-02 -1.00000000E+00
 micro xe abs    micro sm abs   detector xsec   detector flux   inverse vel
0.00000000E+00  0.00000000E+00 -1.00000000E+00 -1.00000000E+00  4.77623230E-09
 sigtr (insc)    sigtr (ousc)
2.70781666E-01  2.70781666E-01
ADFs
0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
LineCurrents
0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
Scattering cross sections
0.00000000E+00  3.00123900E-01
```


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Collision-based Transfer Tallies

- Shift collision tallies are used to compute the transfer rates from one energy group to another

$$RR_{X,\ell}^{g\to g'} = \int_D dV \int_{4\pi} d\Omega \int_{4\pi} d\Omega' \int_{E^g}^{E^{g-1}} dE \int_{E^{g'}}^{E^{g'-1}} dE' \; P_\ell(\vec{\Omega}\cdot\vec{\Omega}')\psi(E,\vec{\Omega},\vec{r}) \sum_i [\sigma_{i,X}(E\to E',\vec{\Omega}\to\vec{\Omega}',T(\vec{r}))N_i(\vec{r})]$$

- (Note collision tallies are slower to converge than path-length tallies)
- TRITON computes relative transfer P0 matrix from the Shift collision tallies

$$NRR_{X,0}^{g\to g'} = \frac{RR_{X,0}^{g\to g'}}{\sum_{g'} RR_{X,0}^{g\to g'}}$$

- TRITON then multiplies the path-length transfer tally by the relative matrix to get the final P0 transfer matrix

$$\Sigma_{X,0}^{g\to g'} = \Sigma_{X,0}^{g} NRR_{X,0}^{g\to g'}$$

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T16 file

- Path length tallies in red box
- Transfer matrix tallies in the blue box

```
Record 1: nblk, lblk, record sizes.
  13  1000  5120    14     4     0     0     0     3   115     0     0     0
Record 2: dimensioning data.
        1         0         1         2         1         6         6         0
        0         6         1         0
Record 6 not currently used.
Record 7: Energy group boundaries.
Energy bounds
92.000000E+07 1.005180E+05 1.000000E-05
Remaining records are written in sets of 4 for each branch calculation
Depletion pass no.    0, branch no.    0
Cross sections
k-eff
1.28564453E+00
Betas
3.04900E-02  2.51151E-01  1.93986E-01  3.23142E-01  1.12965E-01  3.93232E-02
Lambdas
1.28799E-02  3.08094E-02  1.31119E-01  3.32884E-01  1.26662E+00  3.27481E+00
Yields: I,Xe,Pm
6.61114E-02  8.96877E-03  2.11437E-02
Identifier,Number Density,Atom Density
500000000  1.00000E+00  1.00000E+00
 Energy group    1
  total          total-transfer   xe macro         sm macro         capture
2.08166778E-01  3.60213337E-03  0.00000000E+00  0.00000000E+00  1.37940445E-03
 fission          n-2n            transport       nu*fission      kappa*fission
2.22272892E-03 -1.00000000E+00  1.60414025E-01  6.57716626E-03  7.18424547E-14
   nu             chi            diff coeff        flux          elastic scat
2.95905018E+00  9.87645209E-01  2.07795644E+00  5.88952415E-02 -1.00000000E+00
 micro xe abs    micro sm abs   detector xsec   detector flux   inverse vel
0.00000000E+00  0.00000000E+00 -1.00000000E+00 -1.00000000E+00  1.30709965E-09
 sigtr (insc)    sigtr (ousc)
1.60414025E-01  1.60414025E-01
ADFs
0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
LineCurrents
0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
Scattering cross sections
2.00852841E-01  3.71181429E-03
 Energy group    2
  total          total-transfer   xe macro         sm macro         capture
3.06866288E-01  6.74236938E-03  0.00000000E+00  0.00000000E+00  4.94147092E-03
 fission          n-2n            transport       nu*fission      kappa*fission
1.80089858E-03 -1.00000000E+00  2.70781666E-01  5.23435092E-03  6.12847989E-14
   nu             chi            diff coeff        flux          elastic scat
2.90652180E+00  1.23547921E-02  1.23100400E+00  3.34382169E-02 -1.00000000E+00
 micro xe abs    micro sm abs   detector xsec   detector flux   inverse vel
0.00000000E+00  0.00000000E+00 -1.00000000E+00 -1.00000000E+00  4.77623230E-09
 sigtr (insc)    sigtr (ousc)
2.70781666E-01  2.70781666E-01
ADFs
0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
LineCurrents
0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
Scattering cross sections
0.00000000E+00  3.00123900E-01
```


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Outscatter Transport XS and Diffusion Coefficient

- The outscatter transport XS is defined as $\Sigma_{tr}^{g} = \Sigma_{t}^{g} - \bar{\mu}^{g}\Sigma_{X,0}^{g}$
- "total minus mu-bar times transfer"
- Total and transfer are Shift path-length tallies
- Mu-bar, the mean transfer angle, can be derived from Shift collision tallies: $\bar{\mu}^{g} = \frac{\sum_{g'} RR_{X,1}^{g\rightarrow g'}}{\sum_{g'} RR_{X,0}^{g\rightarrow g'}}.$
- Diffusion Coefficient: $D^{g} = \frac{1}{3\Sigma_{tr}^{g}}$

- Verification tests show that this approach is poor for coarse group structures
- Solution: Compute D^{g} over fine group structure and collapse $D^{g} = \frac{\sum_{g_{fine}\in g} D^{g_{fine}}\phi^{g_{fine}}}{\sum_{g_{fine}\in g} \phi^{g_{fine}}}$
- TRITON-Shift currently uses 1000 internally defined fine groups (equal-lethargy widths)

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T16 file

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- Transfer matrix tallies in the blue box
- Diffusion tallies in green box

```
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Record 2: dimensioning data.
        1         0         1         2         1         6         6         0
        0         6         1         0
Record 6 not currently used.
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Energy bounds
92.000000E+07 1.005180E+05 1.000000E-05
Remaining records are written in sets of 4 for each branch calculation
Depletion pass no.    0, branch no.    0
Cross sections
k-eff
1.28564453E+00
Betas
3.04900E-02  2.51151E-01  1.93986E-01  3.23142E-01  1.12965E-01  3.93232E-02
Lambdas
1.28799E-02  3.08094E-02  1.31119E-01  3.32884E-01  1.26662E+00  3.27481E+00
Yields: I,Xe,Pm
6.61114E-02  8.96877E-03  2.11437E-02
Identifier,Number Density,Atom Density
500000000  1.00000E+00  1.00000E+00
 Energy group     1
  total          total-transfer   xe macro         sm macro         capture
2.08166778E-01  3.60213337E-03  0.00000000E+00  0.00000000E+00  1.37940445E-03
 fission          n-2n            transport       nu*fission      kappa*fission
2.22272892E-03 -1.00000000E+00  1.60414025E-01  6.57716626E-03  7.18424547E-14
   nu              chi            diff coeff        flux         elastic scat
2.95905018E+00  9.87645209E-01  2.07795644E+00  5.88952415E-02 -1.00000000E+00
 micro xe abs    micro sm abs    detector xsec   detector flux   inverse vel
0.00000000E+00  0.00000000E+00 -1.00000000E+00 -1.00000000E+00  1.30709965E-09
 sigtr (insc)    sigtr (ousc)
1.60414025E-01  1.60414025E-01
ADFs
0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
LineCurrents
0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
Scattering cross sections
2.00852841E-01  3.71181429E-03
 Energy group     2
  total          total-transfer   xe macro         sm macro         capture
3.06866288E-01  6.74236938E-03  0.00000000E+00  0.00000000E+00  4.94147092E-03
 fission          n-2n            transport       nu*fission      kappa*fission
1.80089858E-03 -1.00000000E+00  2.70781666E-01  5.23435092E-03  6.12847989E-14
   nu              chi            diff coeff        flux         elastic scat
2.90652180E+00  1.23547921E-02  1.23100400E+00  3.34382169E-02 -1.00000000E+00
 micro xe abs    micro sm abs    detector xsec   detector flux   inverse vel
0.00000000E+00  0.00000000E+00 -1.00000000E+00 -1.00000000E+00  4.77623230E-09
 sigtr (insc)    sigtr (ousc)
2.70781666E-01  2.70781666E-01
ADFs
0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
LineCurrents
0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
Scattering cross sections
0.00000000E+00  3.00123900E-01
```


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T16 file

- Path length tallies in red box
- Transfer matrix tallies in the blue box
- Diffusion tallies in green box
- Chi in orange box
- The energy distribution is tallied for all the fission neutrons born in the tally region

```
Record 1: nblk, lblk, record sizes.
  13  1000  5120    14     4     0     0     0     3   115     0     0     0
Record 2: dimensioning data.
        1         0         1         2         1         6         6         0
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k-eff
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Lambdas
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Yields: I,Xe,Pm
6.61114E-02  8.96877E-03  2.11437E-02
Identifier,Number Density,Atom Density
500000000  1.00000E+00  1.00000E+00
 Energy group     1
  total          total-transfer   xe macro         sm macro         capture
2.08166778E-01  3.60213337E-03  0.00000000E+00  0.00000000E+00  1.37940445E-03
 fission          n-2n            transport       nu*fission      kappa*fission
2.22272892E-03 -1.00000000E+00  1.60414025E-01  6.57716626E-03  7.18424547E-14
   nu              chi            diff coeff        flux         elastic scat
2.95905018E+00  9.87645209E-01  2.07795644E+00  5.88952415E-02 -1.00000000E+00
 micro xe abs    micro sm abs    detector xsec   detector flux   inverse vel
0.00000000E+00  0.00000000E+00 -1.00000000E+00 -1.00000000E+00  1.30709965E-09
 sigtr (insc)    sigtr (ousc)
1.60414025E-01  1.60414025E-01
ADFs
0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
LineCurrents
0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
Scattering cross sections
2.00852841E-01  3.71181429E-03
 Energy group     2
  total          total-transfer   xe macro         sm macro         capture
3.06866288E-01  6.74236938E-03  0.00000000E+00  0.00000000E+00  4.94147092E-03
 fission          n-2n            transport       nu*fission      kappa*fission
1.80089858E-03 -1.00000000E+00  2.70781666E-01  5.23435092E-03  6.12847989E-14
   nu              chi            diff coeff        flux         elastic scat
2.90652180E+00  1.23547921E-02  1.23100400E+00  3.34382169E-02 -1.00000000E+00
 micro xe abs    micro sm abs    detector xsec   detector flux   inverse vel
0.00000000E+00  0.00000000E+00 -1.00000000E+00 -1.00000000E+00  4.77623230E-09
 sigtr (insc)    sigtr (ousc)
2.70781666E-01  2.70781666E-01
ADFs
0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
LineCurrents
0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
Scattering cross sections
0.00000000E+00  3.00123900E-01
```


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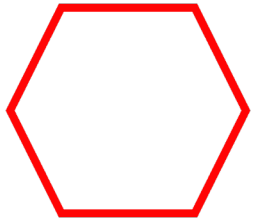
Input Format

Nodal data generation with TRITON-Shift

- **Prerequisites**
  - Sequence name: =t6-depl-shift
  - Global unit boundary is **cuboid** or **rhexprism** (rotated hexprism)

```
global unit 100
   com="LWR assembly"
   cuboid 1 5 -5 4 -4 1 -1
   cuboid 2 6 -6 5 -5 1 -1
   media 4 1 2 -1
   array 1 1 place 1 9 1 0.0 0.0 0.0
   boundary 2
```

```
global unit 100
   com="SFR assembly"
   rhexprism 110 7.50955 10 0
   rhexprism 120 7.90615 10 0
   rhexprism 130 8.12355 10 0
   array 1   110 place 13 13 1 0.0 0.0 0.0
   media 4 1 120 -110 vol=211.7905523
   media 3 1 130 -120 vol=120.71898
boundary 130
```



Nodal data calculation in TRITON-Shift enabled through new FGXS block

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The FGXS Block defines nodal data tallies

```
read fgxs
   shape <type> id=10 <options>
   energy       id=10 1E-5 0.625 20E6 end
   tallyset t16 id=10
   ...
end fgxs
```

- FGXS block can be anywhere in the MODEL block
- Only one FGXS block is allowed
- Nodal tallies are organized through an integer id
- Multiple tallies are allowed (e.g., id=10, id=20, …)

- 4 basic cards to define a nodal tally
  - **shape**: tally region shape
  - **energy**: tally energy grid
  - **tallyset**: tally type (only t16 supported)
  - **mesh**: tally over a mesh (optional)

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FGXS Block (shape)

```
read fgxs
  energy          id=1 1e-5 0.625 20E6 end
  tallyset t16    id=1
  shape cuboid    id=1 5 -5 5 -5 2.5 0
end fgxs

read fgxs
  energy          id=2 1e-5 0.625 20E6 end
  tallyset t16    id=2
  shape rhexprism id=2 1.25 2.0 -2.0 origin x=0 y=0 z=0
end fgxs
```

- Calculation of nodal data for a single region
- syntax:
  `shape <type> id=<ID> <options>`
- **<ID>** must be a positive integer
- **<type>** must one of the following:
  - **cuboid**
  - **rhexprism** (rotated hexagonal prism)
  - **global** (used if mesh will be specified)

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FGXS Block (mesh)

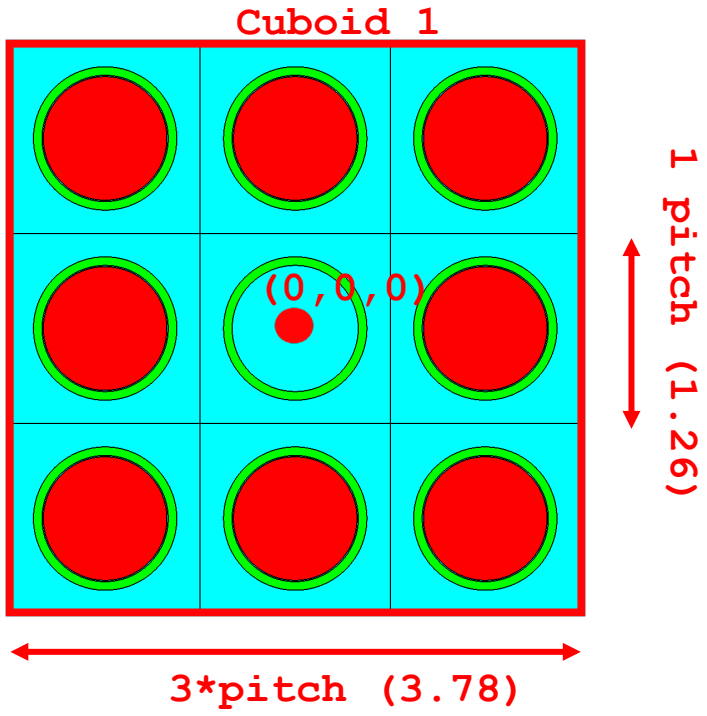
```
read fgxs
  shape global id=10
  energy       id=10 1E-5 0.625 20E6 end
  tallyset t16 id=10
  mesh square  id=10 hpitch=0.63 origin x=0 y=0 dz 0.5 0.5 end
end fgxs
```

- Calculation of nodal data in mesh
- syntax:
  mesh square|hexagonal id=<ID> hpitch=<P> origin x=<X> y=<Y> dz <Z1> ... <ZN> end
- square for square-pitched lattice, hexagonal for triangular-pitched lattice (note that this is a mesh of rotated hexagonal prisms)
- <ID>: must be a positive integer
- <P>: lattice half pitch (cm) used to define the mesh elements in X and Y
- <X> <Y>: coordinates in the global unit coordinate system in which to place the center of a lattice element. Lattice elements are repeated in the negative-x, negative-y, positive-x, and positive-y directions to fill the global unit.
- $<Z_i>$: **relative** axial mesh widths. (Bottom to top) The values must sum to 1. N entries will create N+1 mesh boundaries. The axial mesh boundaries is determined by the relative mesh widths and the bottom and top axial boundaries of the global unit.

FGXS Block (mesh) – Example

```
...
global unit 3
  cuboid 1 4p1.89 2p5
  array 1 1 place 2 2 1 3r0
  boundary 1
...
read fgxs
  shape global id=10
  energy       id=10 1E-5 0.625 20E6 end
  tallyset t16 id=10
  mesh square  id=10 hpitch=0.63 origin x=0 y=0 dz 0.3 0.7 end
end fgxs
```

XY view



- Cuboid 1 defines the global coordinate system with origin (0,0,0)

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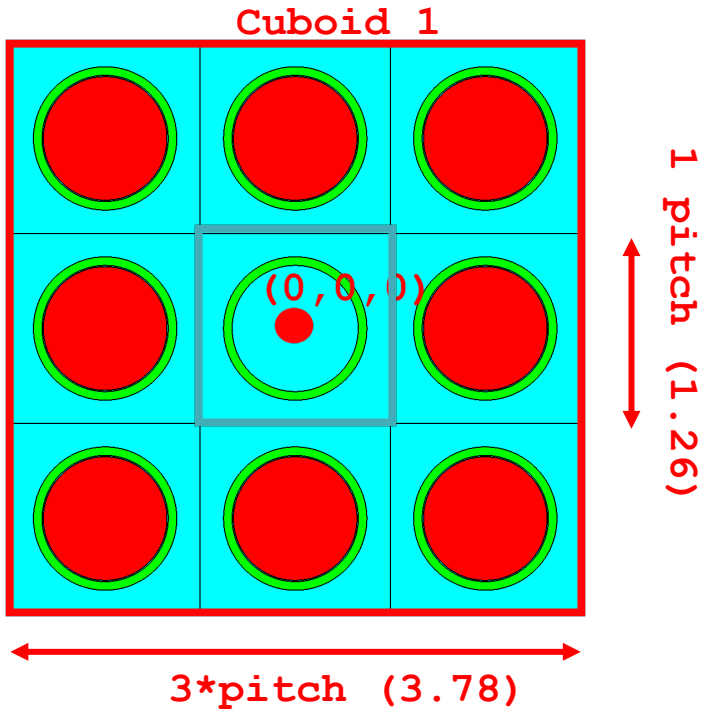
FGXS Block (mesh) – Example

```
...
global unit 3
  cuboid 1 4p1.89 2p5
  array 1 1 place 2 2 1 3r0
  boundary 1
...
read fgxs
  shape global id=10
  energy       id=10 1E-5 0.625 20E6 end
  tallyset t16 id=10
  mesh square  id=10 hpitch=0.63 origin x=0 y=0 dz 0.3 0.7 end
end fgxs
```

XY view



- Cuboid 1 defines the global coordinate system with origin (0,0,0)
- A mesh element is centered at x=0 y=0 with hpitch=0.63

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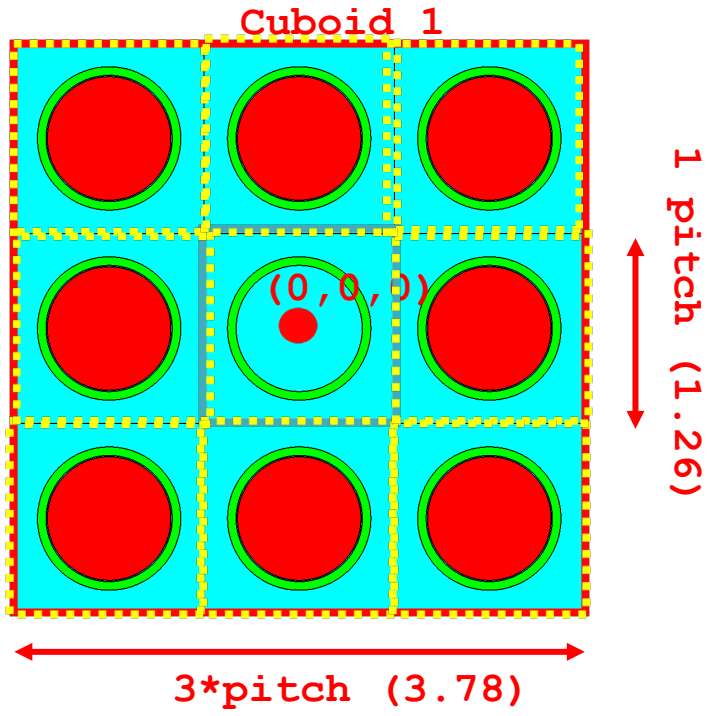
FGXS Block (mesh) – Example

```
...
global unit 3
  cuboid 1 4p1.89 2p5
  array 1 1 place 2 2 1 3r0
  boundary 1
...
read fgxs
  shape global id=10
  energy       id=10 1E-5 0.625 20E6 end
  tallyset t16 id=10
  mesh square  id=10 hpitch=0.63 origin x=0 y=0 dz 0.3 0.7 end
end fgxs
```

XY view



- Cuboid 1 defines the global coordinate system with origin (0,0,0)
- A mesh element is centered at x=0 y=0 with hpitch=0.63
- Additional mesh elements are added until reaching the global boundary

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Nodal Tally Data Output

- A summary of the nodal tally user input is provided in regular out-file
- Nodal data is provided in t16 files:
  - Global nodal tally: ${BASENAME}.id10.t16
  - Mesh-based nodal tally: ${BASENAME}.id10-<I>-<J>-<K>.t16
    - I – goes from 1 to # of tallies in the x-direction
    - J – goes from 1 to # of tallies in the y-direction
    - K – goes from 1 to # of tallies in the z-direction
    - Number of mesh cells in each direction is computed from global boundary shape dimensions and **mesh** card input
    - Detailed description of I/J/K locations for hexagonal meshes printed in the output
- TRITON-Shift t16 files are in the same directory as the output file
- No =shell command is required in SCALE 6.3 to copy t16 files back

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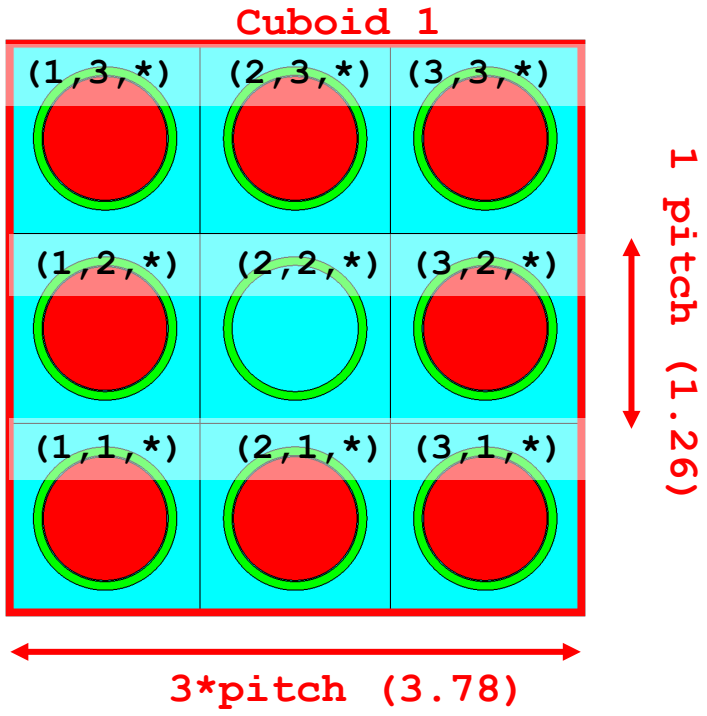
FGXS Block (mesh) – Example

```
...
global unit 3
  cuboid 1 4p1.89 2p5
  array 1 1 place 2 2 1 3r0
  boundary 1
...
read fgxs
  shape global id=10
  energy       id=10 1E-5 0.625 20E6 end
  tallyset t16 id=10
  mesh square  id=10 hpitch=0.63 origin x=0 y=0 dz 0.3 0.7 end
end fgxs
```

XY view



- t16 file name id10-<I>-<J>-<K>
- I and J indices shown on XY view
- K index will be 1 for bottom 30% and 2 for top 70% of the global unit

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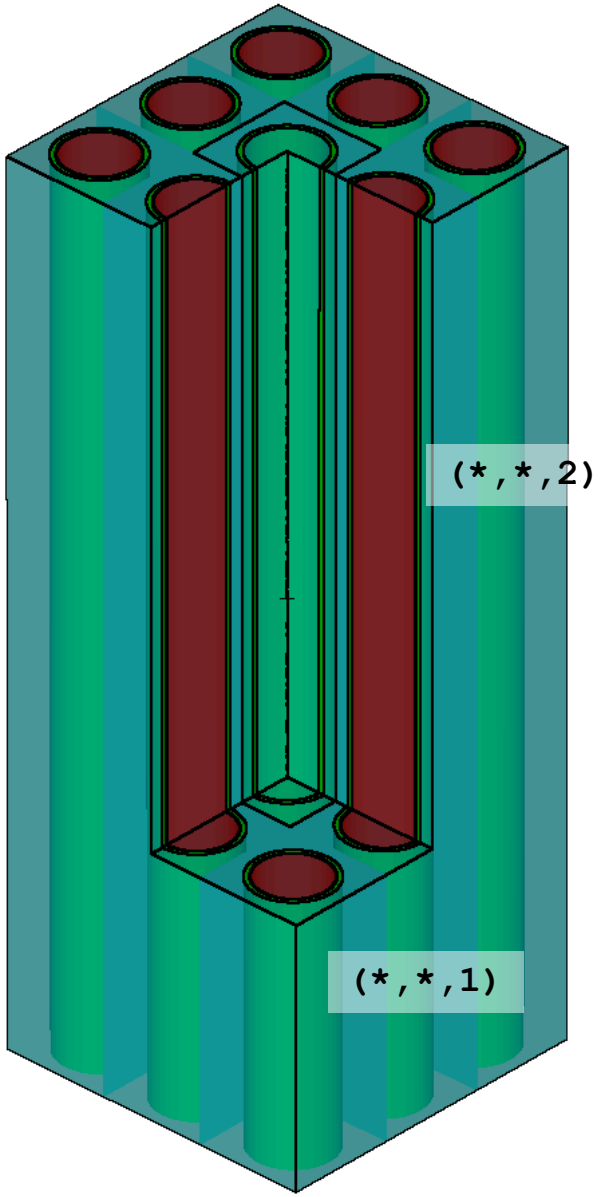
FGXS Block (mesh) – Example

```
...
global unit 3
  cuboid 1 4p1.89 2p5
  array 1 1 place 2 2 1 3r0
  boundary 1
...
read fgxs
  shape global id=10
  energy       id=10 1E-5 0.625 20E6 end
  tallyset t16 id=10
  mesh square  id=10 hpitch=0.63 origin x=0 y=0 dz 0.3 0.7 end
end fgxs
```

3D view



- t16 file name id10-<I>-<J>-<K>
- I and J indices shown on XY view
- K index will be 1 for bottom 30% and 2 for top 70% of the global unit

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Nodal Tally summary in the output file

```
read fgxs
  shape global id=10
  energy       id=10 1E-5 0.625 20E6 end
  tallyset t16 id=10
end fgxs
```

```
==========================================================================
Nodal FGXS Tally Summary
==========================================================================


 Tally ID=10
   tally type: DOMAIN
   tally boundary: CUBOID
   energy grid: 2e+07,0.625,1e-05
   volume mesh planes x: 0,10.75
   volume mesh planes y: -10.75,0
   volume mesh planes z: -5,5
   volume tallies: absorption,fission,flux,kappa_sigma,nu_fission,transfer_1n,transfer_2n,transfer_3n,transfer_4n
   volume tallies on isotopes (nuclide id/reaction mt): 1001/18,1001/101,1001/452,5010/18,5010/101,5010/452,8016/18,8016,
   surface mesh planes x: 1e-06,10.75
   surface mesh planes y: -10.75,-1e-06
   surface mesh planes z: -5,5
   surface tallies: flux
   fine energy grid: 2e+07,1.94415e+07,1.88985e+07,1.83708e+07,1.78577e+07,1.7359e+07,1.68742e+07,1.6403e+07,1.59449e+07,
   fine energy grid volume tallies: flux,absorption,fission,transfer_1n,transfer_2n,transfer_3n,transfer_4n
   volume tally name (shift): domain_nodal_tally_t16_10
   surface tally name (shift): domain_nodal_tally_t16_10_surface
   num tally energy groups: 2
   num tally mesh volumes: 1
   num tally fine energy groups: 1000
   num tally surfaces: 6
```


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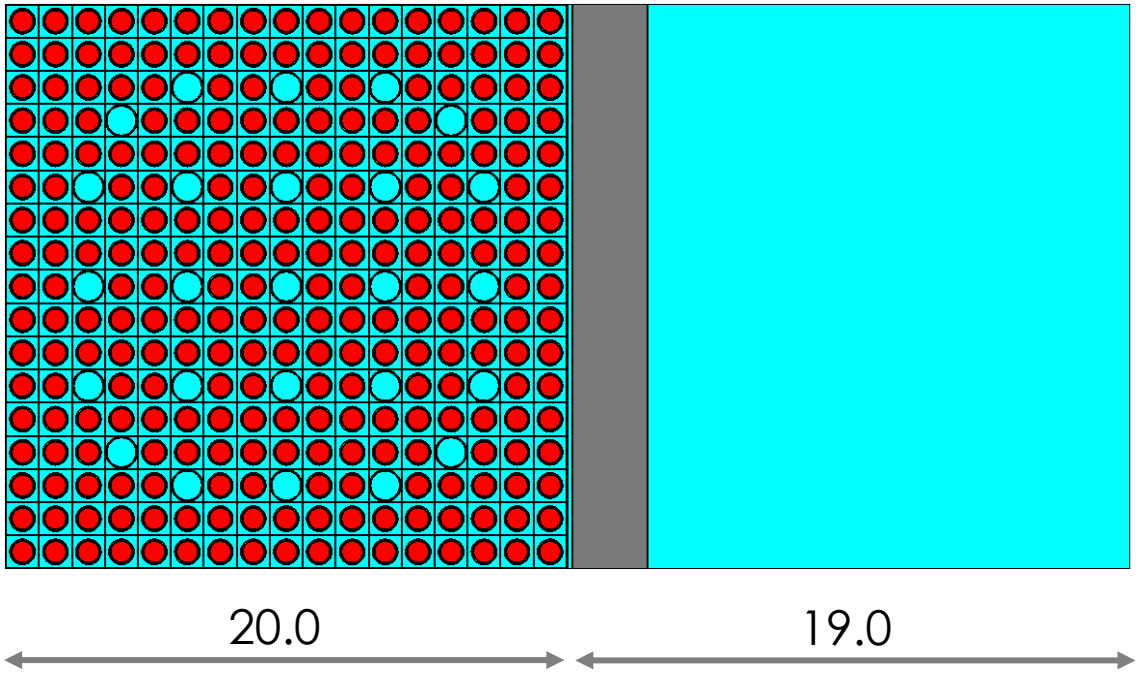
Global Energy and Tally Settings

- Multiple different regions can be tallies in the same FGXS block using special "id=0"
  - Available for energy bins and tallysets
- Useful when nodal needs to be tallied over a nonuniform mesh
- Example: radial reflector

```
read fgxs
  energy       id=0 1e-5 0.625 20E6 end
  tallyset t16 id=0
  shape cuboid id=10 20.0  0.0  10.0 -10.0  1.0 0.0
  shape cuboid id=20 39.0 20.0  10.0 -10.0  1.0 0.0
end fgxs
```



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Comments and Recommendations

Comments and Recommendations

- Runtime can be long when requesting nodal data
  - Use Fulcrum validation when setting up input
  - Run short TRITON-Shift calculation without fgxs block to check input
  - Note that inactive generations can run fast, but active generations take longer
- Observe memory footprint, especially when requesting nodal data on a mesh for a complex geometry
- Statistical uncertainty of nodal data can be determined by running multiple calculations with different random seeds (**`rnd=<seed>`**)
- Volumes in all TRITON calculations:
  - If no volumes are specified and no volume block is found, a volume calculation with many rays is performed which can take a significant amount of time
  - Providing volumes via volume block or by specifying volumes for each media record (**`vol=<val>`**) saves runtime for each transport calculation
- Use "**`burn=0`**" in **`burndata`** block to request transport-only calculation (in that case, consider if you need addnux nuclides)
- Note that ADFs are provided as heterogeneous flux divided by homogeneous flux (NEWT ADF option 3)

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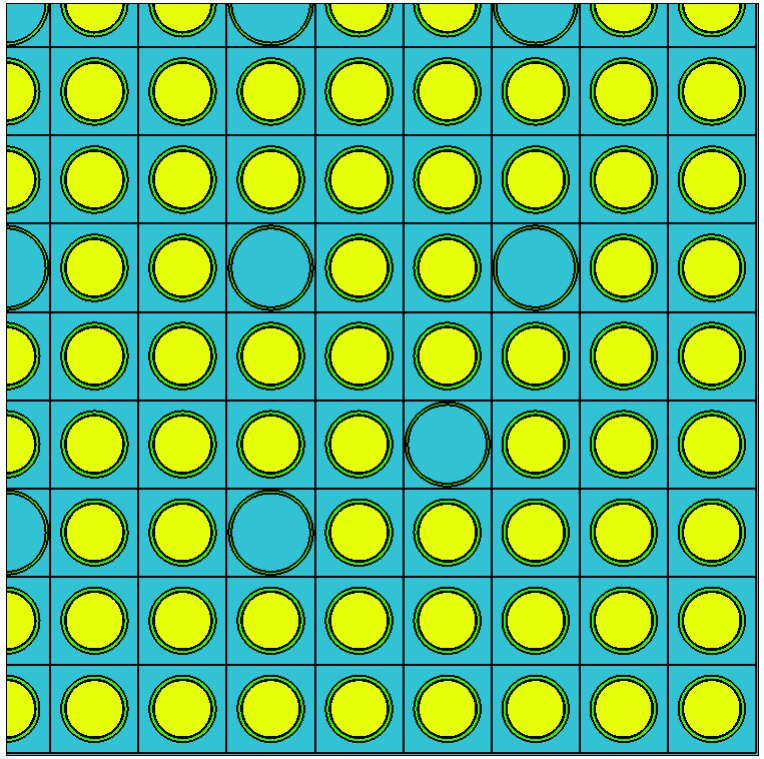
Hands-on Exercises

1. Cuboid Shape
2. Square Mesh
3. Multiple shapes in one block

Exercise 1: Assembly-averaged nodal data

- Model: 17x17 PWR assembly
- Task: get assembly-averaged nodal data
- Starter file: **pwr_w17x17_starter.inp**
- Add FGXS block:
  - Tally ID
  - 2-group structure (1e-5 eV, 0.625 eV, 20 MeV)
  - Geometry: single cuboid shape
  - Tallyset t16
- Examine output:
  - Nodal data print in the out-file
  - How many t16 files were generated?



1/4th PWR assembly

Pin half pitch: 0.63 cm
Assembly half pitch: 10.75 cm

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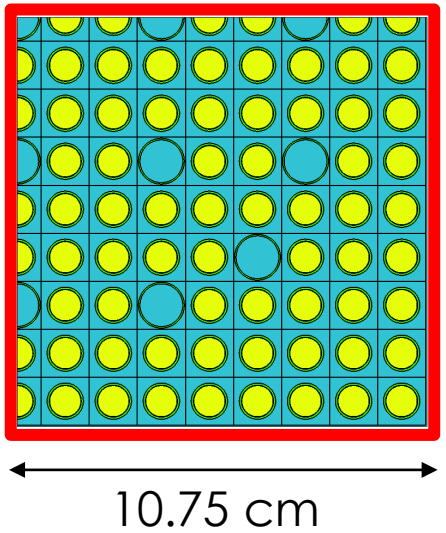
Exercise 1: Results

```
read fgxs
  shape cuboid id=10 10.75 0.0 0.0 -10.75 1 0
  energy       id=10 1E-5 0.625 20E6 end
  tallyset t16 id=10
end fgxs
```



- FGXS block with individual shape **cuboid**
- Nodal data information in out-file starting with "*Nodal FGXS Tally Summary*"
- Generation of one t16 file *pwr_w17x17.id10.t16*
  - 4 burnup steps
  - 2 energy groups
- Examine xs, for example decreasing fission xs with depletion

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Exercise 2: Pin-wise nodal data

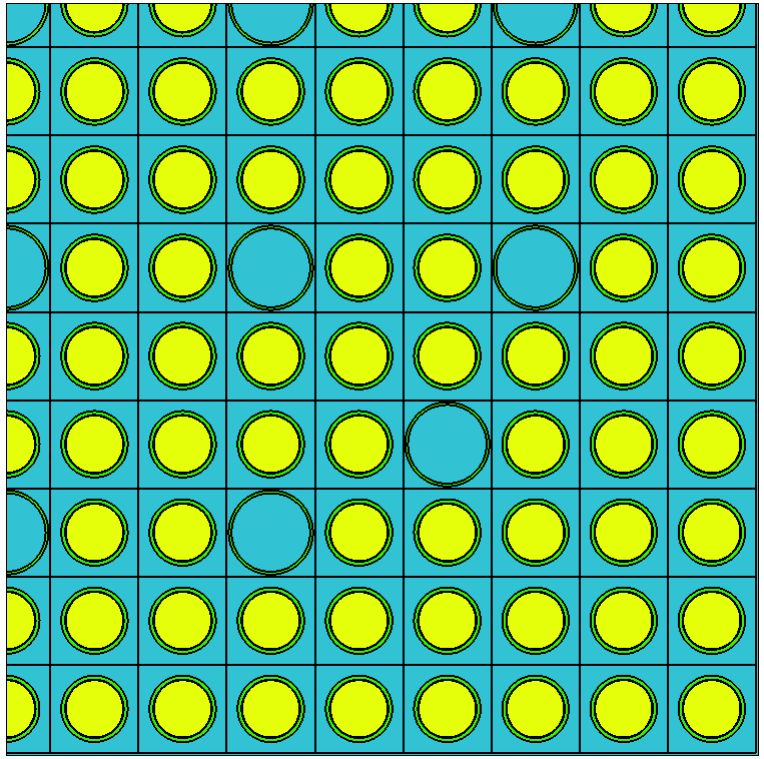
- Model: 17x17 PWR assembly
- Task: get nodal data for each pin in the assembly only for the fresh fuel state (no depletion)

Hint: burn=0

- Starter file: **pwr_w17x17_starter.inp**
- Add FGXS block:
  - Tally ID
  - 2-group structure (1e-5 eV, 0.625 eV, 20 MeV)
  - Geometry: square mesh (hpitch, origin), 1 axial zone
  - Tallyset t16

Is the mesh origin at (0,0,0)?

- Examine output:
  - Nodal data print in the out-file
  - How many t16 files were generated?
  - Use fission cross section to find non-fuel pins



1/4th PWR assembly

Pin half pitch: 0.63 cm
Assembly half pitch: 10.75 cm

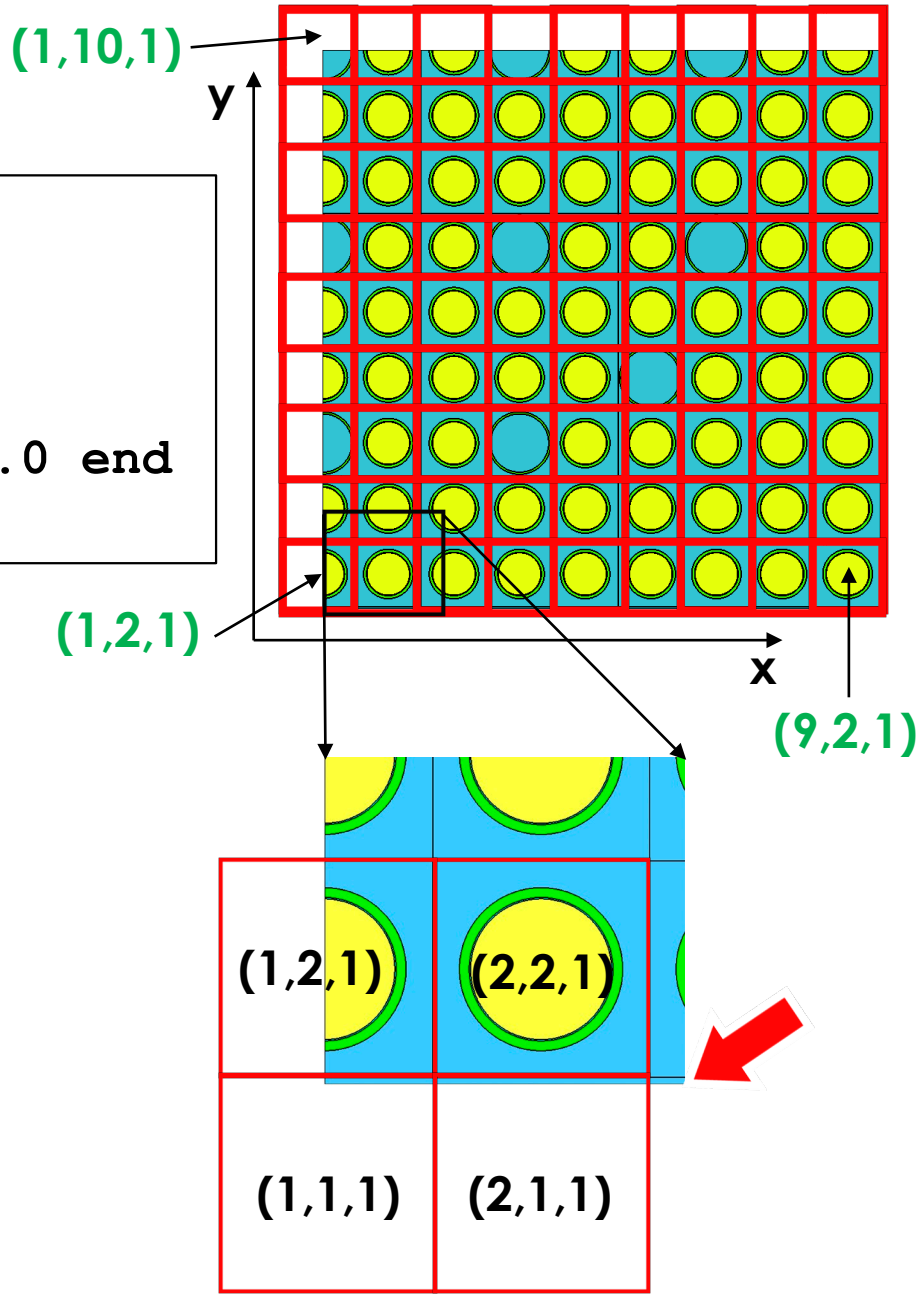
Exercise 2: Results

```
read fgxs
shape global id=10
energy id=10 1E-5 0.625 20E6 end
tallyset t16 id=10
mesh square id=10 hpitch=0.63 origin x=0 y=0 dz 1.0 end
end fgxs
```

- FGXS block with square mesh; origin in any pin center
- *"Nodal FGXS Tally Summary" in out-file:*

```
volume mesh planes x:
0,0.63,1.89,3.15,4.41,5.67,6.93,8.19,9.45,10.71,10.75
volume mesh planes y: -10.75,-10.71,-9.45,-8.19,-6.93,-5.67,-
4.41,-3.15,-1.89,-0.63,0
volume mesh planes z: 0,1
```

- Generation of **100** t16 files *pwr_w17x17_mesh.id10-<x>-<y>-<z>.t16*
- *Confirm fission xs is zero in water channels: (1,4,1), (4,4,1), (6,5,1), (7,7,1)*



Extra mesh cells added because of outer gap!

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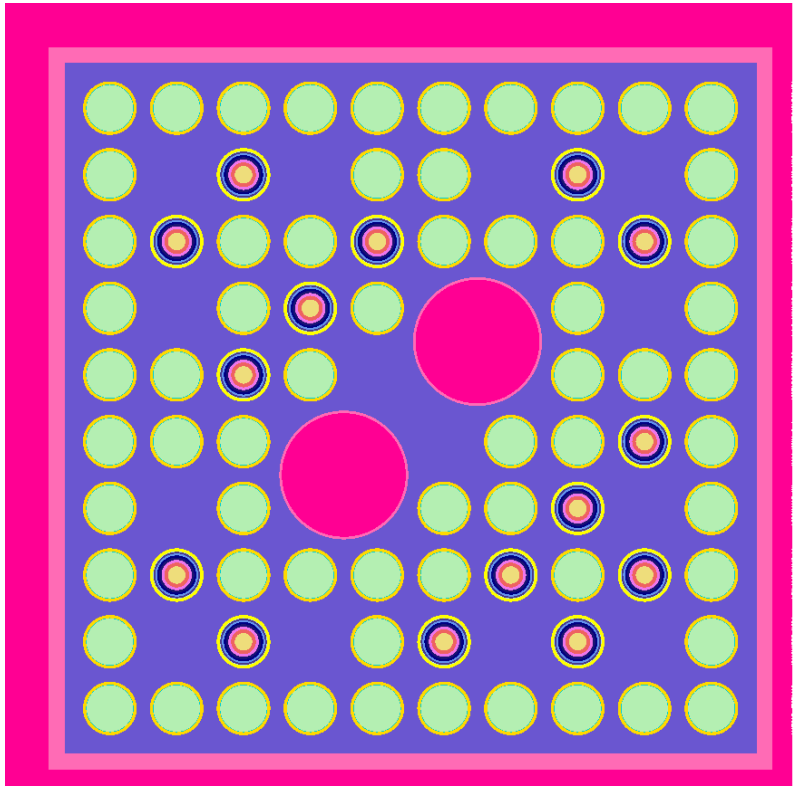
Exercise 3: Nodal data from non-uniform assembly

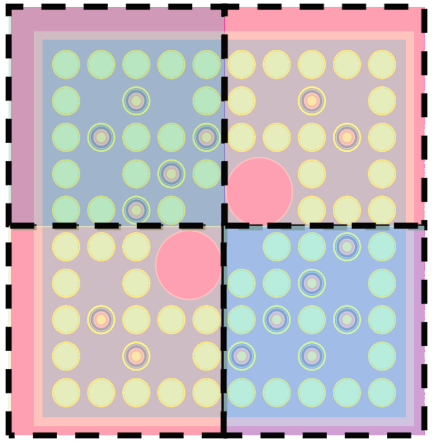
- Model: 10x10 BWR assembly
- Task: nodal data for each quarter of the assembly
- Starter file: **bwr_assembly.inp**
- Add FGXS block:
  - Tally IDs
  - 2-group structure (1e-5 eV, 0.625 eV, 20 MeV)
  - Tallyset t16
  - Geometry: 4 cuboid shapes
  - Use "id=0" where applicable
- Examine output:
  - Nodal data print in the out-file
  - How many t16 files were generated?
  - Compare SW and NE: What would you expect?
- Further questions:
  - What is the best way to determine nodal data for each individual pin/channel in the assembly?



BWR assembly

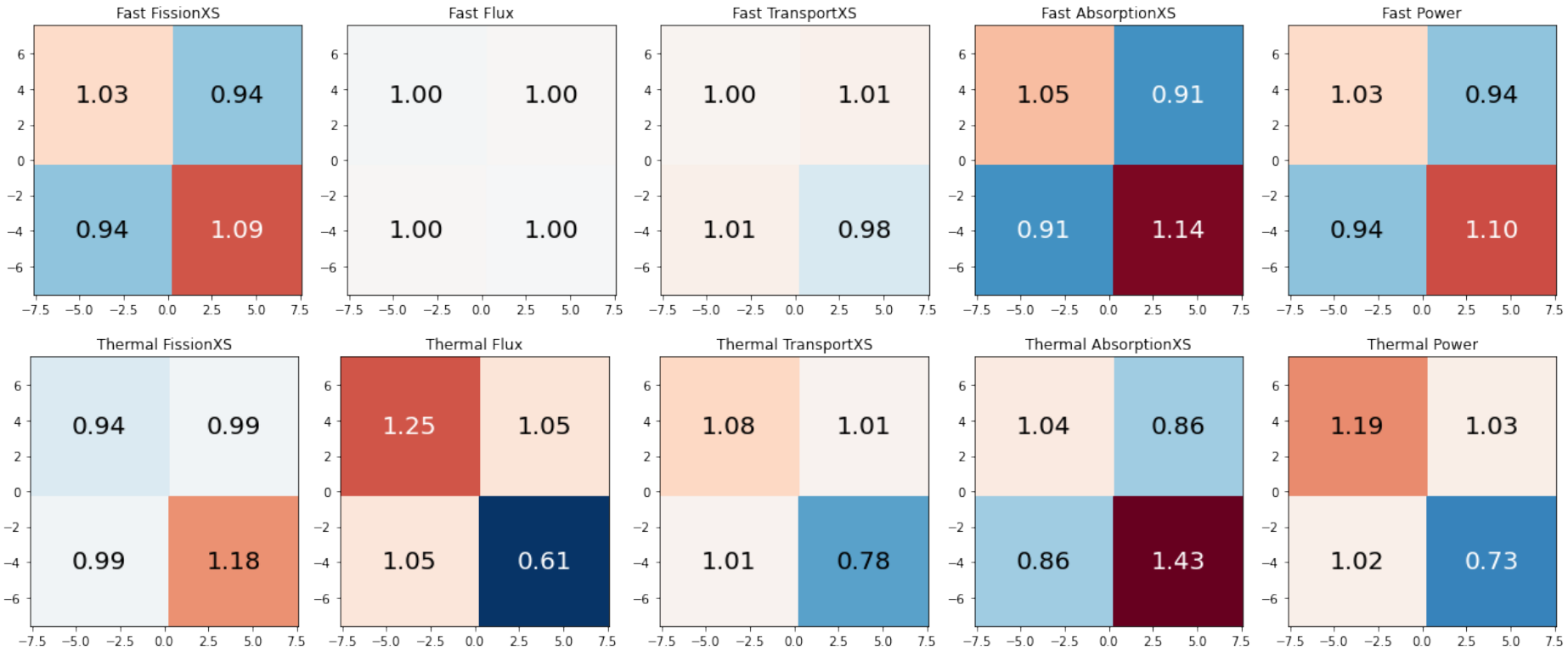
Pin half pitch: 0.6 cm
Assembly flat-to-flat: 14.0 cm
Box thickness: 0.3 cm

Exercise 3 Results



gen=150
npg=50000
nsk=50

- Fission, transport, absorption, kappa*fission, and flux data post-processed from the t16 files. Quadrant power calculated using flux*kappa*fission
- Data provided as a ratio from the global XS data
- NE and SW corner compare well indicated reasonable statistics achieved. Your fast-running simulation results may differ due to statistics! This is especially true for tallies that use the collision estimator as they converge more slowly.
- Some quadrants different significantly from the assembly average data
- NW and SE quadrant yield different results:
  - Fission XS surprisingly higher in the SE corner due to Gd-rod layout
  - Thermal flux much lower in the SE compared to NW due to the non-uniform channel gap, which drive the quadrant power
  - Absorption much higher in the SE corner due to number of Gd rods



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Summary and Outlook

Highlights of TRITON-Shift nodal data capability

- Nodal data generation with TRITON-Shift in continuous-energy mode for complex 3D geometries in SCALE 6.3
- "**T6-DEPL-SHIFT**" input consistent with T6-DEPL (TRITON/KENO) input, plus new nodal data "**fgxs**" block
- Nodal data generated for:
  - Individual cell: cuboid and rotated hexprism
  - Global mesh: Square or rotated hexagonal
  - Multiple cells/meshes in one input
- Tallies:
  - Arbitrary energy group structure
  - Calculation of typical nodal data: few-group cross sections, scattering matrix, kappa-fission, betas, lambdas, micro Xe/Sm absorption
  - ADFs for cartesian geometries

Questions:
scalehelp@ornl.gov

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Outlook to Nodal Data in SCALE 7.0

- Nodal data in HDF5 format (or t16 text files)
- Statistical uncertainty of nodal data
- ADFs for both cartesian and hexagonal geometries
- Mesh types: cartesian, hexagonal, cylindrical
- Nodal data generation with Shift in both continuous-energy and multigroup mode
- Runtime performance improvements
- Nodal data within "tallies" block
  - Flexible control of energy grid, geometry, time array
  - Tallies block already supports flux and fission rate meshes in SCALE 6.3
  - Addition of infinite meshes "NET" and single shapes to definitions block

TALLIES BLOCK

```
read tallies
read fgxs 1
response=macro_nodal
grid=2
time 0 1 2 LAST end
energy=5
end fgxs

read fgxs 2
response=macro_nodal
shape=1
time ALL end
energy=5
end fgxs
end tallies
```

DEFINITIONS BLOCK

```
read definitions
read energyBounds 5
bounds 2e7 0.625 1e-5 end
end energyBounds

read grid 2
type=SQUARE_NET
boundary=GLOBAL_UNIT
pitch=2.5
origin x=0 y=0.5
zplanes 100.0 50.0 0.0 -20.0 end
end grid

read shape 1
cuboid 5.0 -5.0 5.0 -5.0 1.0 0.0
end shape
end definitions
```