Neutronics Analysis for Irradiation Experiment Design

ATR National Scientific User Facility Workshop
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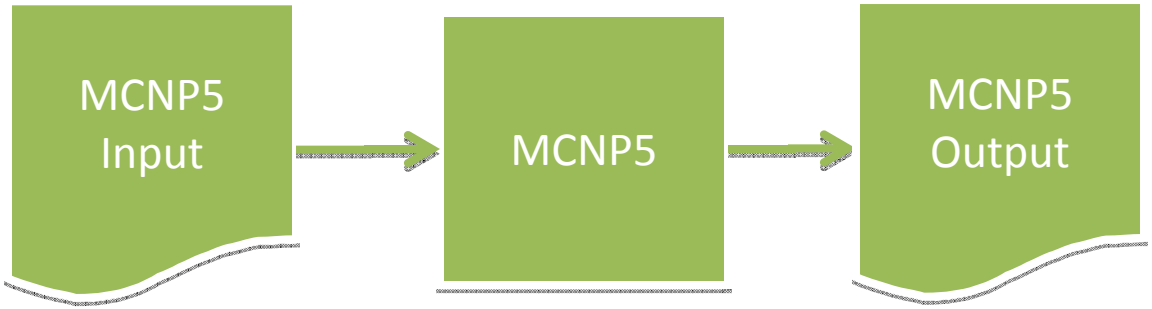
Overview

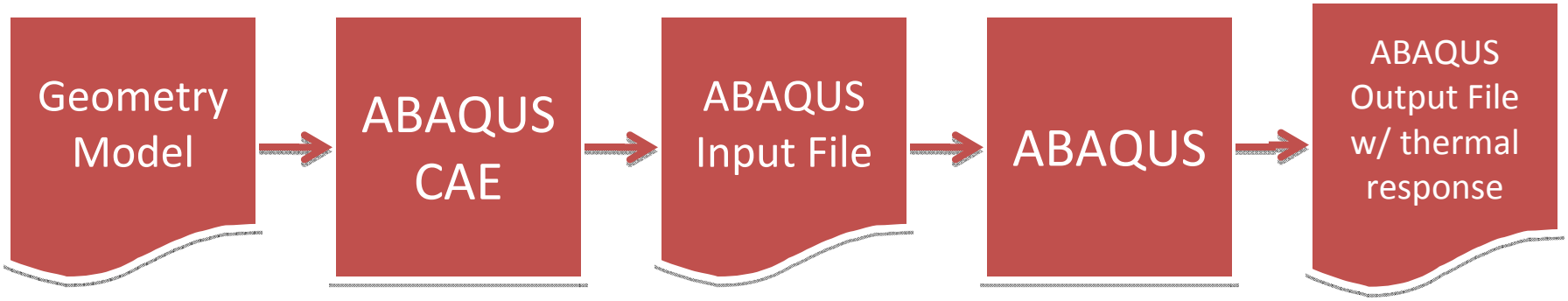
- Motivations
- Substitution Method
- Dagmc workflow front end
- Dagmc workflow backend
- Conclusions

Motivation

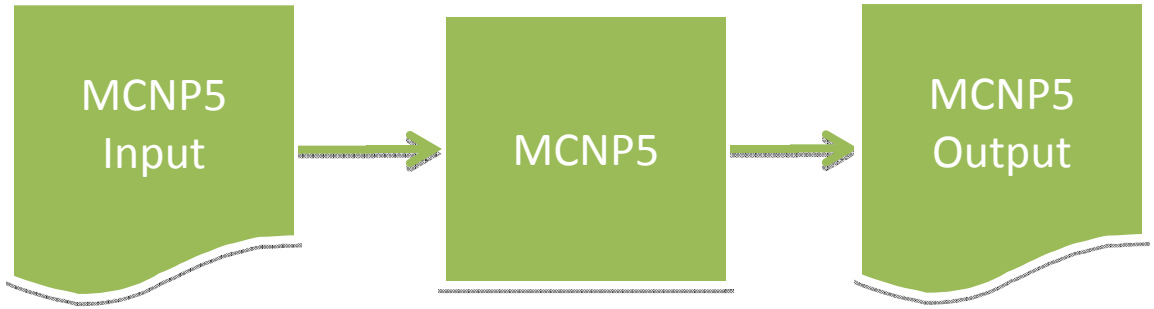
- Create a fast, simple method for experimenters to characterize NSUF experiments with minimal dependence on INL staff
  - focus: support the proposal-writing stage of experiment design
  - fidelity: 10% deviation in major experiment metrics versus full radiation transport analysis
  - ease of use: MCNP5 and CAD-to-DAGMC support, users need only create a stand-alone CAD model of the experimental position
    - Reduce learning curve for new experimenters
    - Reduce computational requirements
    - Increase fidelity of analysis
    - Allow for rapid design iterations

Workflow


MCNP5 Input
MCNP5
MCNP5 Output


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
Moc

BAQUS
tput File
thermal
esponse

Workflow

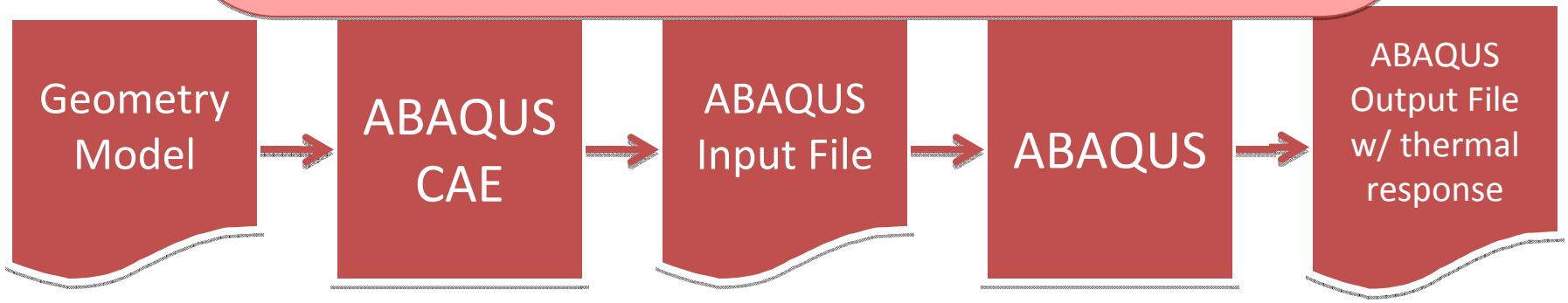
Manual transfer of heating data from MCNP->ABAQUS

Requires

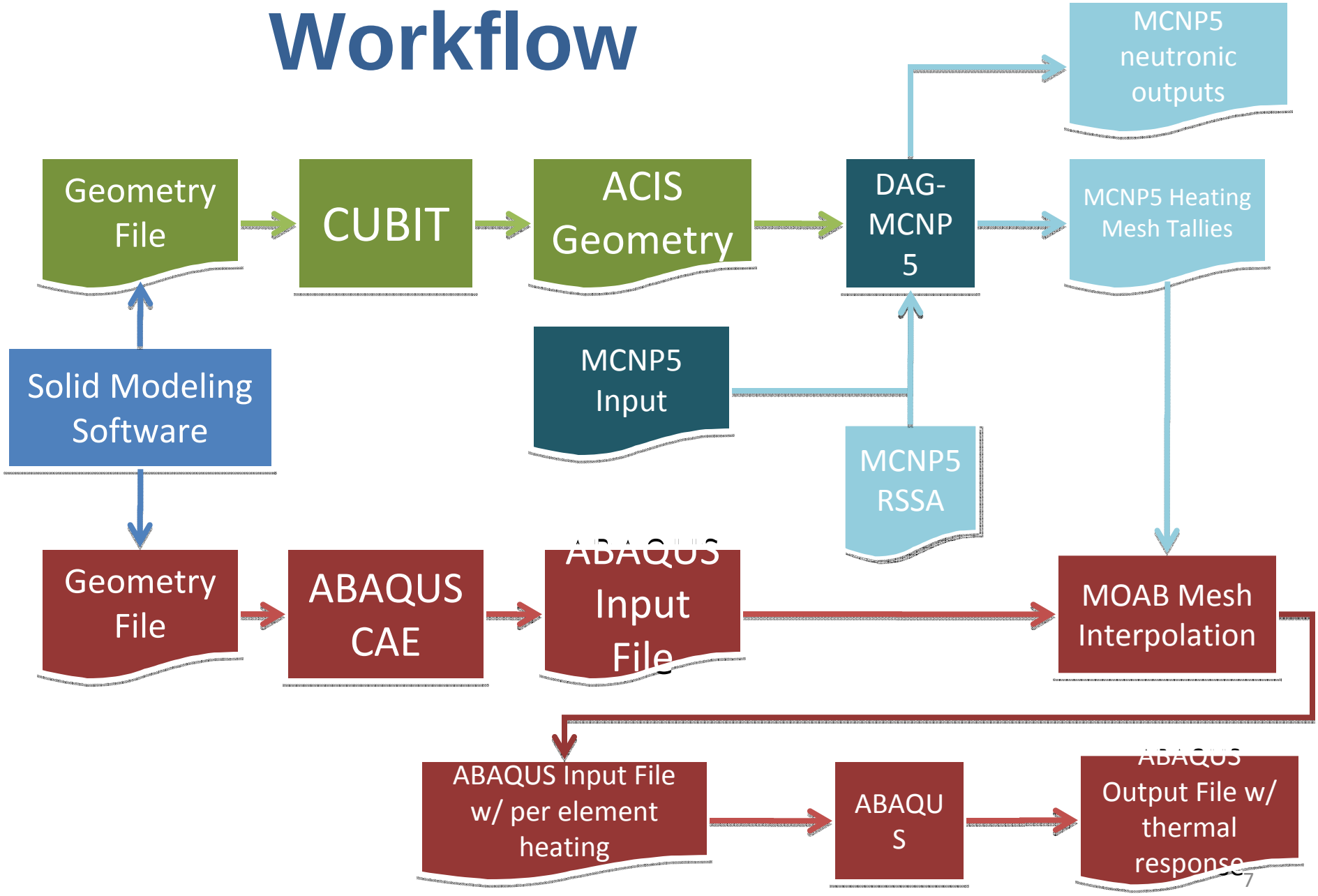
substantial simplification

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 Features: Advanced Geometry

- Replace manual geometry description with CAD-based geometry
  - Assume many experimenters already use solid modeling software in their experiment design
    - (e.g. SolidWorks, Pro/Engineer, AutoCAD)
  - Reduce human effort
  - Reduce error
  - Improve complexity of models
  - Assign materials directly in their solid model

Workflow Features: Local Fixed Source

- Modeling entire reactor requires large computer resources and complex input
- Different experiments have little impact on overall radiation field
- Predefine source based on a nominal experiment configuration
- Re-use as a fixed source
  - Smaller computer resource needs
  - Simpler input

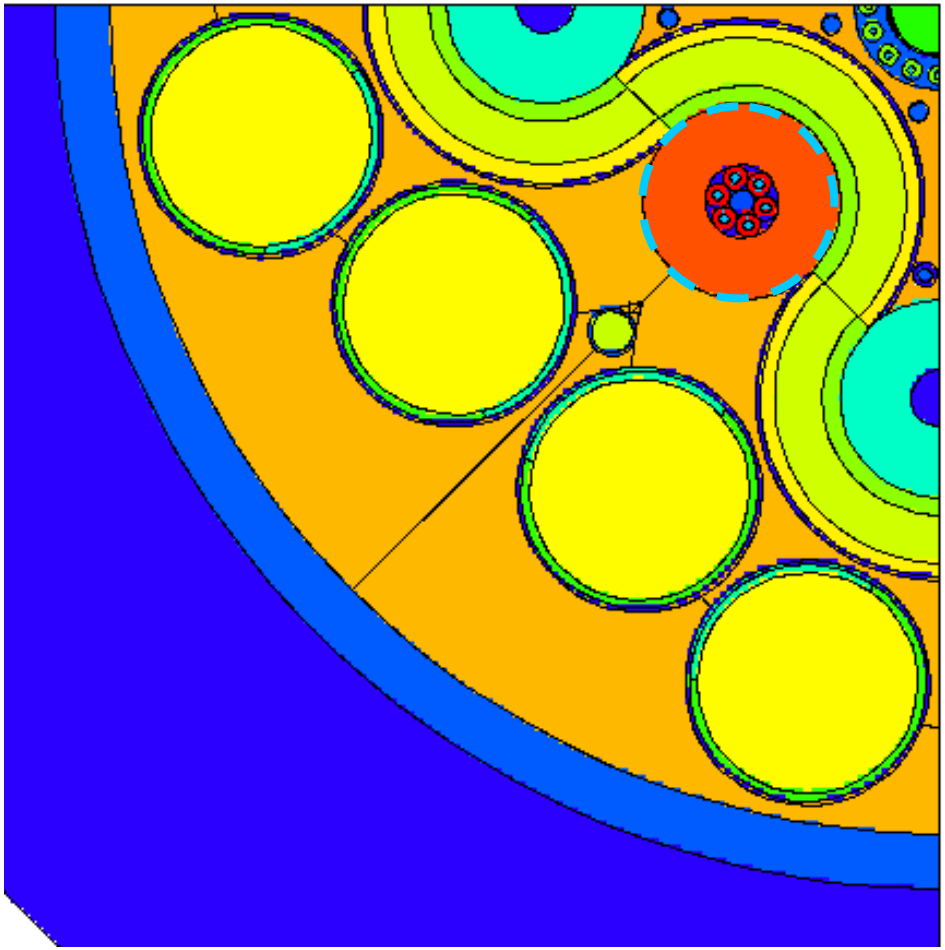
Workflow Features: Coupled High-Fidelity

- Automate transfer of nuclear heating to thermal analysis
- Use same solid model for thermal analysis
- New opportunity for fidelity
  - Local temperature peaks
  - Temperature gradients

Neutronic Analysis: Surface Source "Substitution" Approach

- Overview of the surface source read/write (SSR/W) technique developed to prepare **downloadable MCNP5 surface source files for each experiment position**
  - 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 (or specify them inside CUBIT)*

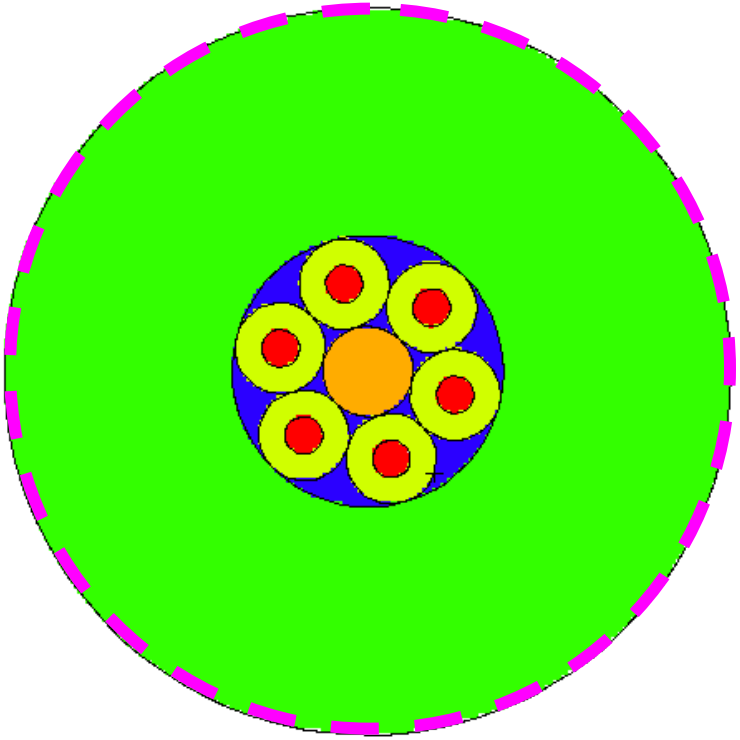
Substitution Approach, Step 1



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 models available to you (CAD & MCNP5) consist only of the region inside SSR surfaces.

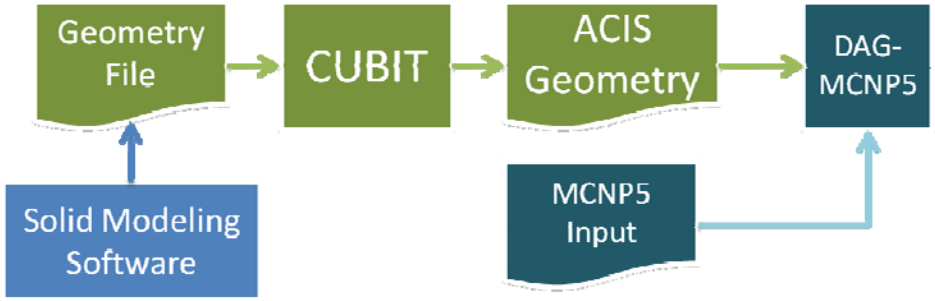
You create your experiment geometries (in MCNP5 or CAD via DAGMC) and run an MCNP5/DAGMC transport calculation using surface sources **(RSSA files)** we supply.

Products

- Downloadable software products supporting this part of the workflow include
  - **The DAGMC software (MCNP5 also required);**
  - **Surface source (RSSA) files ready to be read by MCNP5 or DAGMC;**
  - **Script file for performing CUBIT operations;**
  - **Sample 'legend' file for mapping SolidWorks tags to MCNP5 material identifiers;**
  - **MCNP5 template decks for experiment positions;**
  - **SolidWorks template files for experiment positions.**

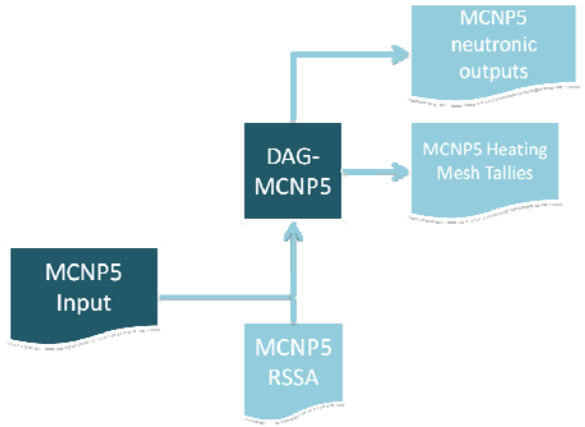
Workflow Components

Geometry: CAD to DAG-MCNP5

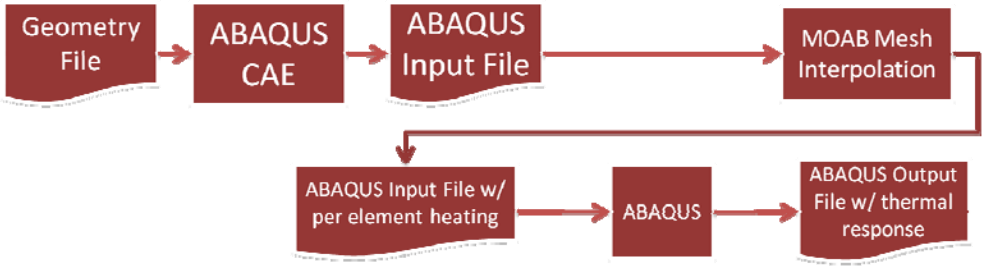


Neutronic Analysis:

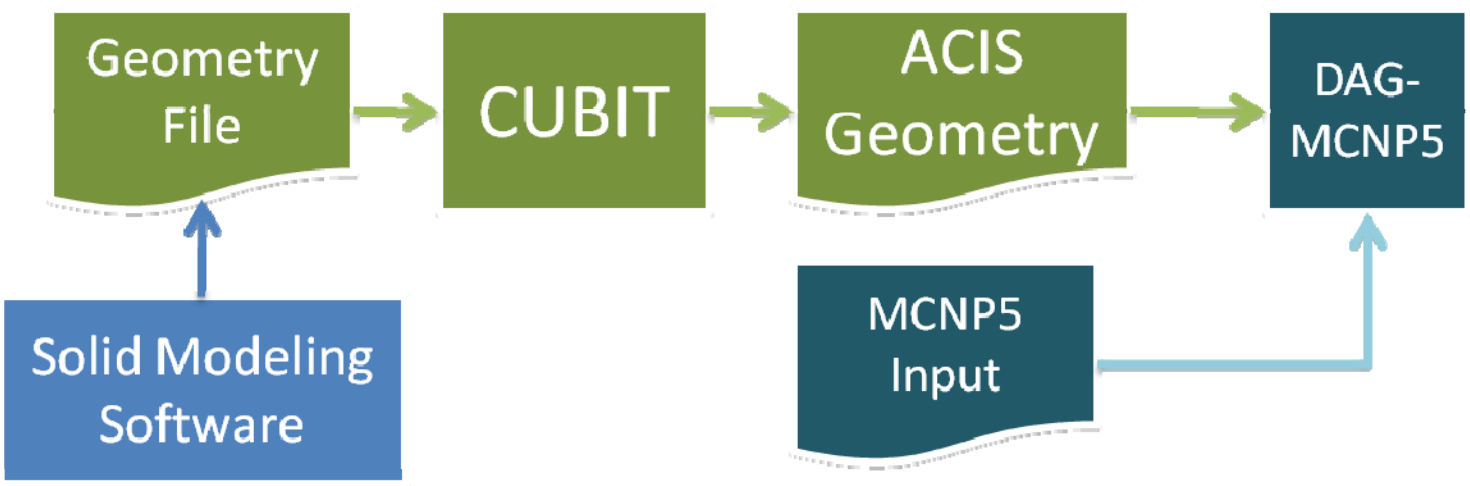
Surface Source Approach



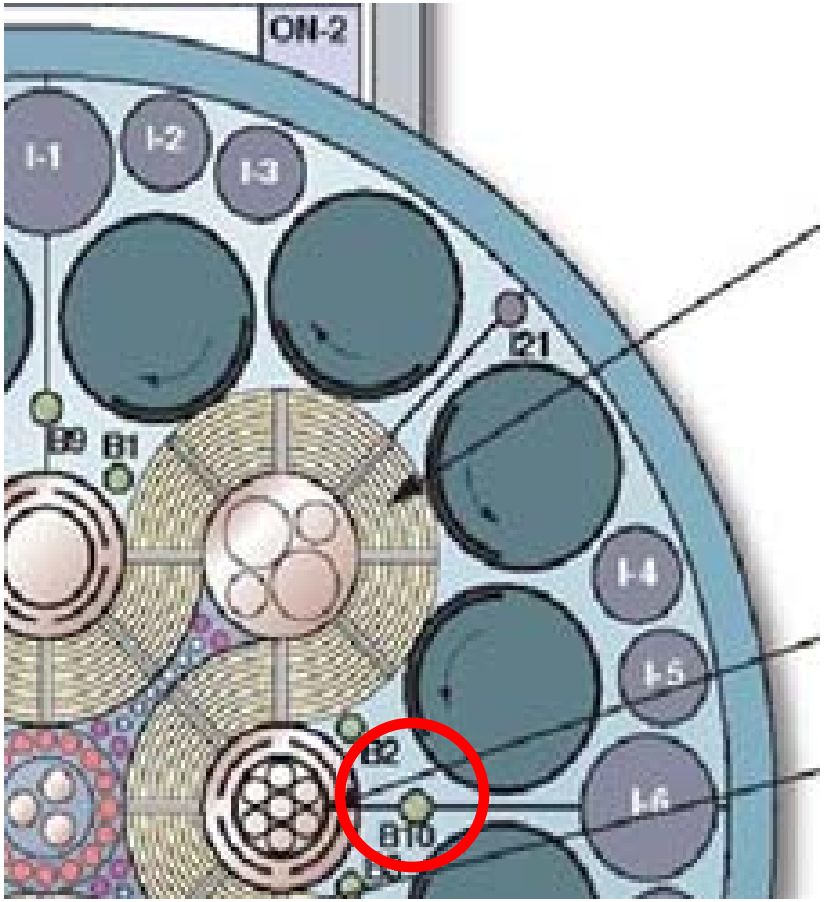
Thermal Analysis: MCNP5->ABAQUS Translation



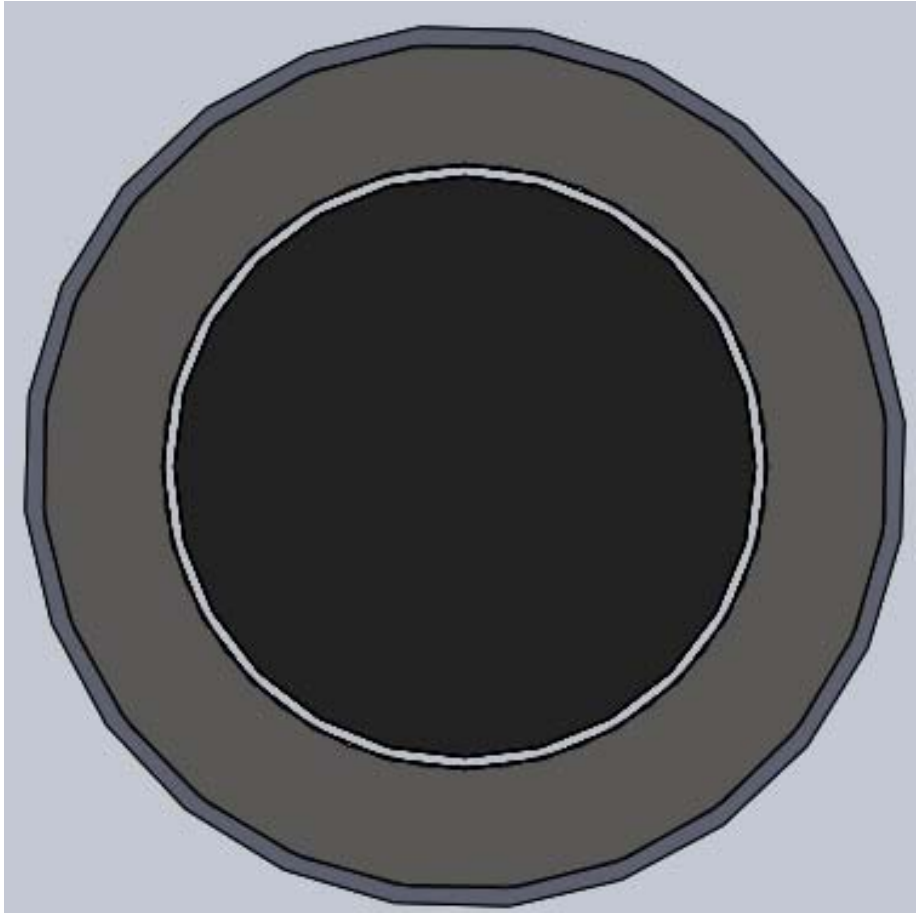
Geometry: CAD to DAG-MCNP5



Example Geometry Location



Example Geometry



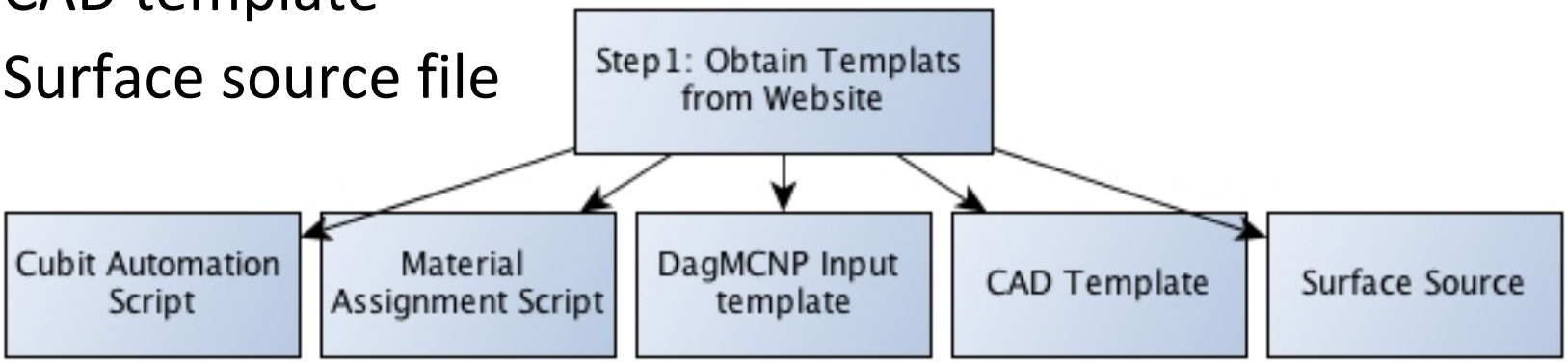
Overview of Neutronic Modeling

- ❑ Obtain Templates from Website
- ❑ Create Geometry
- ❑ Add Materials
- ❑ Specify your outputs
- ❑ Run Dagmc

Step1 Obtain Templates from Website

- Website to download tools for ATR modeling
  http://bit.ly/kbI9gn

- Need to obtain the following files:
  1. Cubit automation script
  2. Material assignment template
  3. DAGMCNP input template
  4. CAD template
  5. Surface source file



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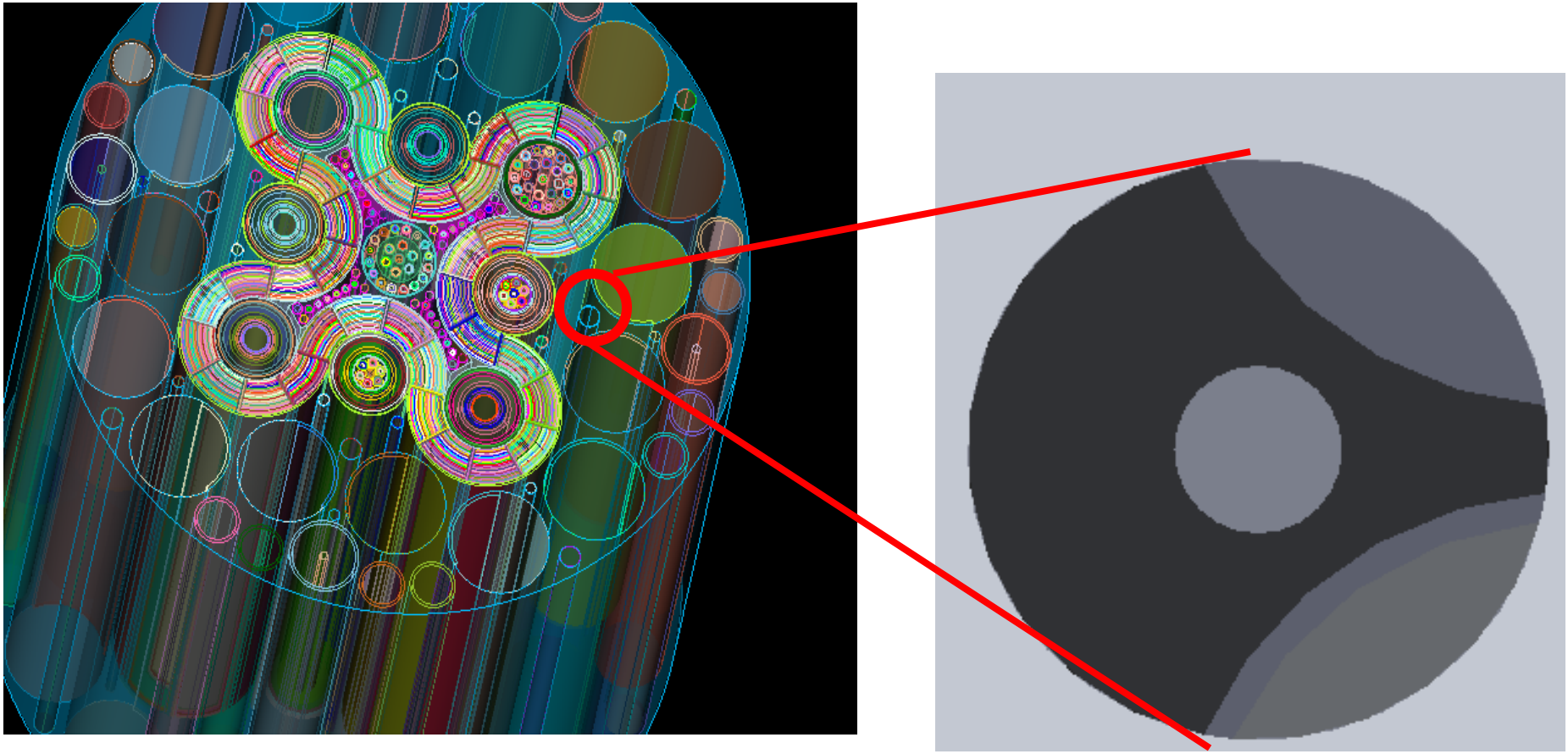
Step 2: Create Geometry (I20)



NOTE: Make sure to fix all cells before adding new experiment to step file

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Step3: Adding Materials

- Add material information to two templates:
  - Dagmcnp template
    - Use Standard AAAZZZ format (Atomic Number, Atomic Mass)
    - Examples
      - Water: H20

        m130 1001 2 8016 1
      - Hf wt% 98% Zr 2%

        m132 72000 -0.98 40000 -0.2
  - Legend template: (units +atms/barn_cm or -g/cc)

    mat_H20 mat_130_rho_.1000

    mat_Hf mat_132_rho_-12.100

*Advanced users can specify materials for specific:

- Temperatures
- Chemical structures (H20, Graphite, etc)
- Type of data (ENDF6, ENDF7, JAERII, KAERI

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Step 4: Specify information needed from the calculation

- Tallies extract useful neutronic outputs from dagmc.
- Put mesh tallies directly into dagmcnp input file
- For individual cell data, you can insert tallies by editing material assignment templates; for example:

```
mat_H20        tally_6_cell.heating_n
mat_Be         tally_7_cell.flux_p
```

Heating rate mesh tallies output

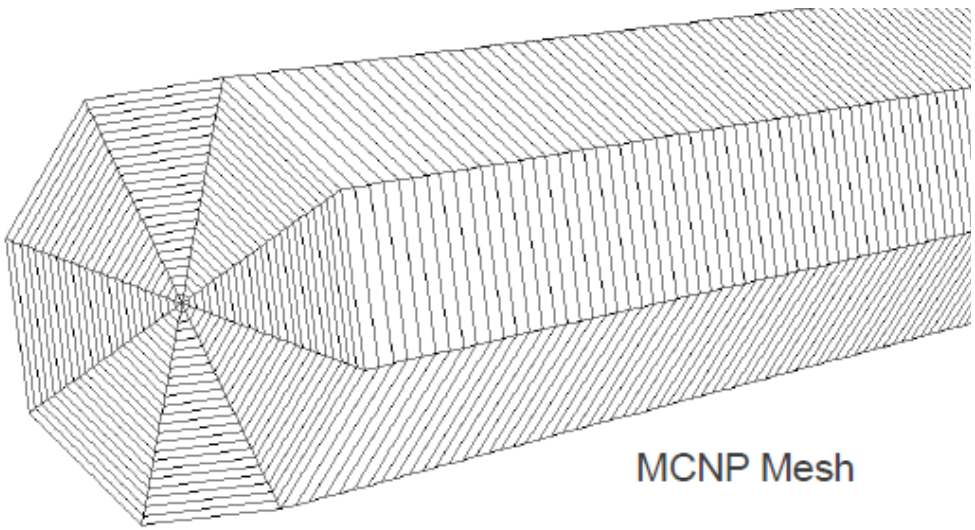
```
fc34 n heating in Glass mesh tally
fMESH34:N GEOM=cyl          ORIGIN=3.92  1.28  -92.7
        AXS=0 0 1           VEC=1 0 0
        IMESH=5.9           IINTS=20
        JMESH=121.92        JINTS=122
        KMESH=1             KINTS=8
fm34 -12150 133 (-1 -4)
```

```
fc114 p heating in water mesh tally
fMESH114:P GEOM=cyl      ORIGIN=3.92  1.28  -92.7
     AXS=0 0 1           VEC=1 0 0
    IMESH=5.9            IINTS=20
    JMESH=121.92         JINTS=122
    KMESH=1              KINTS=8
fm114 -12150 (-5 -6)
```

Normalizations for DAGMC

$$12150\frac{J\left(source\ particle\right)}{MW_{Rx}s}$$

$$7.58E16\frac{neutron\left(source\ particle\right)}{MWs}$$



Overview of Neutronic Modeling

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- ☑ Create Geometry
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- ☑ Specify your outputs
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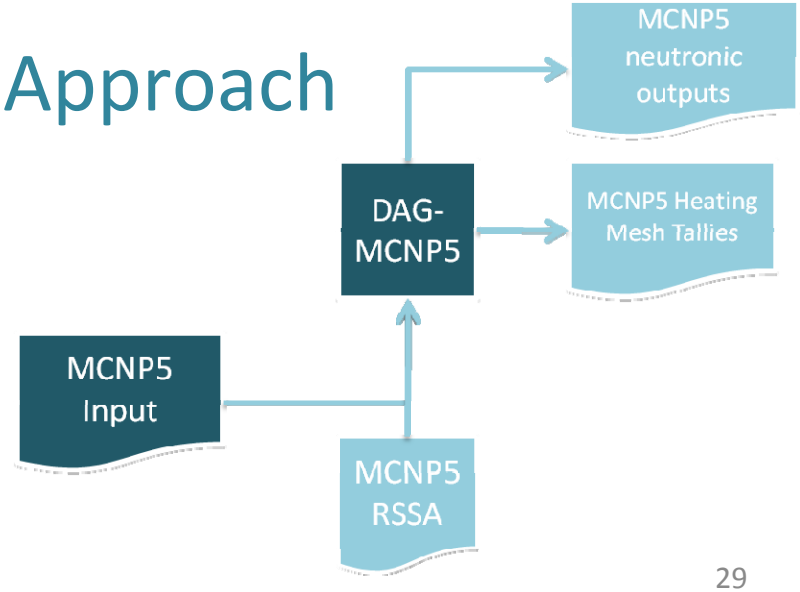
Neutronic Analysis:

Surface Source Approach



Running dagmc

- Python scripit.py [step file] [input file]

Overview of Neutronic Modeling

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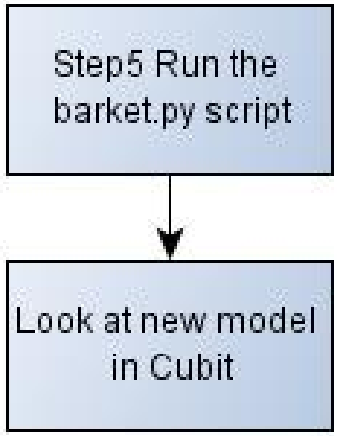
- ☑ Run Dagmc

Step 5: Running DAGMCNP



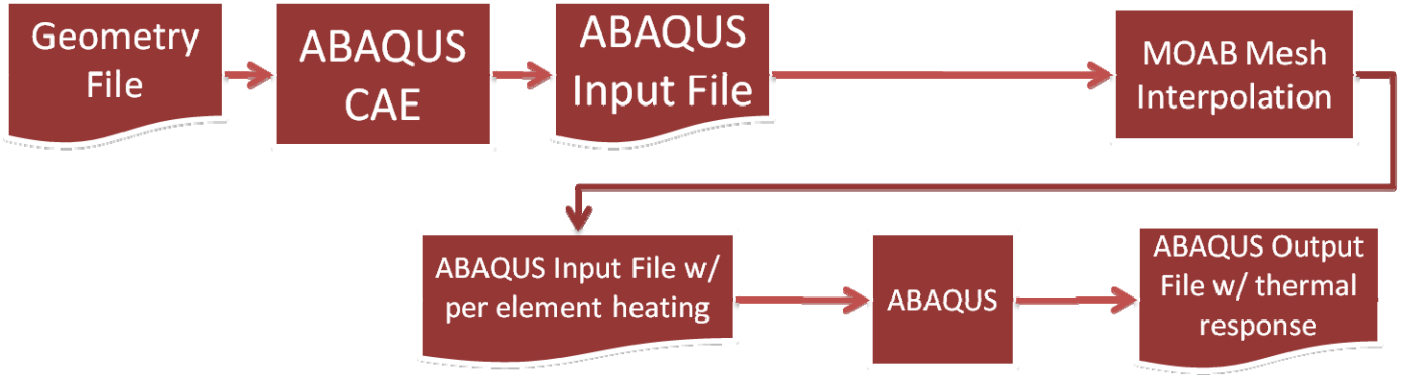
- Type the following to run dagmc:
  - *python barkit.py [GEOM.step] [dagmcnp.i]*
  - The script will open geometry in CUBIT for advanced error checking
    - In cubit type “exit” when done
    - Enter 1 to run dagmcnp
- If you already have the *.sat file processed you can run dagmcnp manually by
  - dagmcnp5 i=input.txt g=geom.sat o=output.txt

Neutron Analysis without DagMCNP

- Advanced users can use surface source files directly with MCNP5 input decks they modify themselves
- MCNP template decks are available on site for supported positions.

Thermal Analysis:

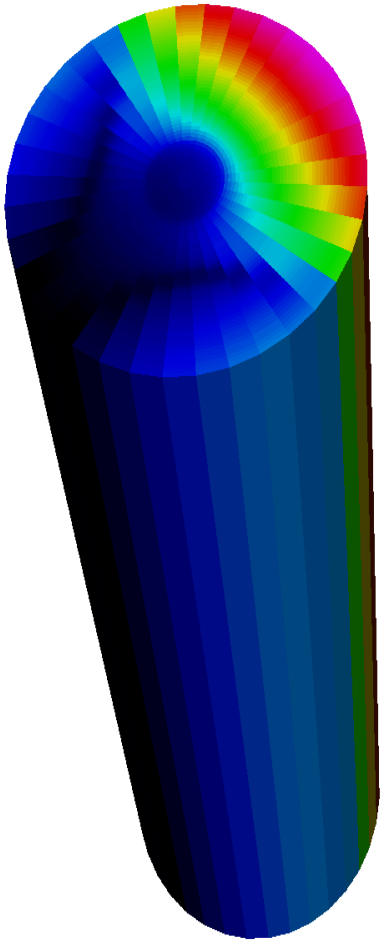
MCNP5->ABAQUS Translation



Outline of Abaqus Preparation

- ❑ Save each part as a STEP file
- ❑ Assign materials
  - Material information
  - Gas gap information
  - Coolant channel information
- ❑ Assign Geometry information
- ❑ Mesh parts and add interactions if needed
- ❑ Add mass flow rate to job input
- ❑ Write out Abaqus input file

MOAB



- Mesh Oreiented dAtaBase

- Used here to convert between two meshes

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

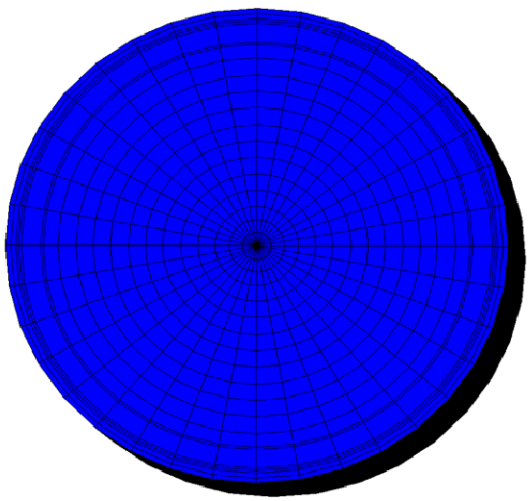
- Native mesh translator included to interpolate MCNP tally geometry onto Abaqus mesh

Mesh Interpolation

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

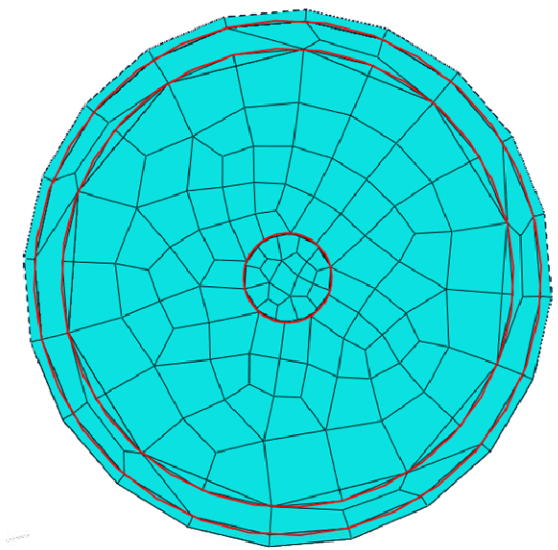
- Via MOAB the problem depicted below is resolved to obtain volumetric power deposition for each Abaqus mesh element:

Body Independent Mesh



MCNP

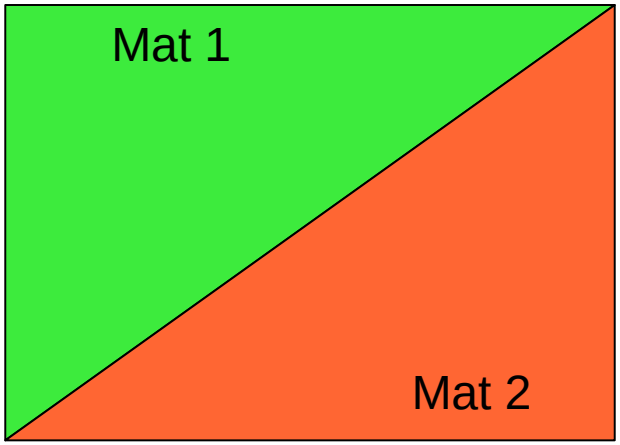
Body Fitted Mesh



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…

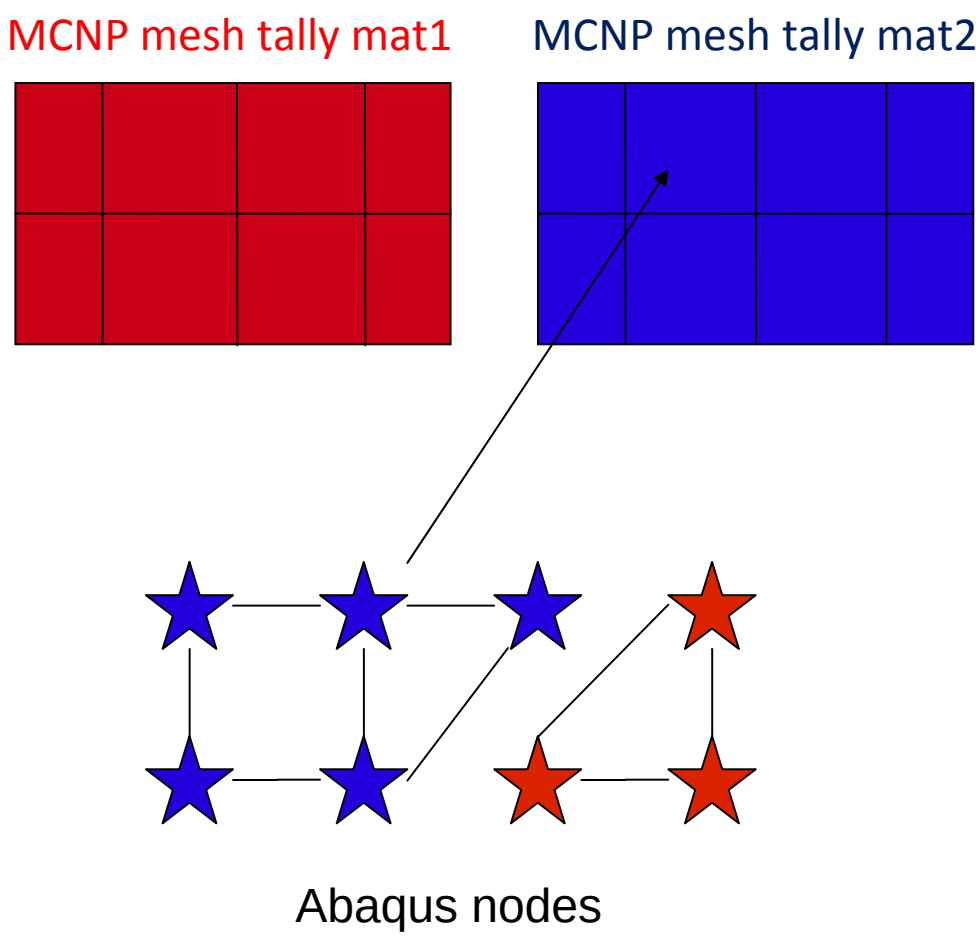
- … each element in Abaqus (green/orange shaded areas) is only comprised of one material

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)



Mesh Interpolation Tool

- Tool used to automatically interpolate mesh tally results onto an Abaqus mesh.
- Requires an Abaqus input file, a mesh tally file, and an mcnp2abq input file.
- Interpolates each material heating results separately.
- Input file is based on keys and values

Mesh Interpolation Output

- 3 directories are made:
- **h5mfiles** – consists of .h5m mesh files created by MOAE during interpolation. These are generally unnecessary for post processing and can be eliminated by giving the '--noh5m' flag during execution.
- **vtkfiles** – consists of .vtk mesh files that are good for visualization. Can also be eliminated by giving the '--novt flag during execution.
- **abqHeatSources** – consists of text files containing abaqus formatted nuclear heat loads. Of most interest is 'combinedSource.abqh' which gives the thermal load for all materials.

Abaqus Input File and Running Abaqus

- Complete the Abaqus text input file by copying the contents of 'combinedSource.abqh' into the load section of the input file

- Run the completed Abaqus input file with the following command:

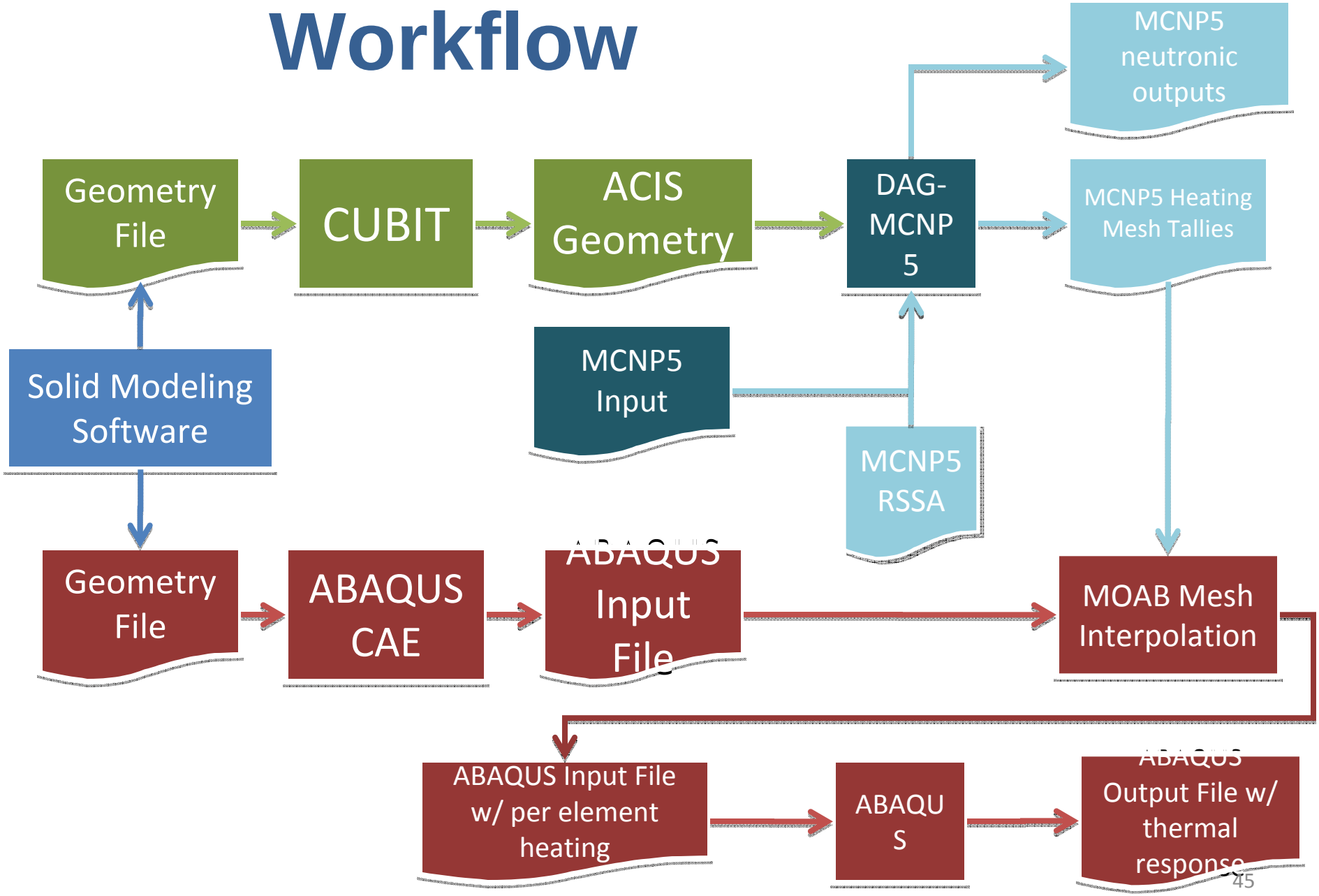
```
abq692 job=vegas.inp
```

Results Post-Processing

- Primary tools – Abaqus Viewer and VisIt

Conclusion

Workflow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Any Questions