A Modern Computational Science and Engineering Effort in Nuclear Engineering

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Motivation for Advanced Simulation

- US can design and build nuclear power plants today
- US has years of operational experience
- Experimentation is possible but is expensive

In the End

Reducing design margin is seen as number one motivation for advanced simulation ($$$$).

Licensing process with reduced experimentation will also motivate advanced simulation

If advanced simulation is to be used to reduce design margins and impact licensing then an appreciable V&V + UQ effort will be required.

Existing DoE Nuclear Programs

- Global Nuclear Energy Partnership (GNEP)
  - Advanced TRU fuels
  - Liquid metal (Na) cooled fast reactor (SFR)
- Next Generation Nuclear Plant (NGNP)
  - High temperature gas (He) cooled reactor (VHTR)
  - Considering pebble bed and prismatic concepts
  - More of a commercialization bent
- GEN IV
  - International agreement
  - Several concepts including SFR and VHTR
  - More of a research bent

Status of Computational Nuclear Engineering

- Sub-fields include computational fluid dynamics and heat transfer, neutral particle transport, structural mechanics, computational materials science
- Not much activity in US over past 2-3 decades
- Much remains 1-D, low-order numerical discretization, more homogenized then necessary, with many things “modeled”.
- CS&E progress made in SciDAC, ASC, and elsewhere can have a positive impact

Examples of Applicable Advances in CS&E

- 3-D turbulent CFD in complex geometries
- Efficient neutron transport methods (vs diffusion)
- Computational materials science
- Parallel computing
- Multiscale and Multiphysics methods
- V&V + UQ

Issues to Keep in Mind for V&V

- Uncertainty in data sets (i.e., neutron cross-sections)
- Inaccuracies in approximate equation sets (i.e., incompressible flow verses low speed compressible flow)
- Applicability of models (turbulence models, flow regime maps …)
- Complex geometries
- Question: How do all of these interact with time and space discretization errors ?

Examples to Highlight Some Issues

1. Time integration error verses uncertainty in data sets: Results from Vince Mousseau

2. Mesh definition and grid refinement studies for complex 3-D flows. Equation set and turbulence model. Results from Kurt Hamman

3. V&V + UQ issues / plans for next generation fuels performance code. Results from Glen Hansen

Time Integration Error (1 of 4)

1. A group of people have been promoting that time integration methods for reactor safety simulation be advanced from 1st order accurate operator split to 2nd order accurate unsplit.

2. A number of parties have made a point that the level of uncertainty in the nuclear cross-section data (and other models) does not warrant accurate time integration.

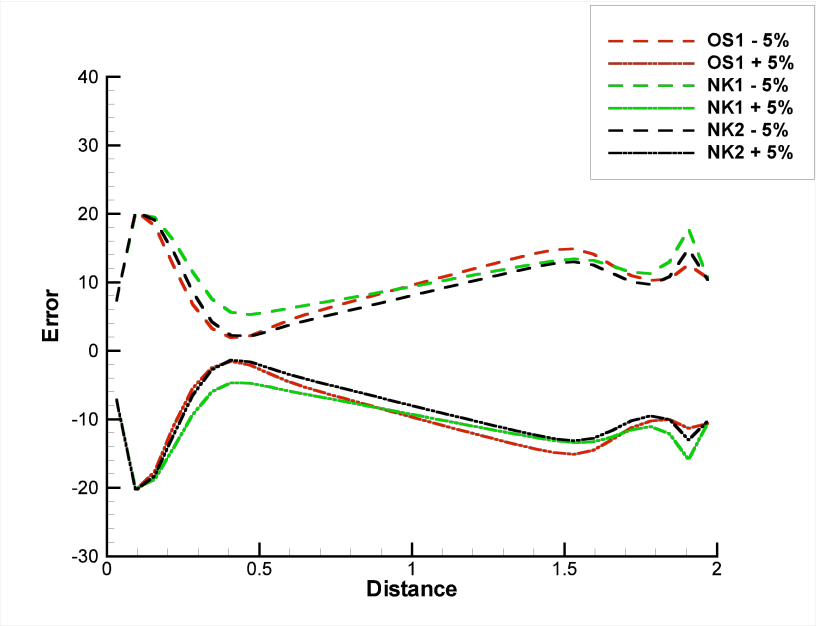
3. This implies that physical model error is much larger than time integration error. Let us do a simple test

Time Integration Error (2 of 4)

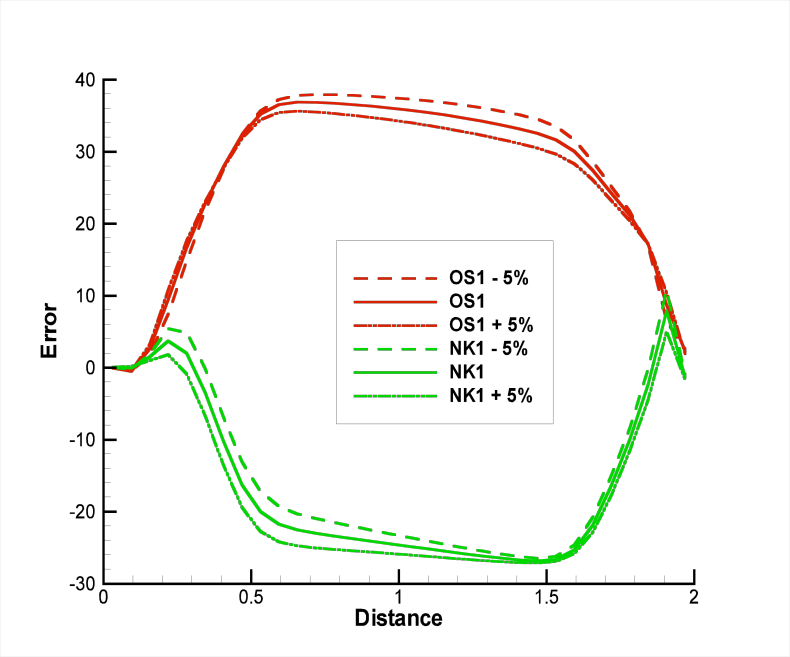
1. The example problem is a model control rod ejection transient in a LWR coming from prototype software for the next generation transient systems simulation code.
2. Mousseau, JCP 2004 (ICONE 2006)
3. +/- 5 % variation in cross-section is compared to 1st order time integration error and operator split numerical error (by removing it). We consider this a “big” variation.
4. Look at difference in clad temperature along fuel at an interesting point in the transient.

Time Integration Error (3 of 4)
Error in clad temperature

Physical model variation



Numerical error



Time Integration Error (4 of 4)

1. Time integration error (1st order or operator split) is same magnitude of variance as is caused by 5 % variation in cross-section.

2. Point 1: All sources of error must be considered / studied when embarking on a V&V campaign

3. Point 2: Time convergence studies must be a part of verification along with space convergence

Complex Geometry (1 of 7)

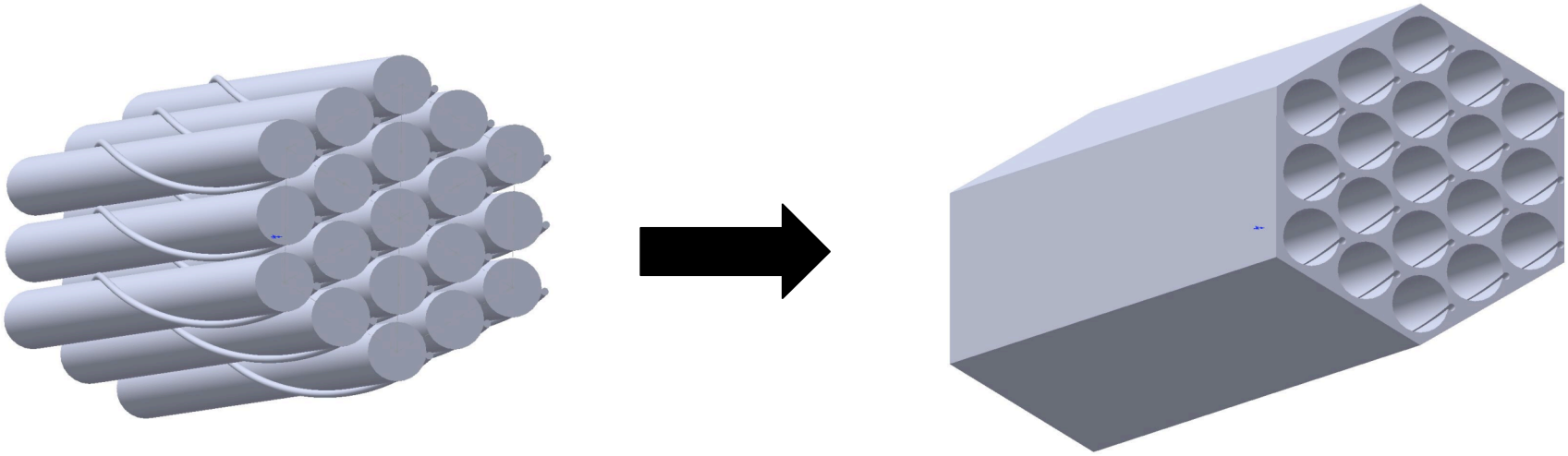
1. Fuel assembly of a SFR will contain 217 fuel pins, each having a small wire wrap, inside of a hexcan.

2. This makes for a very complicated geometry for 3-D turbulent CFD. Especially when attempting to resolve boundary layers

3. What is required to simulate a 19 pin, electrically heated experimental assembly, from a 1980's ORNL experiment (THORS), with a commercial CFD tool

Complex Geom (2 of 7)
CAD Model - SolidWorks

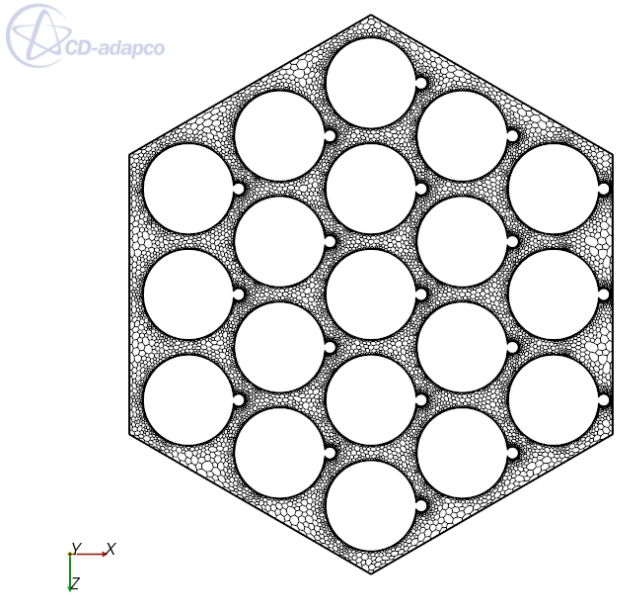
- **Geometry "similar" to Advanced Burner Test Reactor (ABTR)**
  - **Fuelpin Diameter => 0.80 cm (ABTR 0.80 cm)**
  - **Wirewrap Diameter => 0.103 cm (ABTR 0.103 cm)**
  - **Length => 20 cm (ABTR 260 cm)**
  - **Pin to Pin Gap => 0.032 cm (ABTR 0.001 cm)**

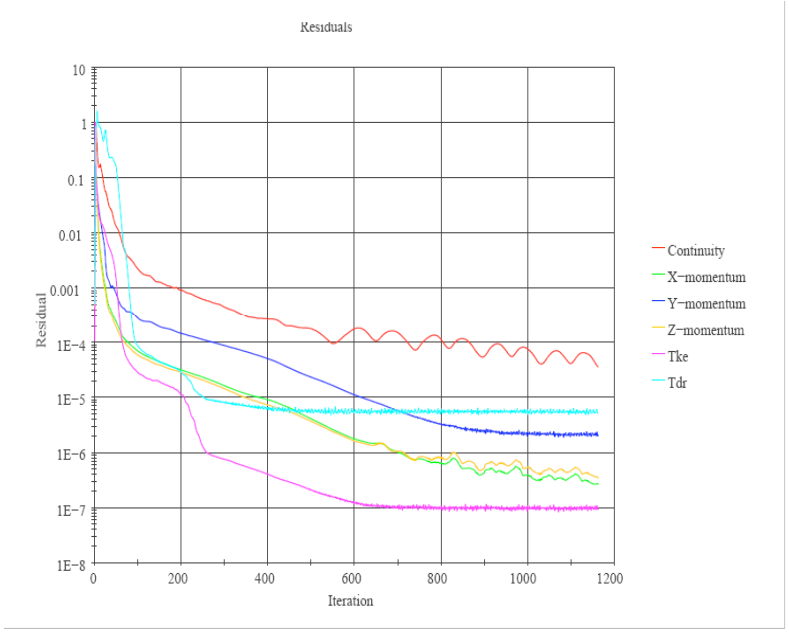


19 Fuelpin Assembly
(ABTR – 217 Fuelpins)

Computational Volume
(Fluid Only)

Complex Geom (3 of 7)
3D Meshing/Simulation

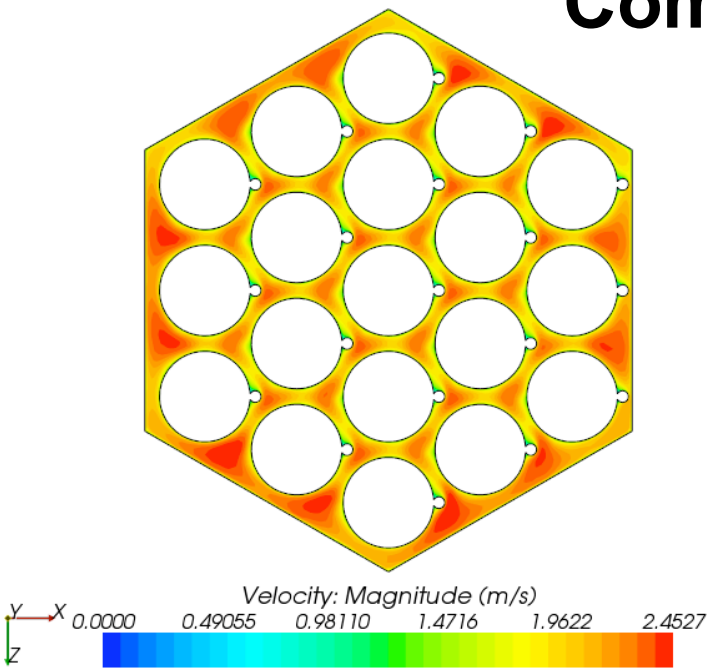


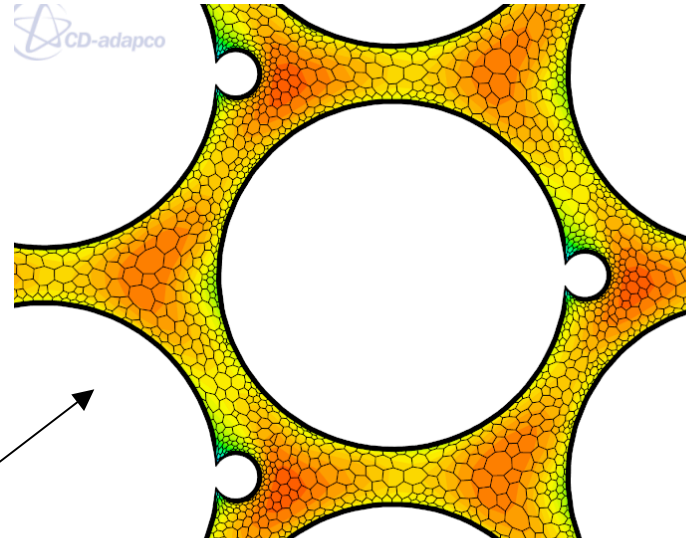


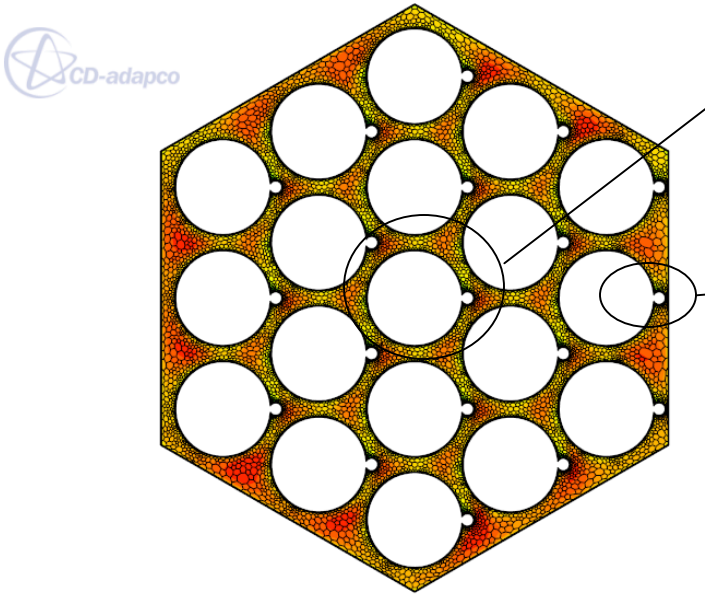
Serial Mesher
65.5 Million Polyhedral Cells
Mesh Time: ~36 hours

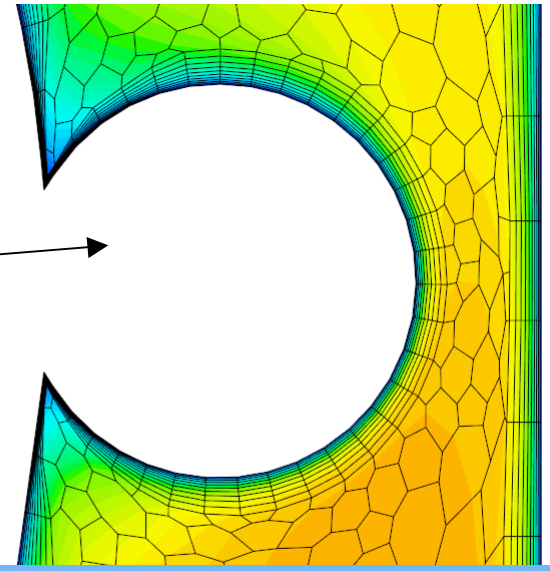
64 Parallel Processors
(Incompressible Turbulent Flow with no H.T.
Inlet Velocity 2 m/s / Outlet Pressure 0 psi)
Simulation Time: ~24 hours/1200 Iterations

Complex Gem (4 of 7)









Complex Geom (5 of 7)
Challenges

- ***Simulation Size (65 - 100 million cells)***
  - Mesh Generation (3D Problem => Wirewrap)
    - **Some Commercial Software**
      - **Could not mesh and/or Labor intensive**
      - **Poor Boundary Layer Control**
    - **CCM$^+$=> Successful (polyhedral cells)**
      - **Less Control over Mesh (unstructured mesher)**
      - **Good Boundary Layer Control**
    - **Memory requirements are large**
    - **Long Meshing Time**

Complex Geom (6 of 7)
Challenges (cont.)

- Commercial CFD Software
  - **Some Software had convergence problems**
  - **Software Capabilities: CCM+ good**
- Visualization of Mesh/Post Processing Results
  - **Tedious and slow (data transmission)**
  - **Extremely Difficult/Impossible to Inspect Mesh**
  - **Need <u>Fast</u> <u>Network</u> <u>Infrastructure</u> for HPC!**
- *Convergence Analyses/Grid Refinement*
- *Validation*

Complex Geometry (7 of 7)

1. Complex geometry combined with boundary layer will add issues to mesh convergence studies and thus verification

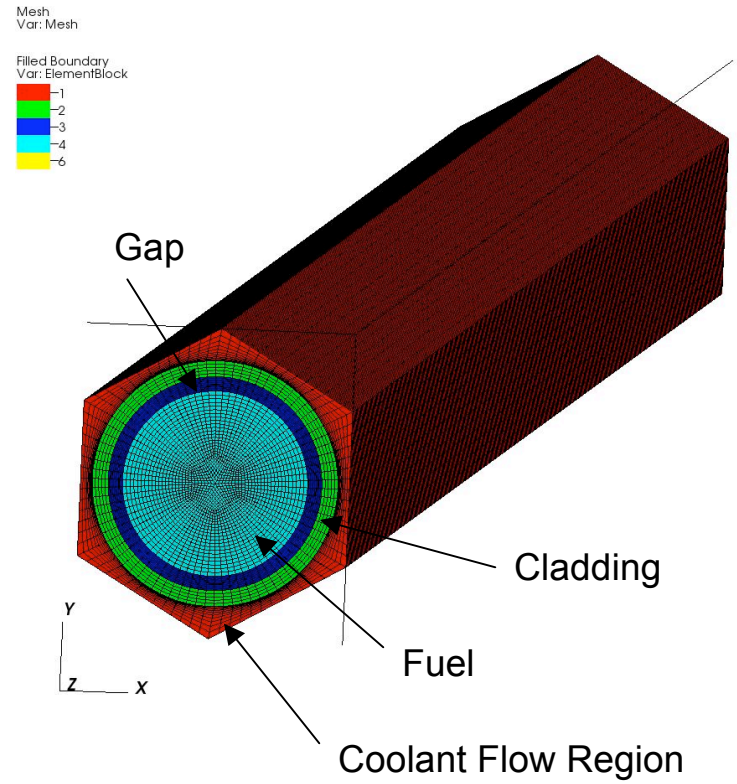
2. Due to the challenging geometries, people will be less likely to consider full Navier-Stokes solvers and use incompressible Navier-Stokes simulations.

3. Improper use of incompressible NS equations can lead to turbulence model validation issues. This results when terms ignored in NS equation have similar order as sensitivity to turbulence models.

4. Issues related to “legacy data” vs “live experiments”

Fuel Performance Simulation (1 of 7)

- Develop a predictive capability for reactor fuel design and analysis
- Design goal - preserve cladding integrity
  - model processes that lead to cladding failure for a nominal pin
  - model failure processes for the first pin to fail
- Actual failure is stochastic - only 1 in one million pins fail



Fuel Performance Simulation (2 of 7)
Predictive Capability

Goal: Predict the behavior of $(U_{0.65}Pu_{0.25}Np_{0.05}Am_{0.05})O_x$

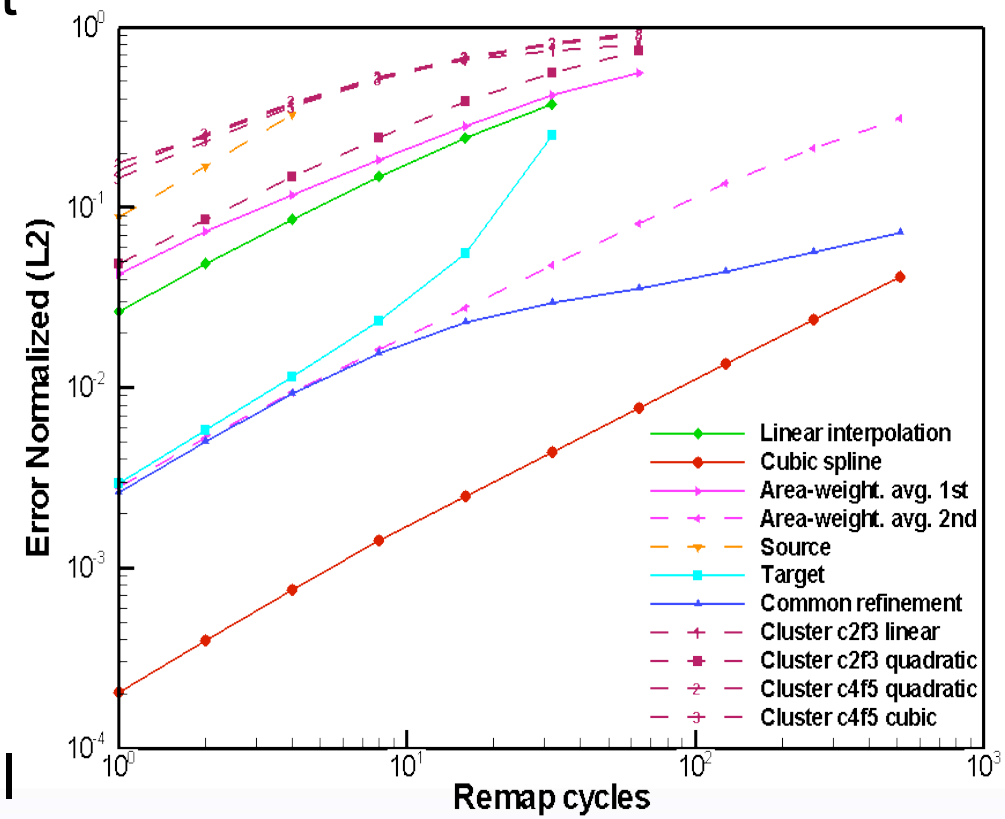
- Given the fuel $(U_{0.7}Pu_{0.25}Np_{0.03}Am_{0.02})O_x$
- Validate the models
  - Incomplete data and understanding of the physics
  - No ready source of fast neutrons for experimentation
- Verify the implementation of the models
- Using the above code, predict the behavior of $(U_{0.65}Pu_{0.25}Np_{0.05}Am_{0.05})O_x$

Fuel Performance Simulation (3 of 7)
Code Design Considerations

- Multiphysics and Multiscale
- Nonlinear thermal/structural response – creep failure
- Fuel matrix/structure degradation (cracking, swelling)
- Chemistry/stoichiometry
- Fission gas production and migration
- Fuel constituent migration – porosity migration
- Radiation damage

Fuel Performance Simulation (4 of 7)
Design Considerations

- Thermal/structural contact (radial/axial growth)
- Each physical model has unique mesh requirements
  - "Remap" the solution between distinct meshes
  - Common mesh for all models; use *hp*-adaptation to provide spatial resolution needed for each model



Fuel Performance Simulation (5 of 7)
Design Considerations

- Predictive capability will require including the meshing process in UQ
  - How sensitive is the coupled solution to perturbations in the mesh?
- Goal-oriented *hp*-adaptation
  - Error metric based on design parameters

Fuel Performance Simulation (6 of 7)
Verification

- Using qualified norms:
  - Individually verify the implementation of the models (unit testing)
  - Verify combinations of the models (integrated testing)
- Build verification tools into the code at design stage
  - a-priori error estimation for testing of component sets
  - a-posteriori error estimation for integrated system testing

Fuel Performance Simulation (7 of 7)
Validation

- LWR fuels data plentiful
  - Experimental
  - Operational
- Lacking data specific to GNEP problem
  - Oxide fuels $(U_{0.65}Pu_{0.25}Np_{0.05}Am_{0.05})O_x$
  - Metal fuels
  - Fast neutron / high temperature environment
- Code to code V&V – legacy codes
  - Simple, LWR focused, models
  - Dated numerical implementations
  - Low dimensionality
  - Legacy codes not always validated nor verified

Conclusion

1. Impact of proper V&V + UQ is significant.
2. New validation oriented experimental program will be needed.
3. Some education of the nuclear engineering community required
4. Need a plan