Algorithmic/Exascale Simulation Opportunities in Modeling of Nuclear Fuel Rods

Phani Kumar V.V. Nukala, Srdjan Simunovic

Computer Science and Mathematics Division
Oak Ridge National Laboratory

Steve Zinkle
Materials Science and Technology Division
Oak Ridge National Laboratory

Larry Ott
Nuclear Science and Technology Division
Oak Ridge National Laboratory

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Nuclear Fuel Cycle

Uranium Ore → (H_2SO_4) → Uranium Oxides (U_3O_8)
U235 (0.7%), U238

↓ Conversion

Uranium hexaflouride (UF_6)

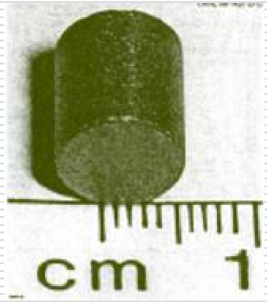
↓ Enrichment

Uranium hexaflouride (UF_6)
U235 (>3.5%), U238

← Uranium dioxide (UO_2)

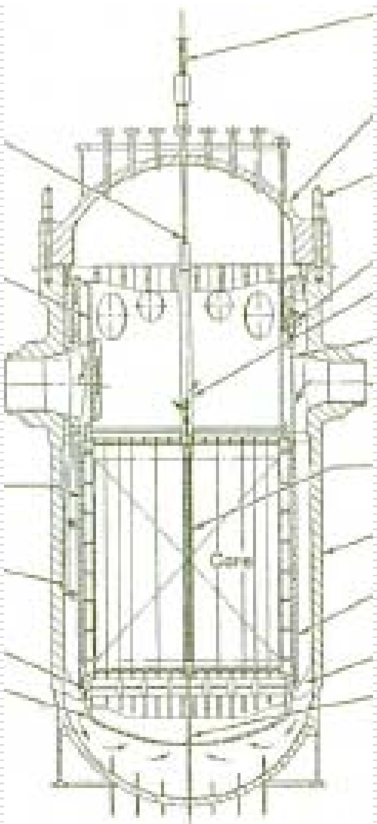
↑ High Temp. sintering furnace

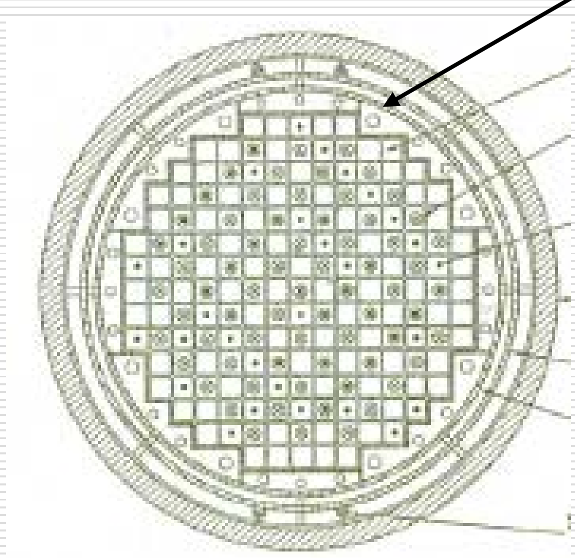
Brittle ceramic pellets



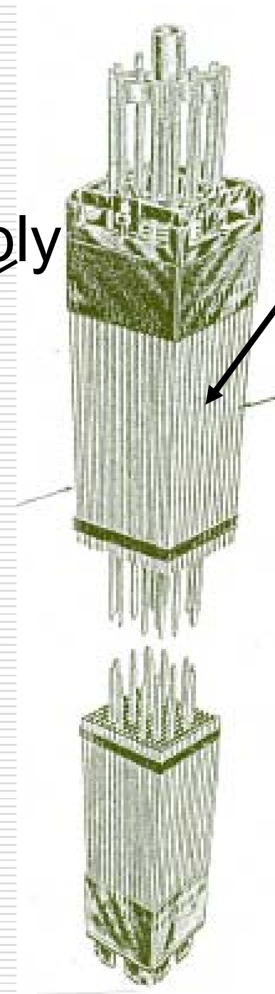
Phani K. Nukala
Oak Ridge National Laboratory
nukalapk@ornl.gov
865-574-7472

Nuclear Fuel Assembly

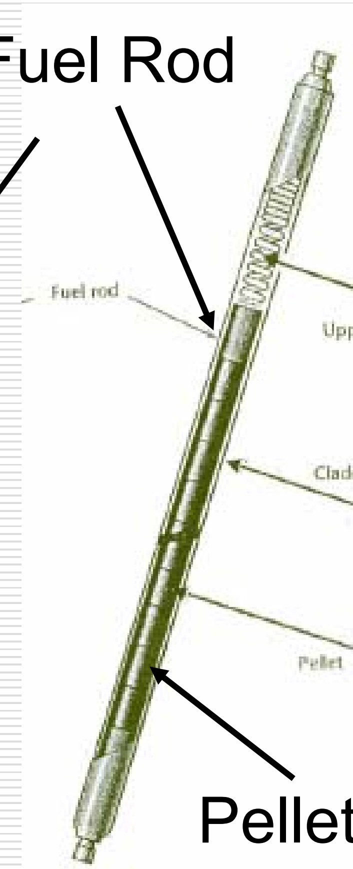




Fuel assembly



Fuel Rod



Pellet

Reactor vessel and internals

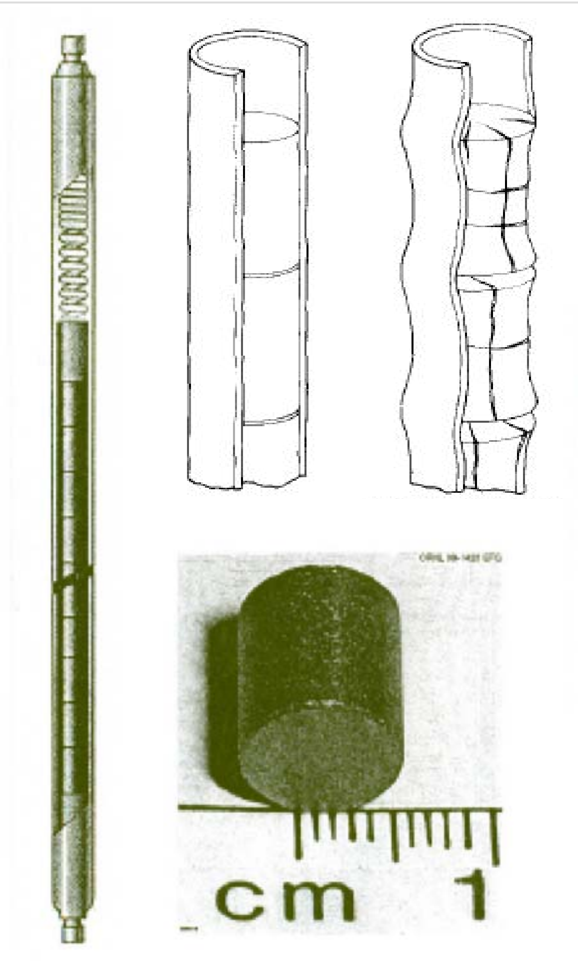
Phani K. Nukala

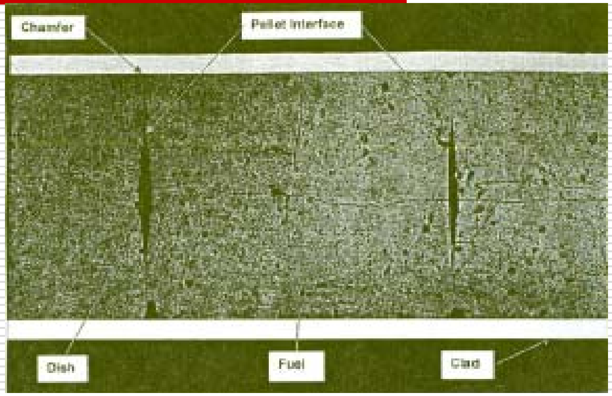
Oak Ridge National Laboratory

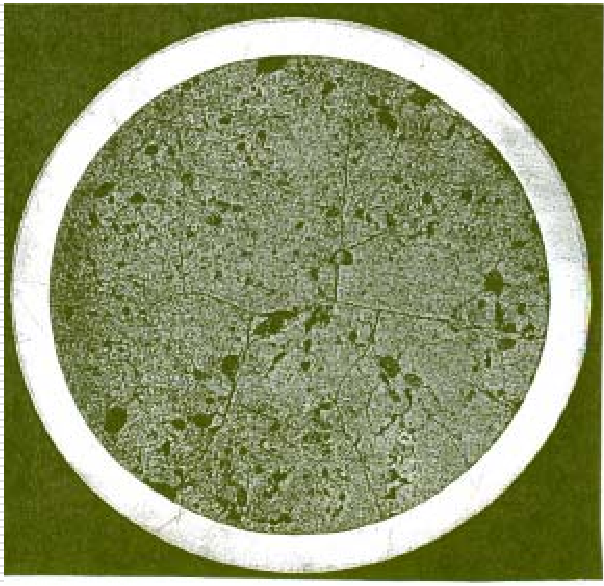
nukalapk@ornl.gov
865-574-7472

Nuclear Fuel Rod

3.6 to 3.8m





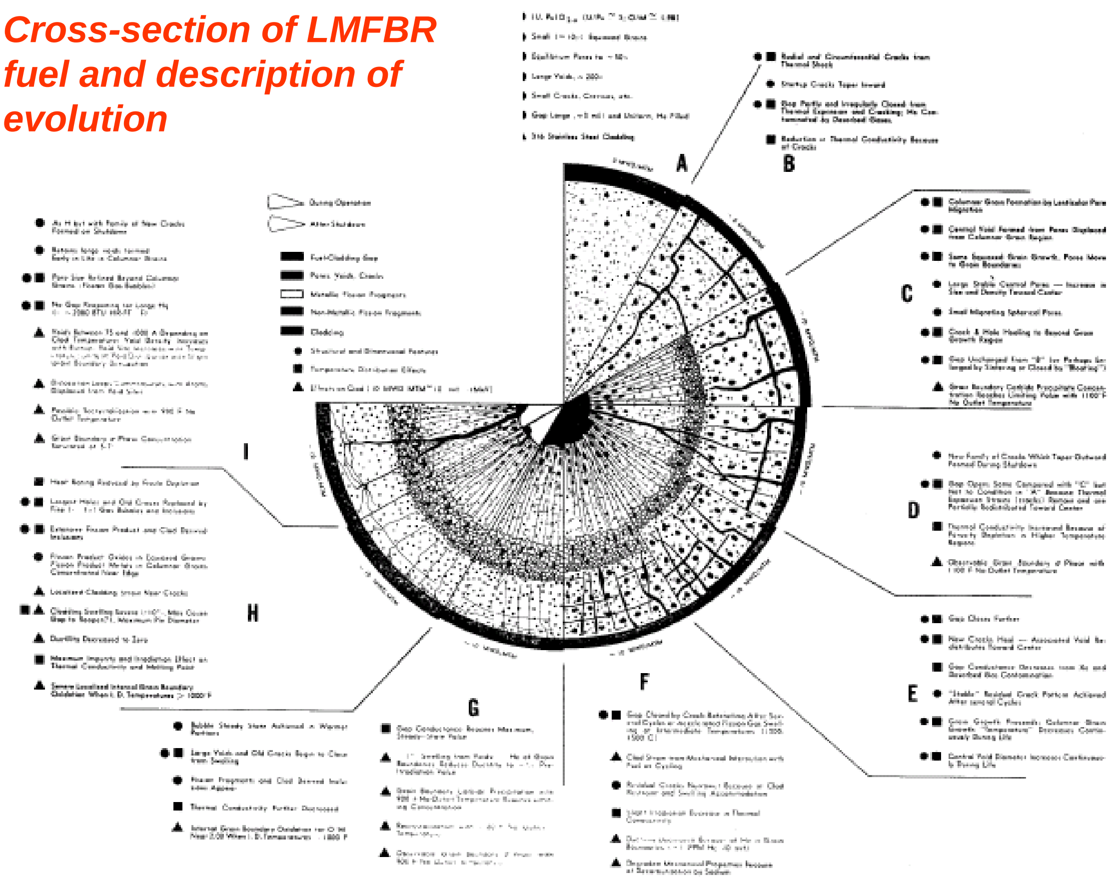


- The fuel pellet undergoes significant physical changes during burn up
- Modeling of pellet deformation requires
  - Fine resolution, and 3D discretization
  - Coupling multi-physics models at multiple scales

Phani K. Nukala
Oak Ridge National Laboratory
nukalapk@ornl.gov
865-574-7472

Complex MOX Fuel Pellet Behavior Seen in Historical LMFBR Studies

Cross-section of LMFBR fuel and description of evolution



- Fuel
  - Swelling due to fission products, irradiation damage
  - phase changes, microstructure evolution
  - Thermal expansion, conductivity, heat generation
  - Cracks and changes in mechanical properties

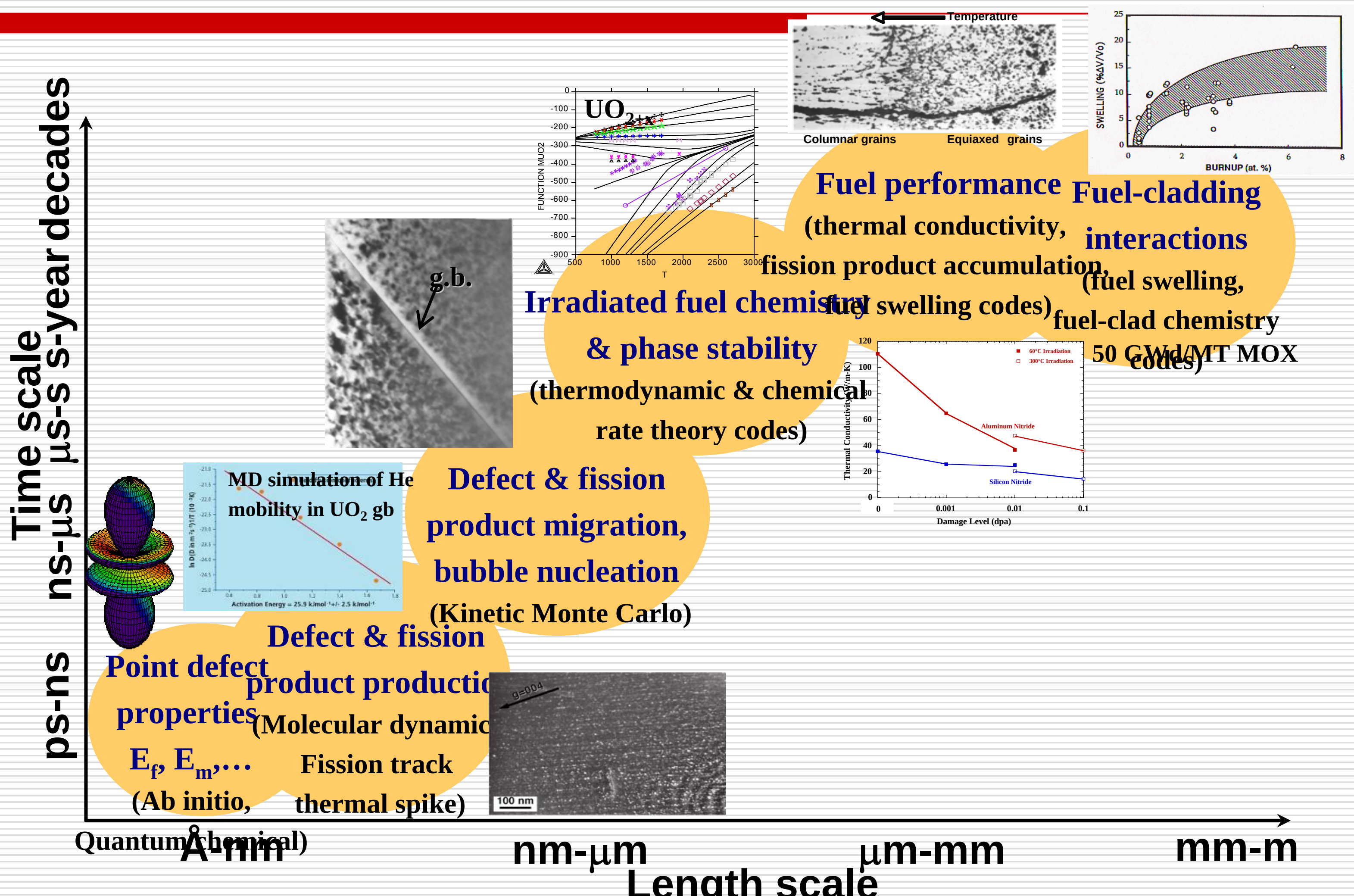
Phani K. Nukala
Oak Ridge National Laboratory
nukalapk@ornl.gov
865-574-7472

Multiple Phenomena

- Thermal conductivity
- Fission gas formation, behavior and release
- Materials dimensional stability
  - Restructuring, densification, growth, creep and swelling
- Defect formation & migrations
- Diffusion of species
  - Pu and Am redistribution
- Mechanical properties
- Thermal expansion
- Specific heat
- Phase diagrams
- Fuel-clad gap conductance
- Radial power distribution
- Fuel-clad chemical interactions

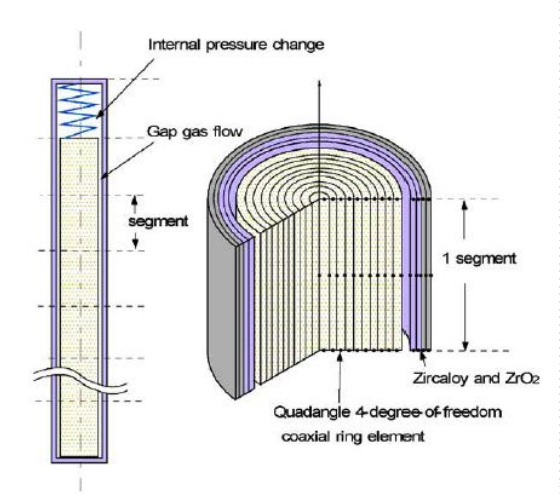
Dynamic properties:
Changes with radiation effects, temperature, and time

Fuel Modeling is inherently Multi-scale



Current State-of-the-Art (NRC Codes)

- Axi-symmetric models (2D)
- Coarse discretization
- Heuristic multi-physics models
- Fundamental nuclear physics occurs at the grain size level (10-20 μm) in the fuel pellet



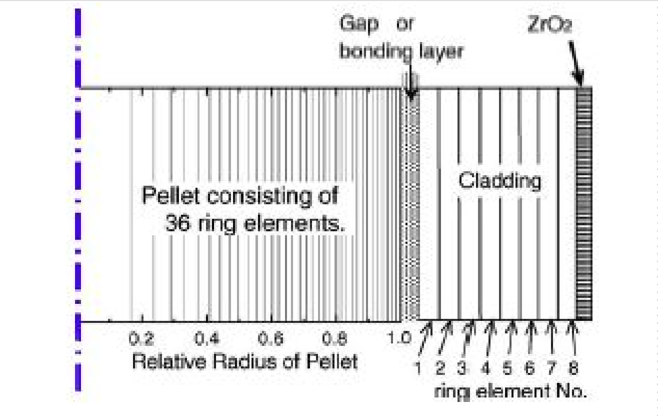


Fig. 2. FEM and thermal analysis meshing geometry of pellet and cladding of one axial segment in the RANNS code.

Simulation & Modeling Motivation

- Predictive capability
  - Reduce fuel development and qualification time by a factor of 3
  - Deliver increasingly accurate simulation capabilities for fuel life cycle performance assessment
  - Address safety concerns during steady state and transients
    - centerline fuel melting and wastage of cladding
  - Address fuel rod behavior in Design Basis Accident scenarios such as loss-of-coolant, reactivity insertion, etc

- TRU fuels
  - Extreme temperatures, irradiation rates, damage
  - New chemistry, physics, material issues that are not considered previously

Motivation for High Performance Computing

- Multi-physics coupling
  - Neutronics, chemistry, fission products transport, heat transfer, thermo-mechanics, thermal-hydraulics etc.
- Modeling of multiple scales in space and time
  - From irradiation point defects, chemistry, microstructure evolution to transport, conductivity and constitutive properties at macro-scale
  - Develop physics-based macroscopic models
- Computational efficiency
  - Provide comparable turn-around time with new codes
  - Design optimization and sensitivities
  - Various loading/boundary conditions scenarios

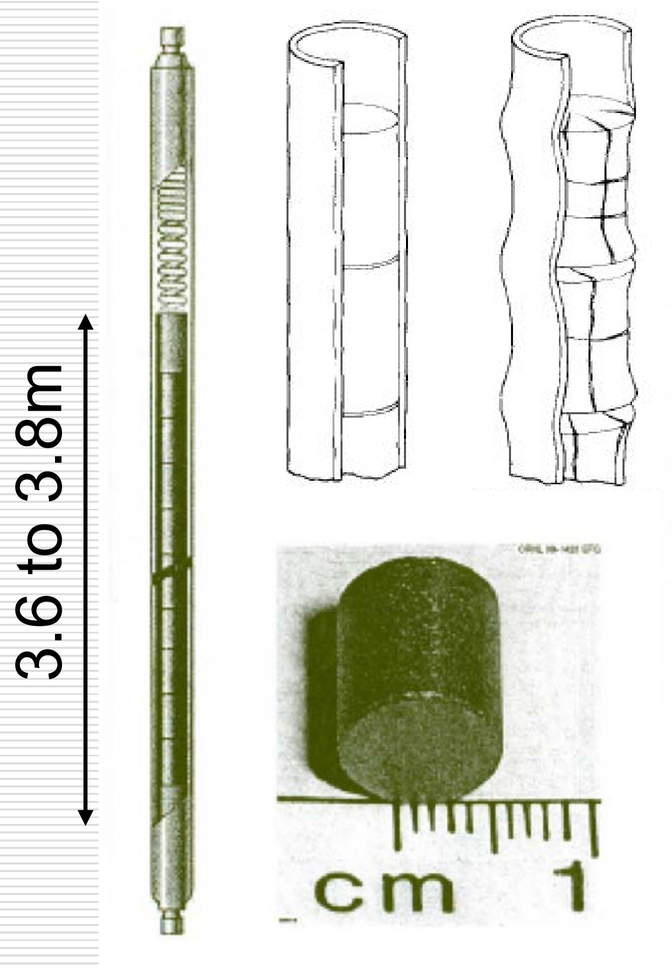
Outline

- High-fidelity, physics-based simulation of nuclear fuel performance requires models with increased spatial and temporal resolution
  - Computational tools for simulation of macroscopic fuel rod models (engineering and design)
  - Computational tools for developing physics-based models (first-principles, molecular dynamics, dislocation dynamics, kinetic Monte Carlo, discrete lattice models)
  - Algorithms for coupling multi-physics based models across length and time scales

nukalapk@ornl.gov
865-574-7472

Relevant Computational Simulations

- Fuel rod / fuel bundle simulations
  - Engineering and design
  - Continuum mechanics based finite element simulations
- Fuel pellet simulations
  - Macroscopic: Finite elements
  - Micro/Mesoscopic: Phase-field, Kinetic Monte Carlo, Discrete dislocation simulations, Discrete lattice models, Molecular dynamics
  - First-principles based simulations: Density functional theory and others



nukalapk@ornl.gov
865-574-7472

Modeling of Fuel Rod

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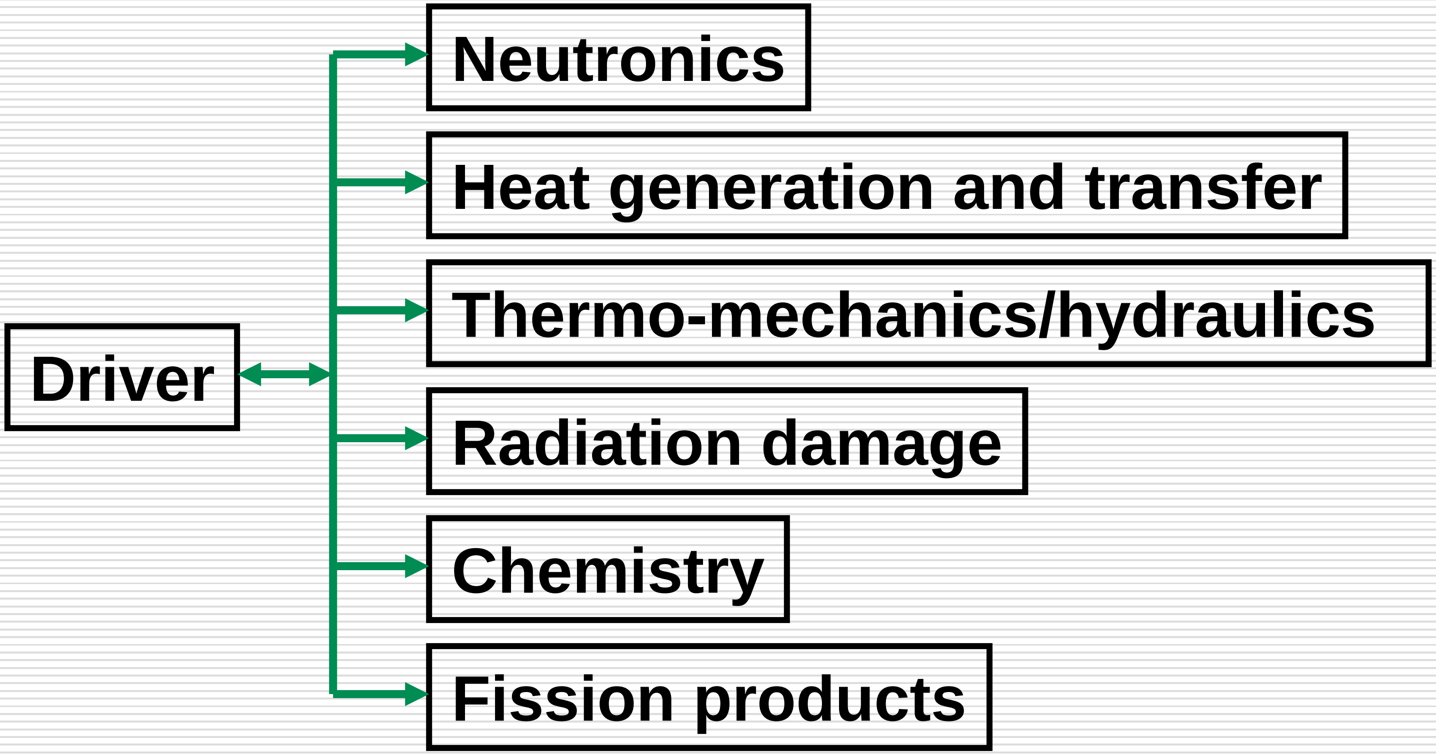
Code Integration - Multi-physics Model

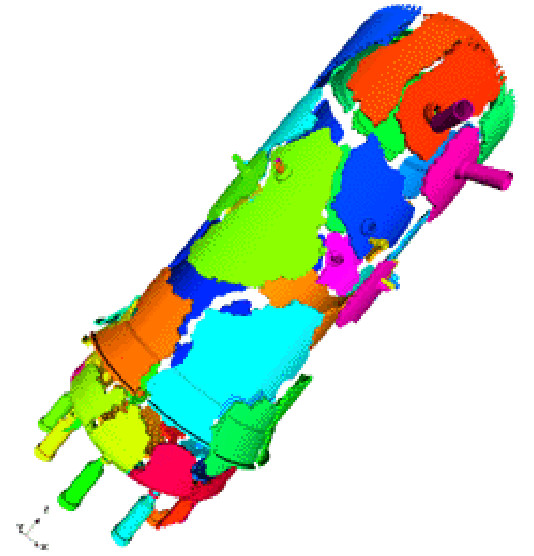


- Base capability
- Depending on the level of coupling one of the modules can become Driver, e.g. FEM Thermo-mechanics module can host chemistry data

Thermo-Mechanical Codes

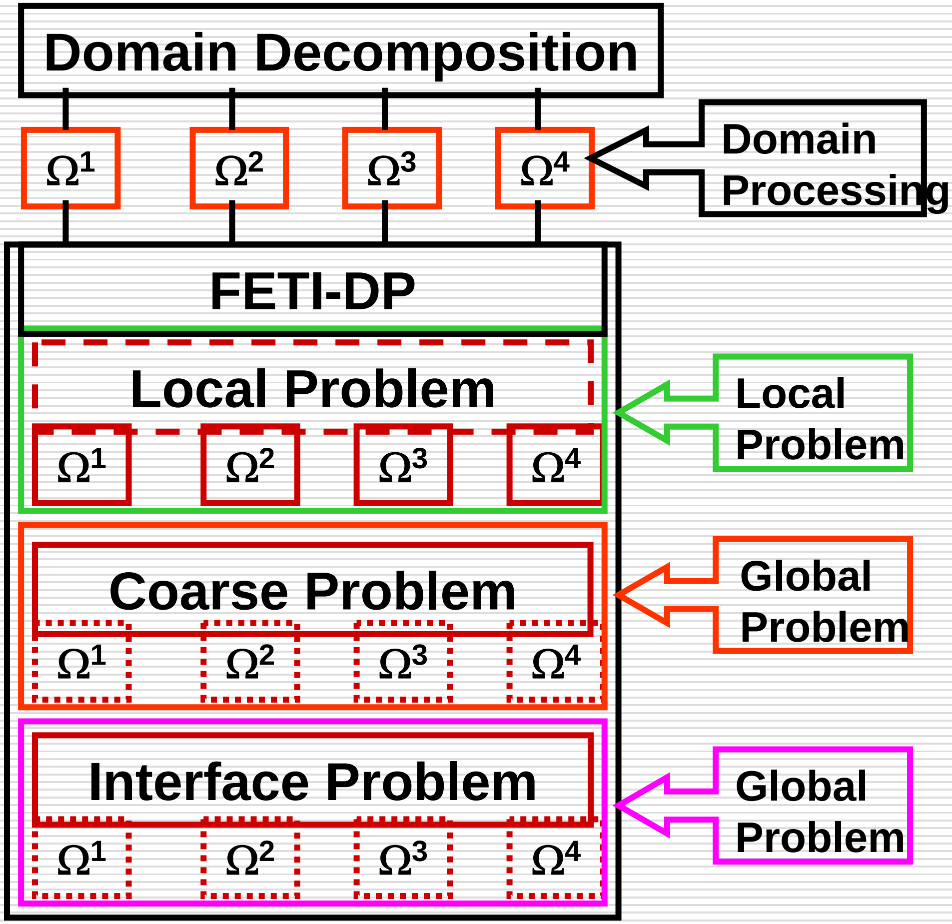
- General-purpose system for large-scale analysis
  - Thermal, and mechanics

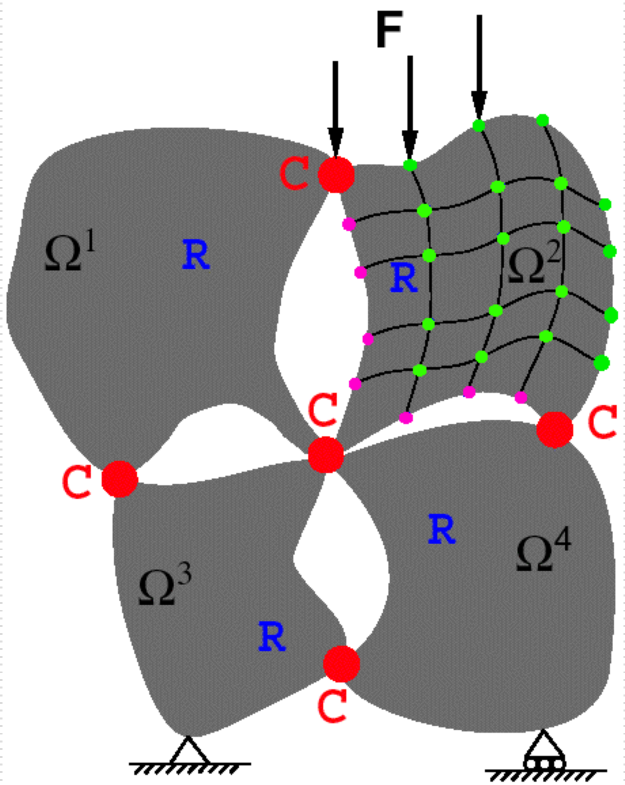
- Employs a hierarchical domain decomposition method (HDDM) to efficiently utilize massively parallel computer resources



✦Partition into non-overlapping sub-domains
✦Analyze sub-domains (fine problem)
✦Enforce compatibility between sub-domains (coarse problem)

FETI-DP/HDDM

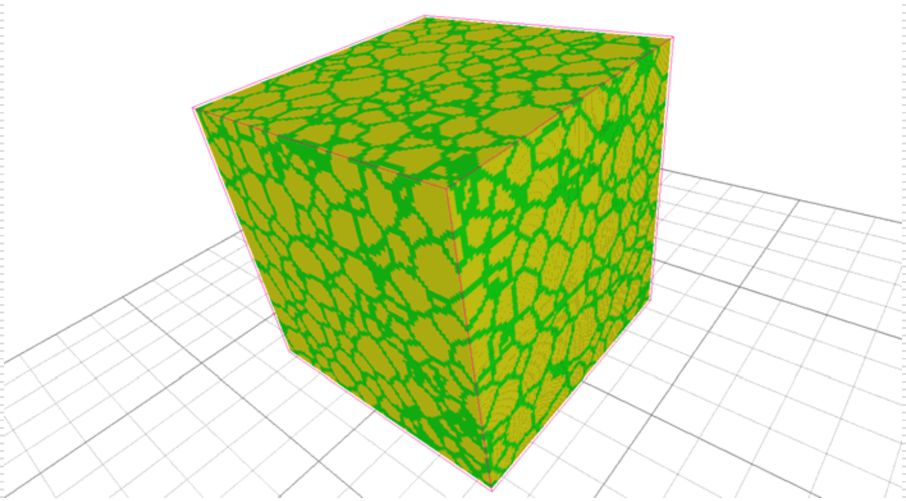


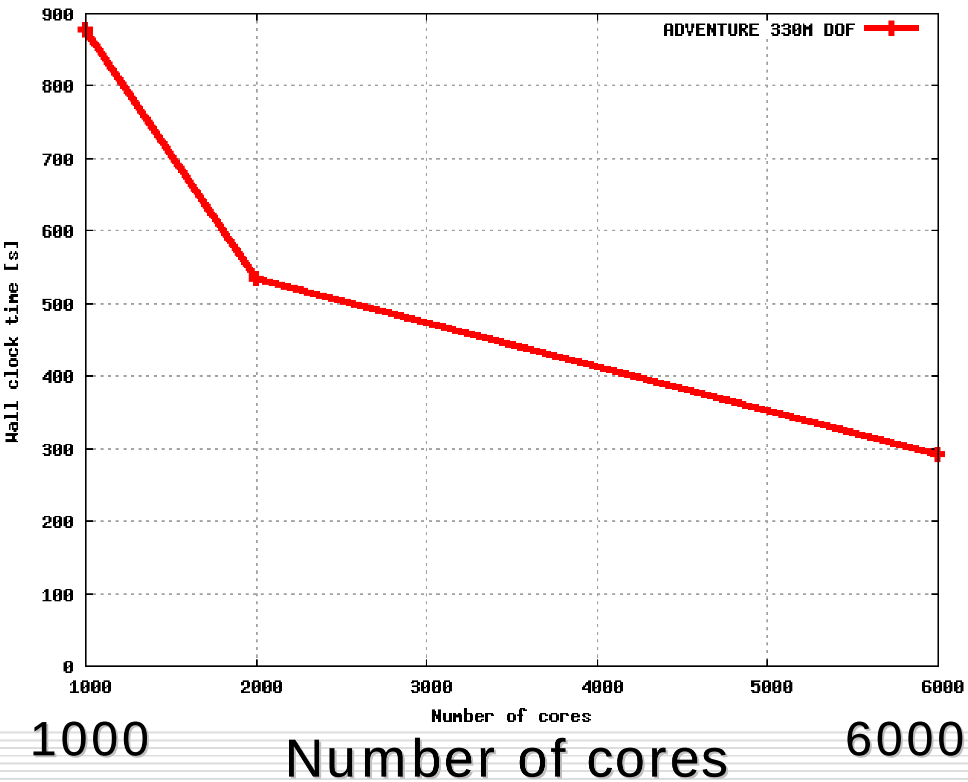


Phani K. Nukala
Oak Ridge National Laboratory
nukalapk@ornl.gov
865-574-7472

Scaling on Cray-XT4

- Scaling up to 6000 cores
- 20% peak efficiency
- Solved up to 300M problem

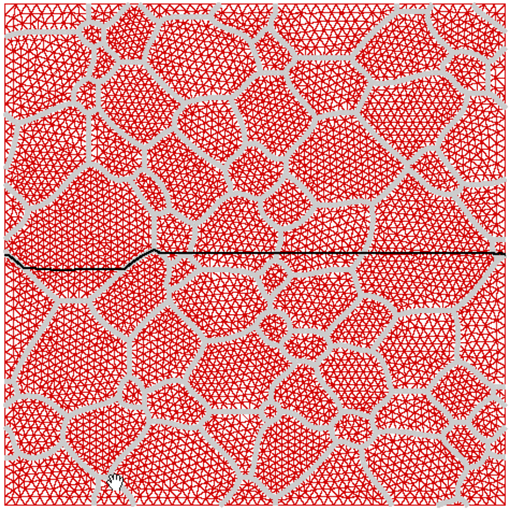


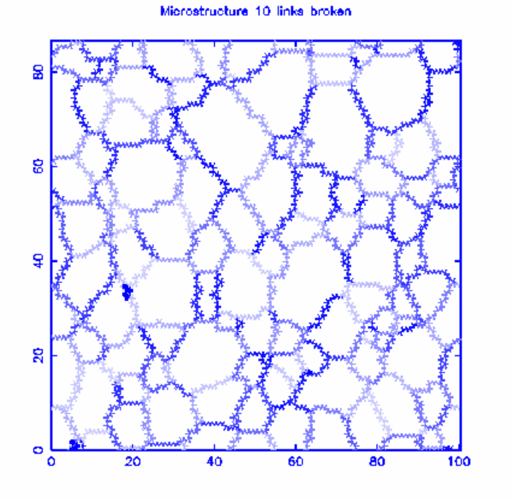


Modeling of Fuel Pellets

Modeling Brittle Fracture of Fuel Pellets

- Fracture due to thermal mismatch and high thermal gradients
- Chemistry/Transport/Diffusion of fission products
- Misorientation dependent low angle grain boundary fracture strength
- Time dependent evolution of grain structures and recrystallization

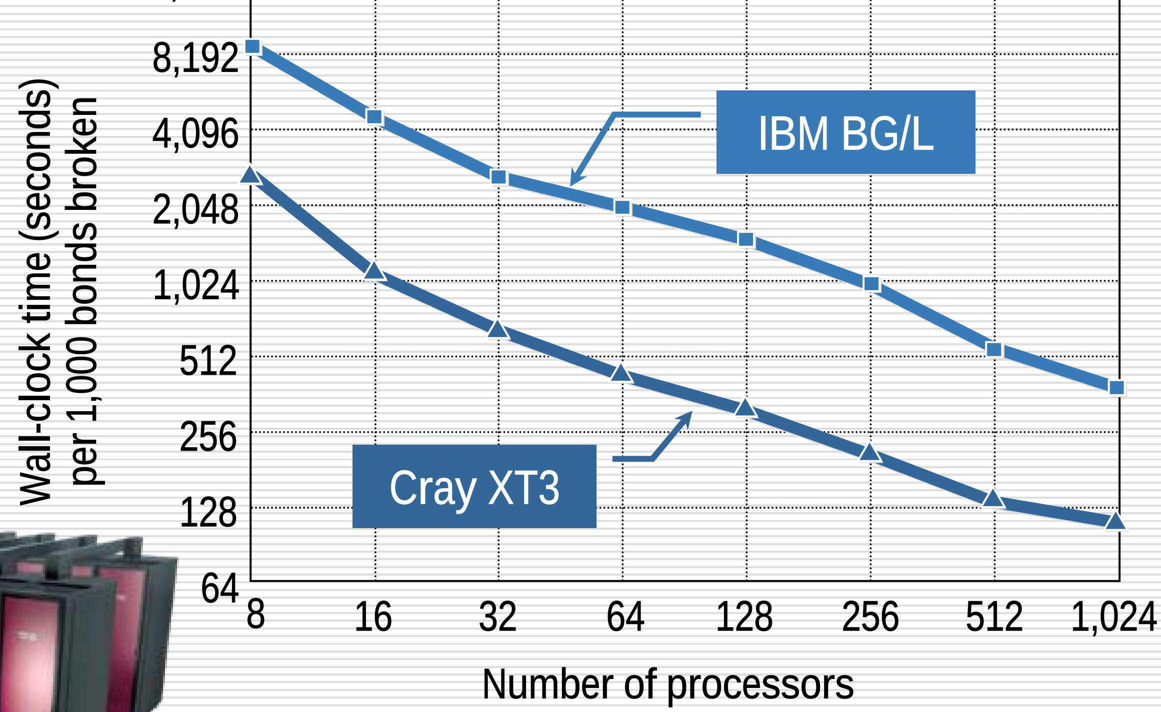




Phani K. Nukala
Oak Ridge National Laboratory
nukalapk@ornl.gov
865-574-7472

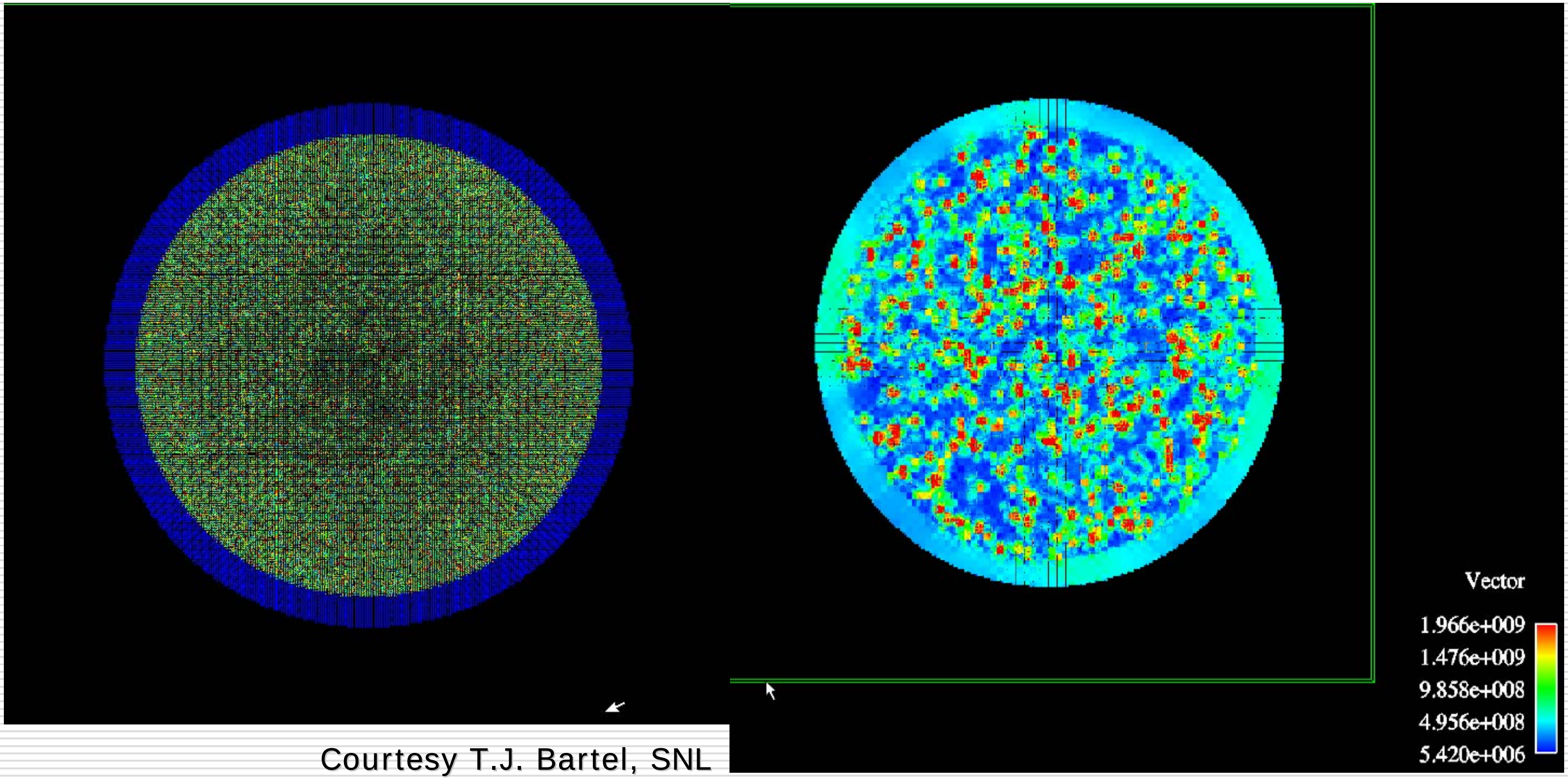
High-performance computing

High-performance computing	Processing time
L = 64 on 128	3 hours
L = 100 on 1024	12 hours
L = 128 on 1024	3 days
L = 200 on 2048	20 days (est.)



Phani K. Nukala
Oak Ridge National Laboratory
nukalapk@ornl.gov
865-574-7472

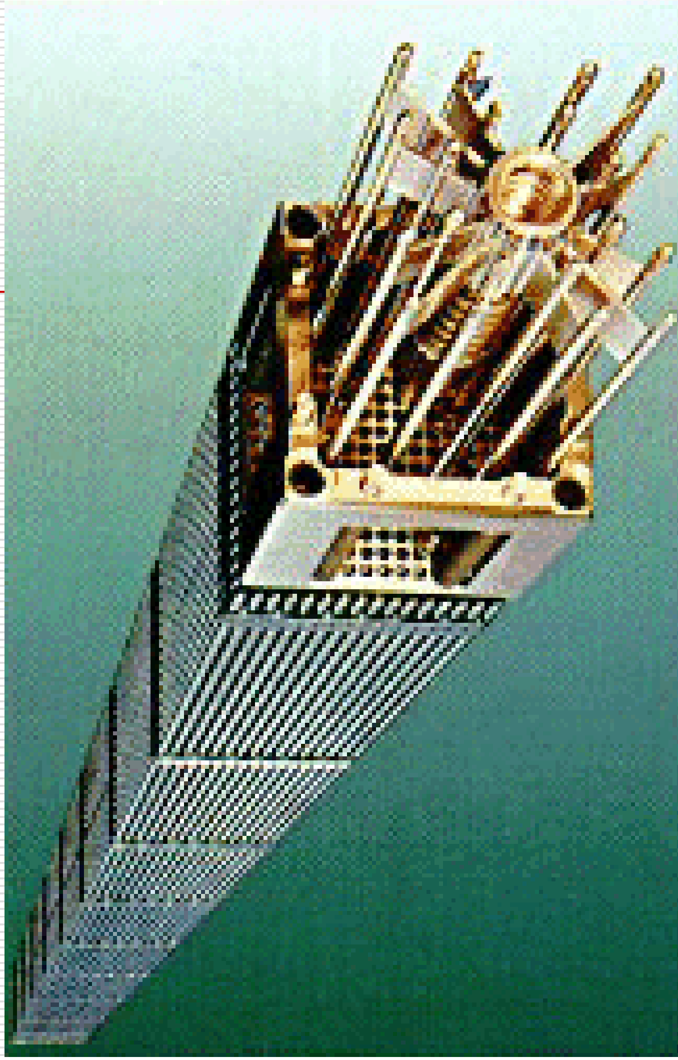
Simulation of Nuclear Fuel Restructuring



Courtesy T.J. Bartel, SNL

- Simulation of fuel swelling due to fission products accumulation in fuel matrix

Exascale Requirements



Fuel Rod/Bundle Simulation

- Solving a 300M problem took 300 seconds on 6000 cores
- Simulation involves 50 steps with 10 iterations per step
- Total time ~ 500 x 300 = 150,000 sec ~ 42 hours
- Assuming a constant efficiency of 20%, a 100,000 core simulation requires approximately
  - (6000/100000) x (42 / 0.2) ~ 12 hours on 500 TF machine
- A bundle of 40 rods requires 12 hours on 20 PF machine
- All this only with thermo-mechanics and no coupling with other multi-physics models

nukalapk@ornl.gov
865-574-7472

Fuel Pellet Simulation

- Solving a 1B problem took 1000 seconds on 8000 cores
- Simulation involves 50 steps with 10 iterations per step
- Total time ~ 500 x 1000 = 500,000 sec ~ 6 days
- Assuming a constant efficiency of 20%, a 200,000 core simulation requires approximately
  - (8000/200000) x (6 / 0.2) ~ 1.2 days on 1 PF machine
- All this only with thermo-mechanics and no coupling with other multi-physics models; No coupling of multiple scales

Additional Details

- Assumed perfect scaling with 20% efficiency!
- Addition of multi-physics models: chemistry, fission products transport, and neutronics will deteriorate the efficiency
- Necessity to run various loading/boundary conditions, and sensitivity studies will require capacity computing with each simulation running at 1 PF.

Final Thoughts ...

- Fuel and cladding behavior is governed by
  - Coupled multi-physics phenomena
  - Feedback from multiple scales
- High-fidelity simulations aiming to resolve these multiple scales and couple multi-physics models demand capability computing
- Development of physics-based models requires higher resolution and larger system sizes
- Coupling of time scales in these multi-physics models requires algorithmic advances
- Faster turn around times, multiple loading/boundary conditions scenarios, and sensitivity studies require capacity computing with each simulation running at a PF.

Algorithmic Challenges: Coupling Multiple Time Scales in MD Simulations

MTS Method

MTS Propagator

$$\Phi_h^{MTS} = \Phi_{h/2}^{*Slow} \circ \left(\Phi_{h/N}^{Fast}\right)^N \circ \Phi_{h/2}^{Slow}$$

↑

Reversible
At least, second-order accurate

- Step 1: ½ kick

$$y_{(1)} = \Phi^{Slow}\left(y^n\right)$$

- Step 2: vibration N steps

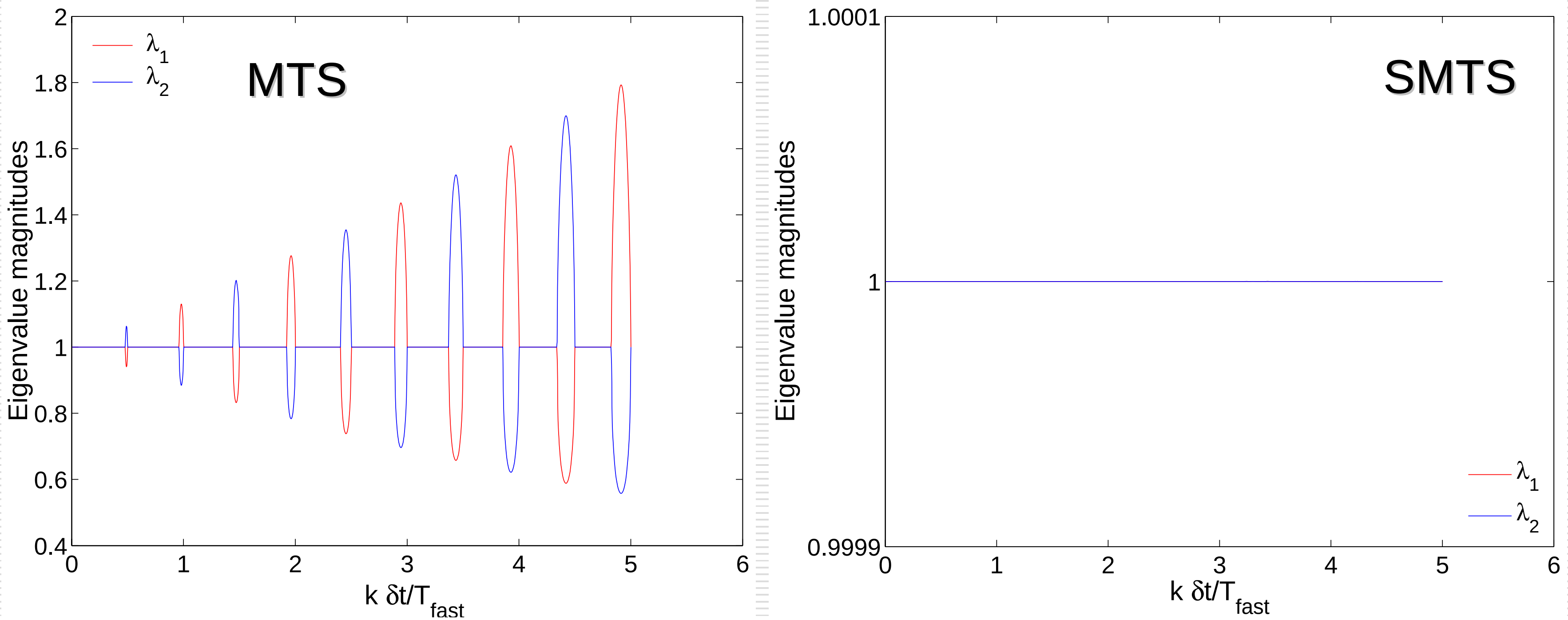
$$y_{(2)} = \Phi^{Fast}\left(y_{(1)}\right)$$

- Step 3: ½ kick

$$y^{n+1} = \Phi^{*Slow}\left(y_{(2)}\right)$$

Stabilized MTS Method Analysis

$$\ddot{q} = -\left(\omega_1^2 + \omega_2^2\right) q \qquad \dot{q} = p \qquad \omega_1^2 >> \omega_2^2$$



- MTS exhibits parametric resonance, whereas SMTS is stable for any time step

Phani K. Nukala
Oak Ridge National Laboratory
nukalapk@ornl.gov
865-574-7472

Stabilized MTS Method Analysis

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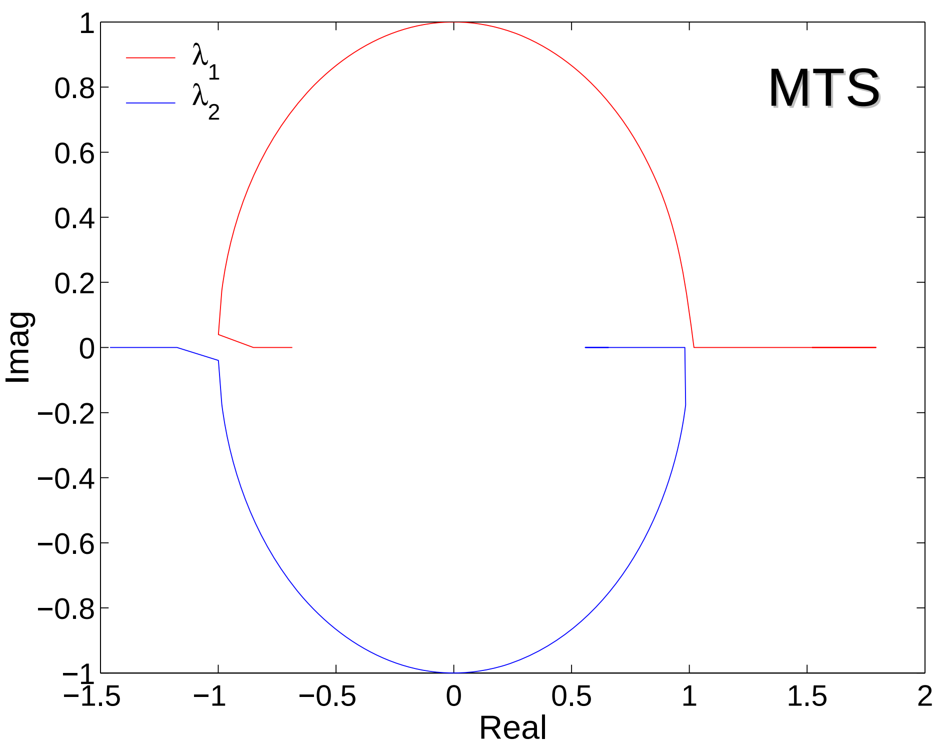
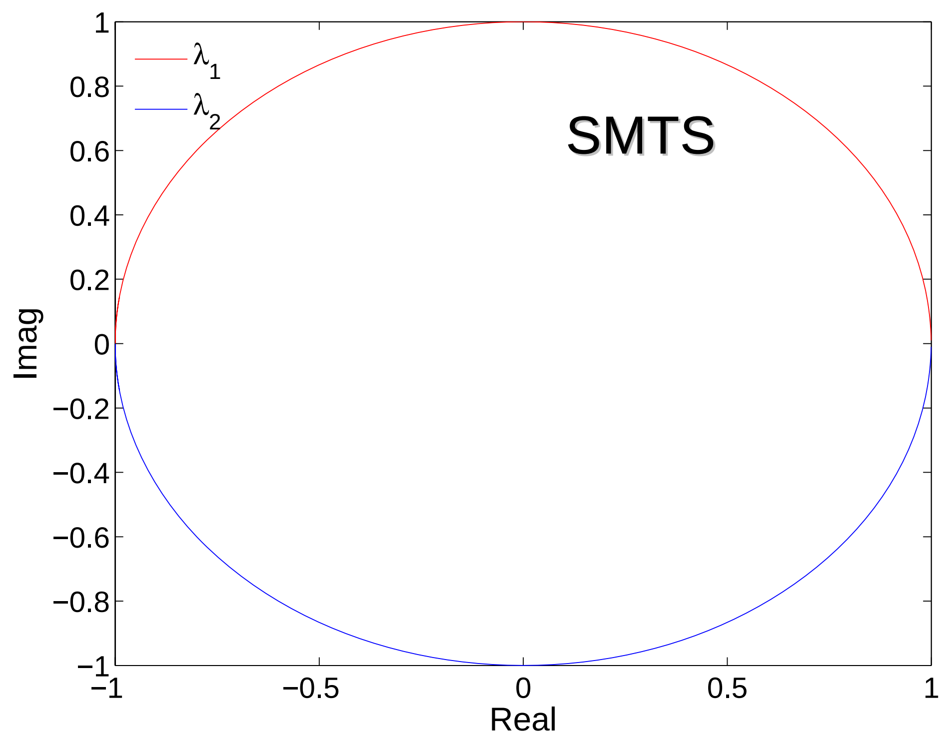
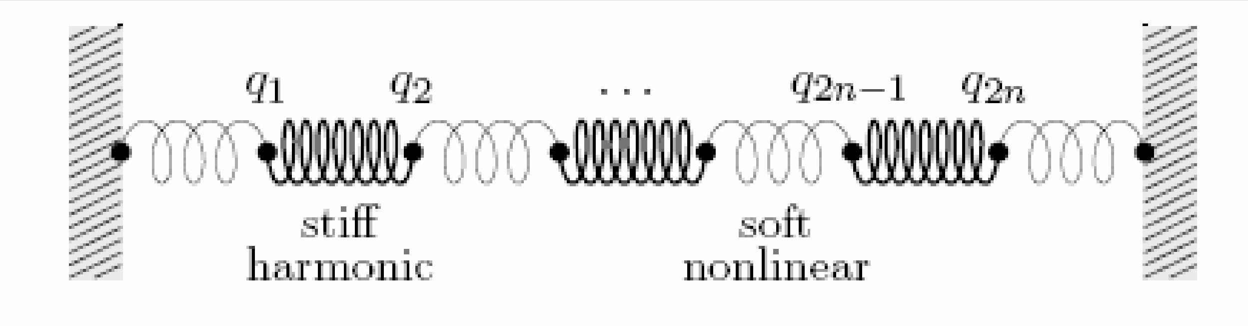




- Collision of eigenvalues leading to instability of MTS is clearly visible

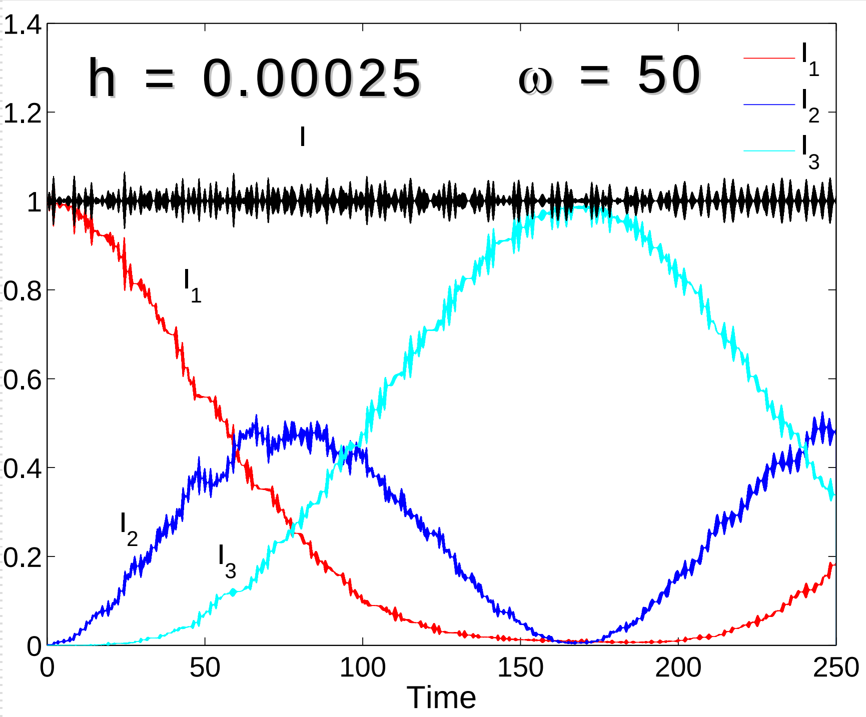
Fermi-Pasta-Ulam (FPU) Problem

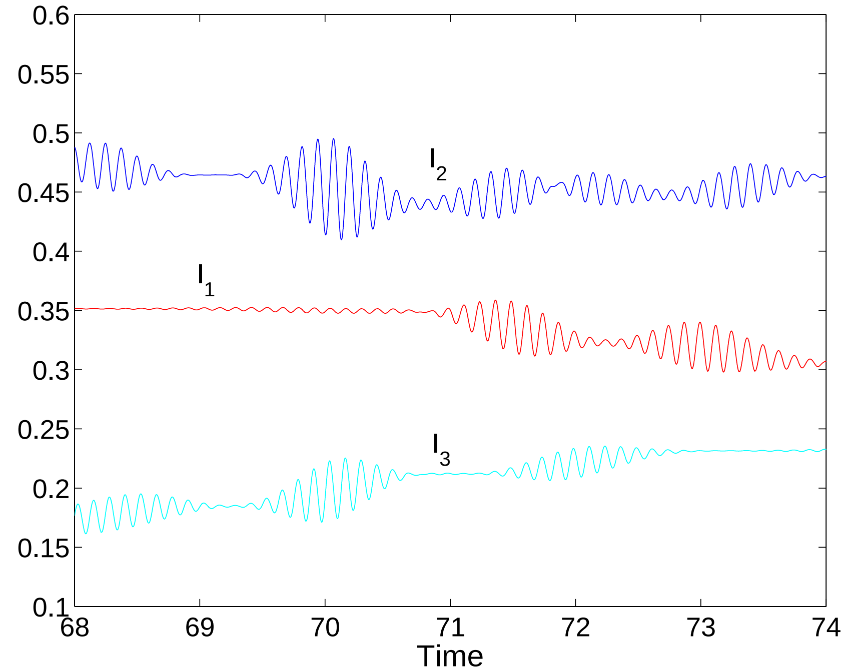


$$H(p,q) = \frac{1}{2}\sum_{i=1}^{n}\left(p_{2i-1}^2 + p_{2i}^2\right) + \frac{\omega^2}{4}\sum_{i=1}^{n}\left(q_{2i} - q_{2i-1}\right)^2 + \sum_{i=0}^{n}\left(q_{2i+1} - q_{2i}\right)^4$$

- Different behavior over different time scales
  - Time scale ω^{-1}: almost-harmonic motion of stiff springs
  - Time scale ω^{0}: motion of soft nonlinear springs
  - Time scale ω: energy exchange among the stiff springs
  - Time scale ω^{N}, $N>1$: $O(\omega^{-1})$ deviations in oscillatory energy

Fermi-Pasta-Ulam (FPU) Problem





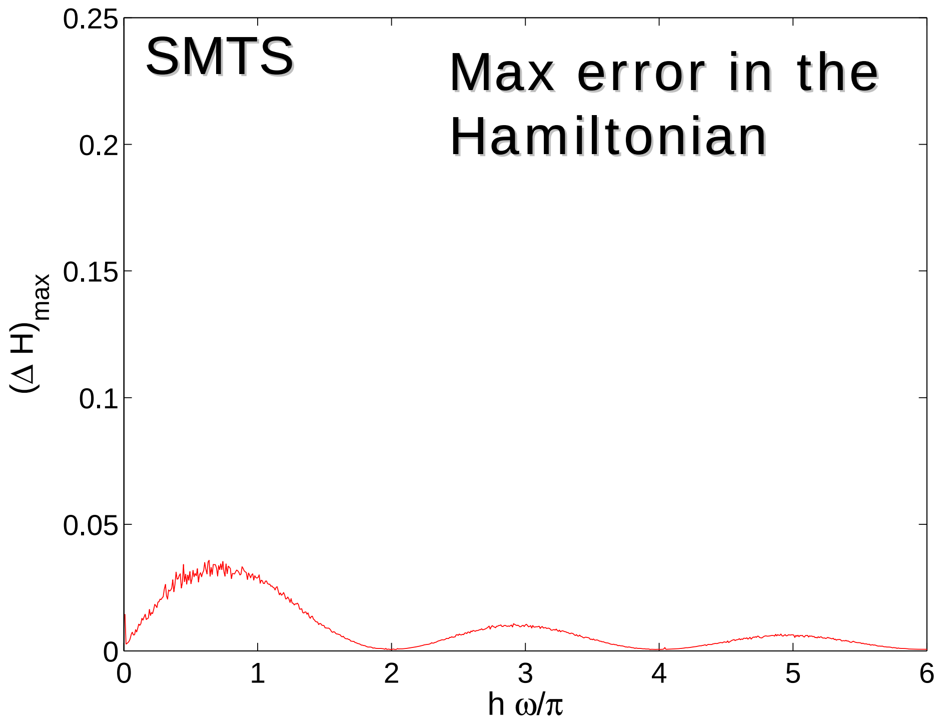
$$y_{n+j} = \frac{(p_{2i} - p_{2i-1})}{\sqrt{2}}$$

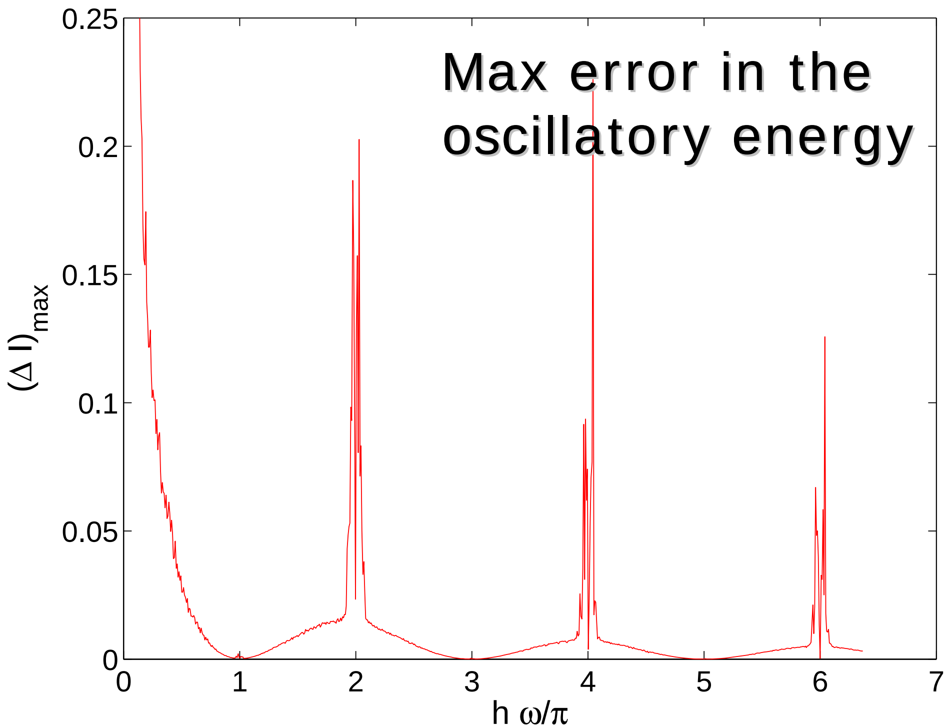
Oscillatory energy

$$I_j = \frac{1}{2}\left(y_{n+j}^2 + \omega^2 x_{n+j}^2\right)$$

$$x_{n+j} = \frac{(q_{2i} - q_{2i-1})}{\sqrt{2}}$$

FPU Problem





- Parametric resonance?
  - No parametric resonance effects in the Hamiltonian
  - Resonance in the oscillatory energy

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