U.S. DEPARTMENT OF ENERGY
Nuclear Energy

The AMP (Advanced Multi-Physics) Nuclear Fuel Performance Code

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Presenting for the entire AMP team:

Developers	Collaborators	Advisors
➢ Oak Ridge National Laboratory ✦ Kevin Clarno ✦ Bobby Philip ✦ Bill Cochran ✦ Srdjan Simunovic ✦ Rahul Sampath ✦ Srikanth Allu ✦ Gokhan Yesilyurt ✦ Jung Ho Lee ✦ Pallab Barai ✦ James Banfield ➢ Los Alamos National Laboratory ✦ Gary Dilts ✦ Bogdan Mihaila	➢ Idaho National Laboratory ✦ Richard Martineau ✦ Glen Hansen ✦ Samet Kadioglu ✦ Ray Berry ➢ Argonne National Laboratory ✦ Abdellatif Yacout ➢ Oak Ridge National Laboratory ✦ Larry Ott ✦ Sreekanth Pannala ✦ Phani Nukala ✦ Jay Billings ➢ Los Alamos National Laboratory ✦ Mike Rogers	➢ Los Alamos National Laboratory ✦ Cetin Unal ✦ Steven Lee ➢ Oak Ridge National Laboratory ✦ John Turner ➢ Idaho National Laboratory ✦ Steve Hayes ➢ Argonne National Laboratory ✦ Marius Stan

Outline

- **FY10 background and plan**
  - **Vision for a predictive Fuels IPSC**
  - **Staged development plan**
  - **Defining the mission to build the code**
    - **Purpose, product, and deliverables**

- **Fulfilling the mission**
  1. **Deliver a useful, new capability to the user community**
     - **Physics incorporated within AMP-0.9**
  2. **Demonstrate an understanding of the coupled physics-simulation process**
     - **Demonstration problems and results**
  3. **Gain experience developing software as a multi-institutional team**
     - **Collaboration approach**
  4. **Enhance our understanding of the software and user requirements**
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Vision for a "predictive" fuel performance and safety code

- **A multi-year effort to provide software that will be used to**
  - **Qualify advanced fuel designs**
    - **to demonstrate that the fuel will perform predictably and acceptably under normal operations and transient conditions**
  - **Design new fuel**
    - **sufficiently predictive to evaluate the potential of novel fuel design options that are beyond the empirical database used to qualify the software**
  - **Enhance embedded engineering codes**
    - **to provide a computationally efficient approximation of the fuel response to a reactor simulation code**

- **Tremendously challenging due to the**
  - **breadth of the fuel/reactor types that must be considered**
  - **extent of micro- and atomistic-scale physics that must be incorporated**
  - **need for a quantified estimate of the uncertainty of the solution to all aspects of the simulation**
  - **need for an interface for a user with limited high-performance computing expertise**

Turner, Clarno, Hansen, "Roadmap to an Engineering-Scale Nuclear Fuel Performance and Safety Code" ORNL/TM-2009/233

Multi-year roadmap to the vision

- **2010**
  - **Design, develop, and deliver the AMP Nuclear Fuel Performance Code**
    - **Nominal operation with UO_2 and MOX fuel in an LWR**
    - **Incorporating material properties and models from FRAPCON**
- **2011**
  - **Understanding the requirements**
    - **How do we couple with the meso-scale simulations?**
    - **What assembly-level effects must be considered (flow, neutronics)?**
    - **How can we integrate chemistry (fuel-clad, clad-coolant)?**
    - **Will contact algorithms converge for hundreds of fractured pellets?**
  - **Getting feedback from the fuel engineering community**
    - **What critical physics is missing?**
    - **How does the user-interface need to change?**
    - **Sensitivity and uncertainty quantification evaluations**
- **2012 – 2015**
  - **Annual releases of the demonstrated capability**
    - **Nominal and transient analyses of a single advanced (transmutation and LWR) fuel pin**
    - **Incorporating on-line simulations of some meso-scale physics to provide continuum-scale properties upon which the solution is most sensitive**
- **2016 – 2022**
  - **Annual releases of the visionary code**
    - **Nominal and transient analyses of fuel in any conceivable composition and configuration**
    - **Incorporating on-line simulations of atomistic, single crystal, and meso-scale physics**

Fuel Performance Code
3D Cylindrical Fuel Geometries

↕

Meso Scale Simulation
Microstructure Evolution

The AMP Nuclear Fuel Performance Code

- **The PURPOSE is to:**
  - **Deliver a useful, new capability to the user community**
    - **For exploratory, not mission-critical, applications**
    - **A vehicle for collaboration with meso-scale developers, fuel designers, and the experimental community**
  - **Demonstrate an understanding of the coupled physics-simulation process**
    - **To ensure we're doing what is needed for the community**
  - **Gain experience developing software as a multi-institutional team**
    - **Trust, understanding, nomenclature, environment**
  - **Enhance our understanding of the software and user requirements**
    - **Software: additional physics, methods of incorporating meso-scale models, handling contact**
    - **User: input and setup, output processing, runtime and performance expectations**

- **The PRODUCT:**
  - **Was conceived, designed, developed, and delivered in FY10;**
  - **Is a 3D coupled thermal-mechanical-chemical code**
    - **with links to existing modularized zero-dimensional solvers,**
    - **as well as a simplified flow and power module;**
  - **Is distributed through the RSICC**
    - **With proper export control protections**
    - **and approval from the legal divisions at each institution**

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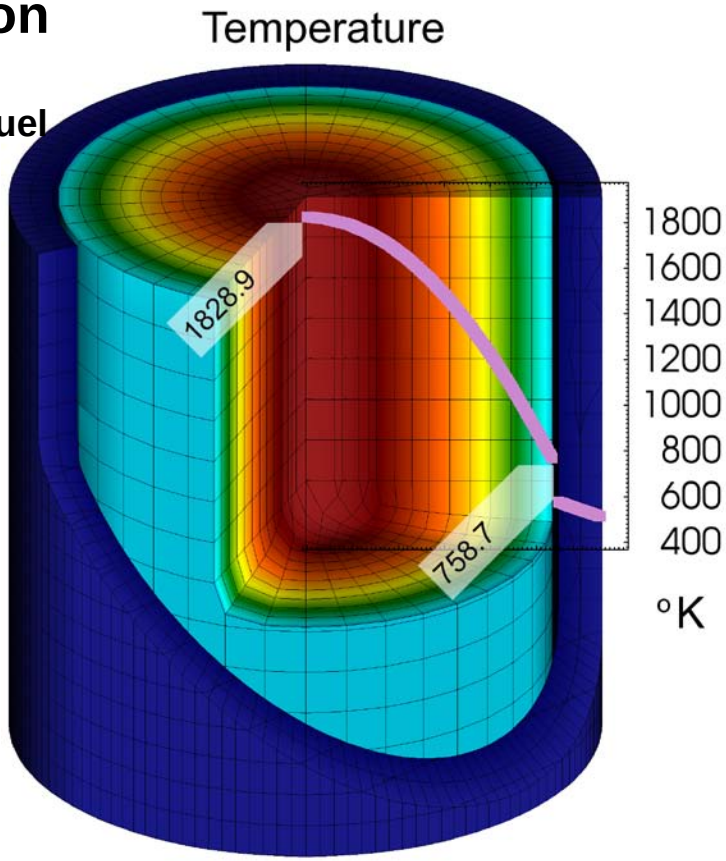
The Physics of AMP-0.9
that may not be fully integrated or validated

- **Pre-processing**
  - **Neutronics**
    - **Power and/or neutron flux**
    - **Isotopic transmutation**

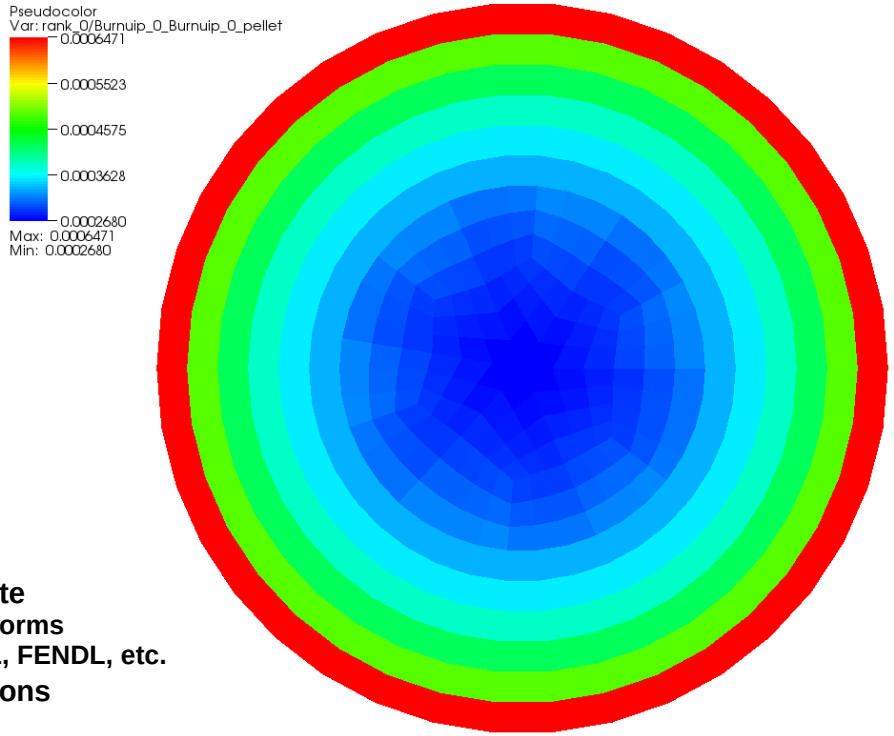
- **Time-dependent, coupled physics simulation**
  - **Heat transfer**
    - **Time-dependent nonlinear thermal diffusion within fuel and clad**
    - **Axially-varying gap conductance**
    - **Quasi-static axial convective coolant flow**
  - **Mechanics**
    - **Small deformation mechanics within fuel and clad**
    - **Accounting for thermal expansion, densification, swelling, relocation, and creep**
    - **No mechanical interaction between bodies**
  - **Oxygen transport**
    - **Time-dependent, or quasi-static, (Fick+Soret) oxygen transport within fuel**

- **Post-processing**
  - **Species formation**



Neutronics
(Preprocessing)

- **Given the user-defined:**
  - **Power (fuel) or neutron flux (clad)**
  - **Piece-wise constant variation in time**
    - **Will add more variations in the future**
  - **Functional variation in space**
    - **Radial rimming effect in thermal reactors**
    - **Axial power peaking factors**
    - **Azimuthal variations due assembly features**



- **Computes the space-time distribution of:**
  - **Specific power (Watts/kg^{Fuel})**
  - **Isotopic/elemental concentrations and rates of change**
    - **eg. kg-U^{235}/kg^{Fuel}**
    - **kg-Xenon/kg^{Fuel}-sec**
  - **Reduced quantity concentrations and rates of change:**
    - **Fission gas (Krypton+Xenon) production rate**
    - **Metal (Thorium, Uranium, Plutonium, …) concentration**

- **Using a modular form of a well-validated code**
  - **ORIGEN-S from the SCALE-6.1 Nuclear Analysis Code Suite**
    - **Countless NUREG and OECD/NEA reports for many fuel forms**
    - **Tracking 1960 isotopes with data from ENDF, JEF, JENDL, FENDL, etc.**
  - **Distributed with multiple prepackages neutron cross sections**
    - **UO_2 in PWR, BWR, or CANDU**
    - **MOX in PWR or BWR**
    - **TRU-Zr in an SFR**

- **Only the specific power is being used by the time-dependent, coupled physics simulation**
  - **Elemental concentrations are used in the post-processing**

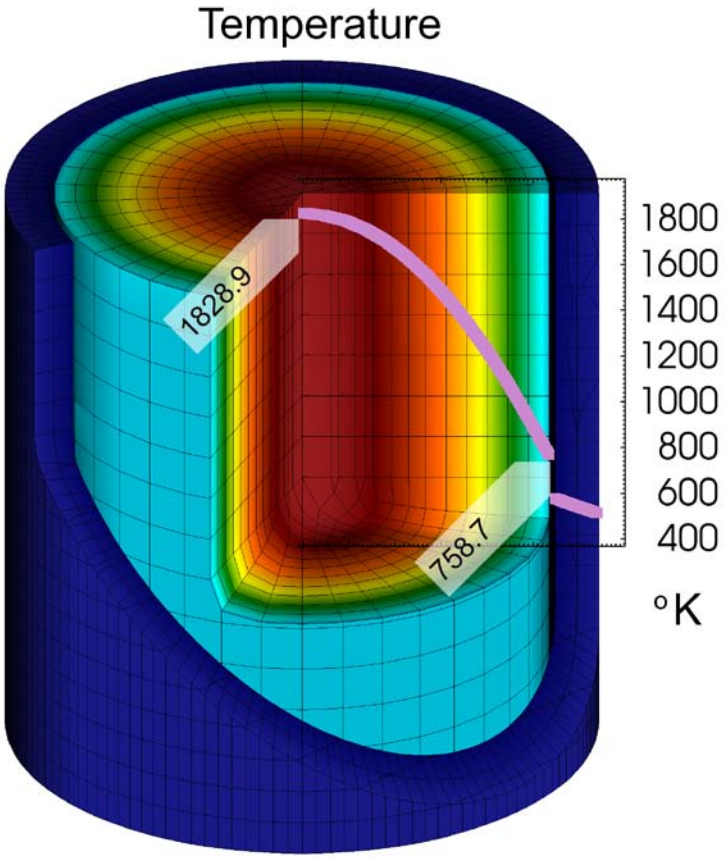
Heat Transfer

- **Time dependent thermal diffusion within a volume**
  - **Conductivity, density, and heat capacity**
    - **A function of variable temperature, burnup, and oxygen concentration**
    - **A function of many other user-defined variables (porosity, etc.)**
  - **Very well tested**
    - **Manufactured solutions with many different boundary conditions**
    - **Used to test many other physics**
      - **Gap conductance, mechanics, flow, etc.**
  - **Time-integration with IDA From SUNDIALS**
    - **Implicit with variable time-stepping**

- **Axial coolant flow**
  - **Map of 2D clad surface to 1D azimuthally-averaged clad surface temperature**
  - **One-dimensional (1D), single phase flow preserves heat balance**
  - **User-defined heat transfer coefficient**
    - **Piecewise-constant in time**

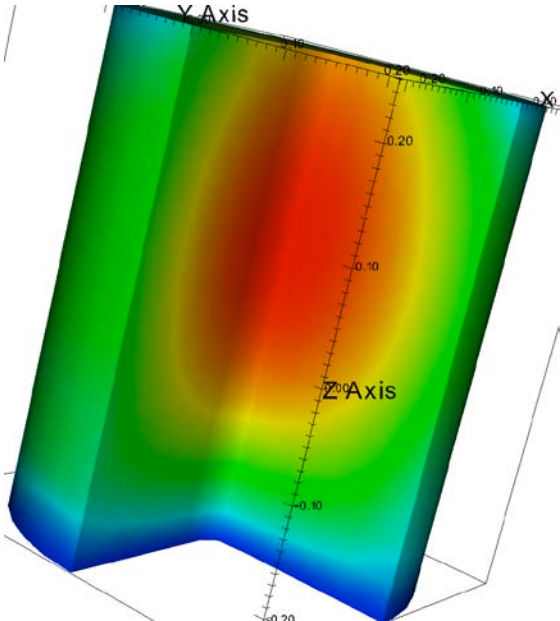
- **Simple gap conductance**
  - **Uses the Map to transfer heat from a single fuel mesh to the clad mesh**
  - **Exactly transfers a heat flux that is (up to) linearly-varying axially and azimuthally-constant.**
    - **Smears any azimuthal variation of the heat flux**
  - **Requires a users-defined heat transfer coefficient**

- **Solution strategy**
  - **Time-dependent or quasi-static**
  - **Fully-coupled or operator split**
  - **Stand alone or with other physics**



Mechanics

- **Elastic-Plastic Mechanics within a volume**
  - **Properties and materials models**
    - **A function of variable temperature, burnup, and oxygen concentration**
    - **A function of many other user-defined variables (porosity, etc.)**
  - **Quasi-static small deformation mechanics**
    - **Small deformation is sufficient for a single pellet/clad**
    - **Neglects the effects of the momentum of one material on another**
  - **Many material models**
    - **Instantaneous:**
      - **Thermal expansion, densification, swelling, relocation**
    - **Implicit (or explicit) creep:**
      - **Mechanical, thermal, irradiation-induced**
    - **Many material models exist, but few are well tested**
- **There is no accounting for mechanical contact**
- **Solution strategy**
  - **Quasi-static with incremental loading**
  - **Fully-coupled or operator split**
  - **Stand alone or with other physics**



Oxygen Transport

- **Time dependent oxygen transport within a volume**
  - **Diffusion coefficient and Soret term**
    - **A function of variable temperature, burnup, and oxygen concentration**
    - **A function of many other user-defined variables**
  - **Oxygen diffusion (Fick-only)**
    - **Uses the same, well tested, coding as the thermal nonlinear diffusion operator**
    - **Is solved with the same, well tested, solvers and time-integrators**
  - **Oxygen transport (Fick+Soret)**
    - **Uses a summation of two nonlinear diffusion operators**
    - **Has been coupled in quasi-static and transient mode with thermal diffusion and mechanics**
      - **Has not been compared with published results or run on the demonstration problem**

- **There is no accounting for oxygen transport between volumes**

- **Solution strategy**
  - **Time-dependent or quasi-static**
    - **In quasi-static mode, the extremely small diffusion coefficient (10^{-18}) seems difficult to converge for Fick-only transport**
  - **Fully-coupled or operator split**
  - **Stand alone or with other physics**

- **The demonstration problem has no experimental or legacy results with which to compare the oxygen**

Material Database

- **Material properties**
  - **Heat transfer**
    - **Heat capacity, conductivity, density, transfer coefficients**
  - **Mechanics**
    - **Density, viscosity, Young's Modulus, shear modulus, Poisson ratio, yield stress, transition stress**
  - **Mechanics models**
    - **Densification, thermal expansion coefficient, strength coefficient, strain hardening exponent, strain rate sensitivity exponent**
  - **Oxygen transport**
    - **Fick coefficient, Soret coefficient, thermal diffusion coefficient**

- **Materials available**
  - **Fuel: UO_2, MOX, U-Zr, U-Pu-Zr**
  - **Cladding: Zircalloy, SS, HT-9**
  - **Coolant: Water, Sodium**
  - **Gap (not used): Helium, Sodium**

Species Formation
(post processing)

- **Equilibrium thermodynamic solver**
  - **Open-source**
    - **Developed by Piro and Thompson (RMC of Canada)**
    - **Advised by Besmann and Simunovic (ORNL)**
  - **Providing a species transport source term**
    - **Given elemental concentrations (U, O, …), temperature, and pressure**
    - **Minimize Gibb's free energy using the "Gibbs Criteria"**
    - **Compute the species formed (UO_2, UO_3, U_4O_9, …)**

- **An initial implementation**
  - **University student developed with substantial limitations and little SQA**

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Test Problem #1
Halden RP Experiment IFA-432

Test Problem #1

- **Purpose:**
  - **Evaluate the accuracy for nominal operation through comparison with experimental data and with respect to a legacy tool**
- **Problem:**
  - **Rod 1 of IFA-432 in the Halden Reactor Project**
  - **Nominal operation**
  - **UO_2 fuel**
  - **Zircalloy cladding**
  - **Many power ramps**
  - **Single pellet/single clad**
  - **Fixed clad outer temperature (513 K)**
- **Metrics:**
  - **Validation with experiment**
    - **Fuel centerline temperature**
  - **Code-to-code comparison**
    - **Temperature distribution**
    - **Mechanical displacement**

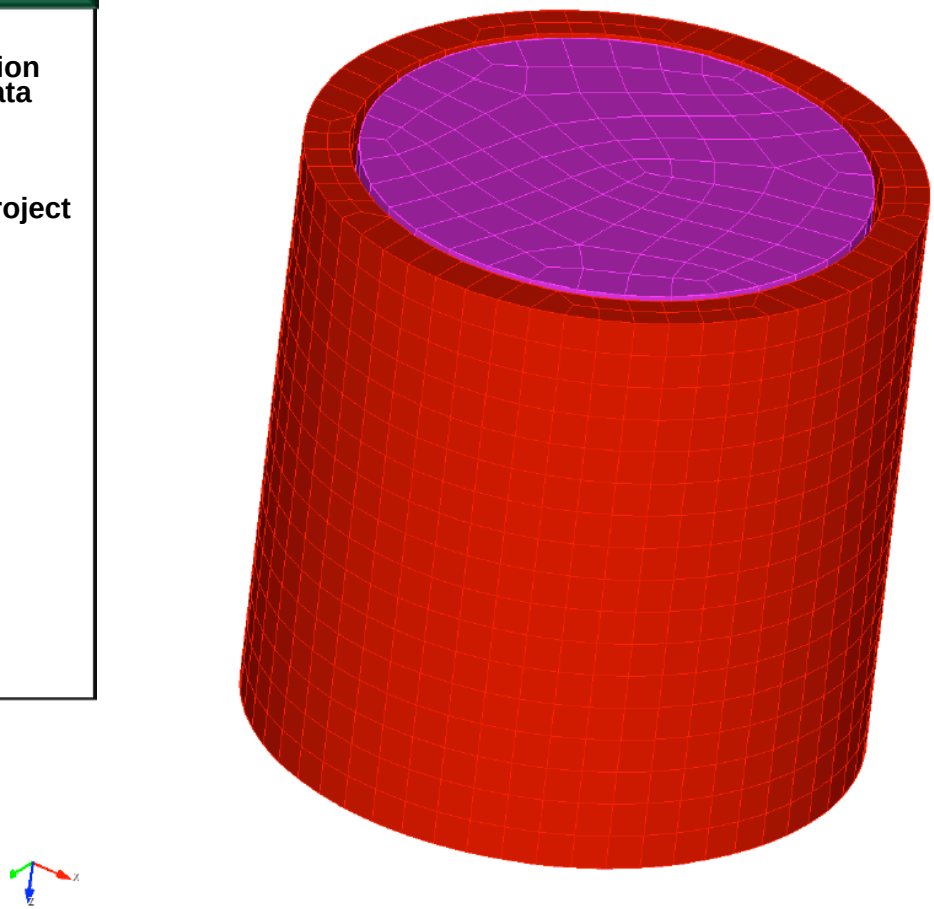
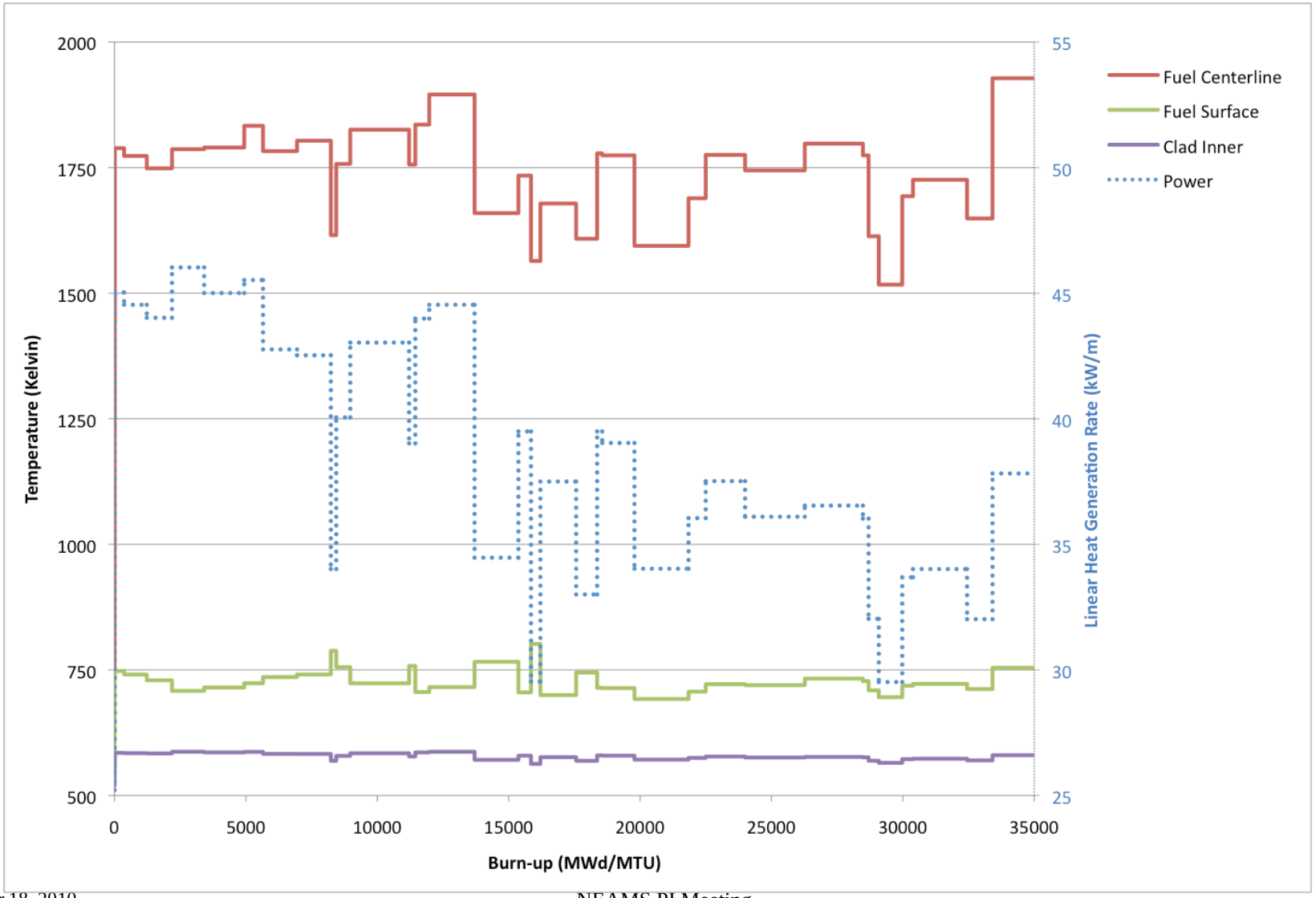
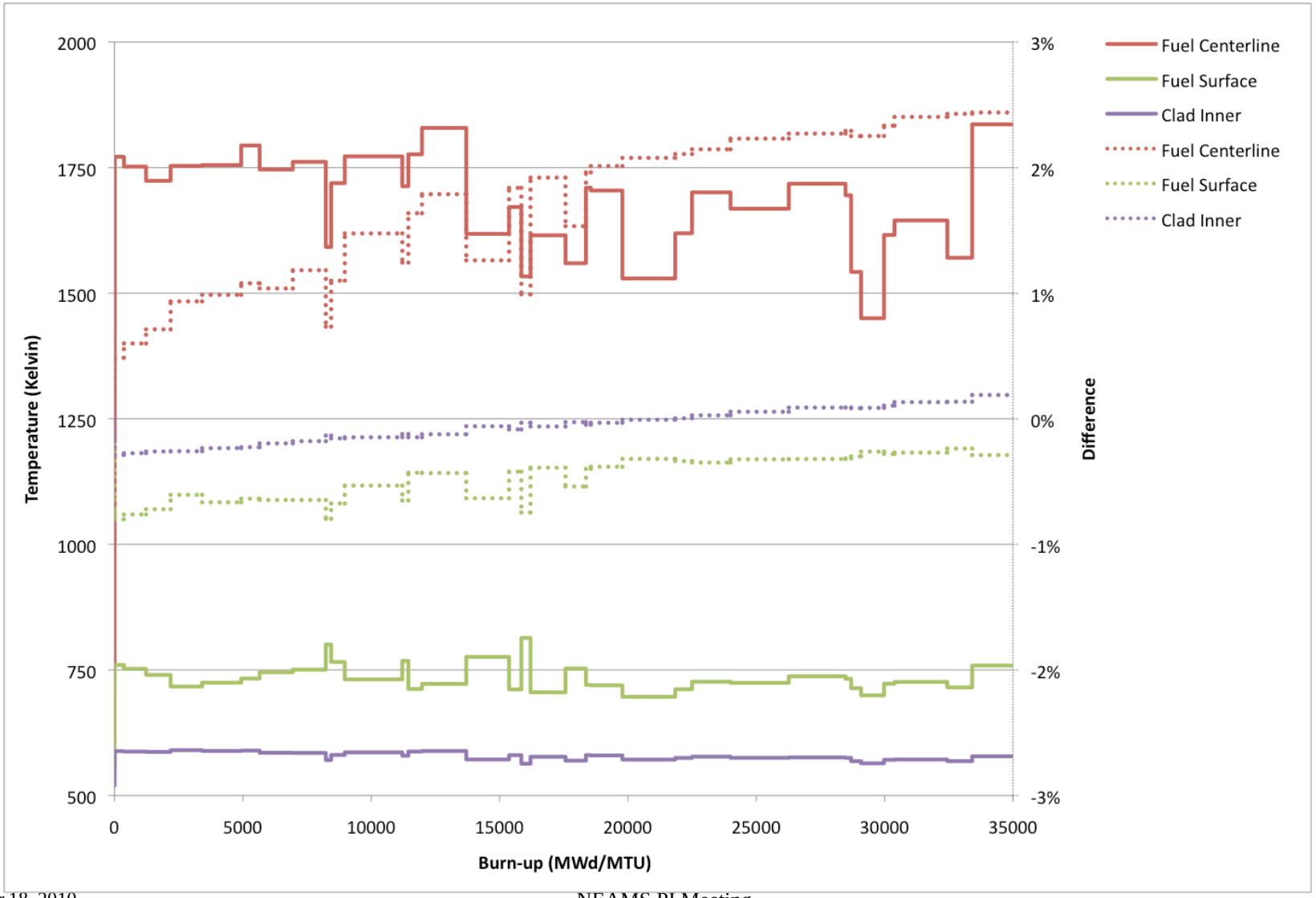


Figure 1: Coarse meshed fuel/cladding geometry, 15 mil gap (Rod 2 in Table 3)

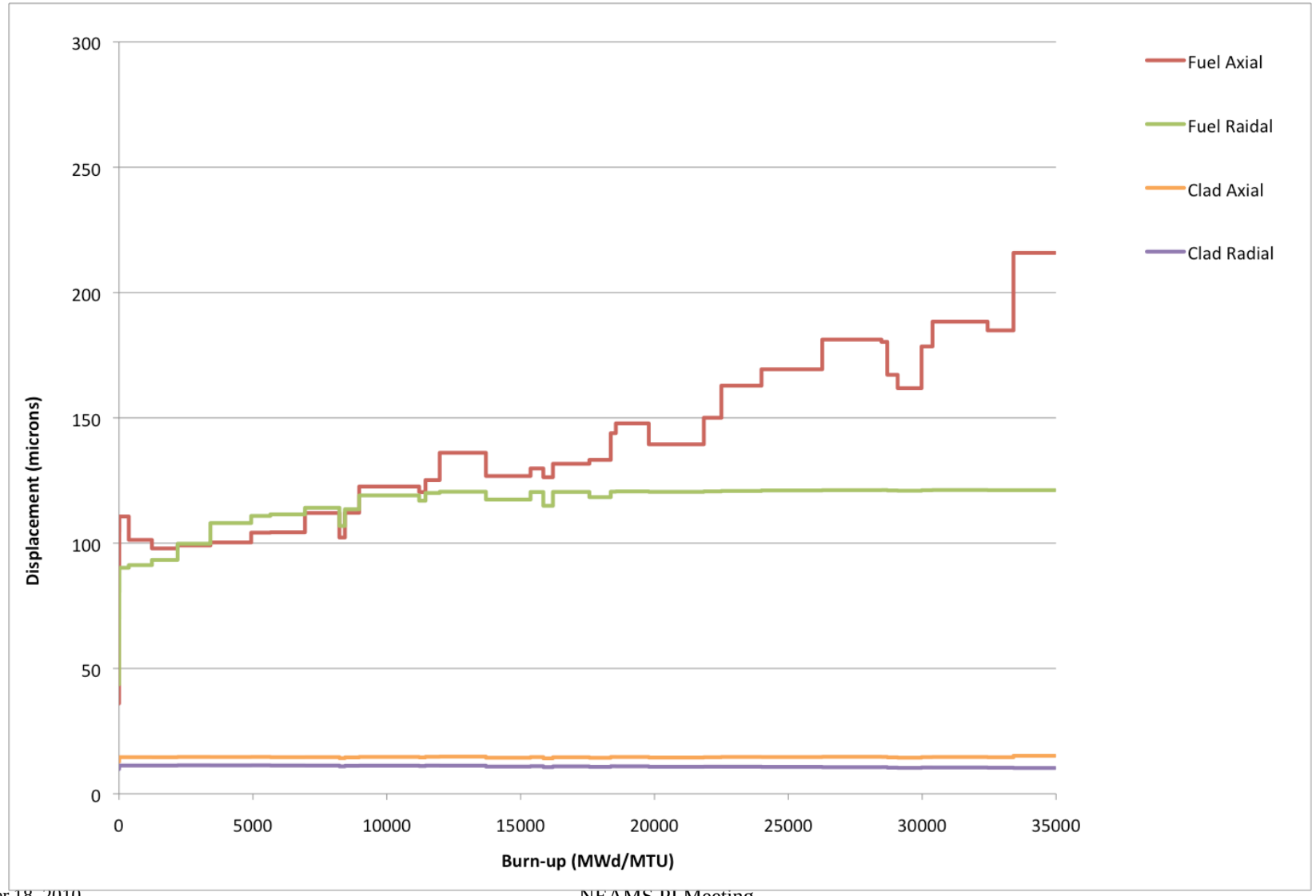
FRAPCON Temperature Distribution



AMP/FRAPCON Comparison Temperature Distribution



FRAPCON Mechanical Displacement



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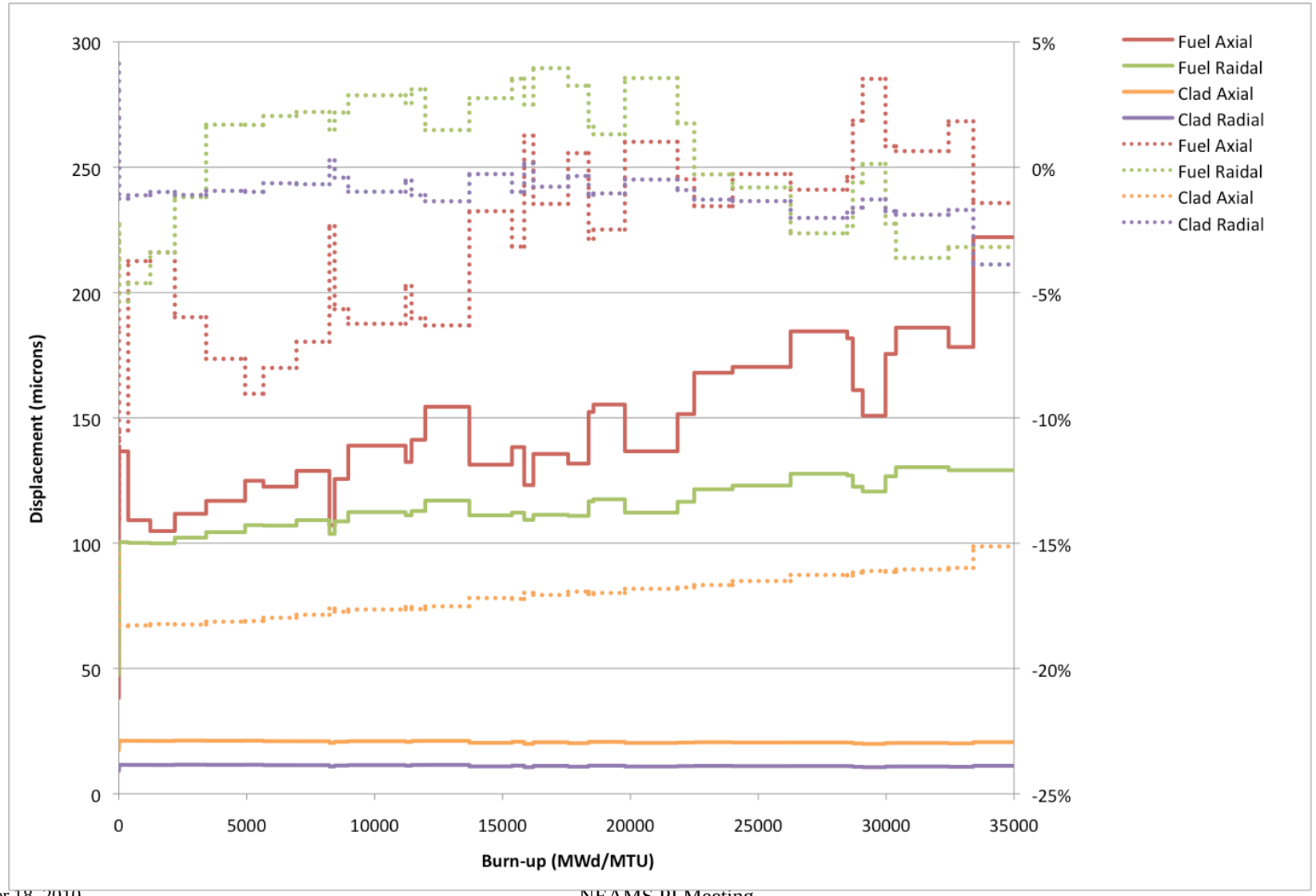
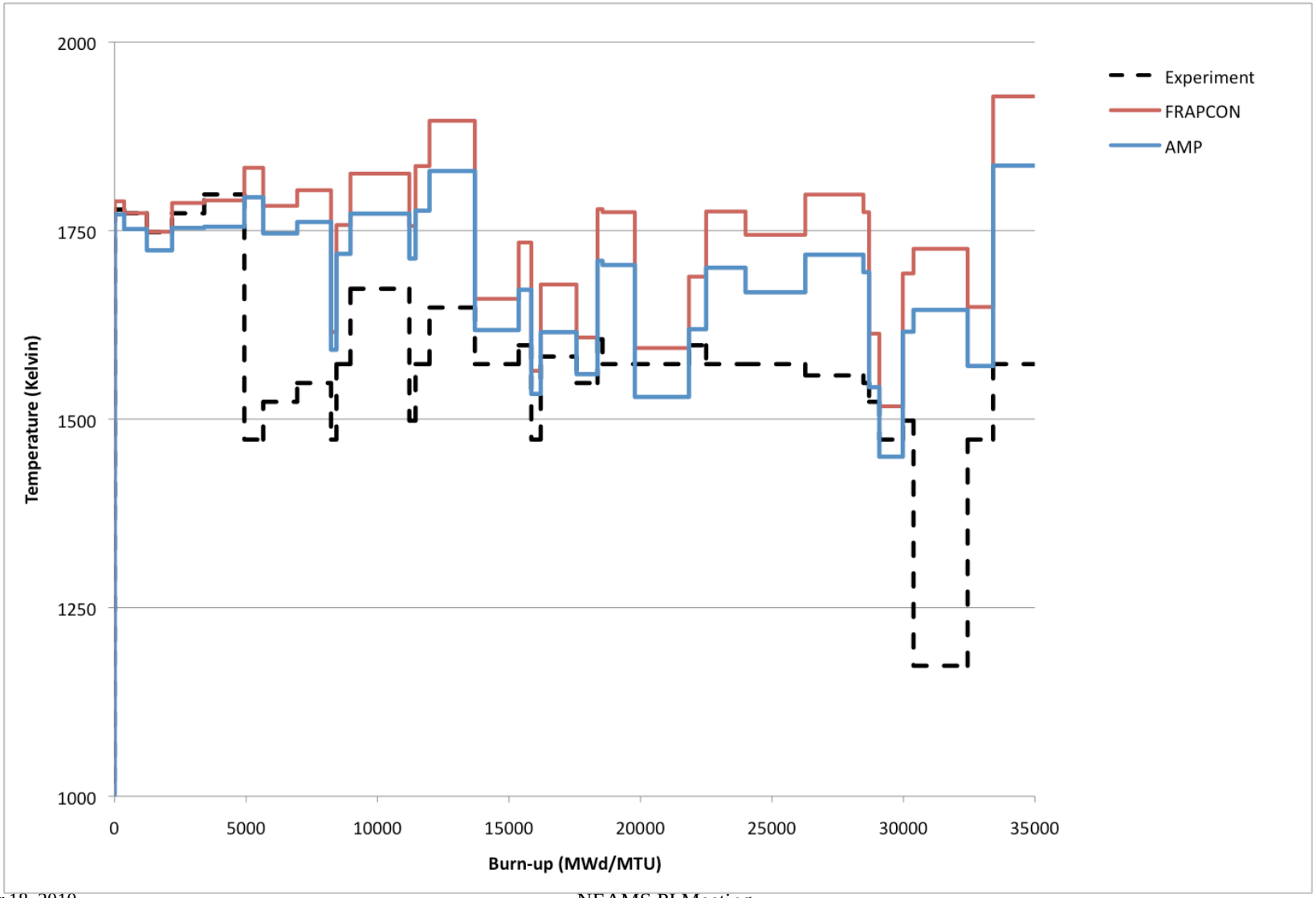


Validation Results
Seeking a Better Experiment



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Test Problem #1 Significance

- **Demonstrating legacy equivalence**
  - **FRAPCON solution was up to 45% different from experimental centerline temperature**
  - **AMP temperature distribution is within 3% of FRAPCON**
  - **AMP mechanics is within 5%, except clad axial**
    - **Anisotropic mechanics will be implemented in FY11**
  - **Substantial extensions required beyond original plan**
    - **Pellet relocation and creep models**
    - **Radial power distribution due to rim effect**

- **Approximate verification of the coding**
  - **Most material models and properties were from FRAPCON**
  - **Results should agree well and generally do**

- **Initial validation results**
  - **AMP was shown to estimate the experimental centerline temperatures with an equivalent accuracy as legacy tools**

Test Problem #1 Insignificance

- **FRAPCON is quasi-static in time**
  - **We did the same for this problem; time-dependent was far too costly for this many power ramps**
- **Mechanical contact did not occur until the last power ramp in the experiment**
  - **Since it didn't occur, our results are accurate despite neglecting it**
- **Many other physics are empirically-embedded within "burnup"**
  - **Neglecting "fission gas release" doesn't effect properties directly**
  - **Gap conductance cannot be computed without fission gas release or gap thickness**
    - **Our user-defined values were derived from the FRAPCON simulation**
- **FRAPCON does not model oxygen transport**
  - **We neglected it for this problem to make the answer's match**
- **This was a poorly characterized experiment**
  - **It does not provide a very good validation evaluation**

Test Problem #2
Axial Peaking within a Pellet

Test Problem #2

- **Purpose:**
  - **Demonstrate 3D capability with a multi-dimensional power distribution**
- **Problem:**
  - **Same problem as Test Problem #1**
  - **Allow the power to vary by a factor of 2 from the top top to the bottom of the pellet**
- **Metrics:**
  - **Visually accurate**
  - **Capable of accounting for the physics**

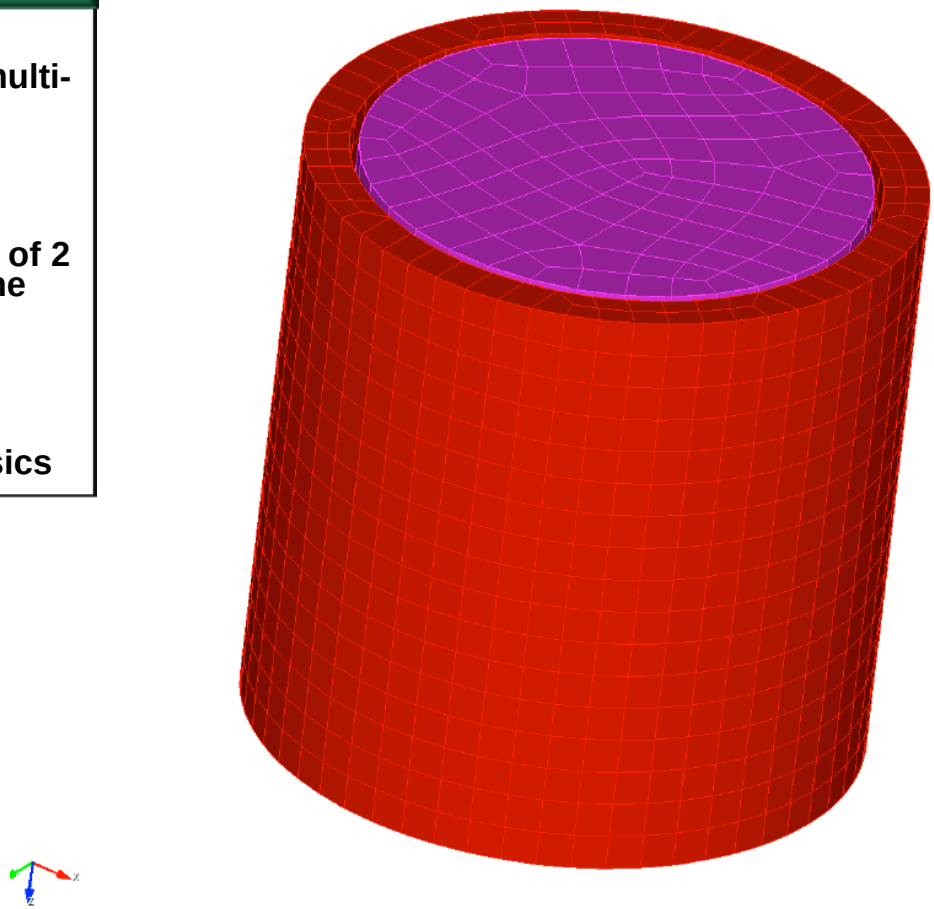


Figure 1: Coarse meshed fuel/cladding geometry, 15 mil gap (Rod 2 in Table 3)

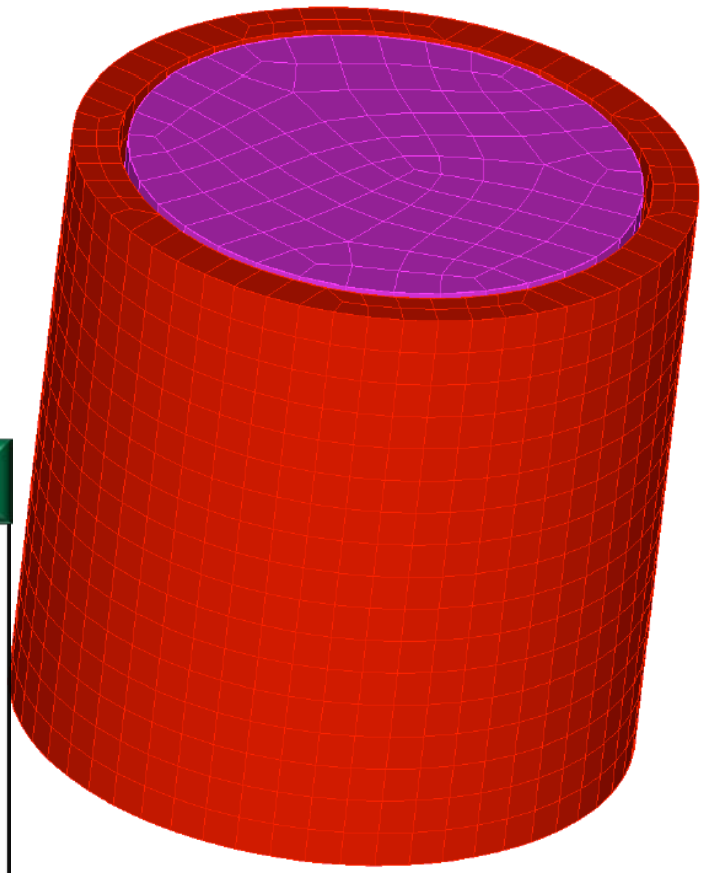
Test Problem #3/4
Radial Offset of a Pellet

Test Problem #3

- **Purpose:**
  - **Demonstrate 3D capability with thermo-mechanical contact**
- **Problem:**
  - **Same problem as Test Problem #1**
  - **Radially-offset pellet to partially close the gap when cold**
- **Metrics:**
  - **Visually accurate**
  - **Capable of accounting for the physics**

Test Problem #4

- **Purpose:**
  - **Demonstrate 3D capability with thermo-mechanical contact**
- **Problem:**
  - **Same problem as Test Problem #1**
  - **Radially-offset pellet to be in contact with the cladding when cold**
- **Metrics:**
  - **Visually accurate**
  - **Capable of accounting for the physics**



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Iterative Development and Team Building

- **AMP Kick-off Meeting**
  - **November 9-10; Los Alamos National Laboratory**
  - **Meet team members, discuss physics, and decompose the problem**
- **Code Camp I**
  - **January 19-22; Idaho National Laboratory**
  - **Technical exchange, demo collaborative environment and initial interface to backplane**
- **Code Camp II**
  - **March 8-12; Oak Ridge National Laboratory**
  - **Demo interface to backplane, mechanics, and materials and created development plan**
  - **Design and refactoring of diffusion and materials**
- **Code Camp III**
  - **April 26-30; Los Alamos National Laboratory**
  - **Diffusion operator is nearly finalized; Single physics solvers is demonstrated.**
  - **Initial release of software to RSICC for legal and export control review**
- **Code Camp IV**
  - **June 22-25; Idaho National Laboratory**
  - **MMS testing of diffusion; demo of multiphysics simulations and time-dependence**
  - **Initial focus on code-to-code comparison and validation of initial time-step results are excellent**
- **Code Camp V**
  - **November 1-5; Los Alamos National Laboratory**
  - **Discovering and debugging multiphysics simulations; initial results for full-benchmark problem**

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FY11 Work Packages

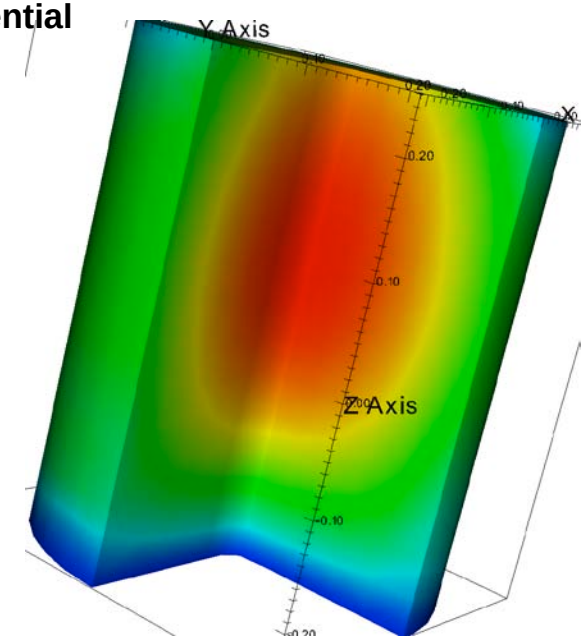
- **Finalize FY10 development efforts**
  - **Substantial testing, integration and documentation**
  - **Refactor software infrastructure to remove shortcuts**
  - **Develop a 3D thermo-mechanical contact capability**
- **Incorporate additional physics**
  - **Fission gas transport and release**
  - **Species formation and transport**
  - **Develop an initial advanced user-interface**
- **Release AMP-1.0**
  - **Additional validation evaluations for oxide and metal fuel**
  - **For use by friendly expert users for exploratory applications**
- **Redefine the long-term vision and roadmap**
  - **AMP and MBM will, together, be a unified predictive code**

Conclusions

- **The multi-lab team is sharing responsibility towards a common goal**
  - **Has developed a common understanding of the problem (physics, nomenclature, coding style)**
  - **Is learning to work (more) efficiently together**
  - **Is working towards a clear long-term development process with achievable goals**
  - **Allows us to interface with fuel designers and material scientists at each institution for rapid feedback and user support**

- **AMP is**
  - **Modeling fully-coupled, implicit thermal-oxygen-mechanics on a single pellet and cladding problem**
  - **Capable of being executed through a simple user interface or an expert developer interface**
  - **Demonstrated for both legacy equivalence and three-dimensional potential**
  - **Capable of being extended to model advanced fuels**
  - **Available through RSICC, to developers, as an export controlled code**
    - **http://rsicc.ornl.gov/rsiccnew/CFDOCS/amprequest_form1.cfm**

- **AMP will**
  - **Be finalized with documentation and thermo-mechanical contact**
  - **Provide a useful, new capability for exploratory fuel simulations**
  - **Serve as a vehicle for addressing M&S needs of all fuel types**



Backup slides

Development Team Members that are Present Today

- **Bobby Philip (The Trail Guide)**
  - **Chief Software Architect**
  - **Lead for multi-physics coupling and time-integration**
  - **Persistently guiding the software to help ensure that the varied, independently-developed components would fully integrate within the time-dependent, multi-physics environment.**
  - **Integrating the components to allow for fully-coupled, implicit time-integration of mechanic, thermal diffusion, and oxygen transport**

- **Bill Cochran (The Foundation)**
  - **Lead for software backplane (interfaces) development**
  - **Anticipating, and responding to, the needs of many distributed software developers to enable efficient coding with little regard to the intricacies of external software packages.**
  - **Hands on assistance for developers in the proper use of the AMP interfaces to the backplane and solvers.**

- **Gary Dilts (Mr. Utility)**
  - **LANL lead**
  - **Lead for development of the diffusion operator used for thermal and oxygen (Fick and Soret) transport**
  - **Also, LANL software architect, build/compile/test external packages at LANL, extensive manufactured solutions of diffusion, scripting, …**

- **Bogdan Mihaila (The Material Scientist)**
  - **Lead for material properties**
  - **Mining and integrating models from many sources and begging for material science end-use applications**
  - **Interface to lower-length-scale modeling efforts to assist with upscaling**

AMP is Designed To:

- **Provide the software infrastructure to perform end to end calculations of time dependent coupled nonlinear multi-physics problems.**
- **Leverage existing investments in software by DOE and others for time integrators, nonlinear solvers, linear solvers, discretizations, and meshing.**
- **Be only loosely coupled to external software packages ensuring that AMP is not tied to the development path or bottlenecks of external packages for time integrators, nonlinear solvers, linear solvers, discretizations, meshing, and materials databases.**
- **Leverage the strengths of multiple packages simultaneously – for example use SUNDIALS, PETSc, and Trilinos at the same time to use their strengths.**
- **Be extensible to allow developers to explore new algorithms for any of the areas mentioned above and use standard interfaces to test their ideas with other parts of the framework seamlessly.**
- **Allow for incremental development in multi-physics problems without having to rewrite code as new physics is introduced.**
- **Allow the development of intrusive and non-intrusive UQ techniques.**
- **Since AMP is only loosely coupled to external packages its long term stability and viability are not restricted or compromised by the existence or non-existence of any external package**

AMP currently implements instantiations of the design in:

- **Time integration:**
  - **SUNDIALS**
  - **AMP (from SAMR)**
- **Nonlinear solvers:**
  - **PETSc SNES (inexact Newton both Jacobian free and with Jacobian)**
  - **AMP nonlinear Krylov acceleration solver (based on NLKAIN)**
- **Linear Solvers:**
  - **Trilinos ML (multigrid)**
  - **PETSc KSP (Krylov) solvers**
- **Linear Algebra:**
  - **PETSc matrices and vectors**
  - **Trilinos matrices and vectors**
  - **SUNDIALS vectors**
- **Discretization:**
  - **libmesh FEM types**
- **Meshing:**
  - **Meshes generated in Exodus format (generally by Cubit)**