

Advanced reactor modeling with TRITON-NEWT

Best Practices for SCALE Modeling & Simulation

SCALE Users' Group Workshop July 27–29, 2020

F. Bostelmann, B. Ade, B. Betzler, M. Jessee

ORNL is managed by UT-Battelle, LLC for the US Department of Energy



Objectives

- Provide modeling recommendation for TRITON-NEWT
 - Cross section library
 - Geometry checks
 - Transport settings
 - Extra tips on hexagonal geometries



Cross Section Libraries

Which multigroup cross section library should I use?

- Depends on:
 - The spectral conditions of the model (thermal vs. fast)
 - The desired solution accuracy
 - The available simulation time
- For thermal systems and with limited applicability for other spectral conditions:
 - If time allows, use the 252-group ENDFB-VII.1 (v7-252) library
 - If a quick answer is needed, use the 56-group ENDFB-VII.1 (v7-56) library
- Additional multigroup libraries to be provided with SCALE 6.3:
 - Very fine group library with 1597 groups
 - **302-group** library optimized for sodiumcooled fast reactor systems



- Especially useful for modeling advanced reactor concepts with non-thermal spectra, such as:
 - Sodium-cooled fast reactors
 - Heat pipe reactor
 - Some molten salt reactors
- Tests with the 1597-group library can be used to increase confidence for current choice of multigroup library



Cross Section Processing

Which cross section processing options should I use?

- The most accurate solution is obtained using CENTRM and a fine-group cross section library
- Latticecell: sufficient for most unit cells
 - Assumes that the fuel pin lies in an infinite lattice of other fuel pins a good assumption in many cases
- Multiregion: to be used if unit cell needs to be divided in multiple rings or more complex scenarios
 - Example: Gadolinium-bearing fuel pins; Gadolinium is a strong absorber of neutrons so the flux shape across the fuel pin changes significantly
 - Example: Ag-In-Cd control rods
 - Example: Complex geometry not easily modeled using Latticecell
- **Doublehet**: to be used for double heterogeneous systems with fuel particles dispersed in a fuel component
 - Allowed fuel components are annular and solid rod, pebble and slab
- All options allow for different lattice specifications: square, triangular (hexagonal), slab cell
- If approximation of infinite lattice of fuel pins is insufficient, modify the **Dancoff factor** for that fuel pin
 - Example: Edge and corner fuel pins in high-void BWR lattices
- If a unit cell geometry is widely different from repeated fuel lattices, try to create a multiregion with
 representative radii and perform thorough comparisons to continuous-energy calculations (see last slide)

- Example: Many molten salt reactor systems have irregular repeating geometries



Cross Section Processing

What are common input errors?

- Check that all necessary lattice parameters are included: all radii, pitches and heights
- Check that boundary conditions are correct (e.g., **right_bdy=vacuum** most likely incorrect)
- Do not confuse pitches (pitch) and half pitches (hpitch) or radii (fuelr) and diameter (fueld)
- For doublehet cells:
 - Specify either volume fraction of fuel particles **OR** number of particles
 - Be aware that coatings can be specified via radius, diameter or thickness: coatr, coatd, coat
 - You need to define a doublehet mixture ID → don't confuse this ID with the fuel mixture ID from a possible CE model
- Triple check material IDs in cell specifications, especially after a copy/paste from an old input



NEWT Geometry Construction

Are there recommendations on how to set up my geometry?

- We recommend giving the unit containing the fuel unit cell the same ID as the fuel material in that cell
 - Helps eliminate confusion
 - Makes lattice array more visibly intuitive in the input file

• Use units

- You could specify everything you need in one global unit, but this can be very confusing
- For each logical building block in the physical model, build a unit
- Use arrays and holes to place all the different units into the global unit
- Example: BWR control blades if they are constructed as different units, you can simply comment them in or out of the global unit to insert or remove them



Geometry Check

How do I check that my geometry is correct?

- 1. Use Fulcrum to check for input validation errors
- 2. Use Fulcrum to view model
- 3. Run TRITON-NEWT with check parameter:
 - =t-newt parm=(check)

CAK RIDGE

- This checks for so far undetected input errors
- Can be used to plot the geometry in conjunction with drawit=yes in the NEWT parameter block
- 4. Also helpful: Use Fulcrum to calculate volumes via "Run"--> "Calculate volumes"





Fulcrum view:

Typical geometry error due to incorrect media placement, undetectable with the validation check

NEWT transport settings

What options should I use in my NEWT transport solution?

- Currently we use and recommend the basic defaults for NEWT, which are a compromise between accuracy and runtime
- At least S₆ should be used for NEWT calculations
- P_0 in the gap, P_1 in fuel, clad and structural materials, and P_2 in moderators
- Spatial mesh of at least 4x4 in fuel cells
- The global grid is sized such that each grid cell is approximately the size of one unit cell
- CMFD is performed on the global grid
- Epsilon = 1e-5



NEWT hexagonal geometries

- Hexagonal geometries are used in many advanced reactor concepts, such as HTGR, FHR, SFR (and also VVER)
- Unit cell level is straightforward:
 - 1. Define appropriate unit cell:

```
latticecell triangpitch hpitch=1.5 1
fuelr=1.0 2 gapr=1.2 3 cladr=1.4 4 end
```

```
latticecell atriangpitch hpitch=1.5 1
fuelr=1.0 2 gapr=1.2 3 cladr=1.4 4 igapr=0.1 5 icladr=0.2 6 end
```

doublehet: rod/pebble + triangpitch/atriangpitch

2. Define appropriate geometry with consistent materials:





CAK RIDG National Laborate

NEWT hexagonal geometries

- Fuel assembly can be trickier, especially if you have an outer wrapper
- Definition of hexagonal array often leads to geometry errors
 → Issues visible in NEWT geometry plot
- hole 5 origin x=0 y=0hole 3 origin x=0.89 y=0hole 1 origin x=0.44 y=0.77hole 1 origin x=1.34 y=0.77hole 4 origin x=0 y=1.55hole 1 origin x=0.89 y=1.55
- Recommendation: explicitly place fuel pin units as **holes** in assembly
- Simplify geometry if possible: reflected assembly can be changed to a rectangular geometry





- Only global grid
- cmfd=rect
- grid_tol=1.0e-5
- cell_tol=1.0e-8
- inrcvrg=yes
- Check NEWT plot of geometry
- Play with grid, npolar, nazim, etc. parameters to check if your solution is converged



Comparisons with Monte Carlo KENO-CE and KENO-MG

I'm doing lattice physics, why do I need Monte Carlo? -> To validate your assumptions!

- CE-KENO compared to MG-KENO:
 - Reveals the bias due to cross section processing and use choice of the multigroup cross section library
 - → Modify the cross section library, or cross section processing options (Dancoff factors, CENTRM options)
- MG-KENO compared to NEWT:
 - Reveals the bias due to geometry approximations
 - → Modify the number of grid cells, angular quadrature, number of sides on cylinders, etc.
- Note: It is relatively easy to generate a KENO model from an existing TRITON model
 - → For hexagonal assemblies, you can easily model a hexagonal array in KENO, i.e., without holes
- SCALE 6.3 will include Monte Carlo code Shift that allows the generation of nodal data in t16 files
 - \rightarrow This provides an additional great opportunity for verification with TRITON

A KENO calculation can offer tremendous help in troubleshooting NEWT models and in verifying your results
→ We strongly recommend to perform comparisons with KENO!





Questions?



