High-Fidelity Coupled Neutronics & Thermal Analysis for ATR Experiments

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Acknowledgements

- This work was funded by the ATR NSUF Faculty Student Team Project Program
- Thanks to INL staff who supported our project:
  - Jim Parry
  - Glenn Roth
  - Scott Davis
  - Jeff Benson

Motivation

- Create a fast, simple method for experimenters to characterize NSUF experiments with minimal dependence on INL staff
  - focus: support the proposal-writing stage of experiment design
  - fidelity: 10% deviation in major experiment metrics versus full radiation transport analysis
  - ease of use: MCNP5 and CAD-to-DAGMC support, users need only create a stand-alone CAD model of the experimental position
    - Direct use of CAD model for analysis
    - Simplified neutronics modeling without full core
    - (Semi-) automated coupling between neutronics and thermal analysis

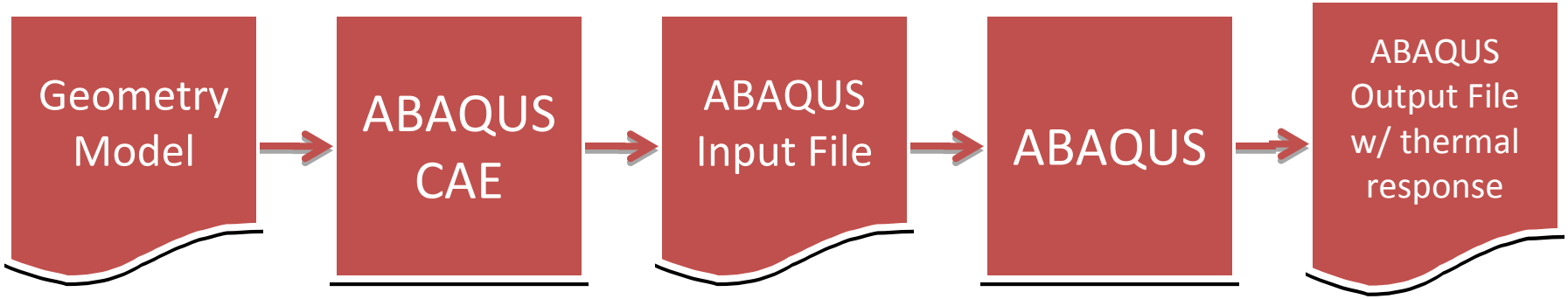
Workflow

Look up nuclear response in material database

1-D or
0-D Excel
Spreadsheet Analysis

Workflow

MCNP5
Input
MCNP5
MCNP5
Input


Geometry
Model
ABAQUS
CAE
ABAQUS
Input File
ABAQUS
ABAQUS
Output File
w/ thermal
response

Workflow

Requires either

<u>substantial simplification</u>

or

<u>large investment in human effort</u>

Skill set unique to nuclear engineering

Geom
Mod

BAQUS
tput File
thermal
sponse

Workflow

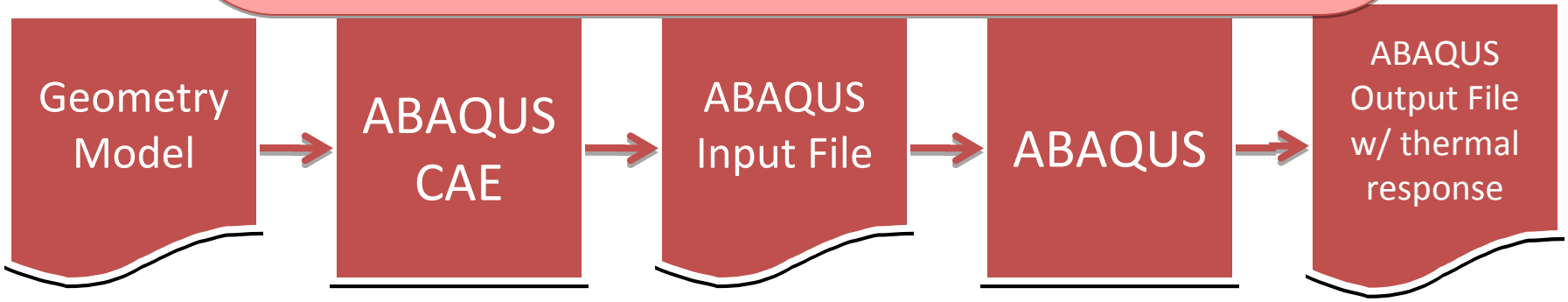
Manual transfer of heating data from MCNP->ABAQUS

Requires

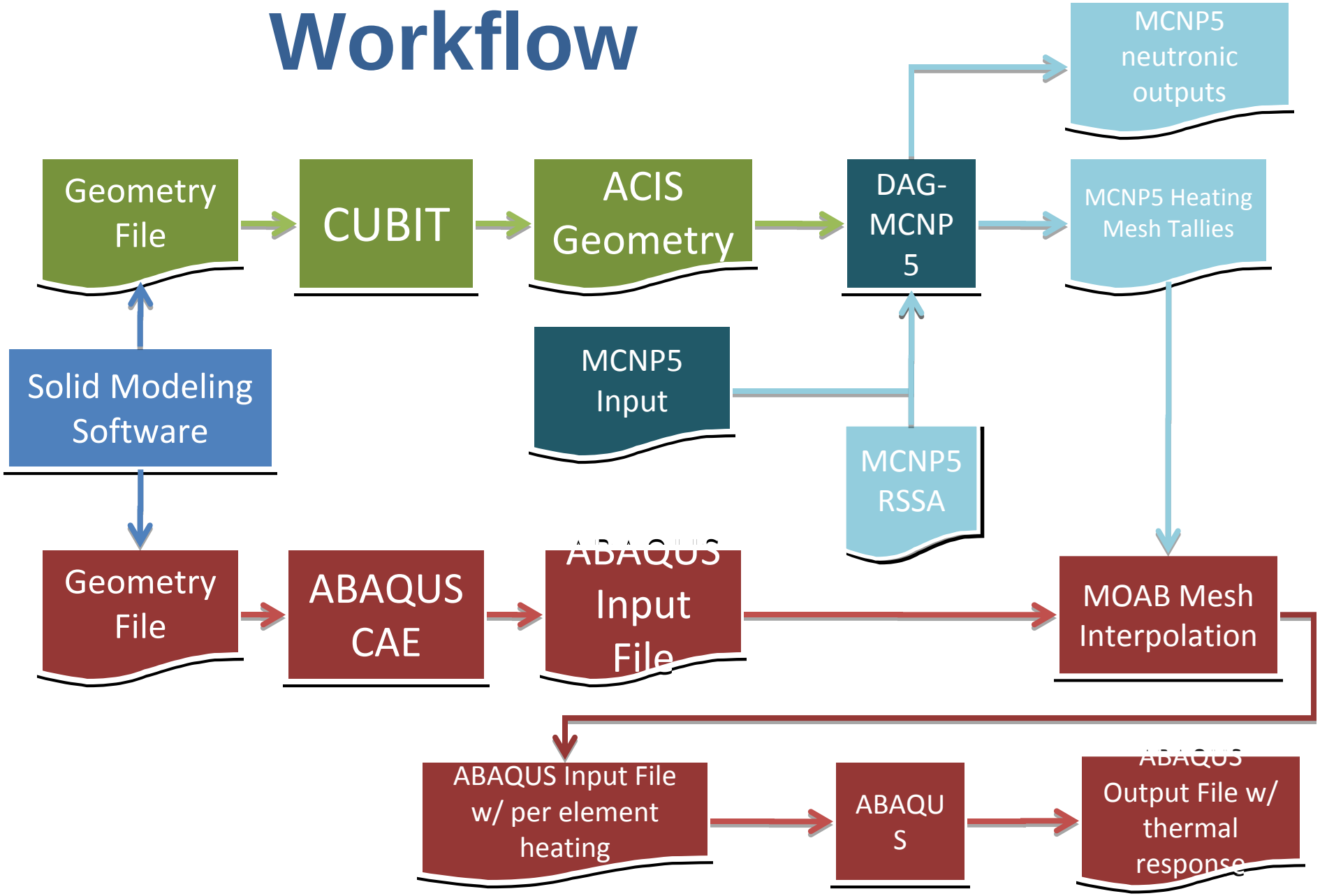
substantial simplification

and/or

loss of fidelity

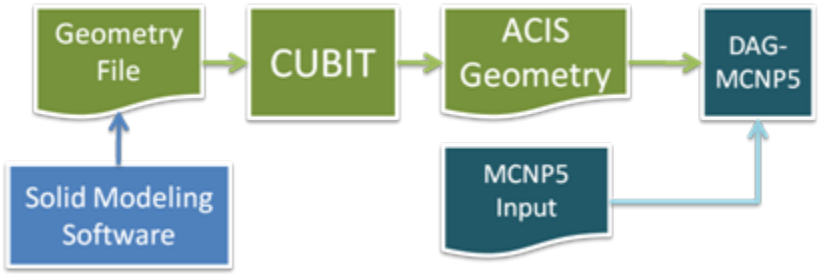


Workflow


MCNP5 neutronic outputs
Geometry File
CUBIT
ACIS Geometry
DAG-MCNP 5
MCNP5 Heating Mesh Tallies
Solid Modeling Software
MCNP5 Input
MCNP5 RSSA
Geometry File
ABAQUS CAE
ABAQUS Input File
MOAB Mesh Interpolation
ABAQUS Input File w/ per element heating
ABAQUS
ABAQUS Output File w/ thermal response

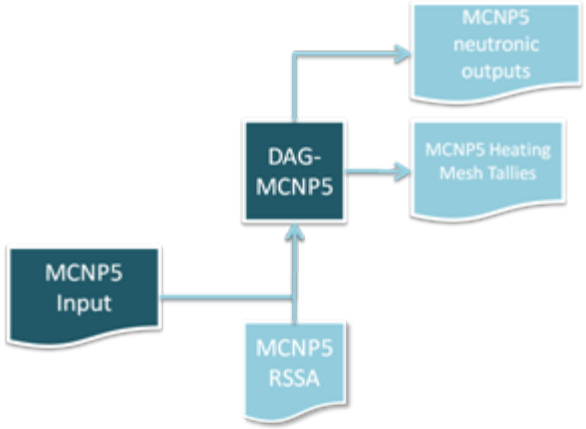
Workflow Components

Geometry: DAG-MCNP5 to the ATR or component

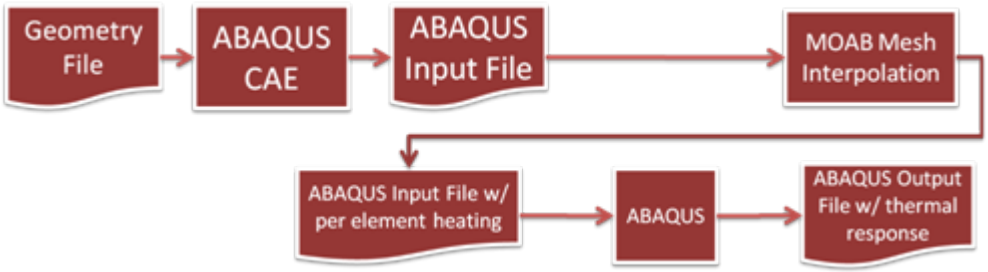


Neutronic Analysis:

Surface Source Approach



Thermal Analysis: MCNP5->ABAQUS Translation

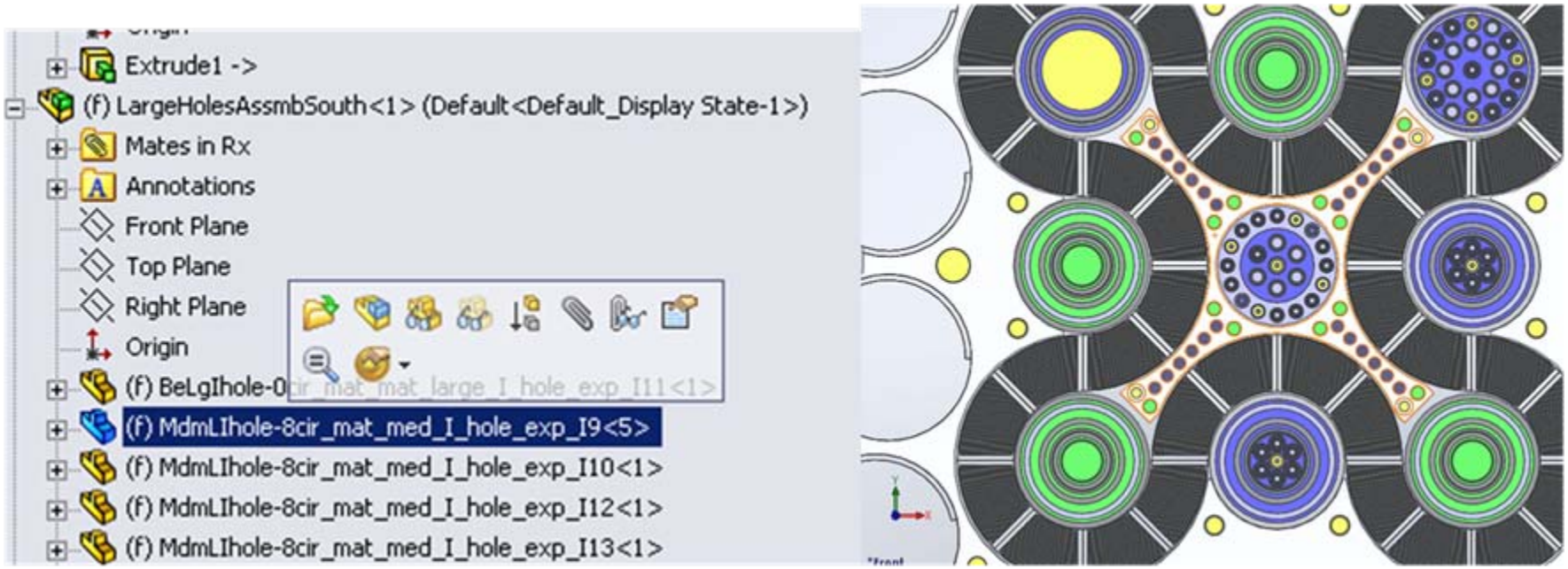


Geometry: CAD-to-MCNP5

- The CAD-to-MCNP5 process involves four steps:
  1. Create geometry in 3D CAD software (e.g. SolidWorks) from a provided template
  2. Import geometry into Cubit to imprint, merge, and add materials *(scripted step involving minimal user interactions)*
  3. Add tallies to MCNP5 template (optional) and execute DAGMC (Direct Accelerated Geometry Monte Carlo) (requires MCNP5 template and Cubit-prepared geometry)
  4. (optional) visualize mesh tally results in VISIT

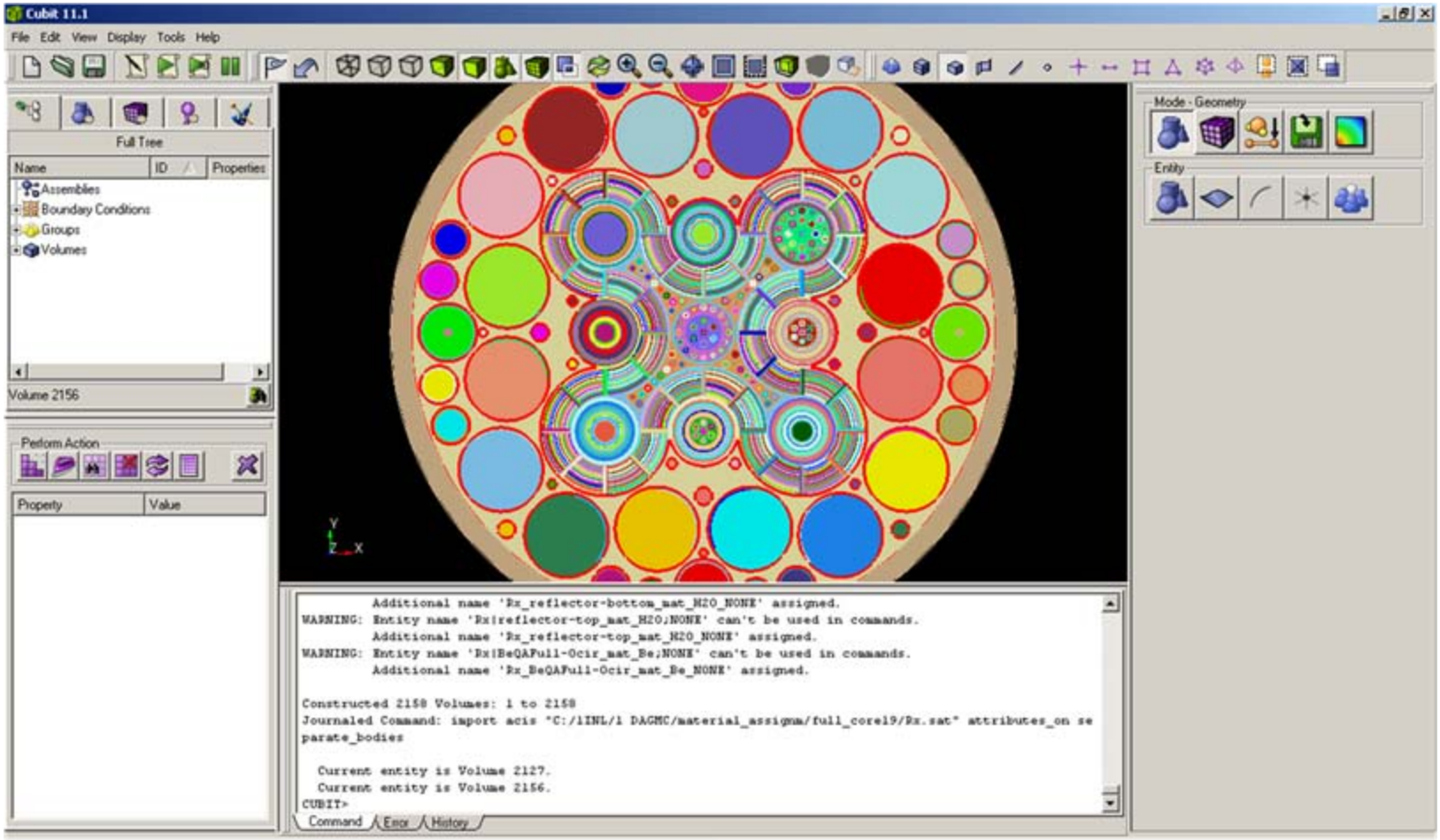
Step 1: Create Geometry in 3D CAD

- Most CAD systems will work for creating the initial model. The screenshot is taken from a SolidWorks full-core ATR model
- Individual parts are associated with material, tally and experiment tags via a naming convention
- It is important that the model has no overlapping surfaces



Step 2: Import into Cubit

- An ‘automated’ step (via script files) that translates the CAD model into the ACIS format suitable for reading by DAGMC



Step 3: Run Radiation Transport Simulation: DAGMC

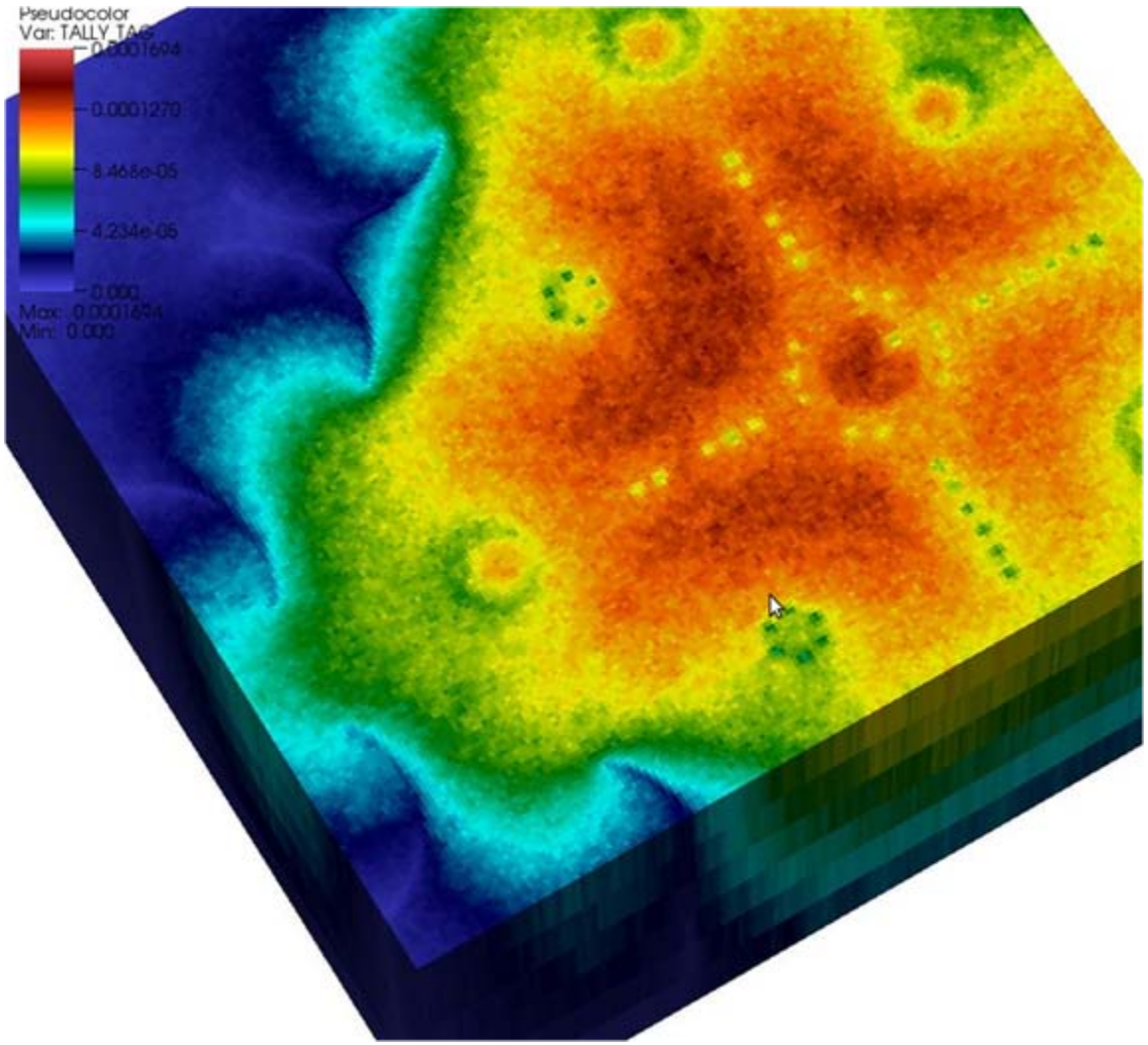
- DAGMC accomplishes ray tracing directly on CAD-based solid models, without translation to MCNP5 input language. DAGMC employs high-fidelity faceting combined with hierarchical trees of oriented bounding boxes for those facets.

- To execute DAGMC, the user must
  - prepare an MCNP input file including only the third block, the data cards.
    - no cell or surface cards are required
  - Run DAG-MCNP5, specifying the geometry and MCNP5 file names and (optional) faceting tolerance, as well as the output facet file name

- DAGMC supports parallel execution and tallies via
  - "groups" created by the user within CUBIT
  - direct tally specification in the MCNP data block.

- Heating mesh tallies serve as input to part 3 of the workflow (ABAQUS thermal modeling)

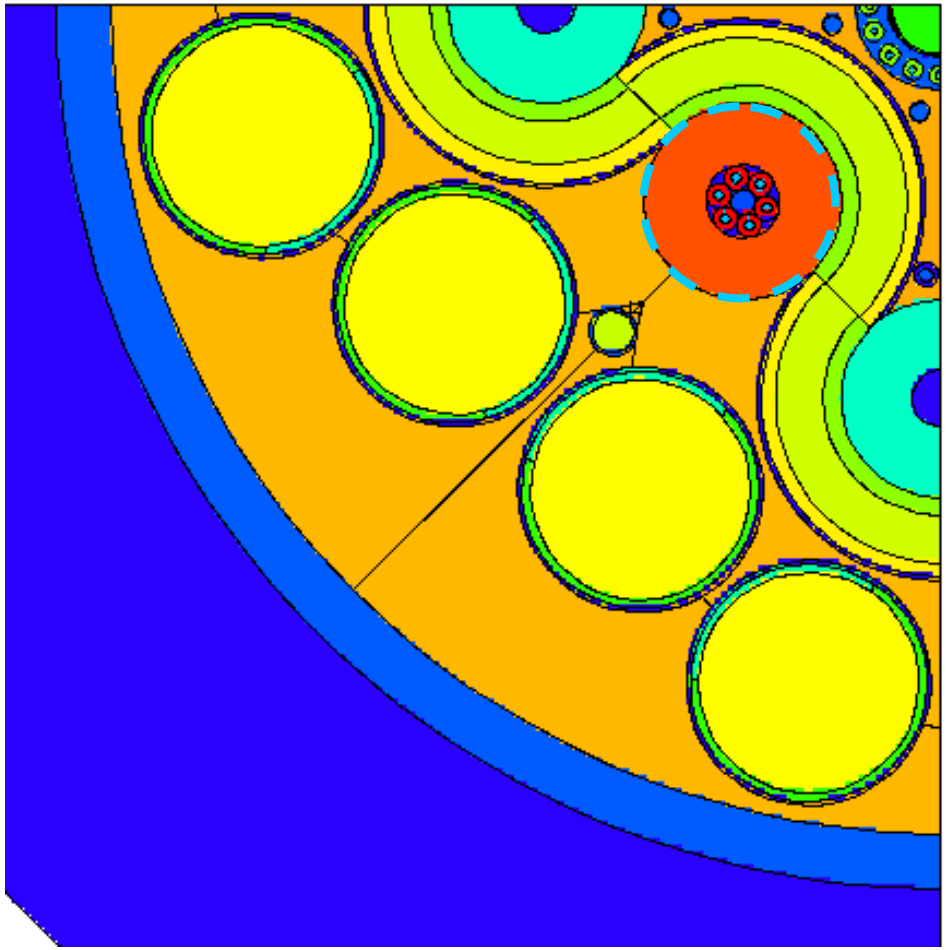
Step 4: Viewing Results in Visit



Neutronic Analysis: Surface Source "Substitution" Approach

- Overview of two surface source read/write (SSR/W) techniques (both available to users; substitution technique is the focus here)
  - Idea: use MCNP5 RSSA files to impose boundary conditions at experiment positions
- Analyses can be carried out
  - **stand-alone:** create geometries within MCNP5
  - **from CAD-software** via interface to DAGMC.
- *Users write their own reaction rate tallies (exception: heating mesh tallies)*

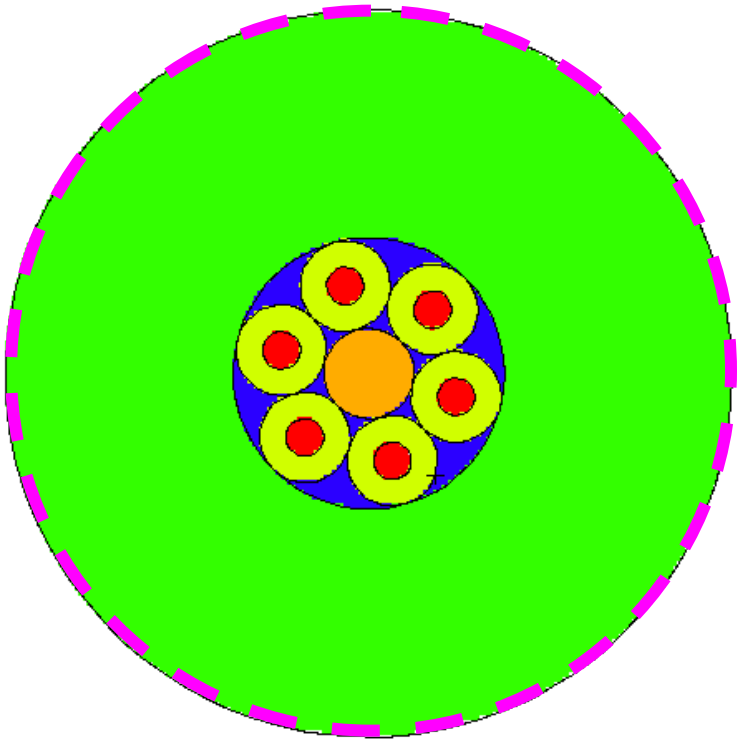
Substitution Approach, Step 1



KCODE (eigenvalue) calculation on full core with representative specimens *(surrogates)* in experiment position

Use SSW to write to surface(s) enclosing position (as many mean free paths from the trap as feasible)

Substitution Approach, 2



This step is completed by users. The model supplied to you (CAD & MCNP5) consists only of the region inside SSR surfaces.

You create your experiment geometries (in MCNP5 or CAD via DAGMC) and run an MCNP5 transport calculation using surface sources **(RSSA files)** we supply.

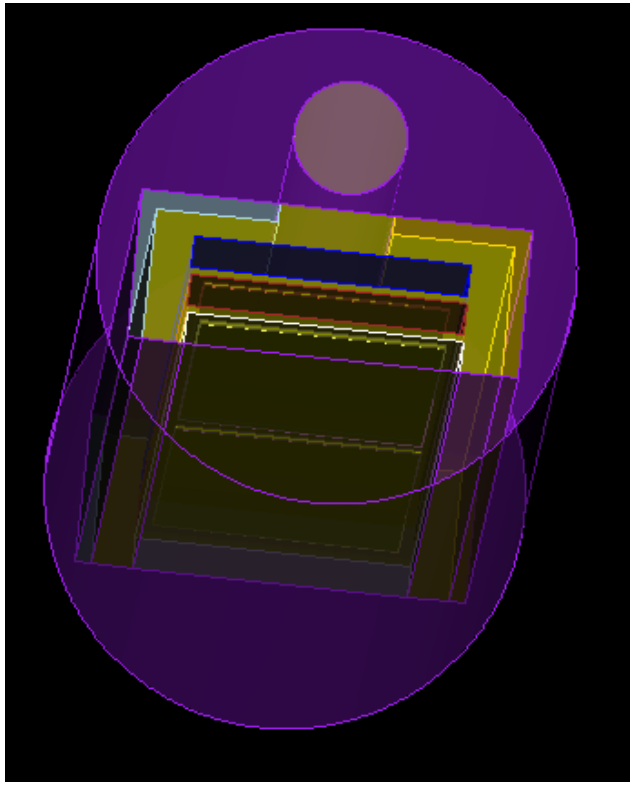
Products

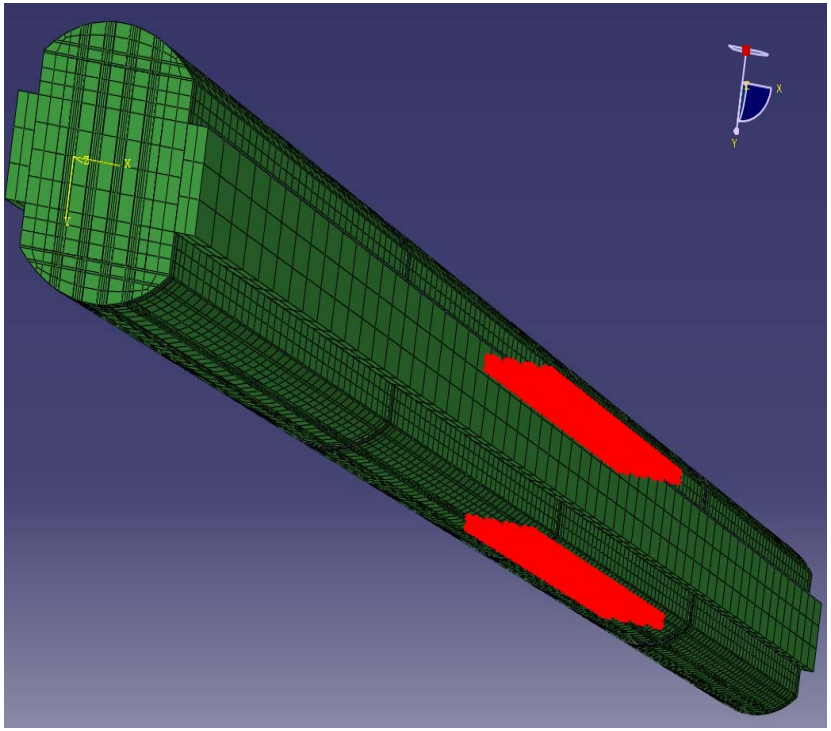
- Software products include
  - **Surface source (RSSA) files ready to be read by MCNP5;**
  - **MCNP5 'template' decks for experiment positions;**
  - **SolidWorks 'template' files for experiment positions.**

- Software is available for
  - large B (B11), small B (B5), an inner and outer A, center, south and southwest flux traps.

- User guide includes walkthrough for using RSSA files and MCNP5 decks

Thermal Analysis: Coupling DAGMC to ABAQUS





Workflow

CAD model
- Describe geometry
- Add material tags

Cubit
- Imprint/Merge
- Assign materials
- Vacuum

MCNP
- Define materials
- Import Source
- Mesh tallies

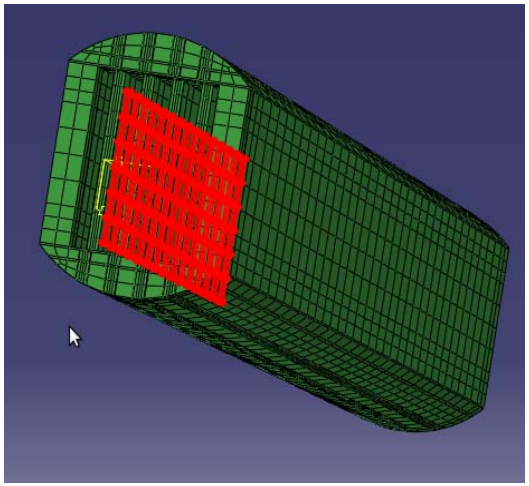
Abaqus
- Tetrahedral mesh
- Create assembly
- Import materials

MOAB
- Common mesh format
- Interpolate between meshes

Abaqus
- Fine resolution heat flux

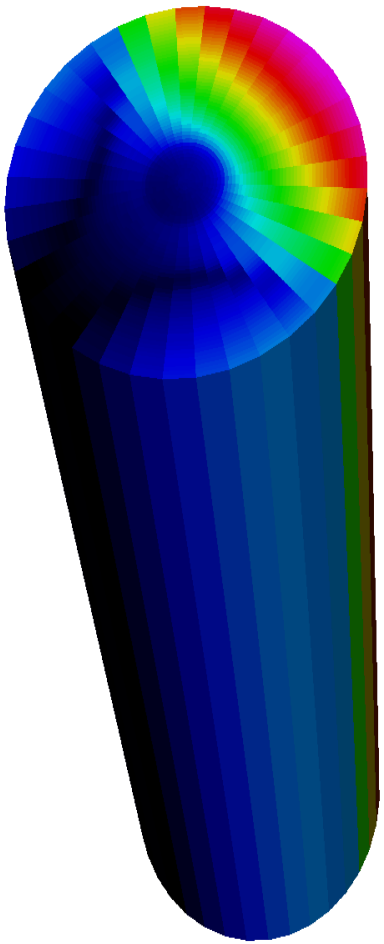
Motivation

- Automate assignment of heat fluxes in Abaqus:
  - support arbitrary mesh resolution
  - (DAG)MCNP heating data supplied via energy deposition mesh tallies



- Use the same geometric model in all steps of the analysis

MOAB



- Mesh Oreiented dAtaBase

- Used here to convert between two meshes

- Interfaces with many different packages:
  - Visit
  - MCNP
  - ExodusII
  - Cubit

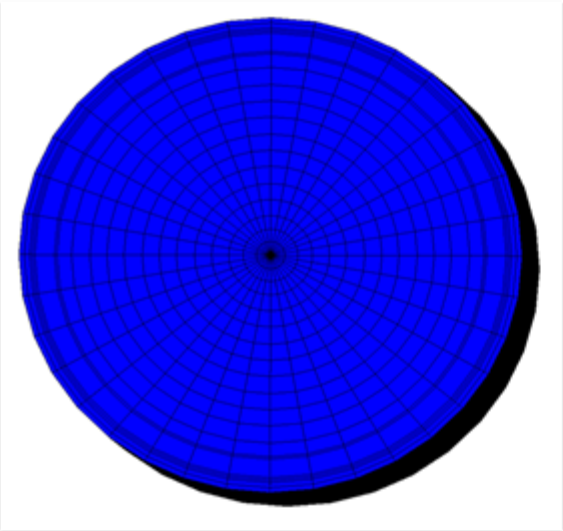
- Native mesh translator included to interpolate MCNP tally geometry onto Abaqus mesh

Mesh Interpolation

- Run MCNP with heating mesh tally and import mesh tally and Abaqus mesh into MOAB

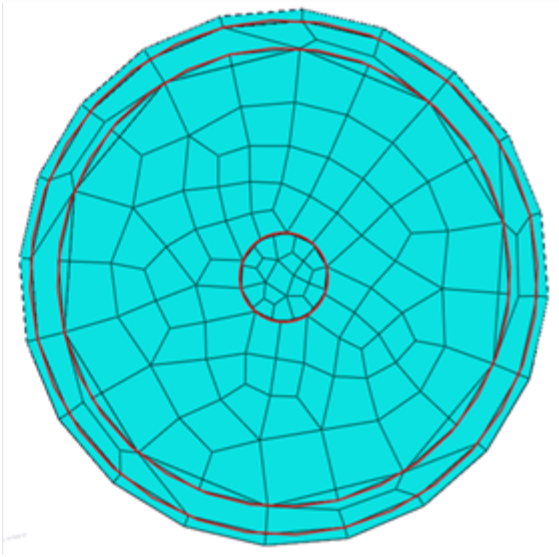
- Via MOAB the problem depicted below is resolved to obtain volumetric power deposition for each Abaqus mesh element:

Body Independent Mesh



MCNP

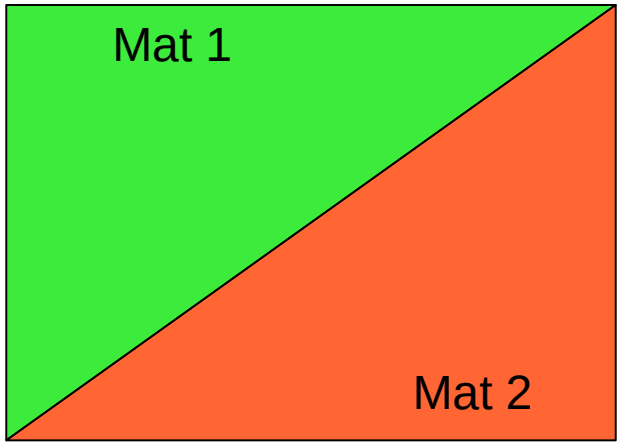
Body Fitted Mesh



Abaqus

Interpolation - The Problem

MCNP mesh element



- **Both mat1 and mat2 contribute to the energy deposition reported in the MCNP mesh tally:**

- the MCNP mesh tally reflects volume-weighted contributions from each material, but…

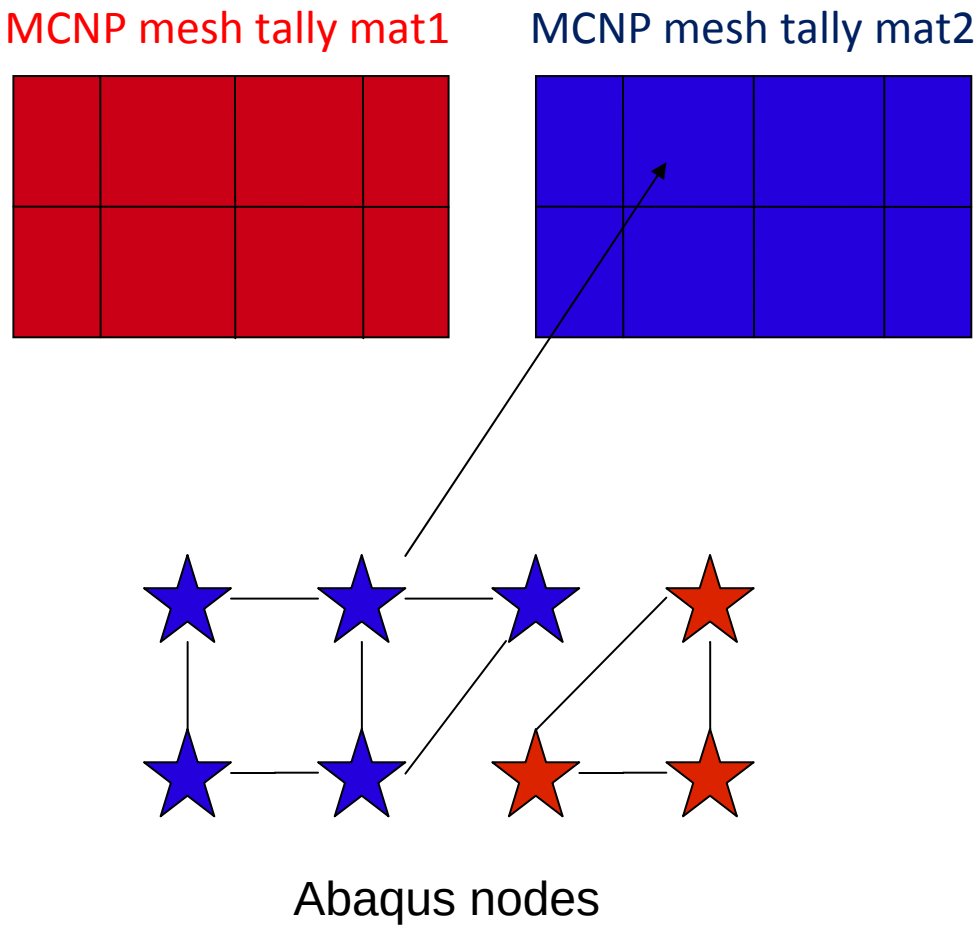
- … each element in Abaqus (green/orange shaded areas) is only comprised of one material

Interpolation – Solution

- Create one MCNP mesh tally for each material in the geometry

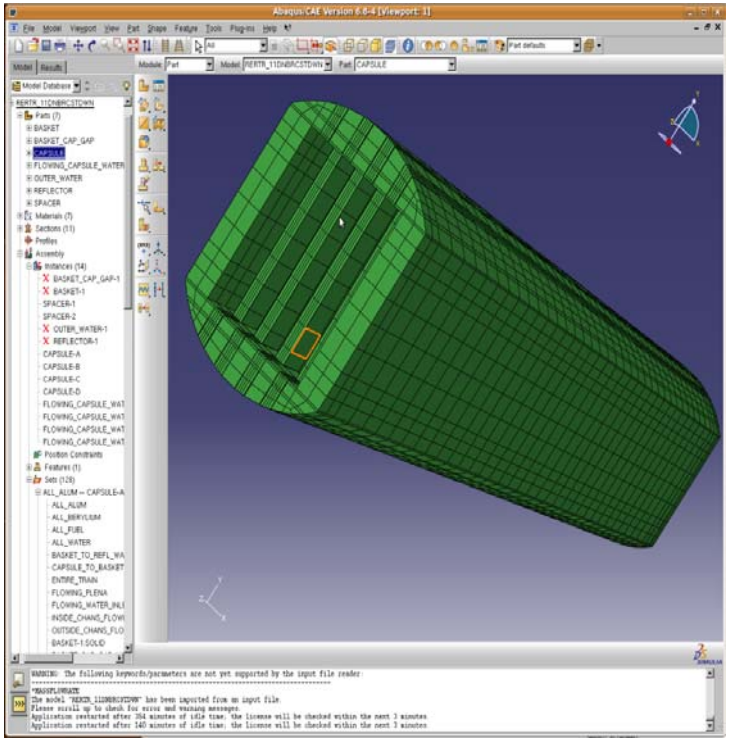
  - MCNP computes the power deposition as if the entire geometry were filled with that material, *independently from its radiation transport calculation*

- Obtain heat flux in each Abaqus node from the mesh tally generated for the material in that abaqus node (red and blue in the illustration)



Process for Abaqus Analysis

- Import CAD geometry
- Add meshes, and create/assign materials
- Create assembly
- Write .inp file and read into MOAB
- Run scripts to interpolate MCNP mesh tallies onto Abaqus mesh
- Write heat data to .inp file
- Add any ancillary inputs to Abaqus model
- Run Abaqus



Resources / References

- DAGMC
  - to obtain DAGMC, please visit http://cnerg.engr.wisc.edu/cgi-bin/index.cgi/wiki?p=DirectAcceleratedGeometryMonteCarlo
  - this site also features walkthroughs for installation, configuration and execution of the software
  - it also provides links to sites hosting the applications **MOAB** and **CUBIT**

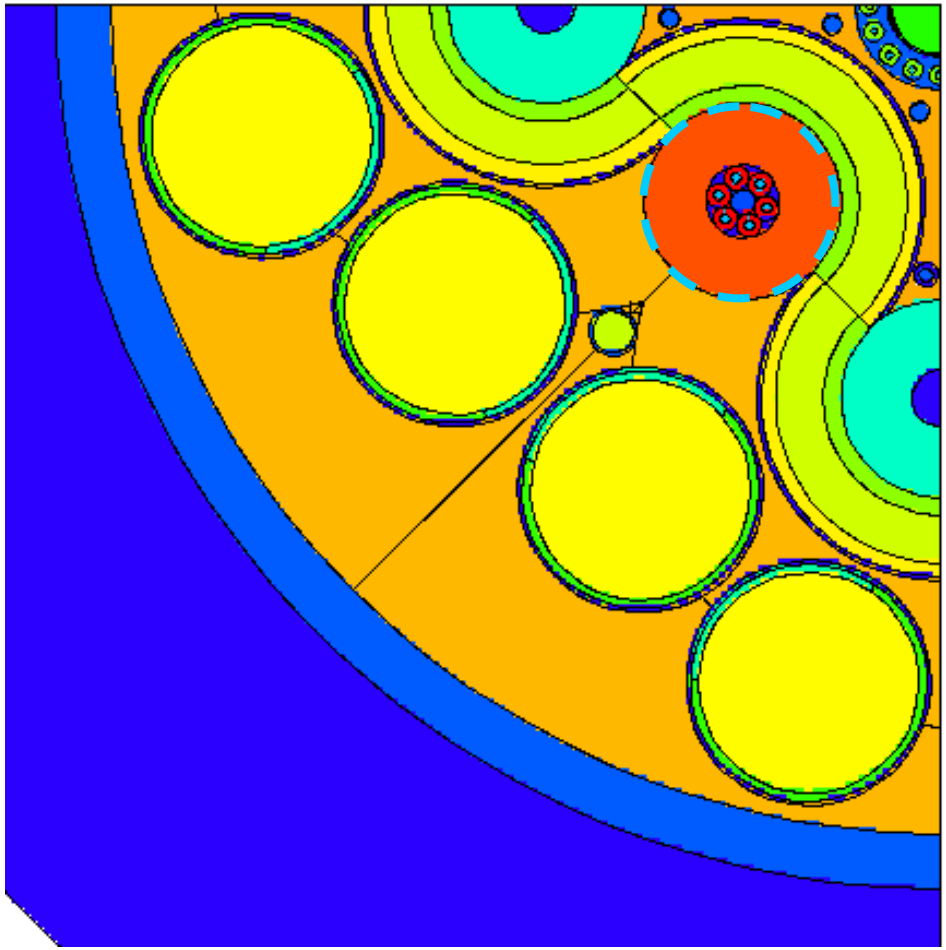
- Full documentation of the workflow and a detailed step-by-step walkthrough may be found in:
  - **P.P.H. Wilson, P. Snouffer, E.A. Schneider, J.L. Peterson, "Demonstrating High-Fidelity Coupled Neutronic and Thermal Analysis of ATR Experiments: A 2009 ATR Faculty Student Research Team Project," technical report (2009).**

- For theoretical background and benchmarking studies on the surface-source method, see
  - **P.P.H. Wilson, P. Snouffer, E.A. Schneider, J.L. Peterson, "A Monte Carlo Surface Source Method for Advanced Test Reactor Experiment Prototyping," Proc. PHYSOR 2010, Pittsburgh, PA, May (2010).**

Neutronic Analysis: Supplemental Information

- Overview of two surface source read/write (SSR/W) techniques (both available to users)
  - Idea: use MCNP5 RSSA files to impose boundary conditions at experiment positions
- Refinement of methods via simulation of existing experiments
- Benchmarking and validation
  - full transport (eigenvalue calculation) versus SSR/W techniques

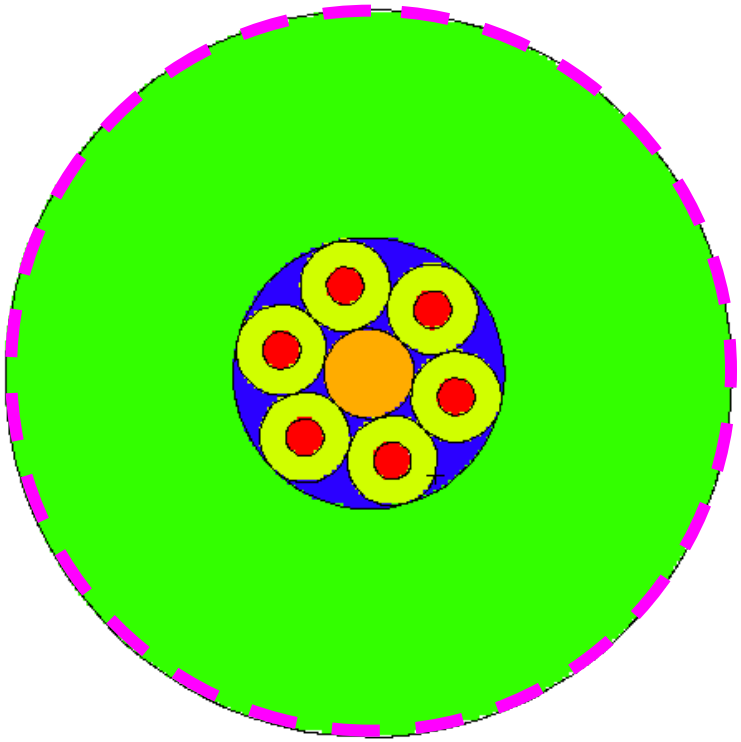
SSW/R Techniques: **Substitution Approach**, Step 1



KCODE (eigenvalue) calculation on full core with representative specimens *(surrogates)* in experiment position

Use SSW to write to surface(s) enclosing position (as many mean free paths from the trap as feasible)

Substitution Approach, 2



This step is completed by users. The model supplied to you consists only of the region inside SSR surfaces.

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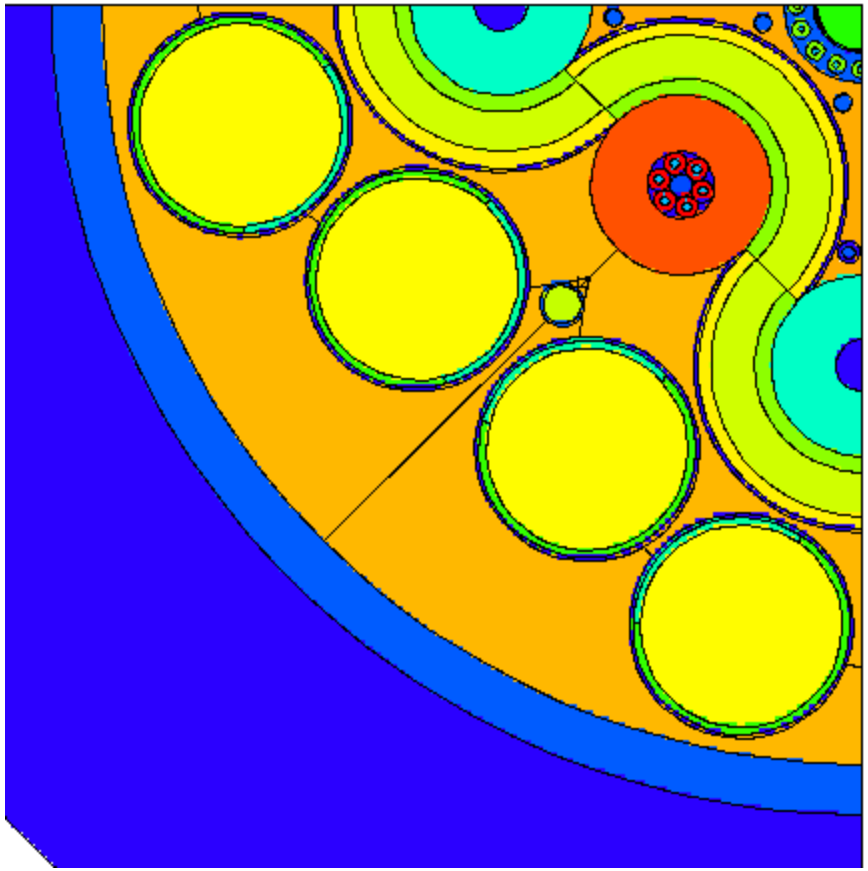
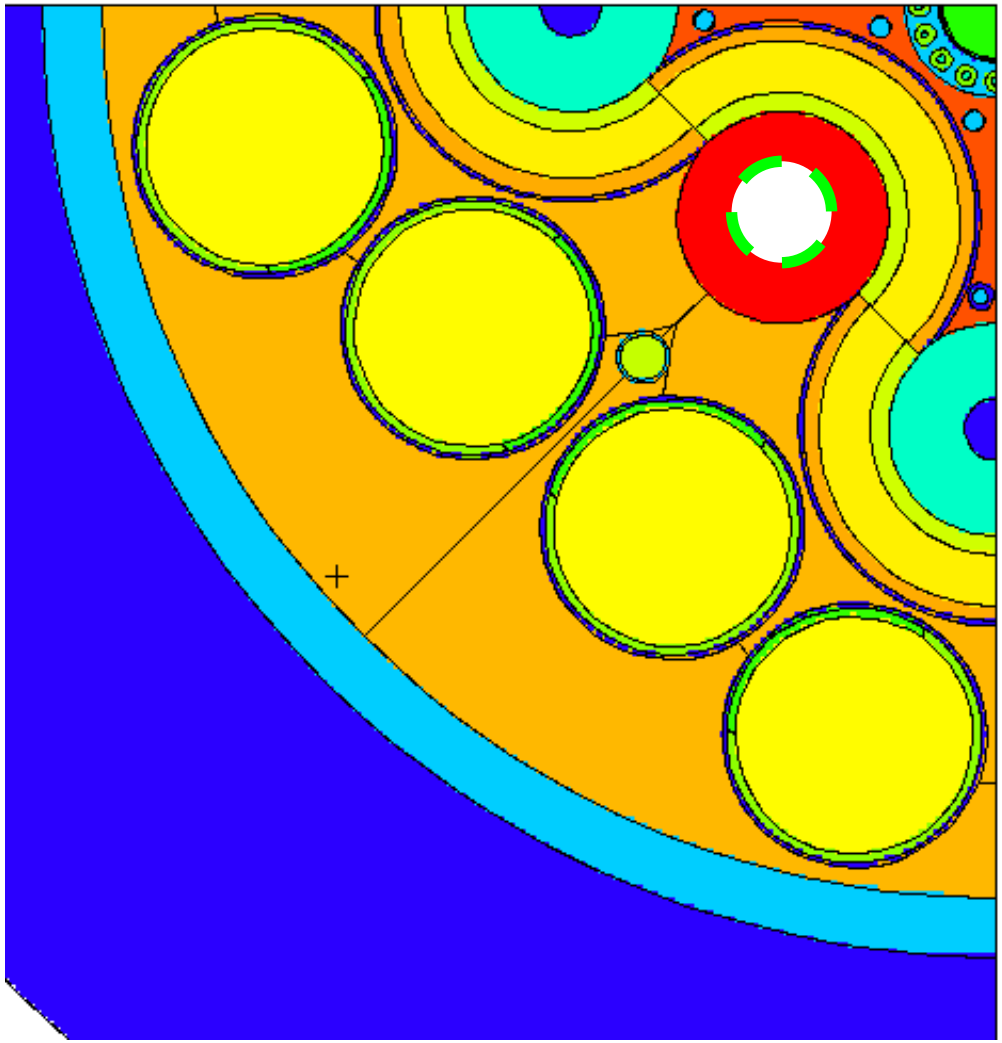
Superposition Approach, Step 1



A KCODE calculation is run on the full core model with default specimens in experiment positions

The MCNP5 SSW CEL command is used to write the fission neutron source distribution. This step must only be done once.

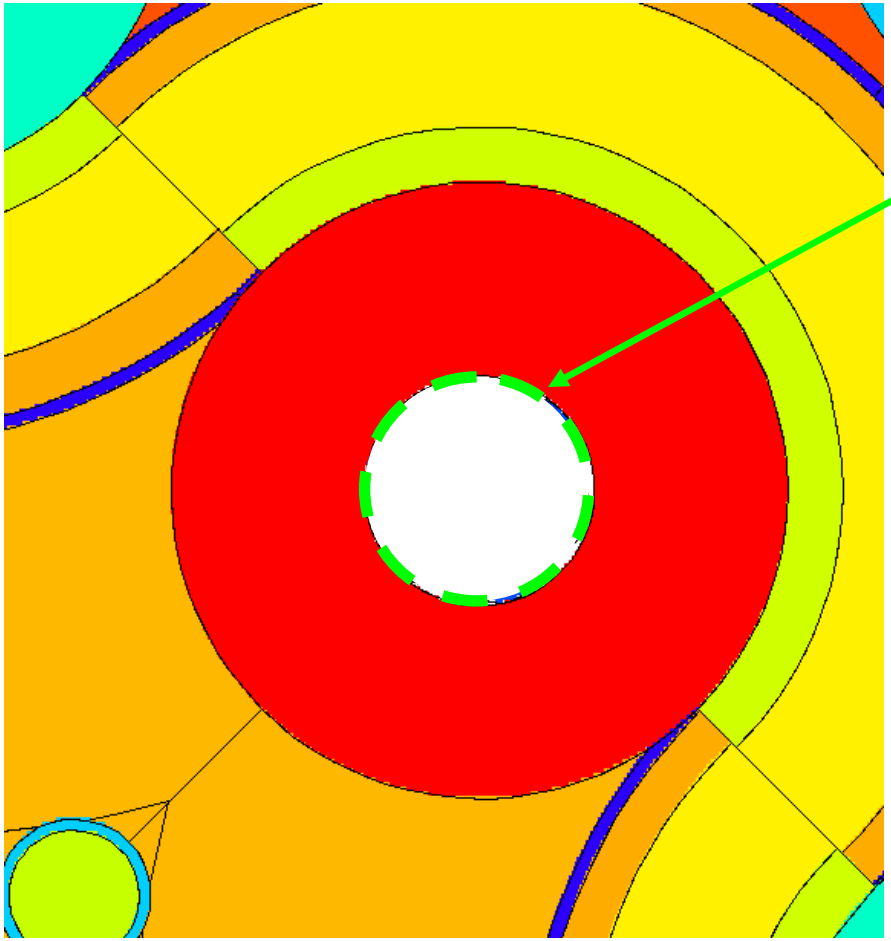
Superposition Approach, 2



SSR calculation on full core with nonu=0 (fission neutrons not produced; prompt gammas produced) to read fission source distribution

Use SSW to write crossings into test region of zero importance (next slide)

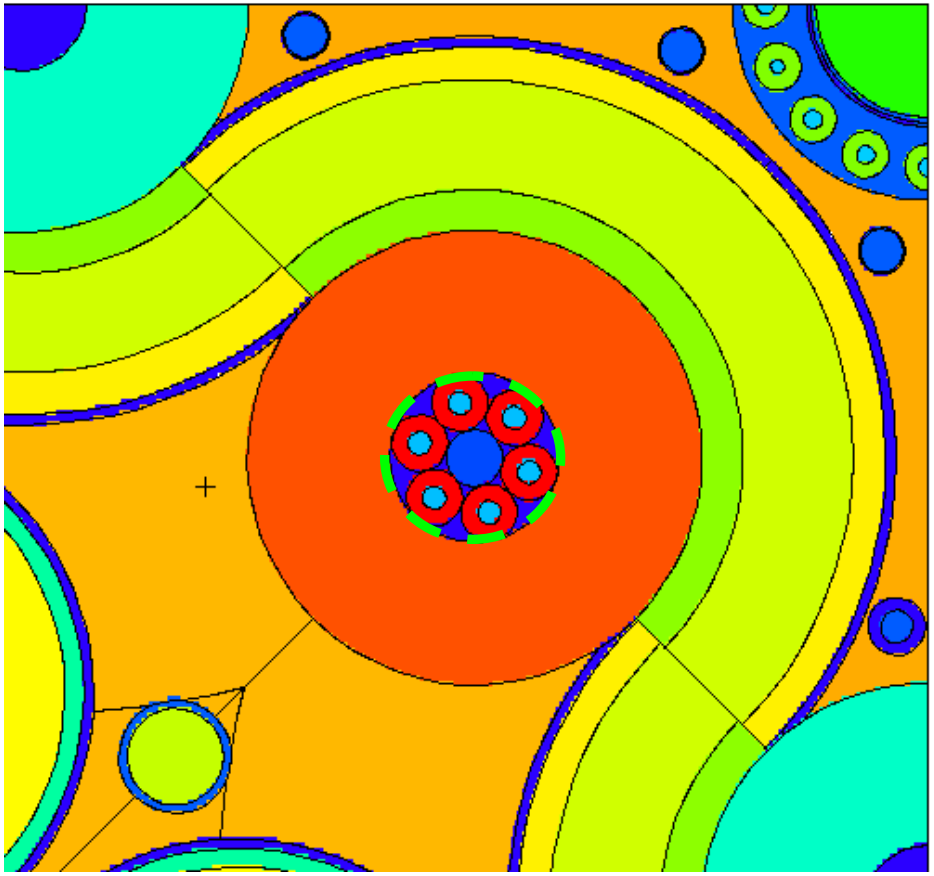
Superposition Approach, 2



In this approach, it's advantageous to 'bank' only particles crossing into the region whose contents might change.

Steps 1 and 2 are carried out in advance. **The user performs only Step 3:**

Superposition Approach, 3



You work with a full core model *but only modify the region within the SSR surface(s)*.

You run a fixed-source calculation using the supplied RSSA file. nonu=0 (no fission n produced) outside the SSR surface(s) and, if necessary, nonu=1 (both n and γ produced) inside

Superposition: Summary

- Summing results of calculations 2) and 3) gives (approximate) full depiction of population in core
  - Like running 1 KCODE iteration
  - Can provide estimate of reactivity worth of experiment
- Advantageous to place SSR/SSW surface as close to samples as possible
  - Substitution functions best when SSR/SSW is far from samples
- Substitution approach aims to capture inside-of-trap transport effects of actual specimen through use of representative surrogates
- Superposition eliminates the need for surrogates but the geometry for the SSR run must extend well beyond the experiment position

Refinement of Methods

- Issues we quantitatively investigated:
  - Substitution
    - Importance of surrogate
    - Sensitivity to size of ‘cutout’ region
  - Superposition
    - Comparison to substitution method
  - Both
    - Applicability to photon as well as neutron transport
- Approach: study existing experiments in a variety of locations, quantify fidelity level

Qualitative Experiment 'Categories'

The fidelity of the substitution approach depends on the choice of surrogate. A surrogate that is qualitatively similar to the experiment being analyzed would be expected to affect the flux at the SSR/W boundary in a similar way.

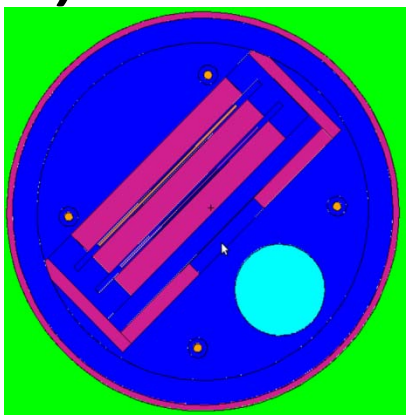
We defined the following four categories and identified surrogates for each from a pool of existing experiments:

	Strong Thermal Absorber Absent	**Strong Thermal Absorber Present**
Multiplying Medium Absent	Aluminum filler rods	Hafnium aluminide experiment
Multiplying Medium Present	AFIP experiment	AFCI experiment (with Cd)

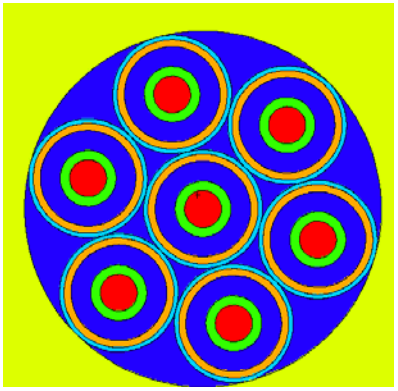
Experiment Models

To investigate the effectiveness of the surrogate approach, additional experiments were modeled and classified by 'category.' These were used to quantify the sensitivity of the substitution method to surrogate 'category.'

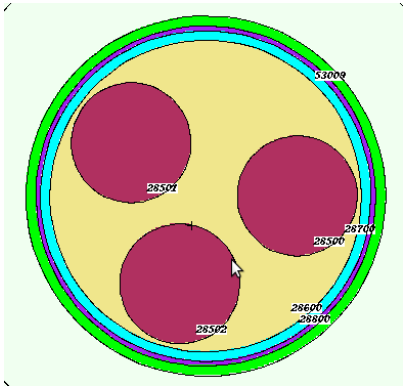
ATR Full Size Plates (AFIP)



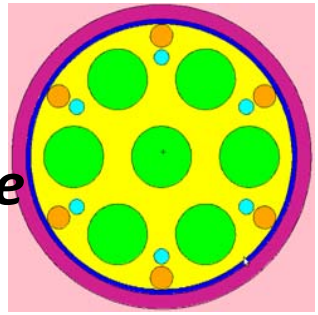
AFCI Metallic Fuel



Advanced Gas Reactor (AGR) Fuel



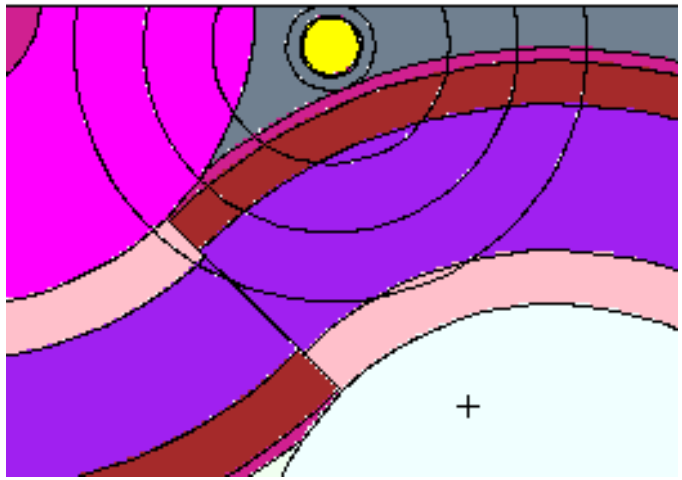
Graphite Irradiation Creep Capsule (AGC-1)



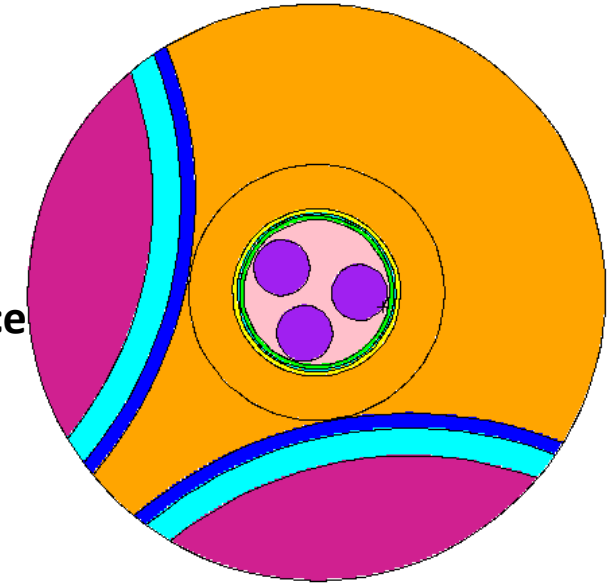
Sensitivity Studies: Surrogates and Radii

	Surrogate	Trial
Non-multiplying, non-absorbing	Aluminum filler rods	Graphite pins (AGC-1)
Non-multiplying, absorbing	Hafnium aluminide experiment	Cobalt rodlets
Multiplying, non-absorbing	AFIP experiment	AGR experiment
Multiplying, absorbing	AFCI experiment (with Cd)	AGR experiment with hafnium shell

Outer A Position: Candidate Surface Source Locations (5)

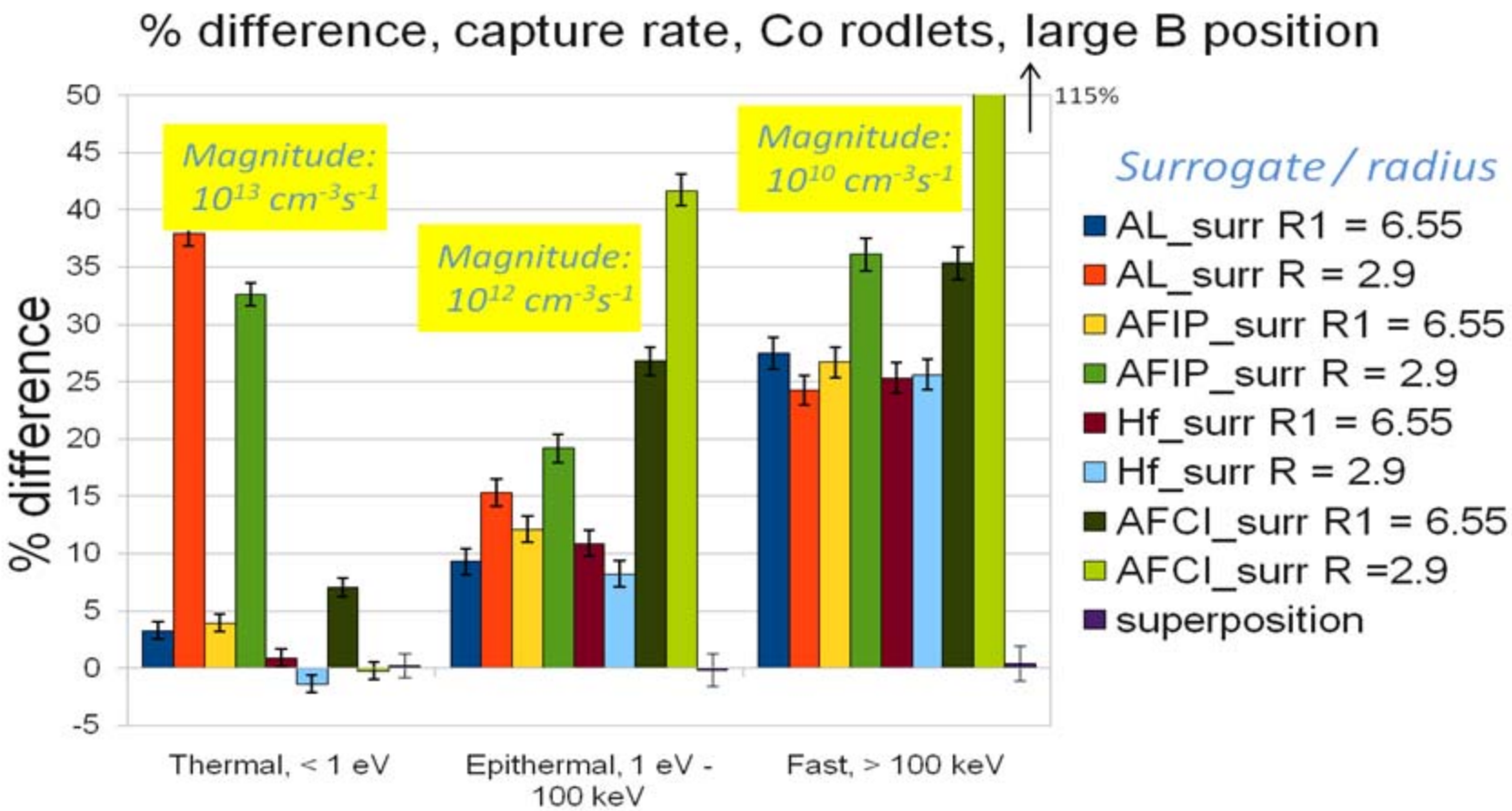


Large B Position: Candidate Surface Source Locations (2)



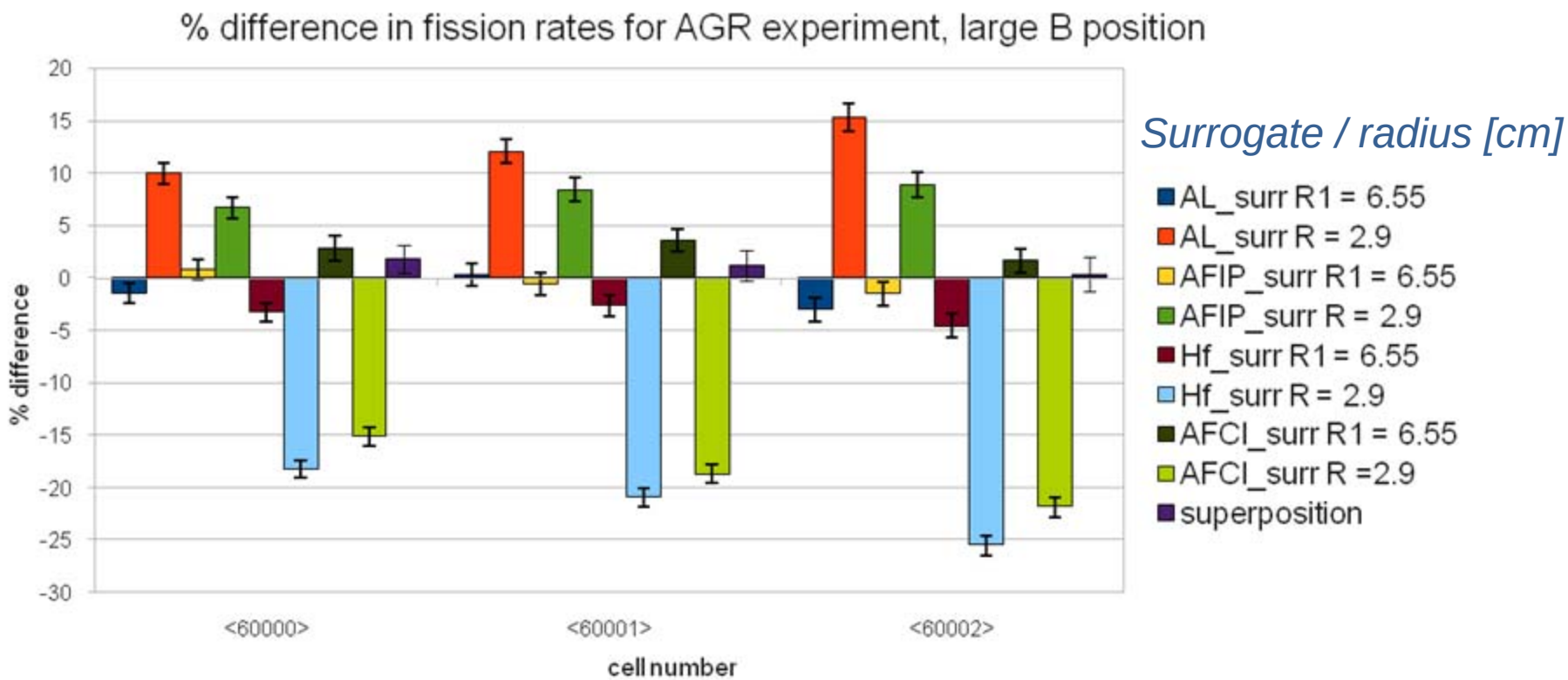
Surrogate & SSW/R Radius I

Cobalt rodlets experiment. The qualitatively 'close' surrogate is Hf, which shows the best agreement at both radii for the substitution approach. Superposition performs well at all flux traps as well as positions farther from the fuel.



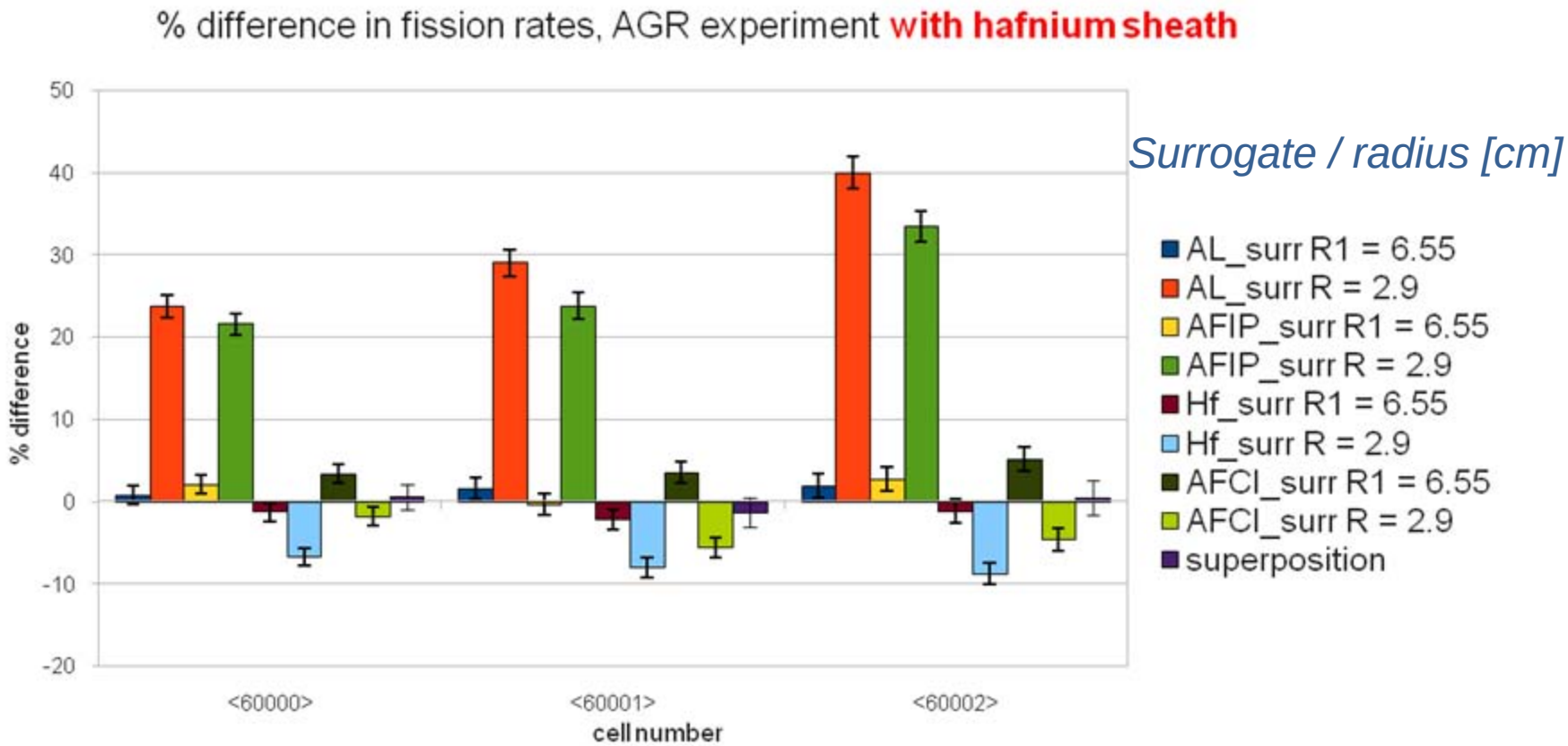
Surrogate & SSW/R Radius II

AGR experiment, no Hf sheath. The figures on this and the next slide illustrate the critical role of the surrogate in the substitution approach, particularly if the volume enclosed by the SSW/R is small. Here the AFIP surrogate is expected to be best.



Surrogate & SSW/R Radius III

AGR experiment, Hf sheath. When the sheath is included, the AFCI surrogate is expected to be most appropriate (and on this occasion, it proves to be the case). Note that the smaller SSW/R (dimension chosen to avoid cutting the adjacent control drum) remains extremely sensitive to surrogate choice.



These tables integrate all experiment / surrogate / radius studies performed for the large B position:

Large B position surrogate study (smaller SSW/R radius: 2.9 cm)

differences: (SSW – benchmark) / (benchmark)

Color codes:
Green: < 10%
Yellow: 10 – 20%
Red: > 20%

% difference in DPA in Iron at r=2.9 cm

		Surrogates			
		Al	AFIP	Hf	AFCI
Experiments	Graphite	2.3	3.9	1.3	36.9
	AGR	5.5	5.7	15.2	1.2
	Co	2.0	4.3	0.4	41.2
	AGR(Hf)	14.8	15.1	5.1	16.1

% difference in TOTAL power deposition at r=2.9 cm (W/cc)

		Surrogates			
		Al	AFIP	Hf	AFCI
Experiments	Graphite	0.6	0.6	2.9	3.9
	AGR	12.3	7.9	21.4	18.4
	Co	7.8	6.4	8.3	2.5
	AGR(Hf)	30.5	25.9	7.7	3.9

% difference in capture rate at r=2.9 cm (capture/cc)

		Surrogates			
		Al	AFIP	Hf	AFCI
Experiments	Graphite	4.8	8.0	32.9	31.6
	AGR	7.5	5.1	21.7	14.7
	Co	33.2	29.8	0.7	8.6
	AGR(Hf)	10.6	16.9	9.4	4.3

% difference in fission rates r=2.9 cm (fission/cc)

		Surrogates			
		Al	AFIP	Hf	AFCI
Experiments	Graphite	n/a	n/a	n/a	n/a
	AGR	12.5	8.0	21.6	18.6
	Co	n/a	n/a	n/a	n/a
	AGR(Hf)	30.9	26.3	7.8	4.0

Large B position surrogate study (larger SSW/R radius: 6.55 cm)

differences: (SSW – benchmark) / (benchmark)

Color codes:

Green: < 10%

Yellow: 10 – 20%

Red: > 20%

% difference in DPA in Iron at r=6.55 cm

		Surrogates			
		Al	AFIP	Hf	AFCI
Experiments	Graphite	1.1	1.1	1.8	3.5
	AGR	1.9	2.7	0.5	6.8
	Co	0.2	1.3	1.0	3.4
	AGR(Hf)	2.6	2.8	1.0	6.9

% difference in TOTAL power deposition at r=6.55 cm (W/cc)

		Surrogates			
		Al	AFIP	Hf	AFCI
Experiments	Graphite	0.9	0.3	1.2	1.3
	AGR	1.6	0.9	3.5	2.6
	Co	5.4	4.8	6.8	1.5
	AGR(Hf)	1.4	1.7	1.5	4.0

% difference in capture rate at r=6.55 cm (capture/cc)

		Surrogates			
		Al	AFIP	Hf	AFCI
Experiments	Graphite	1.2	0.6	3.7	2.2
	AGR	2.1	1.8	4.5	4.3
	Co	4.6	5.7	3.0	11.2
	AGR(Hf)	1.0	2.9	3.0	7.3

% difference in fission rates r=6.55 cm (fission/cc)

		Surrogates			
		Al	AFIP	Hf	AFCI
Experiments	Graphite	n/a	n/a	n/a	n/a
	AGR	1.6	0.9	3.5	2.7
	Co	n/a	n/a	n/a	n/a
	AGR(Hf)	1.4	1.7	1.5	4.0

Conclusion

- Substitution works well (< 10% error) provided that surface source placed far (several mfp) from site of perturbation
- Superposition led to < 10% error in all investigated cases, but requires that users manipulate the full-core model
- Both approaches reduce execution times by about two orders of magnitude (for comparable statistics) as compared to a full KCODE analysis