KENO-VI modeling of double heterogeneous reactor systems using TRISO fuel

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Outline

- Introduction
  - What are double heterogeneous systems?
  - What are the challenges for modeling these systems?
- Modeling double-het systems with SCALE/KENO-VI
- SCALE hands-on: Part 1 (together)
- SCALE hands-on: Part 2 (alone)
- Other SCALE capabilities for double-het systems
- Outlook to SCALE 6.3

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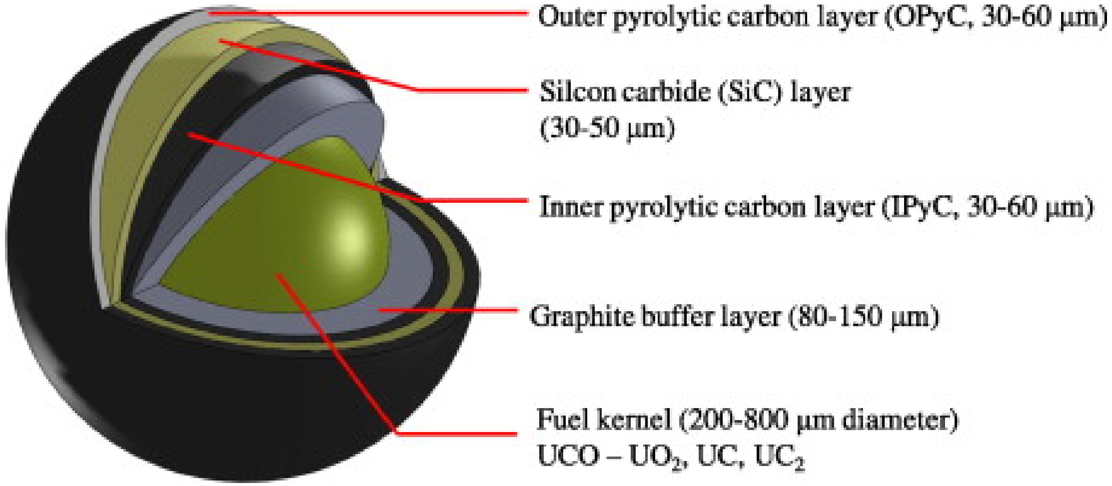
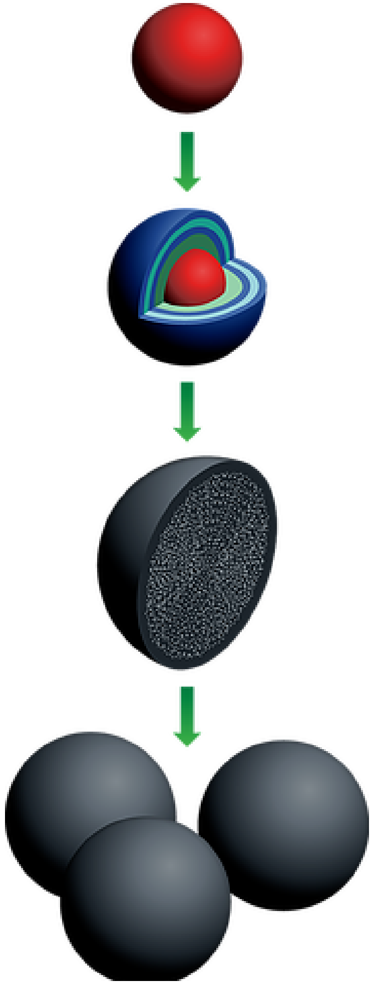
Double heterogeneous systems

(1) Fuel pebble

Tristructural (TRISO) fuel particle





Uranium Oxycarbide (UCO) Kernel
- 10% enrichment

TRISO Particle
- UCO kernel encased in carbon and ceramic layers
- 0.4 mm in diameter

Fuel Pebble
- TRISO particles embedded in graphite
- 25,000 TRISO particles per pebble

Pebble Bed
- 170,000 pebbles per Xe-100 reactor

Figures: Courtesy of M. P. Baker, et al., *J. Nucl. Materials* 432, pp.395-406, 2013; X-Energy website

Double heterogeneous systems

(2) Prismatic fuel block with fuel compacts

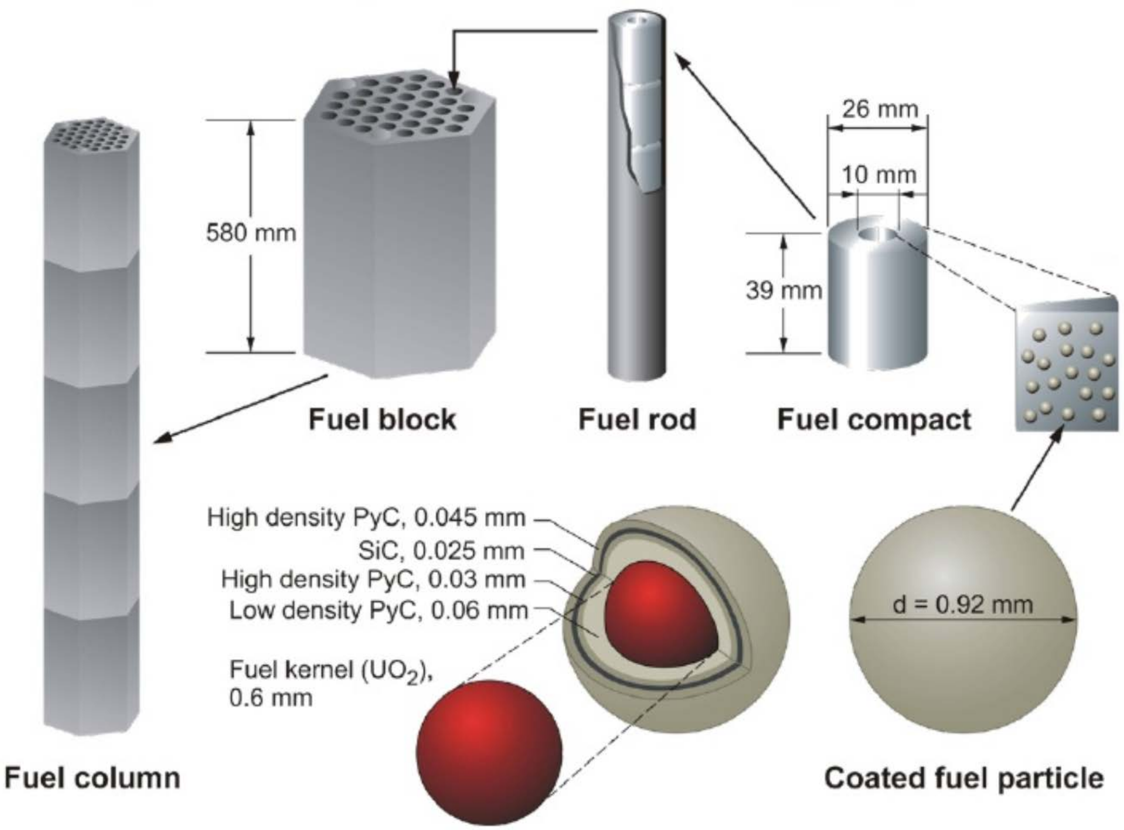
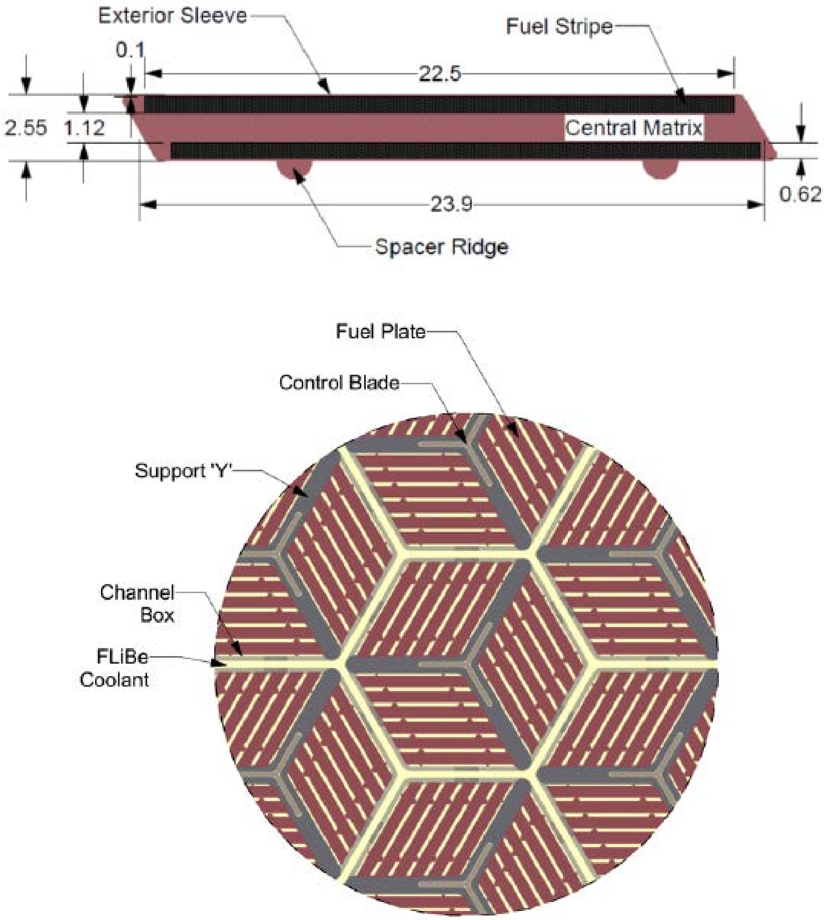


Figure: Courtesy of H. Gougar, NEAMS presentation, January 24, 2016.

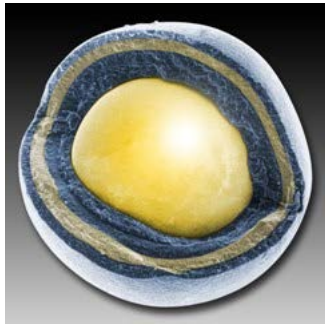
(3) Plate fuel



Figures: D. H. Holcomb, et al., ORNL/TM-2011/365, September 2011.

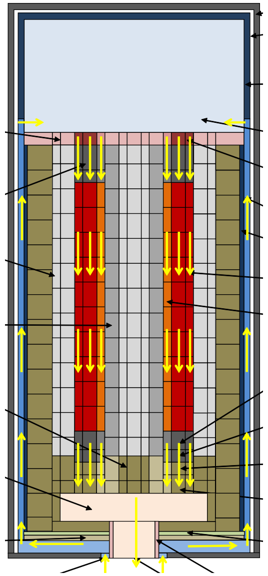
Double heterogeneous systems

- Renewed interest in advanced reactor systems:
  - High temperature gas-cooled reactors (HTGRs); pebbles, prismatic blocks
  - Fluoride salt-cooled high-temperature reactors (FHRs); pebbles, plates, etc.
  - Other designs
- Characteristics:
  TRISO fuel, graphite moderator, helium or molten salt cooled



TRISO particle

Look insight pebble-bed reactor



Prismatic HTGR design

Figures: Courtesy of J. Powers, PhD Thesis, University of California, Berkeley, 2011.

Figure: G. Strydom, F. Bostelmann, INL/EXT-15-34868, Rev. 1, September 2015.

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Modeling challenges of double-het systems

- TRISO particles are randomly dispersed in a graphite matrix

- Criticality calculations:
  - Using continuous-energy (CE) cross section data

    → We can model everything explicitly

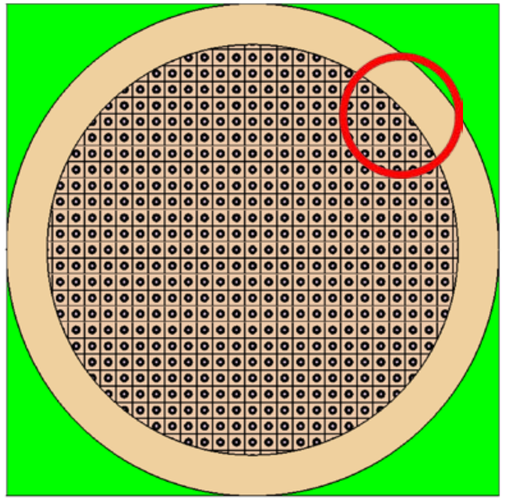
  - Using multigroup (MG) cross section data

    → Problem-independent MG cross sections must be shielded

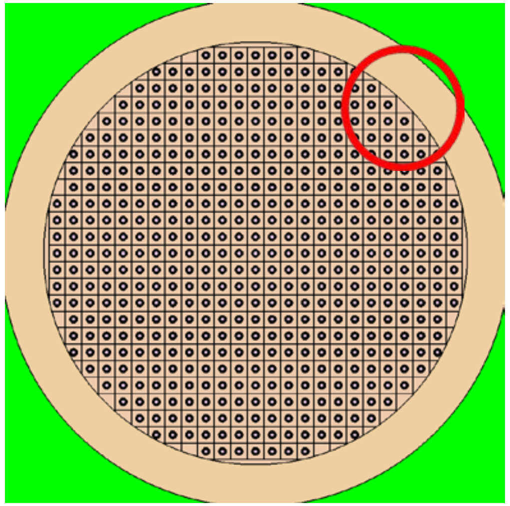
Modeling challenges of double-het systems

- Continuous-energy calculations:

  a) Simplify TRISO particles distributed in array
    - Relatively easy to model
    - Allows for neutron streaming paths
    - Particle clipping recommended to be avoided (adds another unrealistic element and fuel mass might be incorrect)
    - Particles closer together to keep overall packing fraction correct → larger local packing fraction
    - Some codes: on-the-fly random placement of the TRISO particle within its lattice cell



Infinite particle lattice



Lattice without clipping

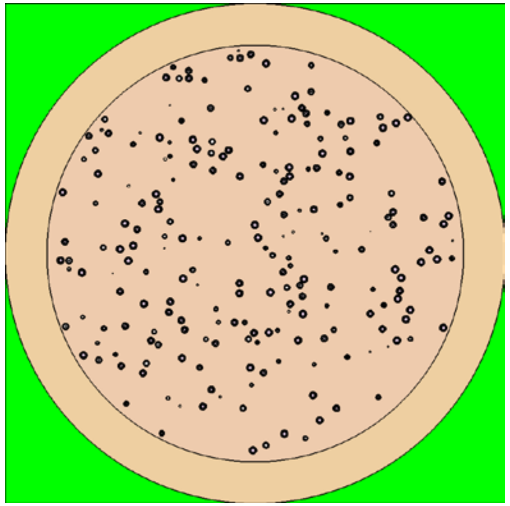
High temperature reactor (HTR) fuel pebble models for CE calculations

Modeling challenges of double-het systems

- Continuous-energy calculations:

  b) Define every single randomly picked position of TRISO particles in fuel region

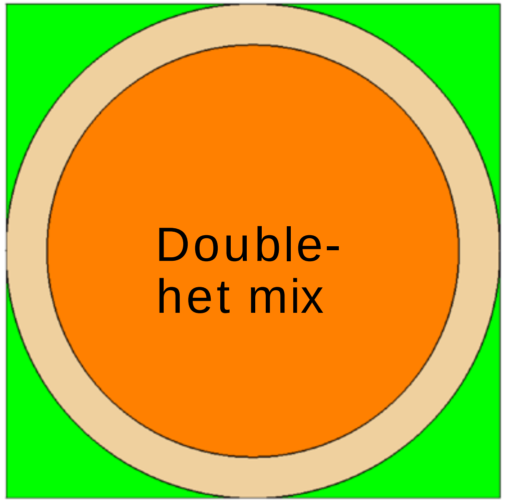
  - A larger modeling effort is required
  - Code might have issues determining initial neutron distribution → some effort has to be spent on defining source
  - An extremely long computation time is required, depending on the number of particles
  - This model is closer to reality, but it still has simplification (cf. particle packing fraction is different in outer zone of fuel pebble)



CE HTR fuel pebble model with randomly dispersed particles

Modeling challenges of double-het systems

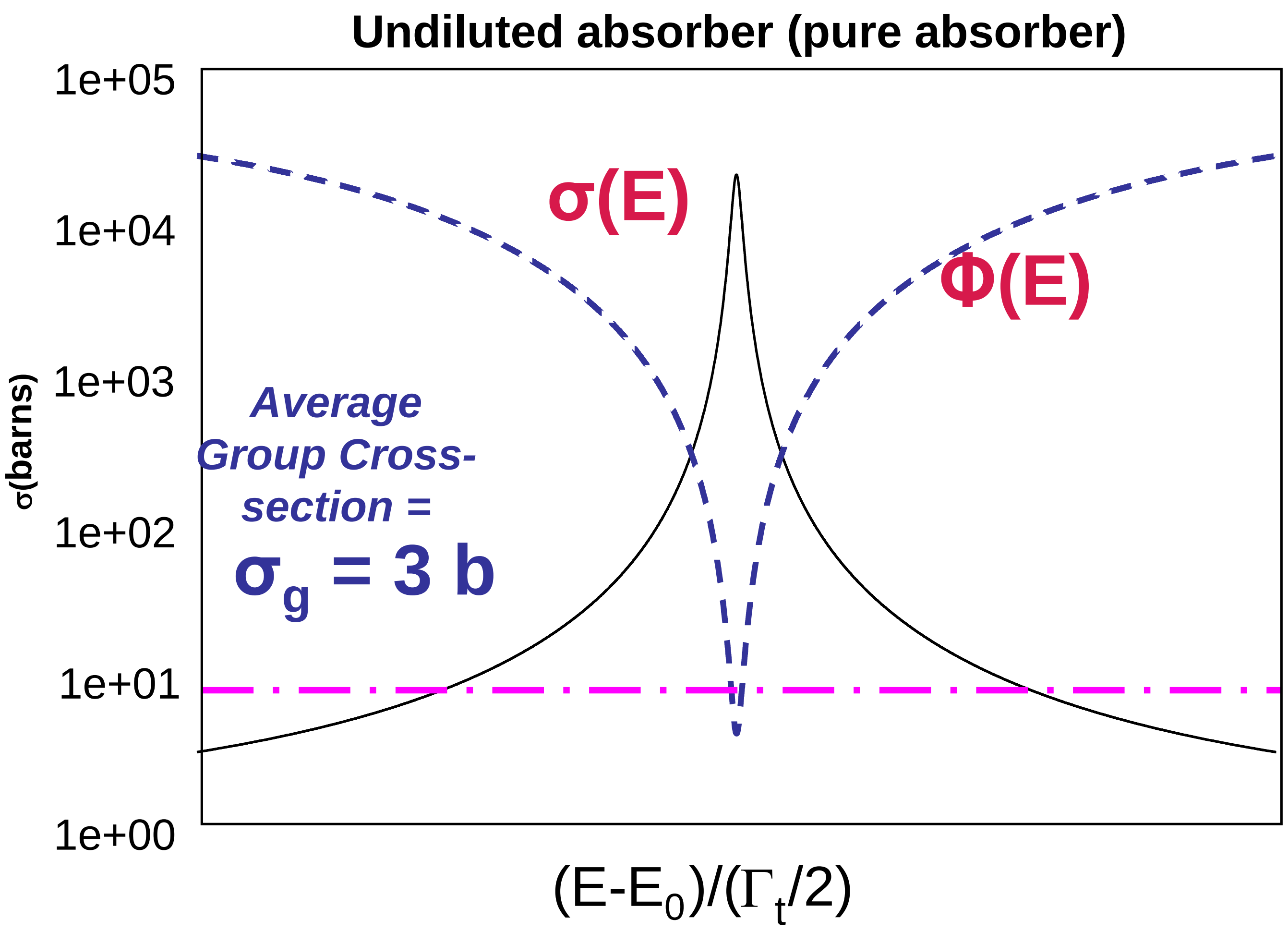
- Multigroup calculations:
  - Generic MG cross sections must be corrected for self-shielding effects in a given application:
    1. TRISO particle in graphite matrix, embedded in fuel pebble/rod/plate
    2. Fuel component in lattice
  - MG calculations allow for simple modeling and fast computation time
  - However, approximation is used, so it always must be validated

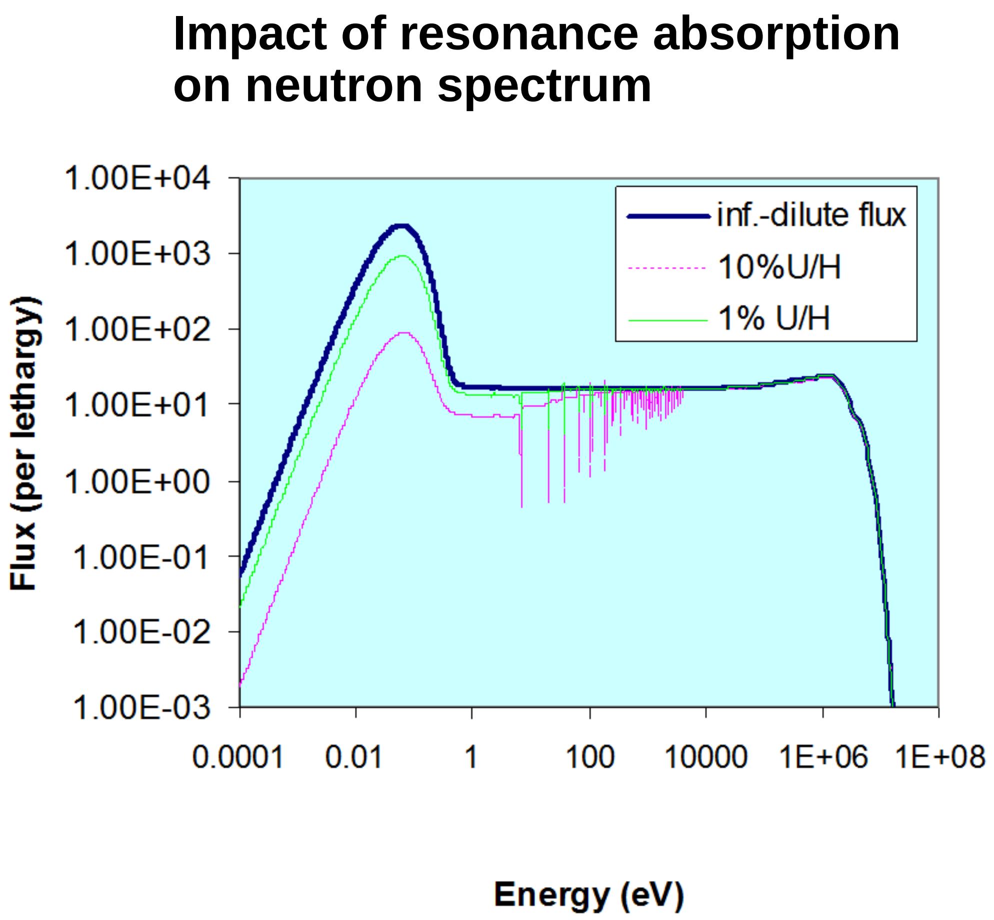


MG HTR fuel pebble model

Modeling challenges of double-het systems

- Self-shielding:





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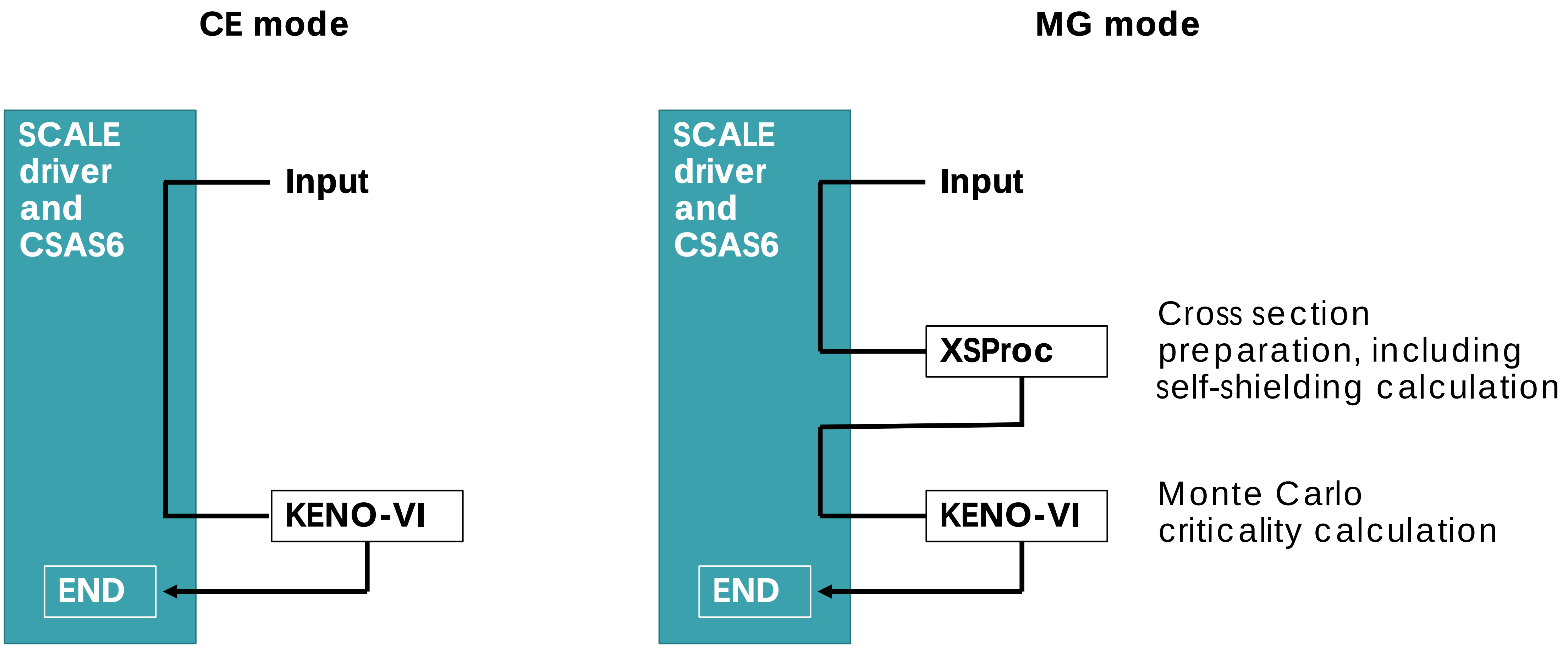
Modeling double-het systems with SCALE

- Criticality calculations with the 3D Monte Carlo code KENO-VI using either CE or MG data
- KENO-VI is used via the CSAS6 sequence that automates the cross section processing

CSAS6 criticality safety sequence



CSAS6 criticality safety sequence

- General structure of CSAS6 input:
  - title
  - cross section library
  - composition
  - cell data for MG self-shielding (only for MG mode)
  - parameters for Monte Carlo calculation
  - geometry description
  - array if applicable (e.g., in CE)
  - boundary condition (always a good idea)
  - end statements

```
=csas6
title
library
read composition
…
end composition
read celldata
…
end celldata
read parameter
…
end parameter
read geometry
…
end geometry
read array
…
end array
read bounds
…
end bounds
end data
end
```

SCALE cross section libraries

- Continuous-energy:
  - ENDF/B-VII.0 (ce_v7.0_endf)
  - ENDF/B-VII.1 (**ce_v7.1_endf**)
- Multigroup:
  - ENDF/B-VII.0: 238-group (v7-238)
  - ENDF/B-VII.1: 56g, 252g (v7.1-56, **v7.1-252**)

Use of ENDF/B-VII.1 data is strongly recommended!

The difference in neutron capture in carbon between the two ENDF libraries can lead to significant eigenvalue differences (>1,000 pcm) in graphite-moderated systems

CSAS6 criticality safety sequence: composition

- There are different ways to define composition via standard composition, atom percent compositions, solutions, etc.
  → Fulcrum's autocompletion can be used for assistance

- Here is one example:
  entering nuclide-wise number densities (atoms/barn-cm):

Nuclide	#mix	0	nuclide_density	temperature	end

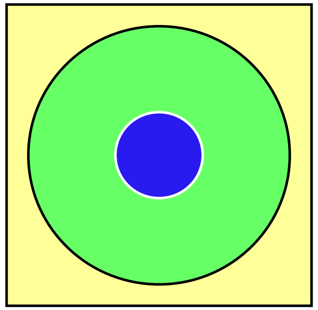
```
h          1  0  0.0667531  300.0  end
pu-238     2  0  4.747e-07  293.0  end
pu-239     2  0  1.068e-04  293.0  end
pu-240     2  0  1.577e-05  293.0  end
pu-241     2  0  5.626e-06  293.0  end
pu-242     2  0  6.187e-07  293.0  end
rh-103     2  0  1.104e-05  293.0  end
```

CSAS6 criticality safety sequence: parameter

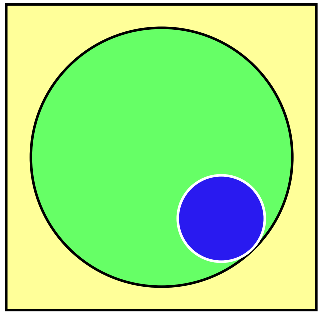
- KENO-VI parameters:
  - numbers of particles per generation (npg)
  - number of total generations (gen)
  - number of inactive generations (nsk)
  - optional: desired eigenvalue uncertainty, random number, doppler broadening rejection correction (DBRC), energy group structure for output when using CE mode, etc.
- Ensure fission source convergence: check convergence tests of Shannon entropy in output file
- Remember statistical uncertainty ~ 1/√N

KENO-VI geometry

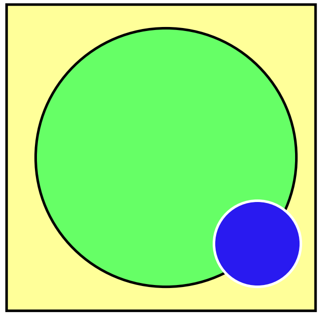
- *Volumes are built in sections called* ***units***. Each unit is independent of all other units and has its own coordinate system
- *Units are built using* ***regions***. Regions are made using the KENO-VI geometry shapes. The unit boundary must fully enclose all defined regions in the unit
- *Regions may share boundaries, may intersect, and may be rotated*



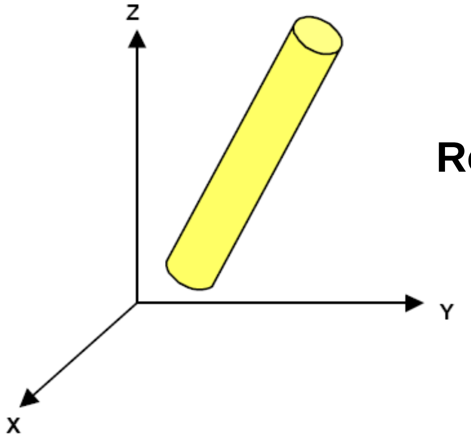
Regions in a unit



Shared boundaries



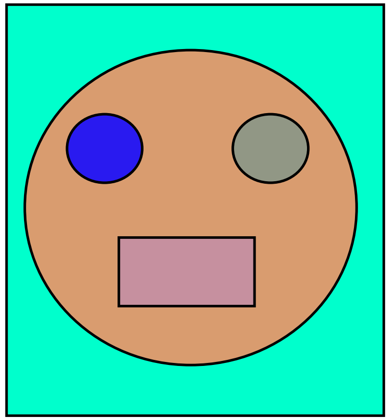
Intersecting regions



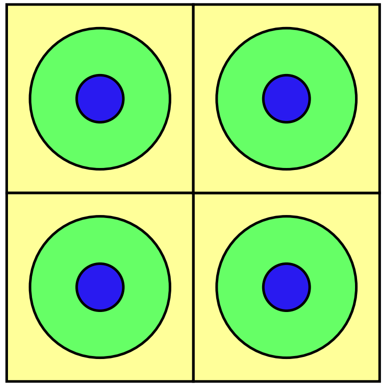
Rotated cylinder

KENO-VI geometry (continued)

- *A* ***hole*** *is used to place a unit within a region of a different unit.* The hole must be completely contained within the region and may not intersect other holes or nested arrays
- *An* ***array*** *is an ordered stack of units.* The touching faces of adjacent units in an array must be the *same size*
- *A* ***global unit*** *that encloses the entire system must be specified.* All geometry data used in a problem are correlated by the global unit coordinate system

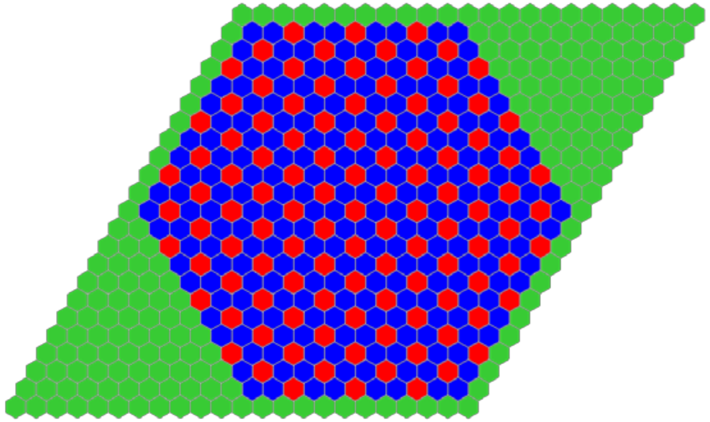


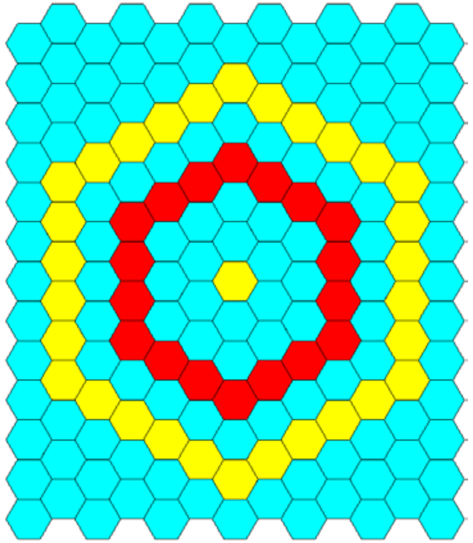
Unit containing HOLES

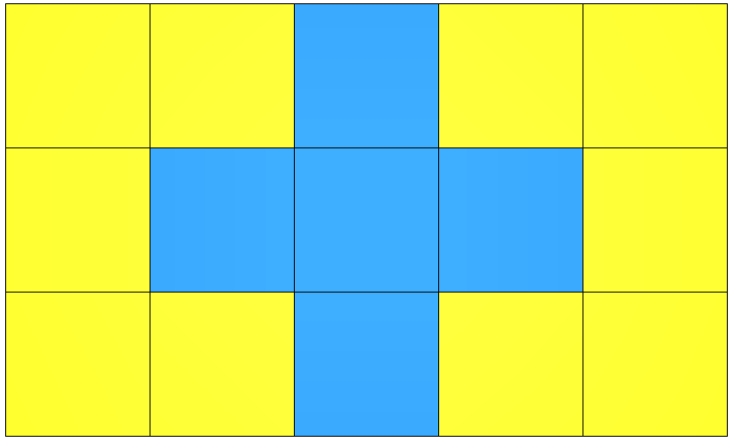


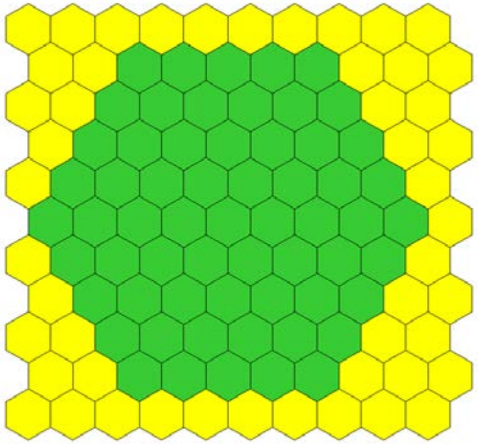
Array of units

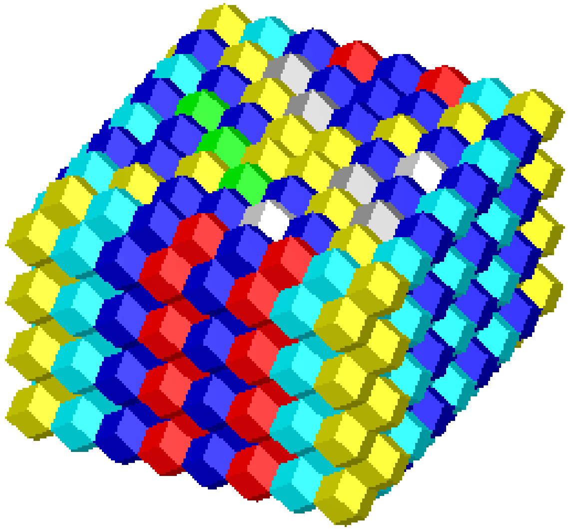
KENO-VI array types


Hexagonal (or triangular)


Rotated hex


Rectangular


Standard hex


Dodecahedral

KENO-VI input records

- Three types of records are used to define the volume, position, and material contents of the regions in a unit
    1. Geometry records
    2. Contents records
    3. Boundary records

```
unit 100
sphere 1 0.0250
sphere 2 0.0340
sphere 3 0.0380
sphere 4 0.0415
sphere 5 0.0455
cuboid 6 6p0.097634150
media 100 1 1
media 101 1 2 -1
media 102 1 3 -2
media 103 1 4 -3
media 104 1 5 -4
media 105 1 6 -5
boundary 6
```

KENO-VI input records

- Three types of records are used to define the volume, position, and material contents of the regions in a unit
  1. **Geometry records**
  2. Contents records
  3. Boundary records

- Geometry keyword
- Geometry record label
- Geometry boundary definitions
- Geometry modification data

```
unit 100
sphere 1 0.0250
sphere 2 0.0340
sphere 3 0.0380
sphere 4 0.0415
sphere 5 0.0455
cuboid 6 6p0.097634150
media 100 1 1
media 101 1 2 -1
media 102 1 3 -2
media 103 1 4 -3
media 104 1 5 -4
media 105 1 6 -5
boundary 6
```

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cuboid 6 6p0.097634150
media 100 1 1
media 101 1 2 -1
media 102 1 3 -2
media 103 1 4 -3
media 104 1 5 -4
media 105 1 6 -5
boundary 6
```

- Contents keyword (array, hole, media)
- ID number (array #, unit #, mixture #)
- Bias ID number (media only)
- Region definition vector (array, media)

KENO-VI input records

- Three types of records are used to define the volume, position, and material contents of the regions in a unit
  1. Geometry records
  2. Contents records
  3. **Boundary records**

Specify the overall volume of a unit:

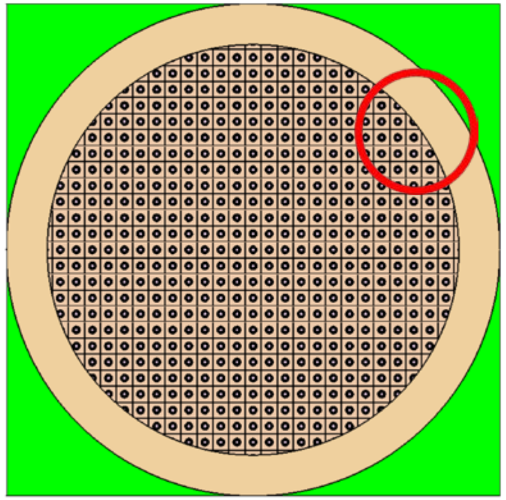
- ***One and only one boundary record*** is required for each unit
- Only the volume defined in the region definition vector of the unit's boundary record is contained within the unit
- Volumes outside the boundary record's region definition vector are not included in the unit

```
unit 100
sphere 1 0.0250
sphere 2 0.0340
sphere 3 0.0380
sphere 4 0.0415
sphere 5 0.0455
cuboid 6 6p0.097634150
media 100 1 1
media 101 1 2 -1
media 102 1 3 -2
media 103 1 4 -3
media 104 1 5 -4
media 105 1 6 -5
boundary 6
```

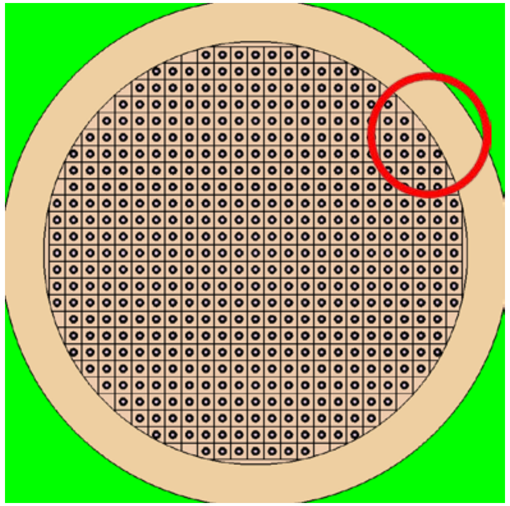
SCALE/KENO-VI double-het CE model

SCALE/KENO-VI double-het CE model

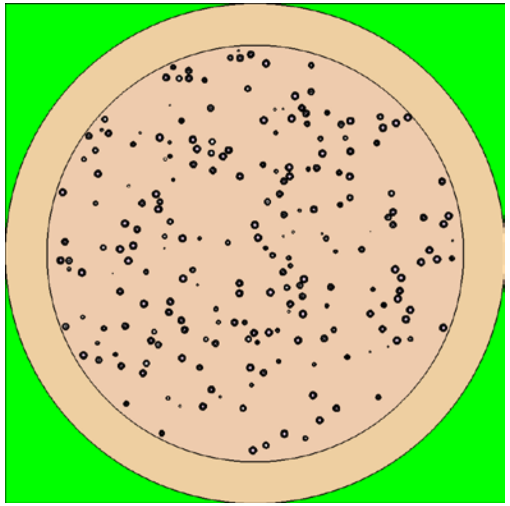
- Continuous-energy modeling:
  - Infinite particle array
  - Particle array with particles removed to avoid clipping
  - Explicit placement of randomly dispersed particles (not covered here)
  - Random distribution within mesh cells to improve runtime (not covered here)



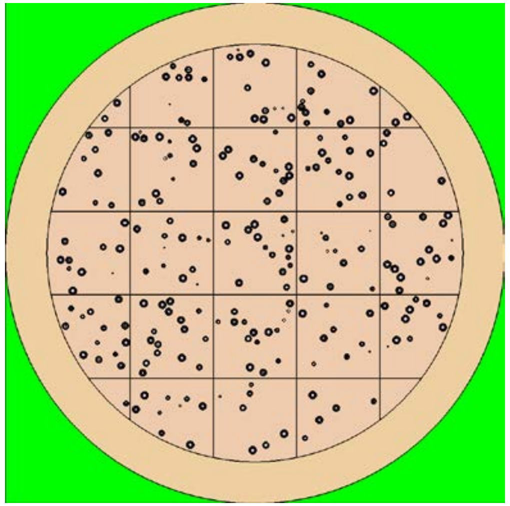
Infinite particle lattice



Lattice without clipping



Truly random



Random-mesh

SCALE/KENO-VI double-het CE model: TRISO particle

1. **TRISO particle** in its cuboid lattice cell
   – cuboid side length is lattice pitch of particle array

```
unit 100
sphere 1 0.0250
sphere 2 0.0340
sphere 3 0.0380
sphere 4 0.0415
sphere 5 0.0455
cuboid 6 6p0.097634150
media 100 1 1
media 101 1 2 -1
media 102 1 3 -2
media 103 1 4 -3
media 104 1 5 -4
media 105 1 6 -5
boundary 6
```

2. Lattice cell filled with graphite only

```
unit 200
cuboid 1 6p0.097634150
media 105 1 1
boundary 1
```

SCALE/KENO-VI double-het CE model: particle array

- **Infinite** TRISO particle **array** definition:

```
read array
  ara=1 nux=27 nuy=27 nuz=27 typ=cuboidal
  fill
    100 100 100 100 100 […] 100 100 100
  end fill
end array
```

- Better fill using fido input “f”:

```
read array
  ara=1 nux=27 nuy=27 nuz=27 typ=cuboidal
  fill f100 end fill
end array
```

In this way, the particles are clipped by the outer cylinder/pebble/plate in which this array is placed

SCALE/KENO-VI double-het CE model: particle array

- TRISO particle array **without particle clipping:**

```
read array
  ara=1 nux=27 nuy=27 nuz=27 typ=cuboidal
  fill
    200 200 200 200 200 […] 200 200 200
    200 200 200 100 100 […] 200 200 200
    200 200 100 100 100 […] 100 200 200
    200 100 100 100 100 […] 100 100 200
    […]
    200 200 200 100 100 […] 200 200 200
    200 200 200 200 200 […] 200 200 200
  end fill
end array
```

Place pure graphite cells in outer area of array

- Better repeat unit numbers

```
read array
  ara=1 nux=27 nuy=27 nuz=27
  typ=cuboidal
  fill
    27r200
    3r200 21r100 3r200
    2r200 23r100 2r200
    200   25r100 200
    […]
    3r200 21r100 3r200
    27r200  end fill
end array
```

SCALE/KENO-VI double-het CE model: particle array

- Fuel component:
  - Place fuel particle array into volume
  - Add the other materials
  - Place fuel component into array, declare as global unit, etc.

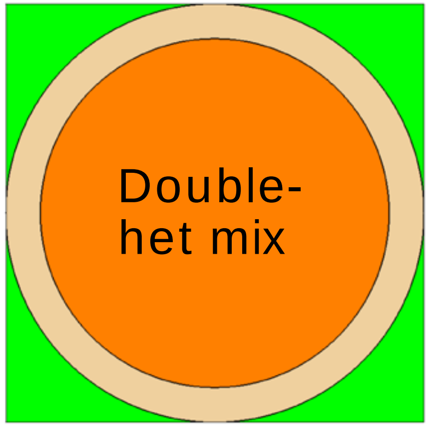
- Fuel pebble:

```
global unit 1
sphere 1 2.5
sphere 2 3.0
cuboid 3 6p3.0
array 1 1 place 14 14 14 0 0 0
media 106 1 2 -1
media 300 1 3 -2
boundary 3
```

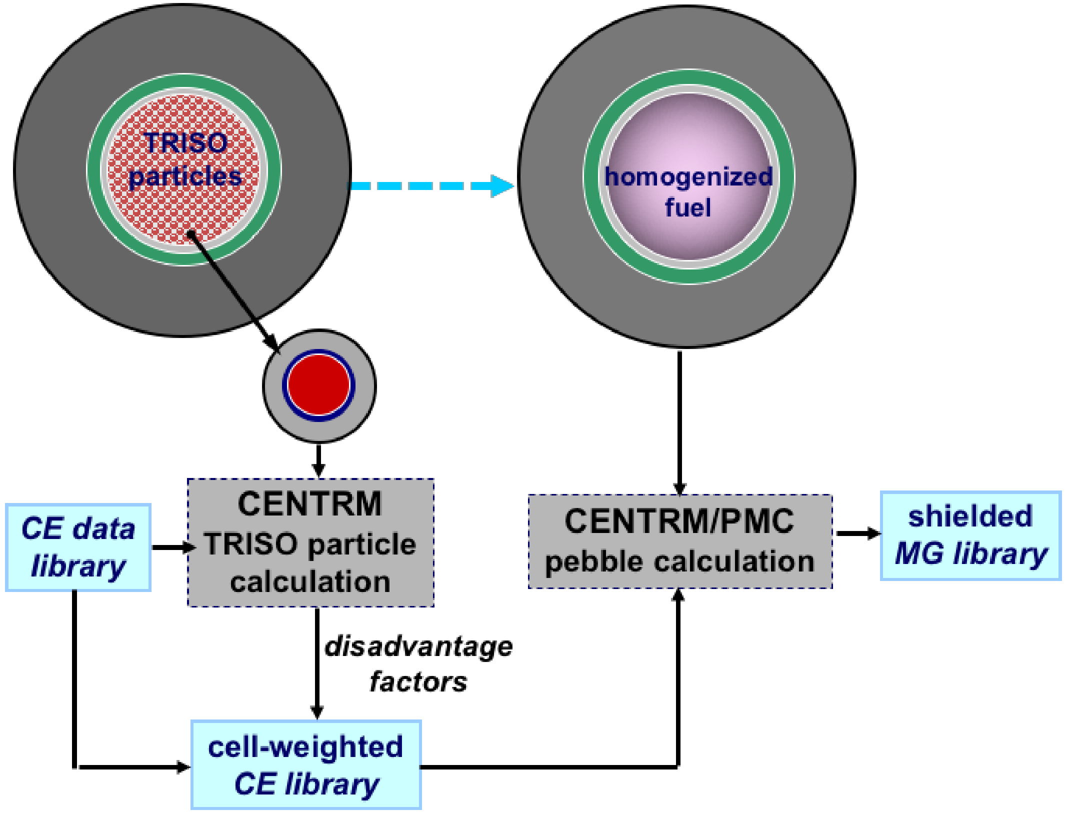
SCALE/KENO-VI double-het **multigroup** model

SCALE/KENO-VI double-het multigroup model

- Addition of cell data block:
  - Double heterogeneous self-shielding cell
  - Basically two self-shielding calculations
  - Simple user input in cell block for self-shielding
  - Creates one mixture to be placed in geometry model

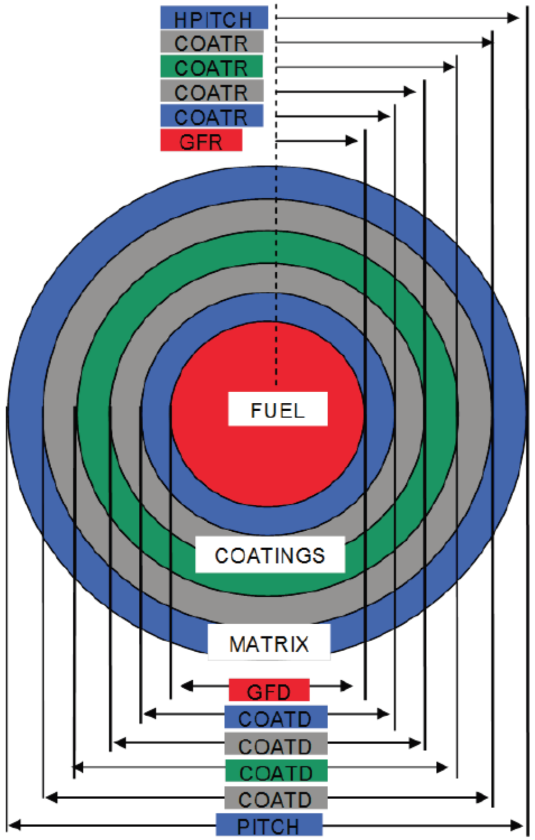


MG HTR fuel pebble model

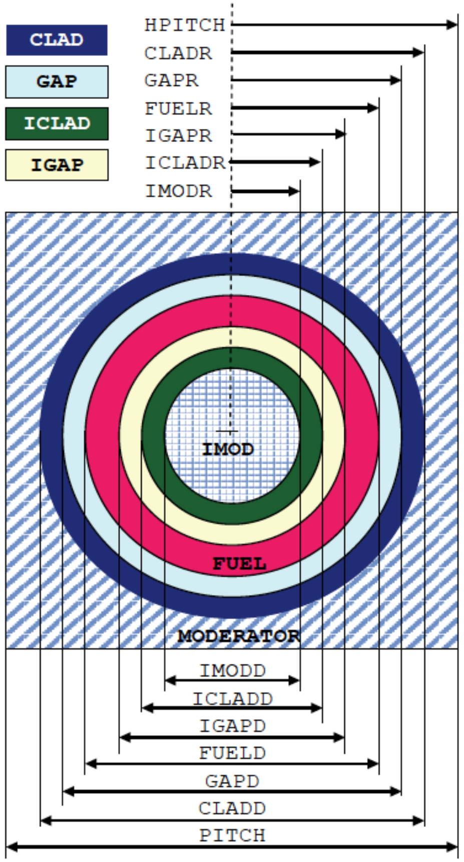


Double-het computational procedure for a pebble fuel component with SCALE

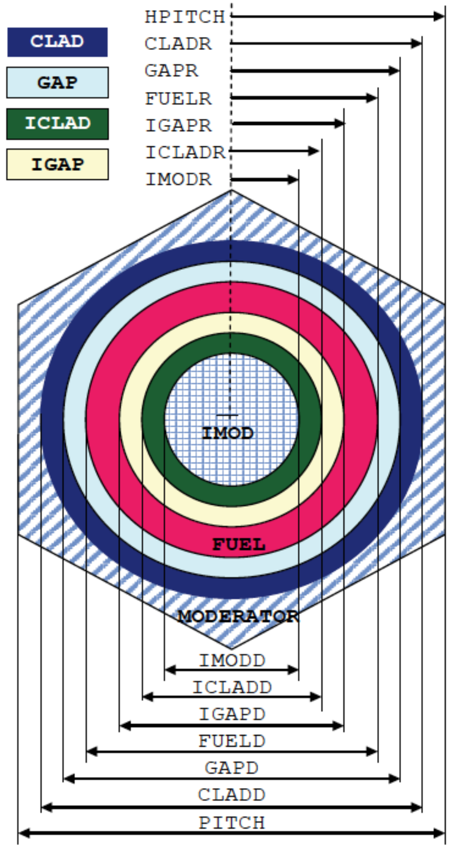
Unit cell geometries for MG double-het fuel components



Particle

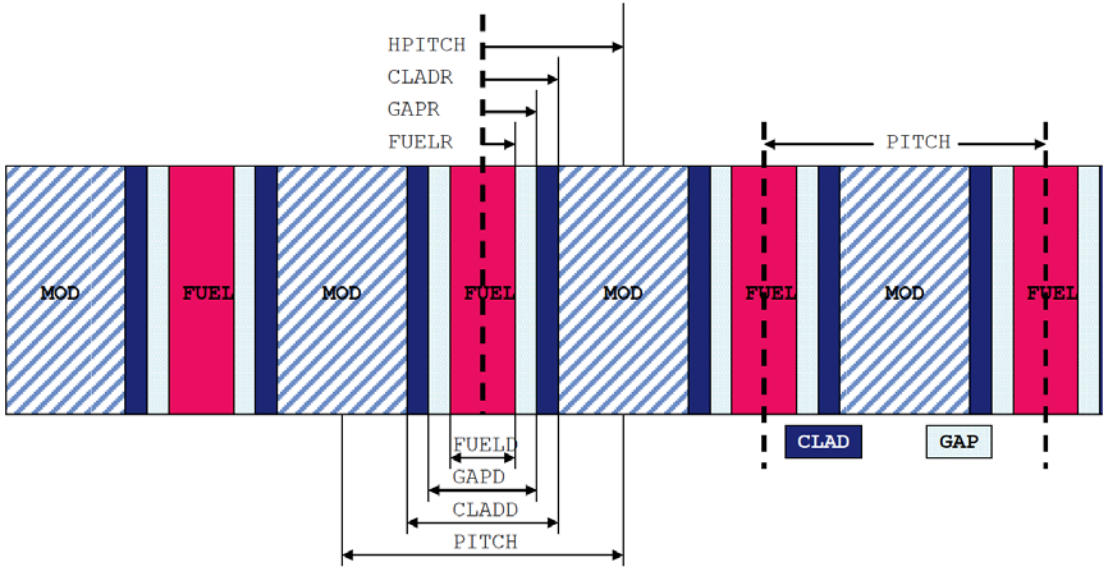


Unit cell for (annular) cylindrical rods in a square pitch or spherical pellets in a cubic lattice

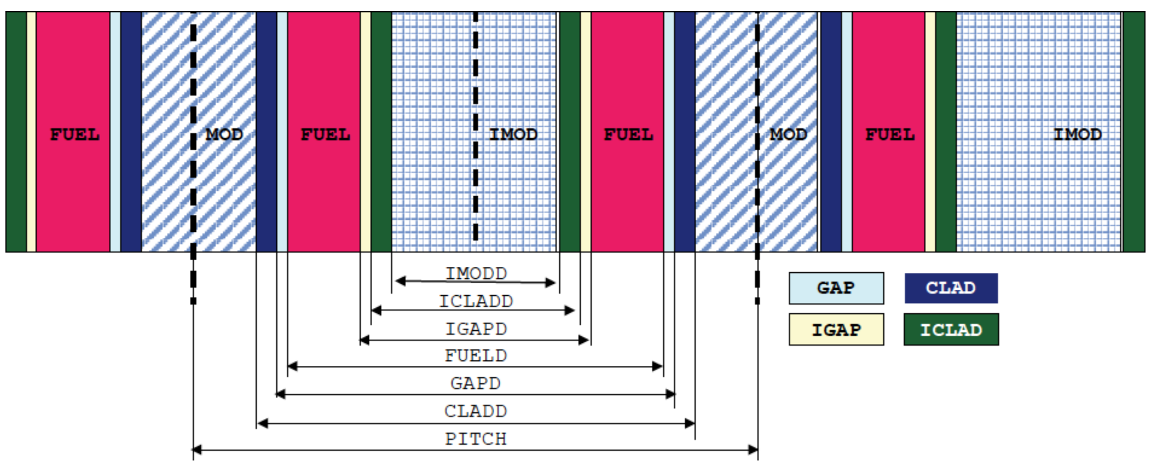


Unit cell for (annular) cylindrical rods in a triangular pitch or spherical pellets in a bi-centered or face-centered hexagonal close-packed lattice

Unit cell geometries for MG double-het fuel components



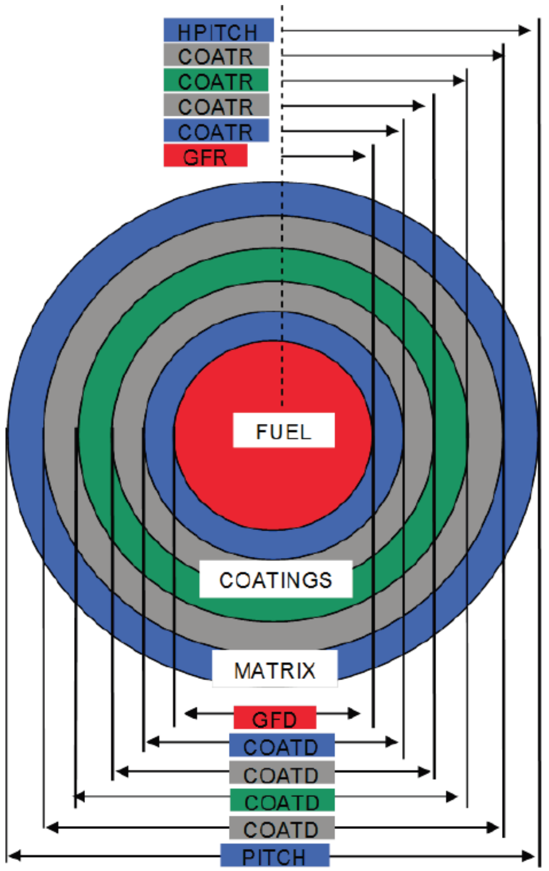
Symmetric array of slabs



Periodic but asymmetric array of slabs

Note: Plate-fuel double-het cells are not yet extensively tested

Cell data for MG double-het fuel component



Particle

- **gfr/gfd**: fuel grain radius/diameter
- **coatt/coatr/coatd**: coating thickness, radius, diameter
- **numpar**: number of particles
- **vf**: packing fraction

Don't fall into the d/r/t-trap:

d: diameter
r: radius
t: thickness

Often both **d** and **r** are possible, and for coating, additionally **t**

```
doublehet
right_bdy=white
fuelmix=10 end

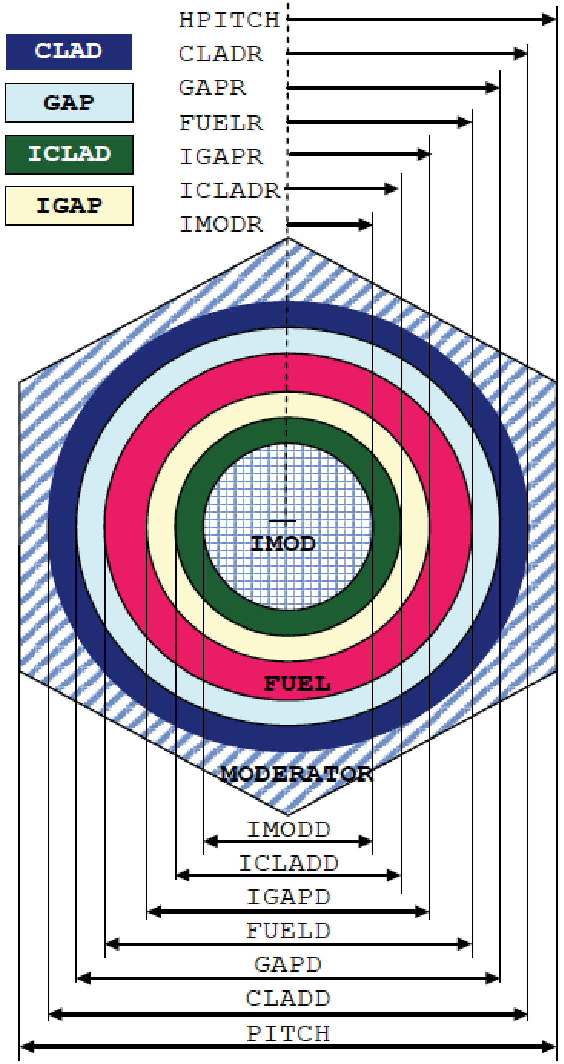
gfr=0.1 1
coatt=0.2 2
coatt=0.3 3
coatt=0.4 4
coatt=0.5 5
matrix=6
numpar=15000
vf=0.1
end grain
```

particle (grain)

```
rod
triangpitch
right_bdy=white
left_bdy=reflected
hpitch=5.0 7
fuelr=1.0
cladr=2.0 8
fuelh=3.0
end
```

rod/plate/1pebble

Cell data for MG double-het fuel component



Fuel component

- **hpitch/pitch:** (half) pitch of fuel component infinite lattice
- **fuelr/fueld:** fuel component radius/diameter
- **cladr/cladd:** cladding radius/diameter
- **fuelh:** fuel component height

- Others: gaps, central hole

```
doublehet
right_bdy=white
fuelmix=10 end

gfr=0.1 1
coatt=0.2 2
coatt=0.3 3
coatt=0.4 4
coatt=0.5 5
matrix=6
numpar=15000
vf=0.1
end grain
```

particle (grain)

```
rod
triangpitch
right_bdy=white
left_bdy=reflected
hpitch=5.0 7
fuelr=1.0
cladr=2.0 8
fuelh=3.0
end
```

rod/plate/pebble

SCALE/KENO-VI double-het multigroup model

- Steps
  1. Create double-het cell block
  2. Place fuel mix into volume that includes the particles

- Fuel pebble

```
global unit 1
sphere 1 2.5
sphere 2 3.0
cuboid 3 6p3.0
media  10 1 1
media 106 1 2 -1
media 300 1 3 -2
boundary 3
```

Outline

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  - What are double heterogeneous systems?
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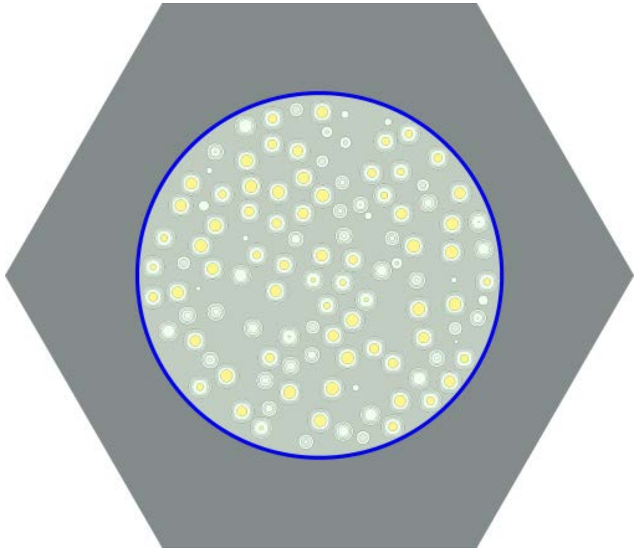
- Outlook to SCALE 6.3

High-temperature gas-cooled reactor (HTGR) prismatic pin cell in infinite lattice



MHTGR pin cell

1. Multigroup model using the double-het cell
2. Continuous-energy model using an infinite array of particles

Use provided SCALE composition block
→ *htgr-prismatic-pin-cell-composition.txt*

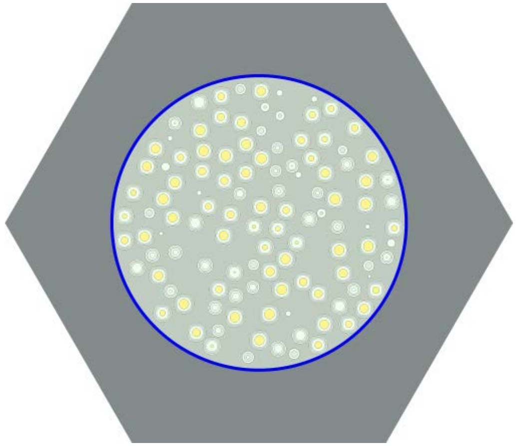
Use Fulcrum's auto-completion!

Ref.: G. Strydom, F. Bostelmann, INL/EXT-15-34868, Rev. 1.

HTGR prismatic pin cell in infinite lattice

Dimensions for MHTGR pin cell

Parameter		**Dimension (cm)**
TRISO fuel particle	$UC_{0.5}O_{1.5}$ kernel radius	2.125E-02
	Porous carbon buffer layer outer radius	3.125E-02
	Inner PyC outer radius	3.525E-02
	SiC outer radius	3.875E-02
	Outer PyC outer radius	4.275E-02
Average TRISO packing fraction		0.35
Fuel compact outer radius		0.6225
Fuel/helium gap outer radius		0.6350
Large helium coolant channel radius		0.7940
Unit cell pitch		1.8796
Fuel compact height		4.9280



MHTGR pin cell

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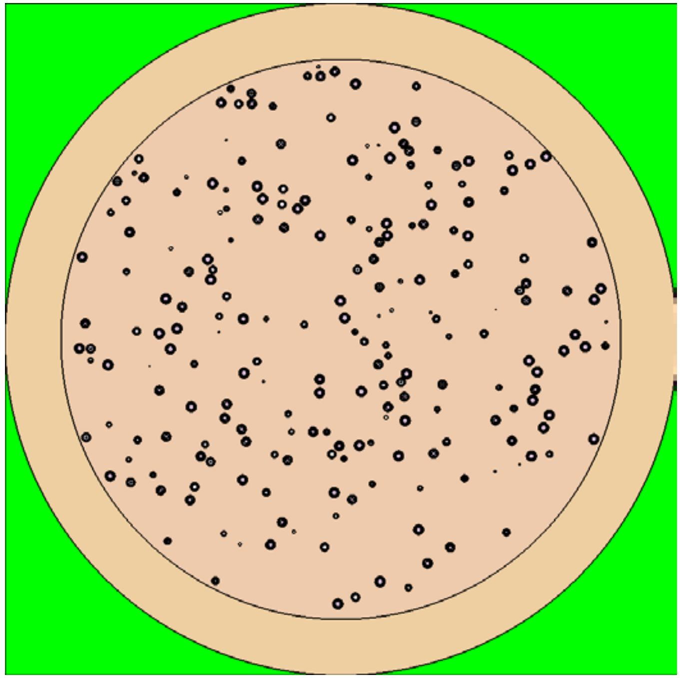
HTGR fuel pebble in infinite cubic lattice

1. MG model using the double-het cell
2. CE model using an infinite array of particles



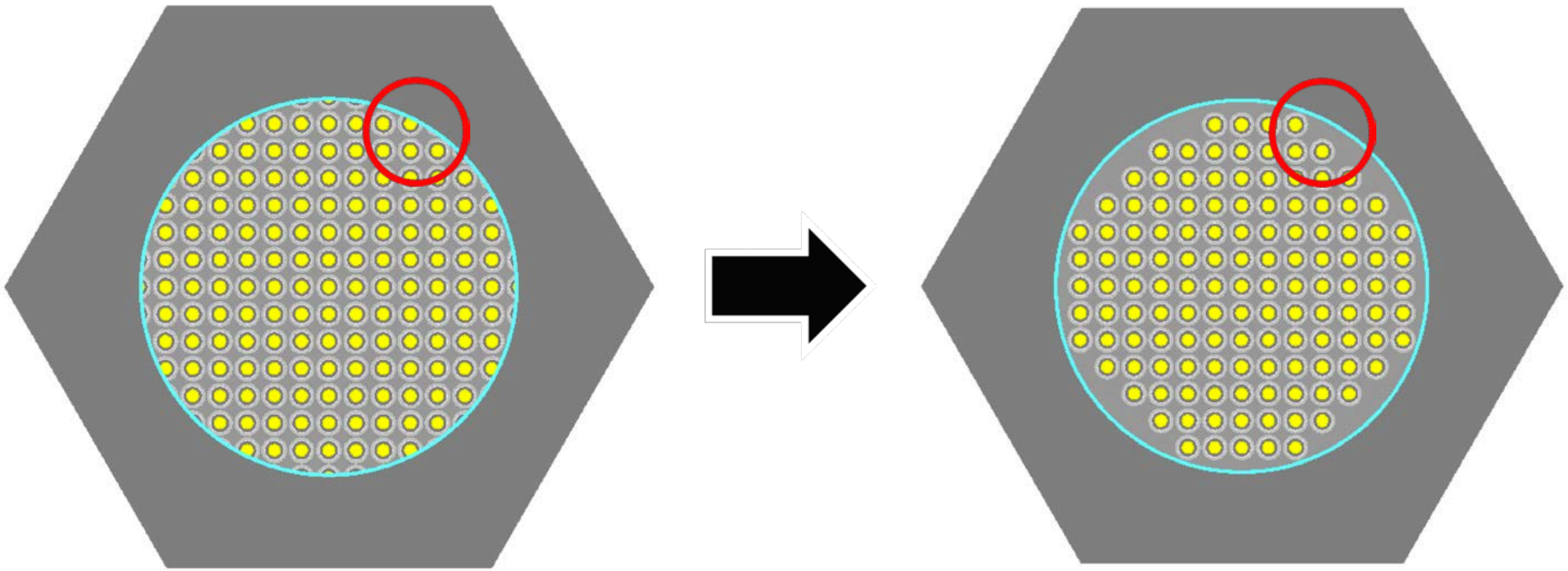
HTR fuel pebble

UO_2 fuel density (g/cm^3)	10.4
Uranium enrichment	17 wt.%
Fuel kernel radius (cm)	0.025
Fuel particle coating layer materials (starting from kernel)	Buffer/PyC/SiC/PyC
Fuel particle coating layer thicknesses (cm)	0.009/0.004/0.0035/0.004
Fuel particle coating layer densities (g/cm^3)	1.1/1.9/3.18/1.9
Number of particles in pebble	8,385
Diameter of fuel pebble (cm)	3.0
Diameter of fuel zone in pebble (cm)	2.5
Graphite matrix and fuel pebble outer shell density (g/cm^3)	1.73

Use provided SCALE composition block
→ *htgr-fuel-pebble-composition.txt*

HTGR prismatic pin cell in infinite lattice

3. Modification of CE model of prismatic pin to avoid particle clipping



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What else can we do with double-het systems in SCALE?

- 2D deterministic code calculations using NEWT
- Depletion calculations using Triton in combination with NEWT and KENO-VI (both MG and CE)
- Uncertainty and sensitivity analysis:
  - Perturbation theory: CE TSUNAMI (using KENO-VI CE as transport code)
  - Random sampling: Sampler (using either NEWT or KENO-VI MG)

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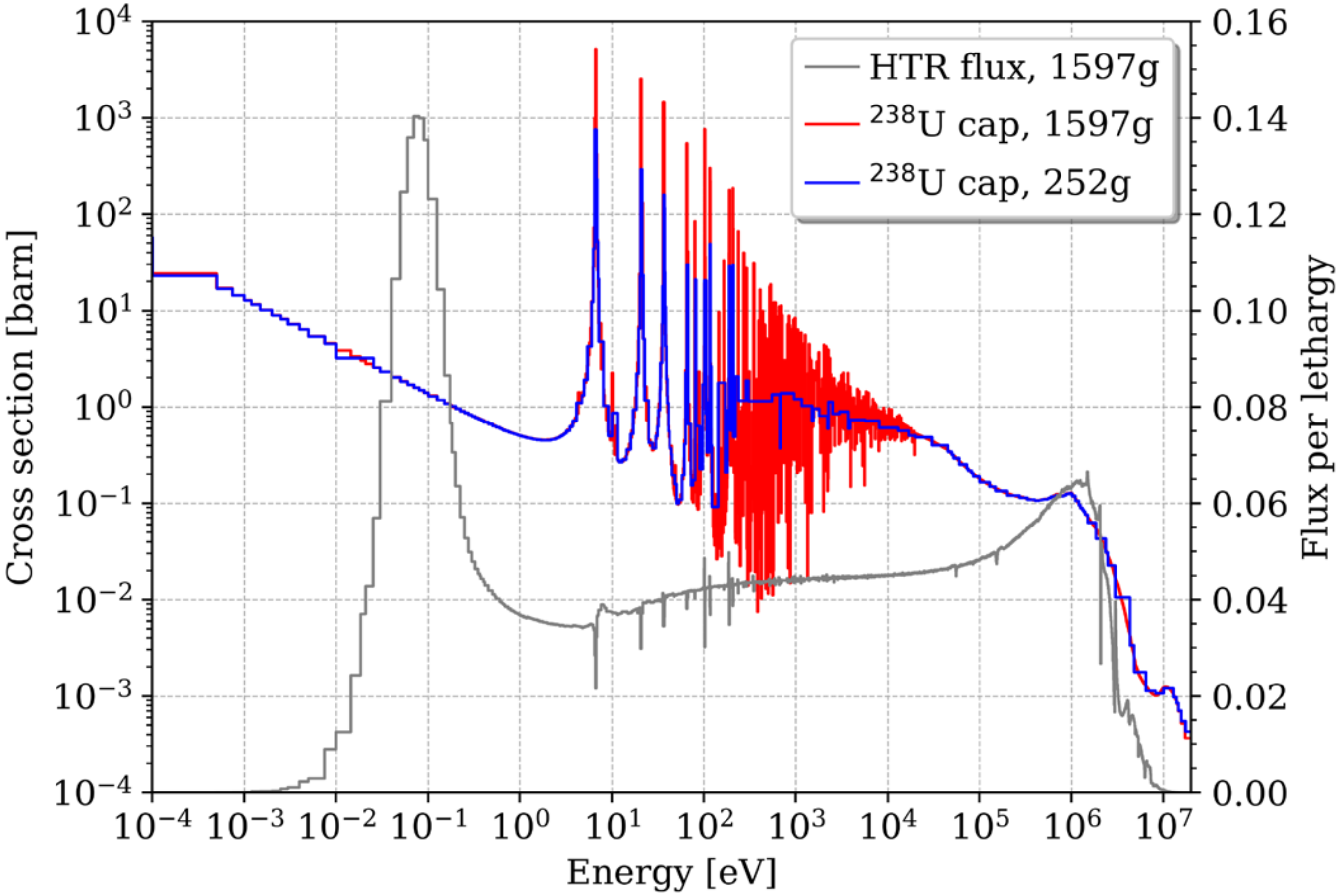
- **Outlook to SCALE 6.3**

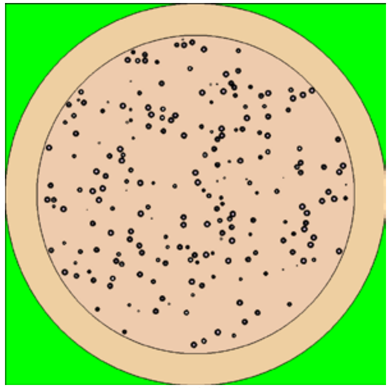
Outlook to SCALE 6.3

- New data libraries:
  - 1597-group cross section library
  - ENDF/B-VIII.0 data, offering graphite as perfect crystal, with 10% and 30% porosity
    (→ cf. presentation about SCALE double-het capabilities)

^{238}U capture cross section; HTR neutron flux



Outlook to SCALE 6.3



- New Monte Carlo code Shift
  - MG and CE calculations
  - Use of KENO-VI input via CsasShift sequence (*csas6-shift*)
  - Other supported input formats: own format and MCNP input
  - **New block to simplify random placement of particles in CE mode:**

```
unit 1
com=‘TRISO particle'
sphere 1 2.50e-02
sphere 2 3.40e-02
sphere 3 3.80e-02
sphere 4 4.15e-02
sphere 5 4.55e-02
media 100 1 1
media 101 1 2 -1
media 102 1 3 -2
media 103 1 4 -3
media 104 1 5 -4
boundary 5
```

```
read randomgeom
randommix = 'trisos'
type=random
units=1 end
pfs=0.05054954 end
clip=no
seed=1111
end randommix
end randomgeom
```

```
global unit 10
com=‘fuel pebble'
sphere 1 2.5
sphere 2 3.0
cuboid 3 6p5.0
media 105 1 1
randommix='trisos'
media 106 1 2 -1
media 300 1 3 -2
boundary 3
```