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Title: MCNP6 Element-Wise Densities and Temperatures

Author(s): Vaquer, Pablo Andres

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MCNP6 Element-Wise Densities and Temperatures

Pablo A. Vaquer

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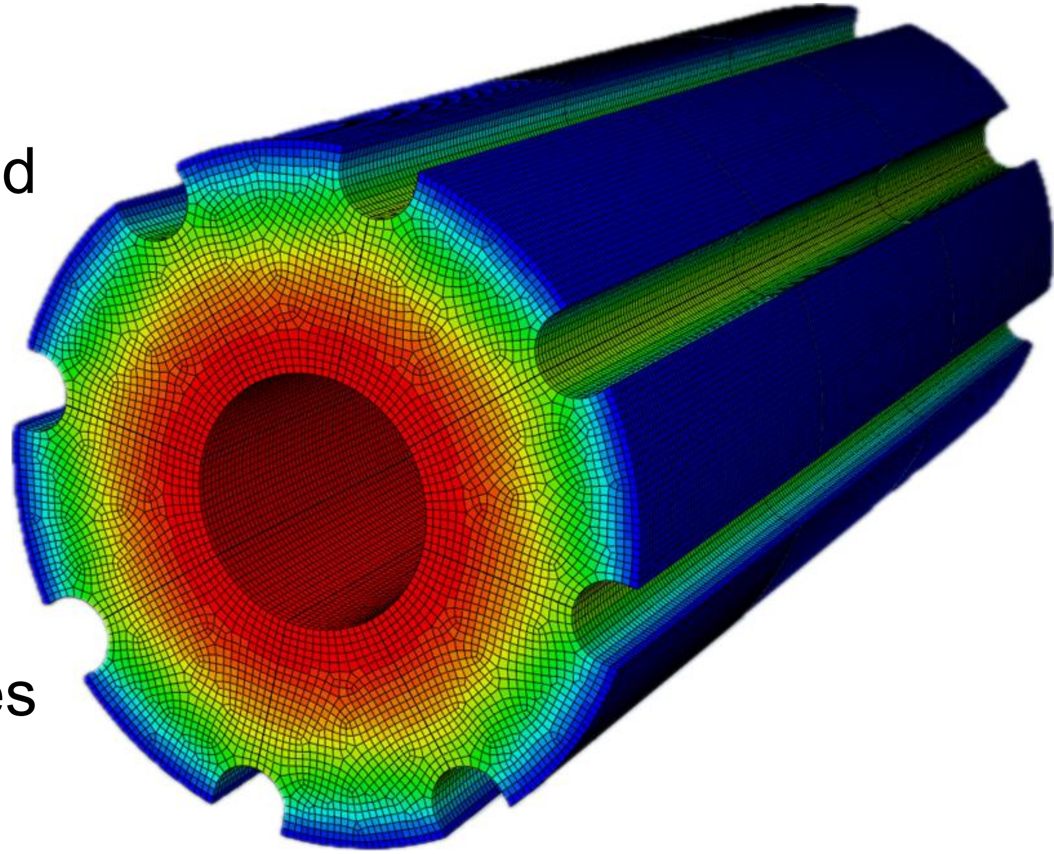
Goal: higher-fidelity multi-physics simulations

- Individual elements in MCNP6 unstructured meshes can now be tagged with unique densities and temperatures
  - This capability is currently available in "devel" branch
  - It will be included in MCNP6.4+
- Densities and temperatures no longer need to be averaged onto a coarser spatial resolution (pseudocells)



Example of an element-wise temperature distribution that can be imported in MCNP6.4+ via an HDF5 mesh file

The MCNP UM HDF5 file was modified to include element-wise densities and temperatures

- The material group in the new MCNP UM HDF5 file ***must*** contain the following attributes and datasets:
  - **material_id**: a 1D dataset composed of a single integer
  - **density_by**: an ASCII string (either “element” or “pseudocell”)
  - **density**: a 1D dataset of non-negative real numbers
  - **temperature_by**: an ASCII string (either “element” or “pseudocell”)
  - **temperature**: a 1D dataset of non-negative real numbers

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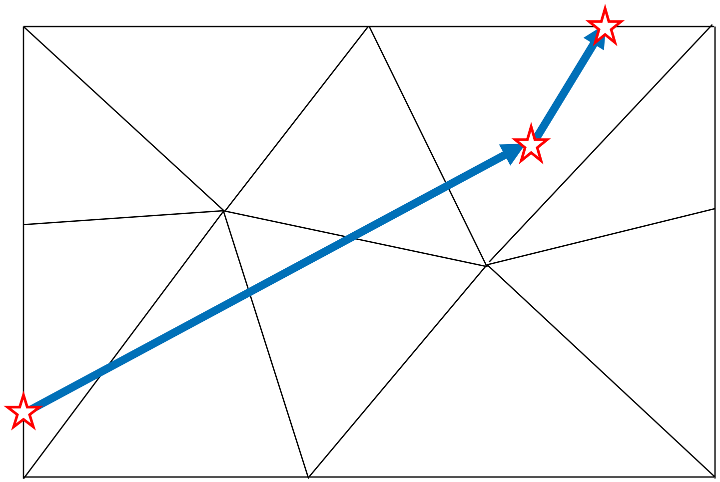
Examples of element-wise densities and temperatures are included in the test suite

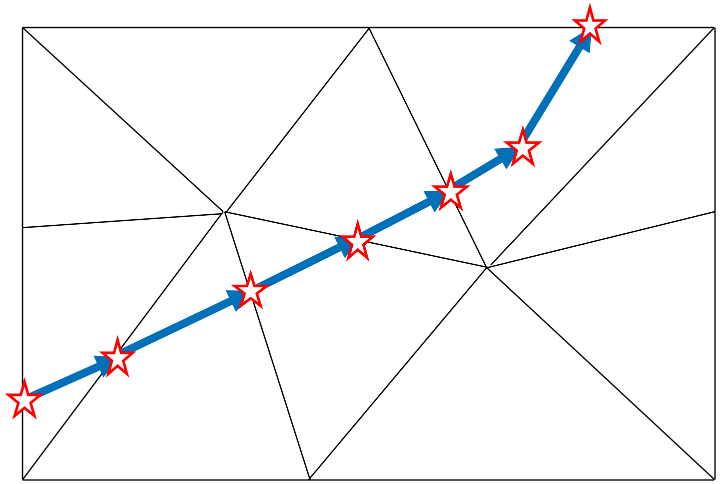
- Example using element-wise densities:
  - mcnp6/Testing/features/unstructured_mesh/hdf5_input10
- Example using element-wise temperatures:
  - mcnp6/Testing/features/unstructured_mesh/hdf5_input11
- Examples using element-wise densities and temperatures:
  - mcnp6/Testing/features/unstructured_mesh/hdf5_input12
  - mcnp6/Testing/features/unstructured_mesh/hdf5_input13

If there are element-wise differences in material properties, particle tracking behavior is modified

If there **are no** element-wise differences



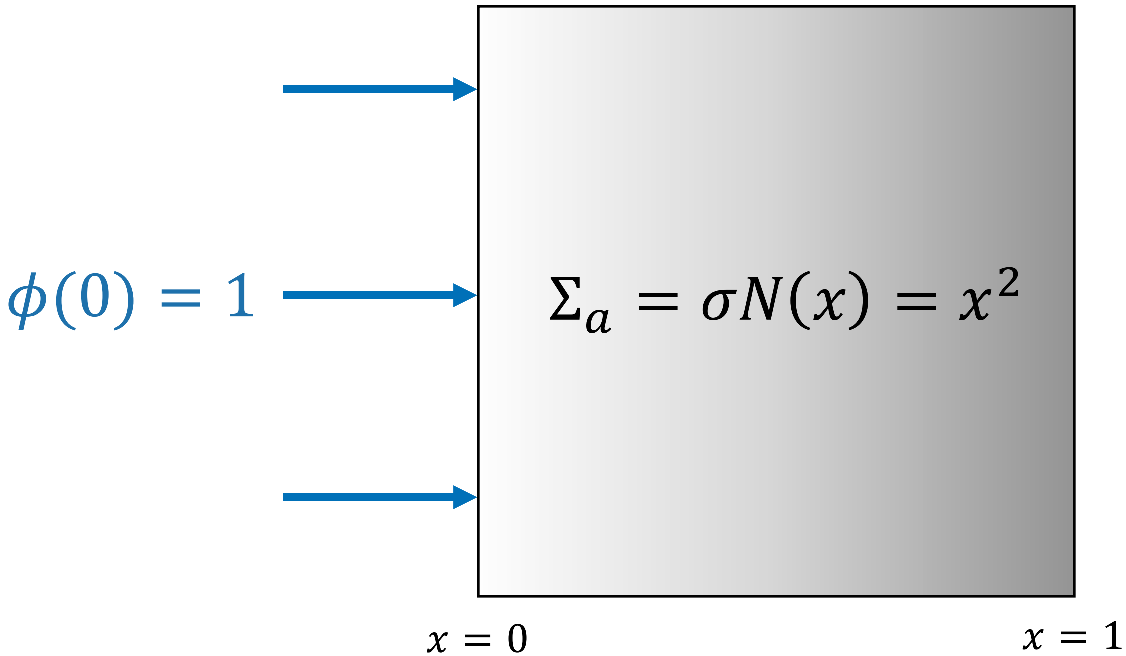
If there **are** element-wise differences



→ represents particle tracks

☆ represents material property look-ups & resampling of distance-to-collision

Analytical test problem 1: A cube (1 cm^3) with density varying in the x-dimension

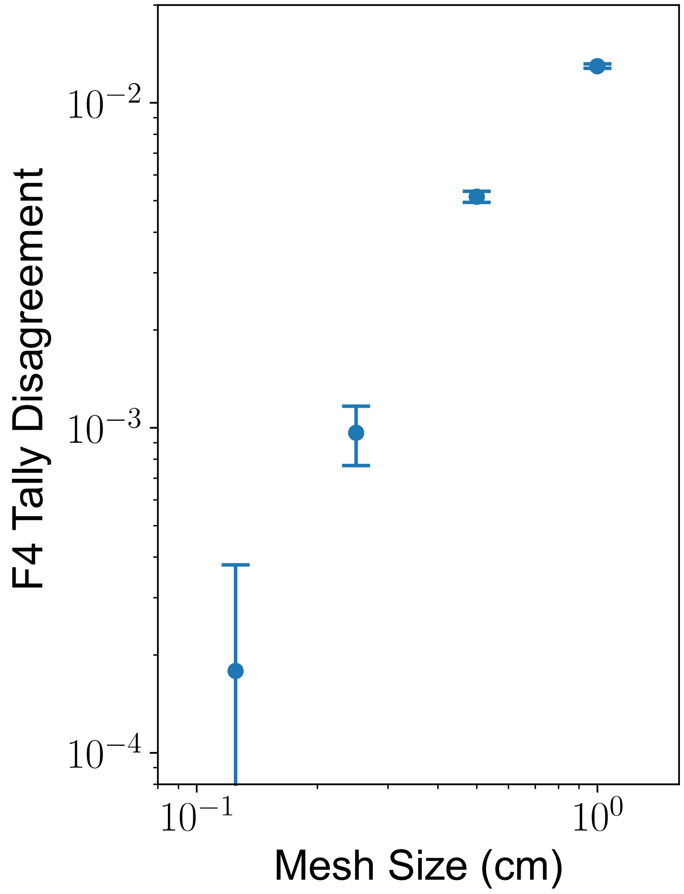


Analytical result for volume-averaged flux (F4) for the cube:

$$\overline{\phi} = \int_0^1 dx \exp\left(-\int_0^x dx' \, \Sigma_a(x')\right) \approx 0.924023$$

Analytical test problem 1 convergence study: simulation error as function of mesh resolution

Mesh Size (cm)	Number of Tetrahedra	Disagreement ± Noise
1	12	$1.3\times10^{-2} \pm 2\times10^{-4}$
0.5	49	$5.1\times10^{-3} \pm 2\times10^{-4}$
0.25	430	$9.7\times10^{-4} \pm 2\times10^{-4}$
0.125	4051	$1.8\times10^{-4} \pm 2\times10^{-4}$



- **Disagreement:** relative error between MCNP and analytical result
- **Noise:** one standard deviation of statistical uncertainty in MCNP

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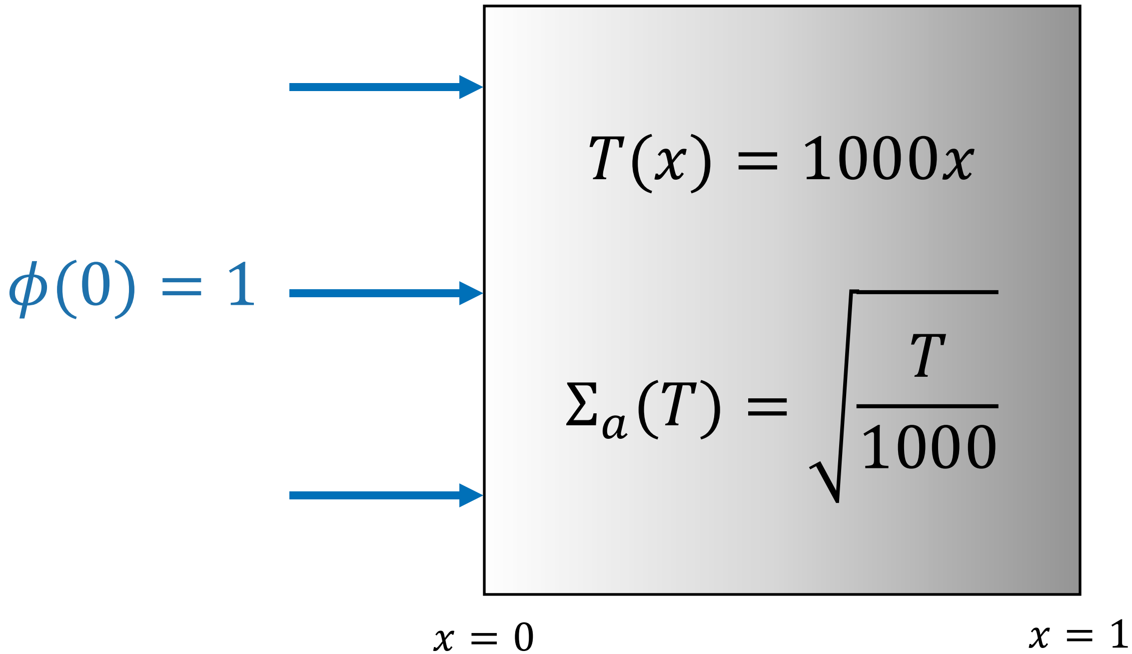
Analytical test problem 2: A cube (1 cm^3) with temperature varying in the x-dimension

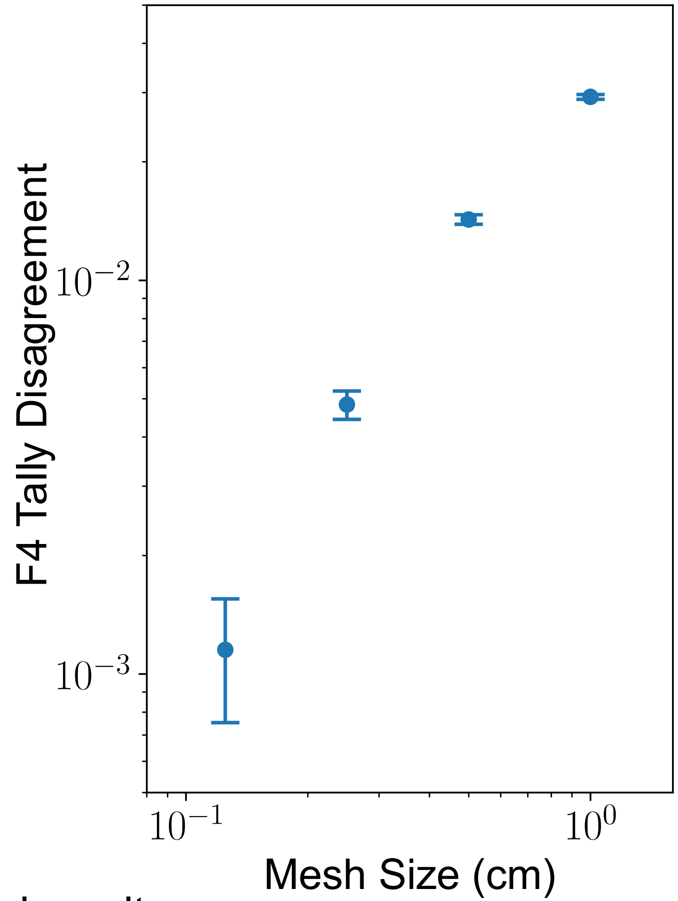


Analytical result for volume-averaged flux (F4) for the cube:

$$\overline{\phi} = \int_0^1 dx \exp\left(-\int_0^x dx' \, \Sigma_a(x')\right) \approx 0.780968$$

Analytical test problem 2 convergence study: simulation error as function of mesh resolution

Mesh Size (cm)	Number of Tetrahedra	Disagreement $\pm$ Noise
1	12	$2.9\times10^{-2} \pm 4\times10^{-4}$
0.5	49	$1.4\times10^{-2} \pm 4\times10^{-4}$
0.25	430	$4.8\times10^{-3} \pm 4\times10^{-4}$
0.125	4051	$1.2\times10^{-3} \pm 4\times10^{-4}$



- **Disagreement:** relative error between MCNP and analytical result
- **Noise:** one standard deviation of statistical uncertainty in MCNP

Considerations for element-wise temperatures

- Specifying temperatures in the HDF5 mesh file is equivalent to specifying values using the TMP card
- By itself, the TMP card only modifies:
  - the neutron *elastic-scattering* cross section
  - the sampling of target nuclide velocity from the free-gas scattering model
- The DBRC and OTFDB card can be used to improve sampling of target nuclide velocity and improve cross sections for *several* reactions
- The NJOY software can also be used generate cross section data at specific temperatures
  - However, the only way to implement element-wise cross sections with NJOY2016 is to *convert each UM element into a separate pseudocell* and then generate corresponding cross sections

DBRC card

- The DBRC card uses temperatures provided in the TMP card
- It corrects for inaccuracies in the TMP-card model to obtain improved sampling of target nuclide velocity based on a more accurate free-gas scattering model

OTFDB card

- The OTFDB card still uses temperatures provided in the TMP card, but loads a **precomputed regression model** to replace cross section values for:
  - total cross section (MT 1)
  - elastic scattering cross section (MT 2)
  - fission cross section (MT 18)
  - first-chance neutron-induced fission (MT 19)
  - neutron disappearance (MT 101)
  - total gamma production (MT 202)
  - energy release due to total cross section (MT 301)

$$\sigma_x(T, E_p) = \sum_{i=-N}^{N} a_{p,i}\, T^{i/2}$$

E_p is the energy grid point

$a_{p,i}$ is the i^{th} coefficient of the regression model for grid point p

Flowchart for generating an HDF5 mesh file with element-wise densities and temperatures

CAD model

Use CUBIT to generate unstructured mesh

Use Python pre-processor to convert a CUBIT Abaqus file into an MCNP Abaqus file

Run MCNP in “i” (input only) mode to convert Abaqus file into an HDF5 mesh file

Use a 2nd Python pre-processor to add densities/temperatures to elements/pseudocells in the HDF5 mesh file

Conclusions

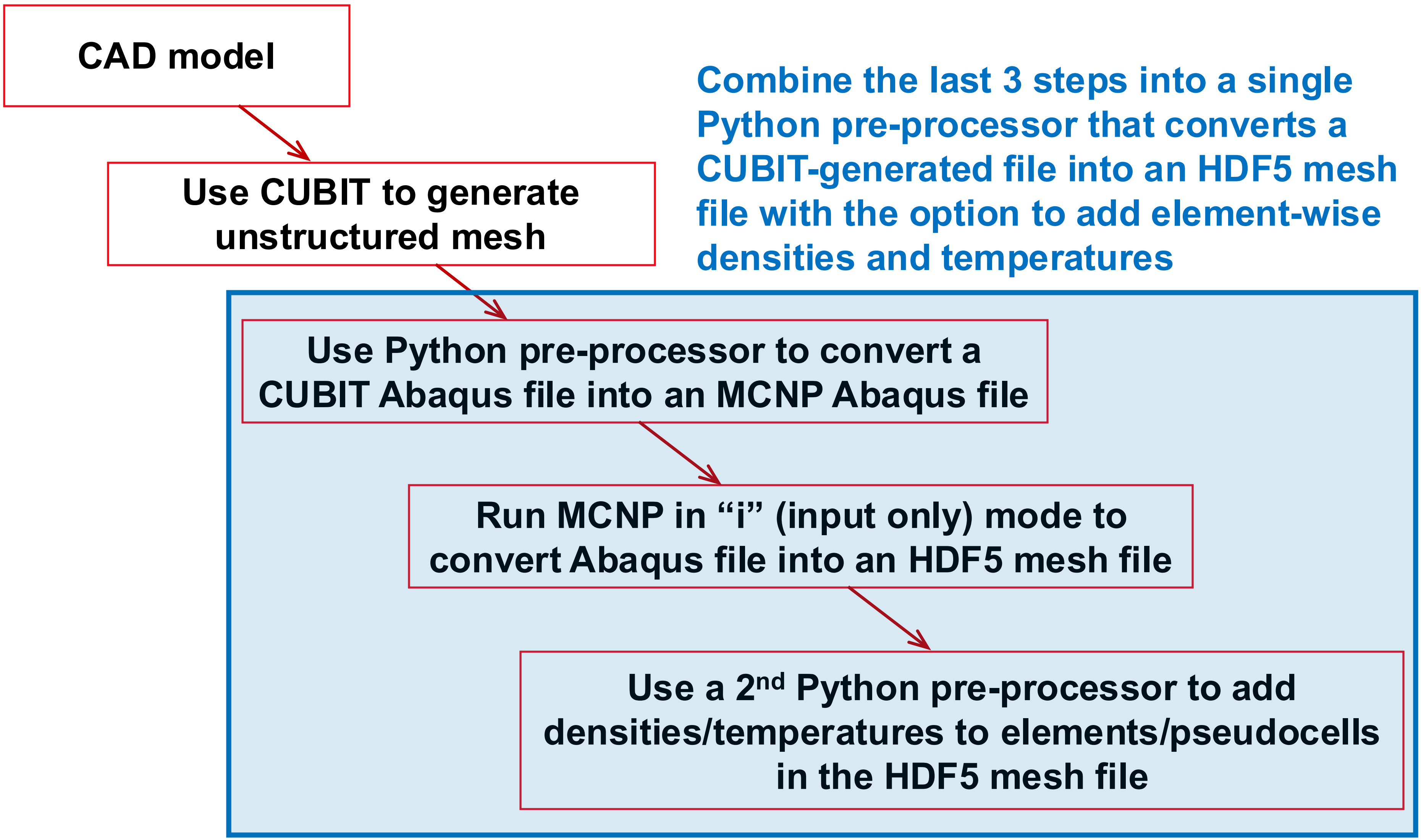
- Element-wise density and temperature specification were successfully implemented in the MCNP code
  - In MCNP6.4, a user will be able to specify element-wise densities and temperatures in the MCNP UM HDF5 file
  - Two analytical verification problems demonstrated mesh convergence for MCNP simulations with element-wise densities and temperatures
  - The code implementation was also verified by the MCNP test suite
- When using element-wise temperatures, consider using DBRC and OTFDB cards as well

Ideas for future work: new EMBED-card options

```
embed1  meshgeo = hdf5
        mgeoin = hdf5_input.h5
        filetype = ascii
        hdf5file = hdf5_output.h5
        meeout = hdf5_output
        background = 50
        matcell = 1 10 2 20 3 30 4 40
        hdf5temperatures = True
        hdf5densities = True
```

By default, these options would be set to False, and temperatures/densities are read from the MCNP input file

Ideas for future work: a new Python pre-processor



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Questions?

Thank you!

vaquer@lanl.gov