INL/MIS-23-71297-Revision-0

Accelerated Griffin Training (focused on eVinci-like microreactors) Part 1: Workflow

January 2023

Changing the World's Energy Future

Vincent M Laboure

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Idaho National Laboratory
Idaho Falls, Idaho 83415

http://www.inl.gov

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Accelerated Griffin Training (focused on eVinci-like microreactors) Part 1: Workflow

Vincent Labouré (INL)

NEAMS Nuclear Energy Advanced Modeling and Simulation

January 31st, 2023

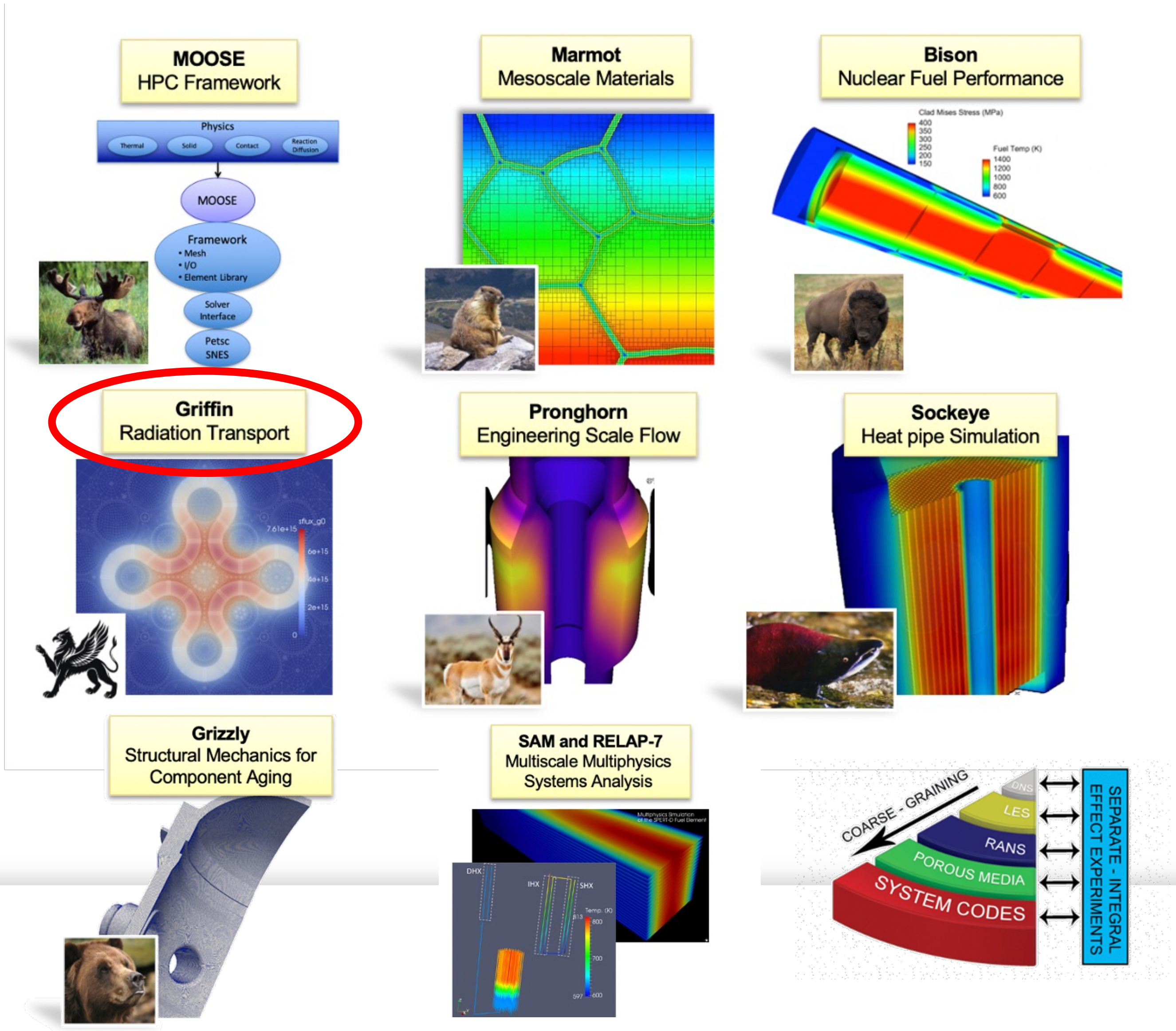
Training Outline (all times are ET)

- Part 1: Workflow (focused on homogeneous SPH and heterogeneous paths) – 1:40-2:10PM
- Part 2: Mesh generation with MOOSE – 2:10-2:40PM
- Break – 2:40-3:10PM
- Part 3: Defining XS/material regions –3:10-3:40PM
- Part 4: Heterogeneous transport solver with criticality search – 3:40-4:10PM
- Break – 4:10-4:20PM
- Part 5: Considerations for multiphysics coupled simulations – 4:20-4:50PM
- Discussion/additional questions – 4:50-5:00PM

Part 1 (Workflow) Outline

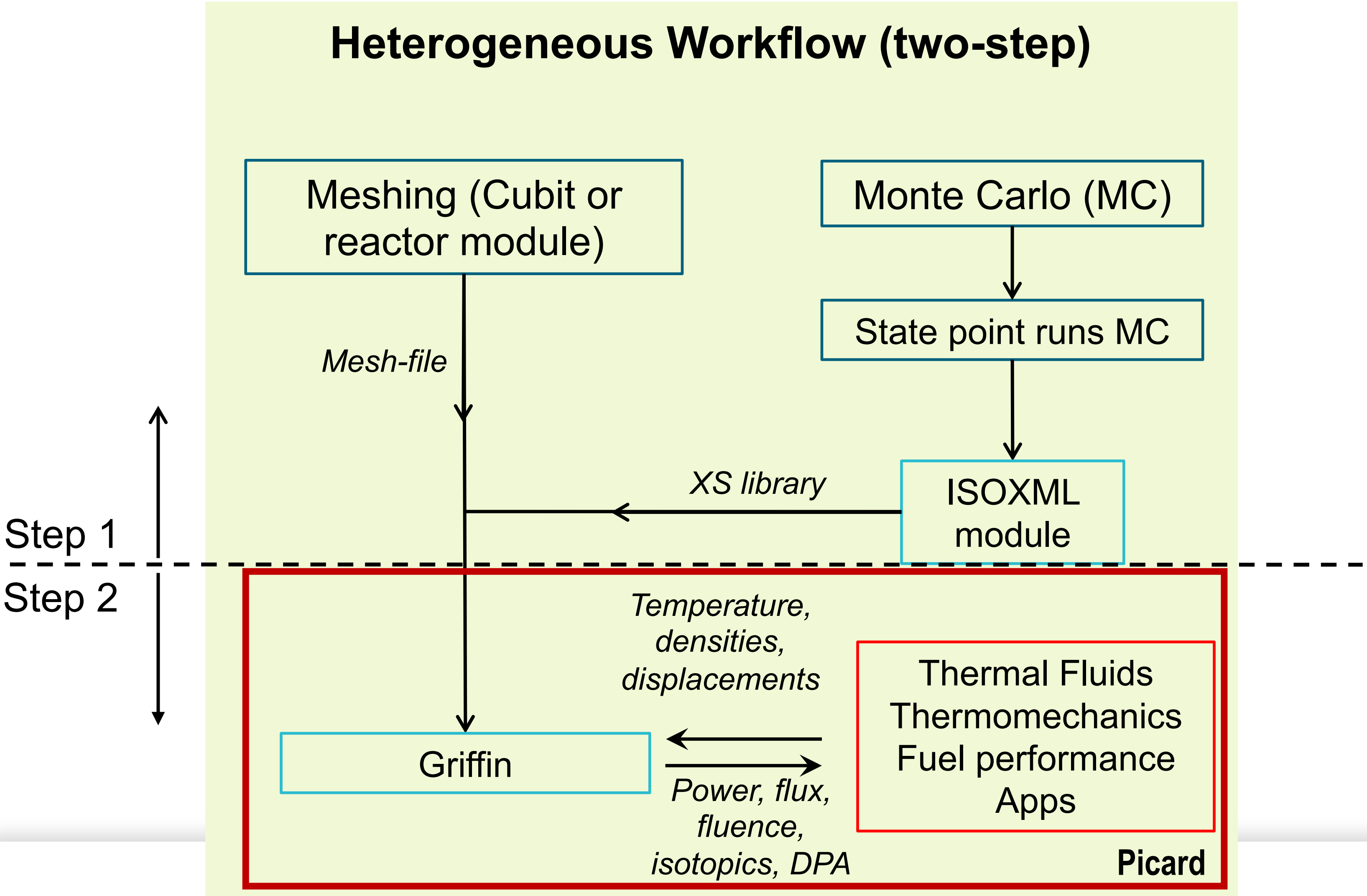
- Heterogeneous two-step workflow (DFEM-SN + CMFD)
- Homogeneous SPH two-step workflow
- Typical procedure before running a multiphysics transient
- How to run Griffin on INL HPC

DOE NEAMS MOOSE Based Applications



- **NEAMS**: The Nuclear Energy Advanced Modeling and Simulation Program
- **MOOSE**: Multi-physics Object Oriented Simulation Environment
- **Flexible**
  - 1D, 1DR, 2D, 2DRZ, 3D,
  - Huge variety of physics
  - Adaptive time stepping and sub cycling
  - Multiscale trough Multiapp system
  - Easily Extendible to new physics and sales
- **Tunable fidelity**
  - 0D scalar lumped parameters problem
  - 1D systems models
  - Multi D Intermediate “homogenized” geometry
  - High-fidelity “explicit” Geometry
- **Scalable**
  - MOOSE supports hybrid parallelism
  - Scales well on workstation and HPC
  - 2D/RZ models execute in minutes
  - High-fidelity 3D models execute on HPC

Two-Step Heterogeneous Workflow



- Focus of this training
- Mesh contains XS (or material) IDs
- State points capture the XS dependency on various parameters (Tfuel, Tmod, control drum angle, etc.)
- Transport solver used (typically DFEM-SN + CMFD)

XS Library Preparation

Serpent model

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%% Core control
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

set pop 1000000 100000 100
set bc 1

%       fuel, moderator, monolith, HP,  Be,  B4C, air, Be (axial reflector only)
set gcu 1001  1002       1003      1004 1005 1006 1007 1008
```

Convert to ISOXML format

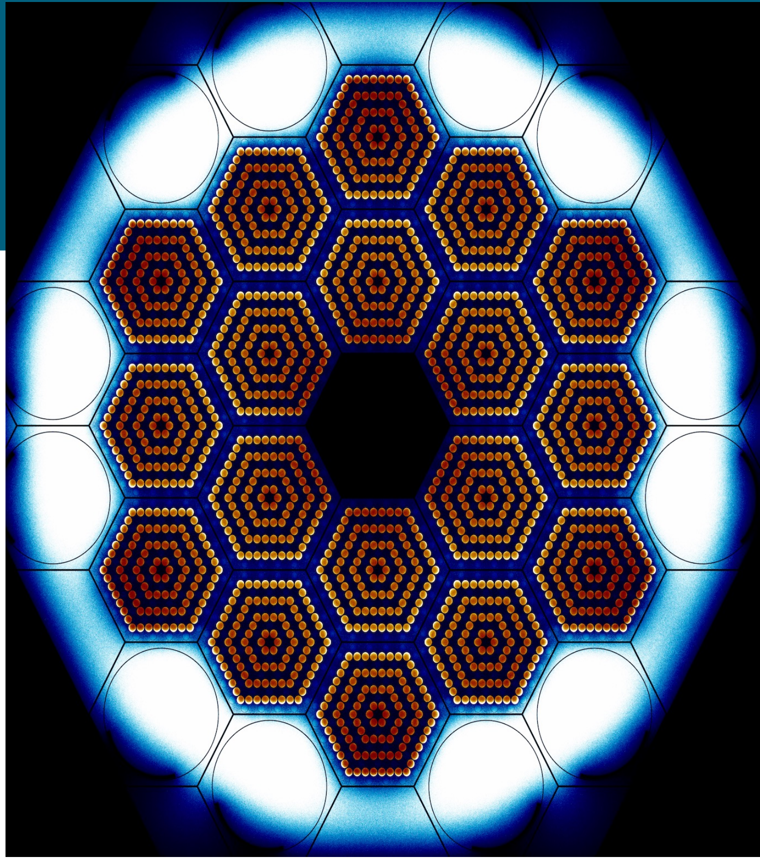
```
<ISOXML Format="SERPENT2" Name="empire_core_modified_11G" NGroup="11" ND

<Librarywise DataType="macro" L="1" LType="1" Transient="true">
  <Tabulation>Tfuel Tmod Trefl</Tabulation>
  <Tfuel>800 1000 1200 1400</Tfuel>
  <Tmod>800 1000 1200</Tmod>
  <Trefl>600 1000</Trefl>
  <BaseFile>empire_core_modified</BaseFile>
  <BaseExtension>sss</BaseExtension>
</Librarywise>

</ISOXML>
```

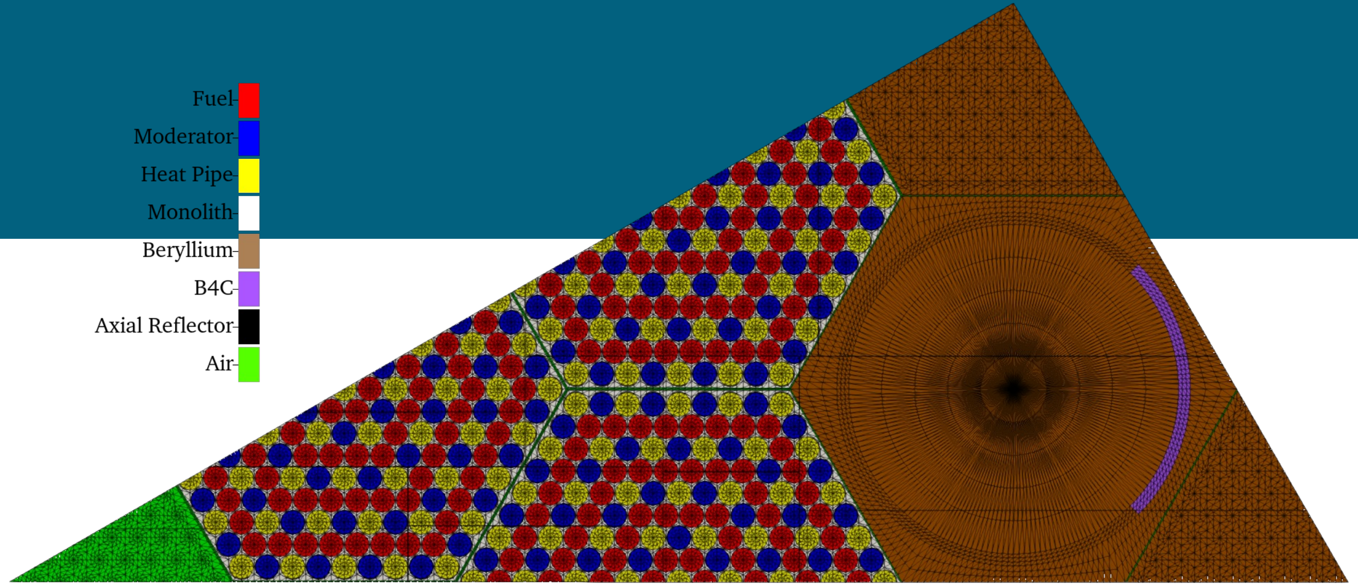
Griffin input

```
[Materials]
  [fuel]
    type = CoupledFeedbackNeutronicsMaterial
    block = '1 2' # fuel pin with 1 cm outer radius, no gap
    material_id = 1001
    library_file = '../../isoxml/empire_core_modified_11G.xml'
    library_name = empire_core_modified_11G
    densities = 1.0
    isotopes = 'pseudo'
    grid_names = 'Tfuel Tmod Trefl'
    grid_variables = 'Tfuel Tmod Trefl'
    is_meter = true
    plus = true
  []
[]
```



- For each state point, run Serpent calculation with gcu card
- Convert to a XS library containing all the state points
- Use library in NeutronicsMaterials (material ID = XS ID = universe ID in Serpent, see Part 3 of training)

Heterogeneous Path

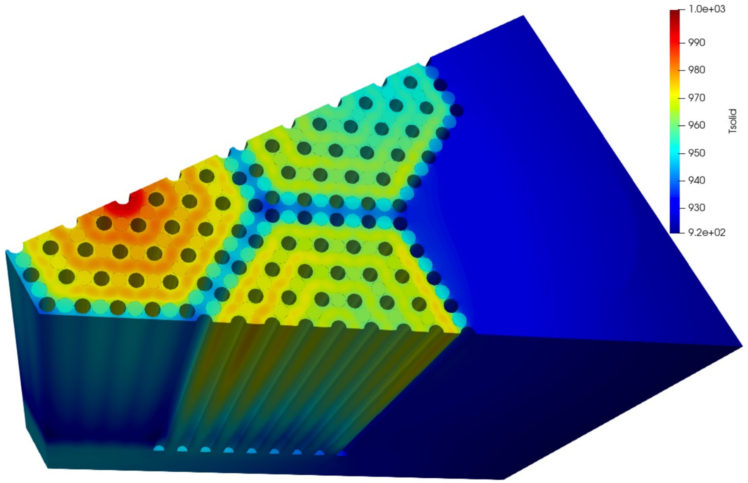


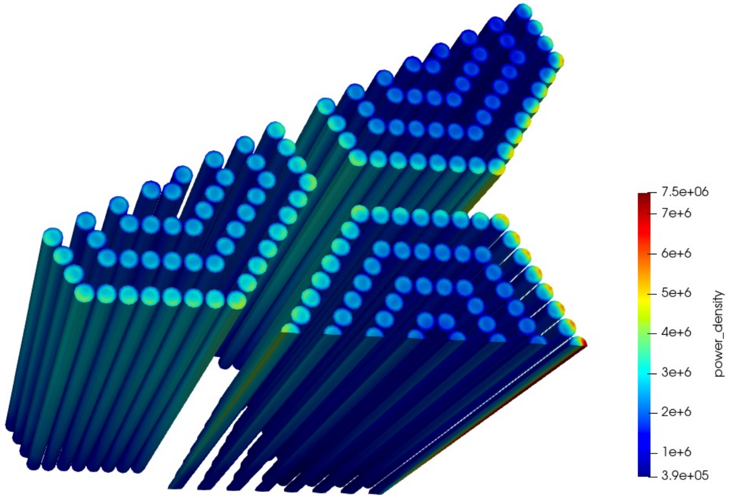
❑Pros:

- XS do not vary as much as SPH factors
  (could require less state points)
- Pin power reconstruction not needed
- Simpler workflow
- Kinetics parameters might be improved

❑Cons:

- Finer mesh needed
- Much more unknowns to solve for
  (but runtime can remain reasonable)





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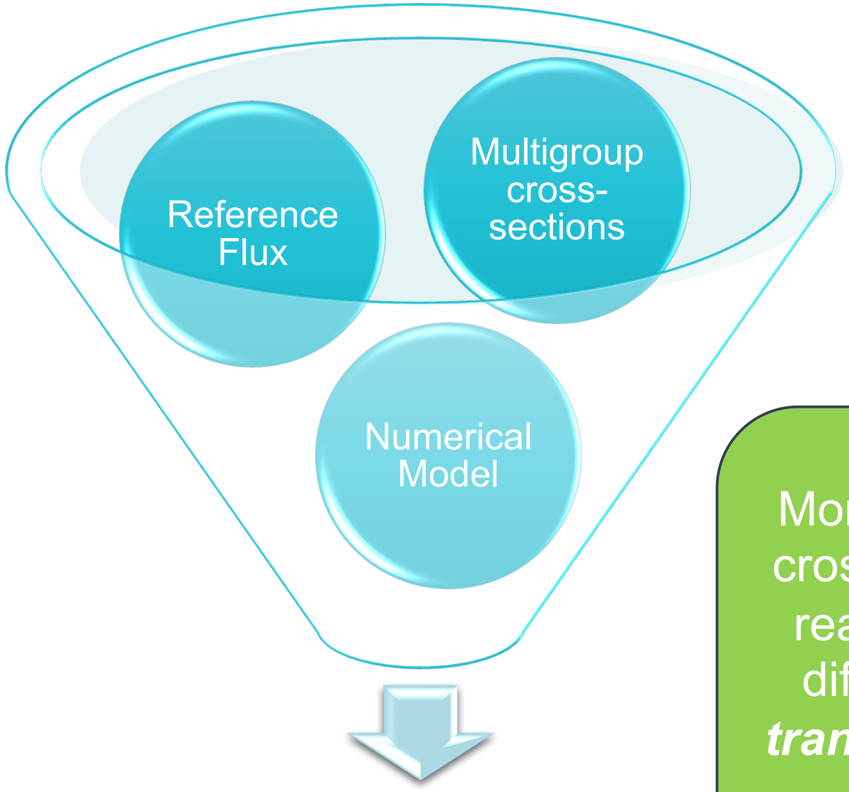
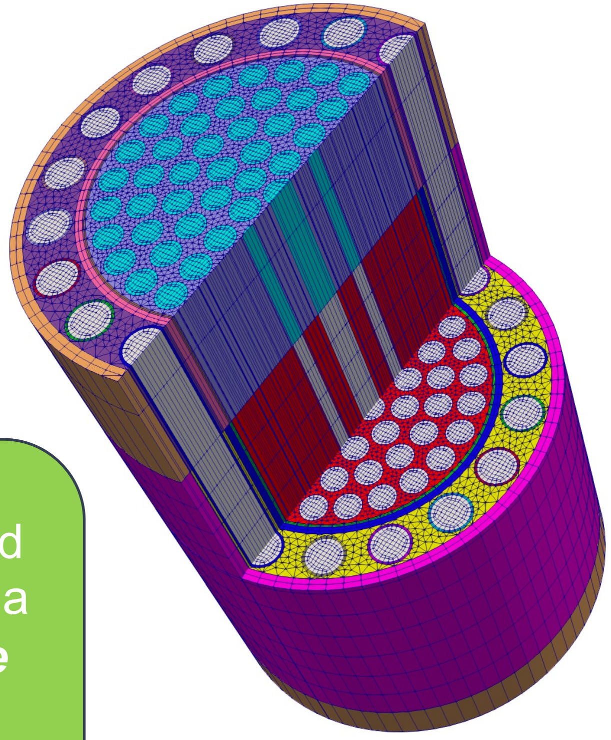
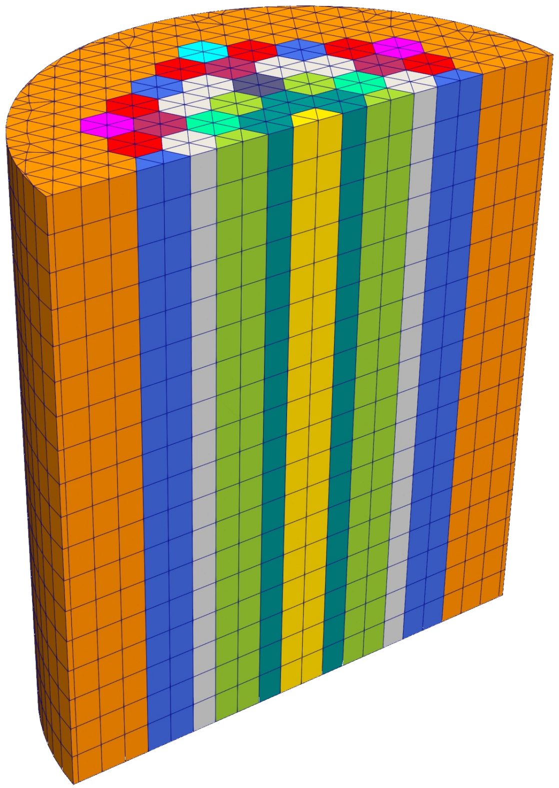
Physics-based Reduced Order Model: Super-Homogenization (SPH) Diffusion Path



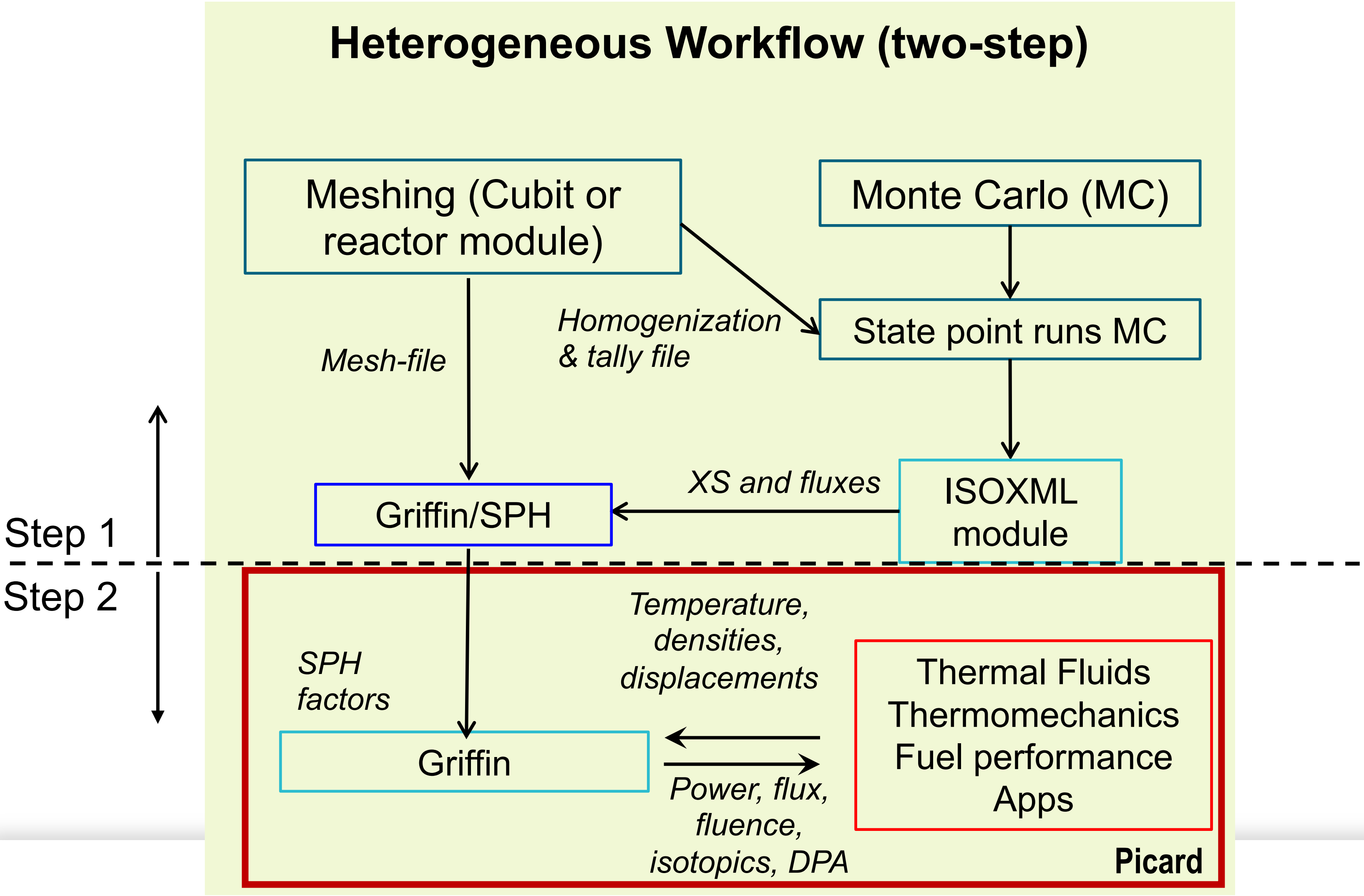
SPH-corrected library

Monte-Carlo corrected cross sections to use a reasonably ***accurate*** diffusion scheme for ***transients*** *on a* ***coarse*** *mesh*





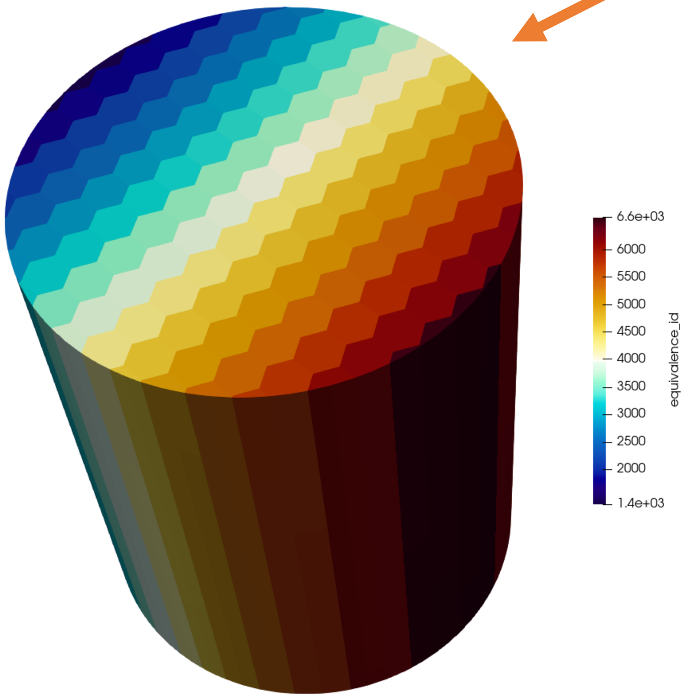
Two-Step Homogeneous SPH-Diffusion Workflow



- Corresponds to current eVinci model
- Coarse mesh contains XS (or material) IDs and flux (or equivalence) IDs
- State points capture the XS and flux dependency on various parameters (Tfuel, Tmod, control drum angle, etc.)
- Diffusion solver used

Homogeneous Meshing for SPH Diffusion Path

NEMO
(meshing scripts)




```
%Add gcu card for cross section regions
set gcu 11 12 13 21 22 23 31 32 33 41 42 43 51 52 53 61 62 63

%Add SPH flux detectors for each axial layer
det     1 dl hex_lat_1 de eg1 dz 0.0 10.0 1
det     2 dl hex_lat_2 de eg1 dz 10.0 60.0 5
det     3 dl hex_lat_3 de eg1 dz 60.0 70.0 1
```

- Meshing done along with detector definition to ensure the SPH regions are ordered in the same way MC tallies are
- Long-term plan is to have NEMO replaced with MOOSE reactor module

Generating/Using the SPH Factors

- Need to generate the SPH factors at each state point before using them

Reference XS & Fluxes → SPH correction → Match eigenvalues → Griffin multiphysics

```
[Equivalence]
  type = SPH
  transport_system = diff
  equivalence_library = '<fluxes>.xml'
  library_name = 'empire_core_modified_11G'
  compute_factors = true
  equivalence_grid_names = 'Tfuel Tmod Trefl'
  equivalence_grid = '4 2 1'
  updated_equivalence_library = '<SPH library>.xml'
  sph_initialization = <fSPH_file>.i
  sph_block = '<SPH blocks>'
[]
```

```
[Equivalence]
  type = SPH
  transport_system = diff
  equivalence_library = '<SPH library>.xml'
  library_name = 'empire_core_modified_11G'
  compute_factors = false
  equivalence_grid_names = 'Tfuel Tmod Trefl'
  equivalence_grid = '4 2 1'
  sph_block = '<SPH blocks>'
[]
```

```
[Equivalence]
  type = SPH
  transport_system = diff
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  library_name = 'empire_core_modified_11G'
  compute_factors = false
  equivalence_grid_names = 'Tfuel Tmod Trefl'
  equivalence_grid_variables = 'Tfuel Tmod Trefl'
  sph_block = '<SPH blocks>'
[]
```
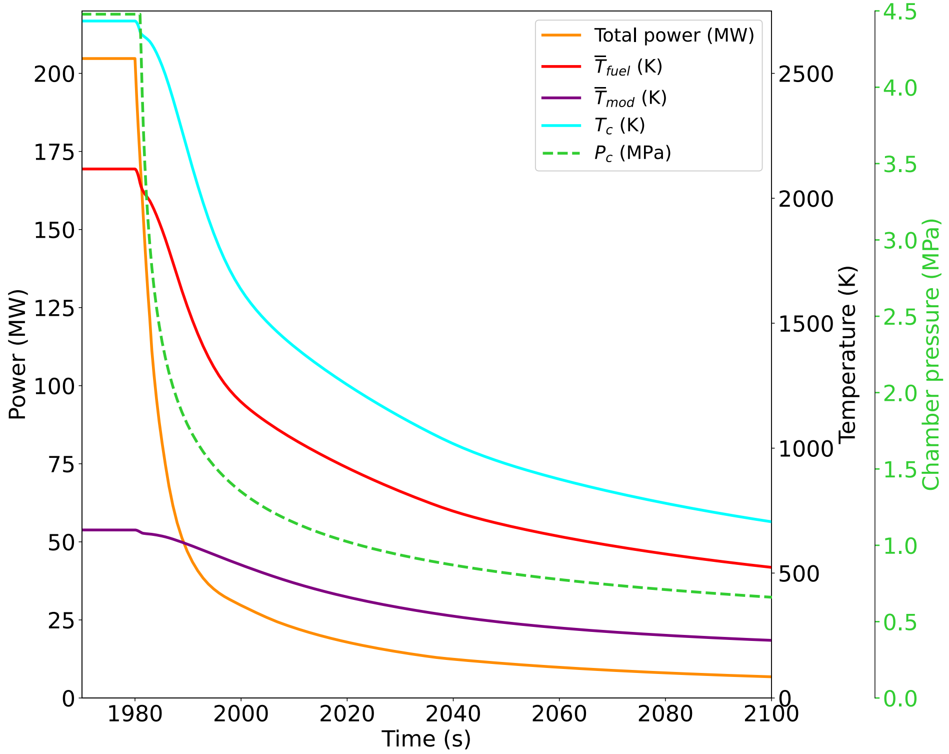
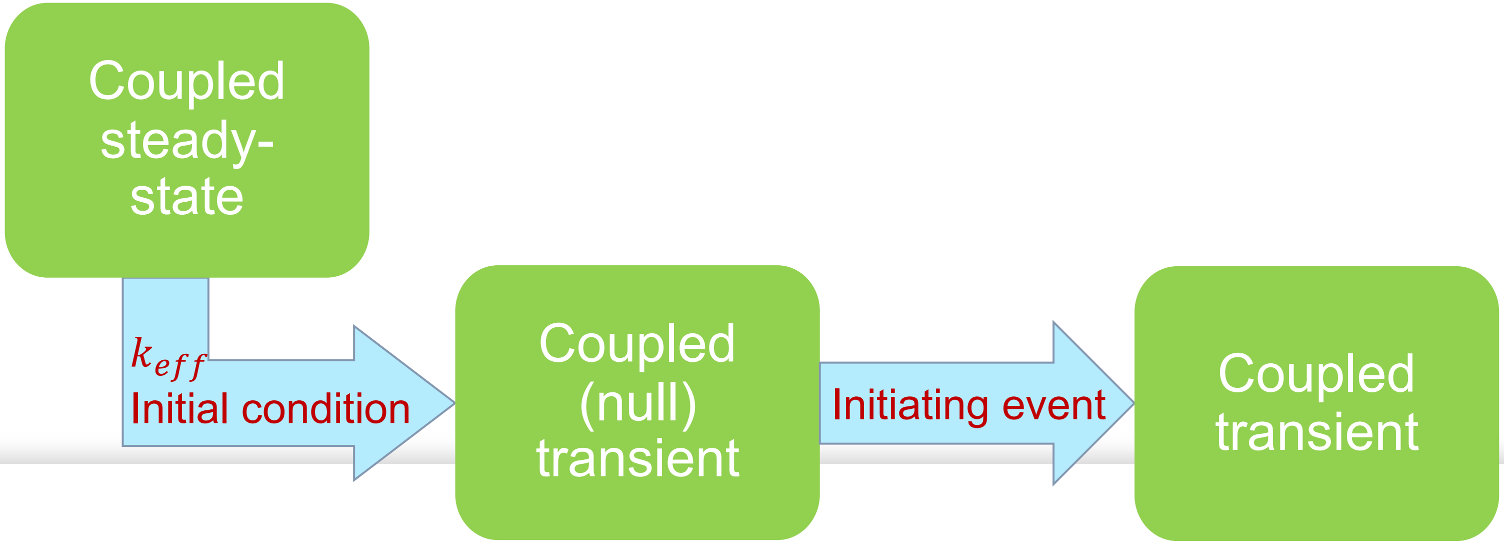

Step 2 Standard Approach: Steady-State Precedes Transient Calculations

- Even if a (real) reactor is critical, numerical eigenvalue ≠ 1.00000
- Scaling with k_{eff} (multiplication factor) is required to start from a self-sustaining solution
- Otherwise, bias in initial reactivity
- Highly recommended to check that a null-transient can be maintained





Running precompiled Griffin/ISOXML on INL Sawtooth HPC

- https://griffin-docs.hpc.inl.gov/latest/getting_started/index.html

```
> module load use.moose moose-apps
> module load griffin
> mpiexec griffin-opt –i <input_name>.i
```

Replace griffin with dire_wolf to run DireWolf

- https://griffin-docs.hpc.inl.gov/latest/isoxml-user-manual/getting_started_isoxml.html

```
> griffin-opt --isoxml-input -i <input_name>.xml
```

Single processor! But ability to merge the outputs from multiple calculations.

Conclusion

- Focus of this training will be Two-Step Heterogeneous with DFEM-SN + CMFD acceleration
- Current eVinci models use Two-Step Homogeneous SPH Diffusion approach
- Workflow similar with a few extra steps for the latter.
- Hands-on tutorials and documentation are available on the Griffin website (griffin-docs.hpc.inl.gov/latest).
- Many other capabilities in Griffin already available or under active development will be left for a more comprehensive training (pin power reconstruction, microdepletion, HFEM-PN, IQS, online XS generation, GPU acceleration, etc.)

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Questions?

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