Nuclear Fuel Performance

NE-533

Spring 2023

Last Time

- We derived two analytical solutions for the stress in a pressurized cylinder
  - Thin walled cylinder
  - Thick walled cylinder
- Increases in temperature cause most materials to expand
- We call this thermal expansion, which is a strain that doesn't inherently cause stress
- Thermal expansion can cause stress when
  - Deformation is constrained
  - There are gradients in the expansion coefficient
  - There is a temperature gradient
- We have analytical equations for thermal stresses in the cladding and in the fuel

The gap changes as a function of time

- Both the pellet and the cladding swell

$$\Delta\delta_{gap} = \delta_{gap} - \delta_{gap}^{0}$$
$$\Delta\delta_{gap} = \Delta\bar{R}_C - \Delta R_f$$
$$\frac{\Delta R_f}{\bar{R}_C} = \alpha_f\left(\bar{T}_f - T_{fab}\right)$$
$$\frac{\Delta R_C}{\bar{R}_C} = \alpha_C\left(\bar{T}_C - T_{fab}\right)$$
$$\Delta\delta_{gap} = \bar{R}_c\alpha_C\left(\bar{T}_C - T_{fab}\right) - \bar{R}_f\alpha_f\left(\bar{T}_f - T_{fab}\right)$$

- But, as the gap decreases, the temperature changes, which again makes the gap change
- The solution using the analytical equations is iterative, due to the dependence of the gap size and temperature

Example

Calculate the steady state temperature profile in the rod, including thermal expansion

- LHR = 200 W/cm, δ^0_{gap} = 30 μm, R_f = 0.6, T_{co} = 600 K, $T_{EXP,0}$ = 373 K, k_{gap} = 0.0026 W/cm-K, t_C= 0.06 cm, α_f = 11.0e-6 1/K, α_C = 7.1e-6 1/K

$$\Delta\delta_{gap} = \bar{R}_c \alpha_C \left(\bar{T}_C - T_{fab}\right) - \bar{R}_f \alpha_f \left(\bar{T}_f - T_{fab}\right) = \Delta R_c - \Delta R_f$$

$$\Delta T_{gap} = \frac{LHR}{2\pi R_f k_{gap}/\delta_{gap}}$$

- So, T_{IC} = 600 + 11.2 = 611.2 K, T_s = 672.4 K, T_0 = 1232.0 K
- First, we will deal with expansion in the cladding
  - Av(R_c) = 0.6 + 30e-4 + 0.06/2 = 0.633 cm
  - Av(T_C) = (600+611.2)/2 = 605.6 K
  - ΔR_c = 0.633*7.1e-6*(605.6 – 373) = 0.001 cm

Calculate the steady state temperature profile in the rod, including thermal expansion

- Second, we deal with the fuel
  - Av(Tf) = (1203 + 672.4)/2 = 937.7 K
  - ΔR_f = 0.6*11e-6*(937.7 – 373) = 0.0037 cm

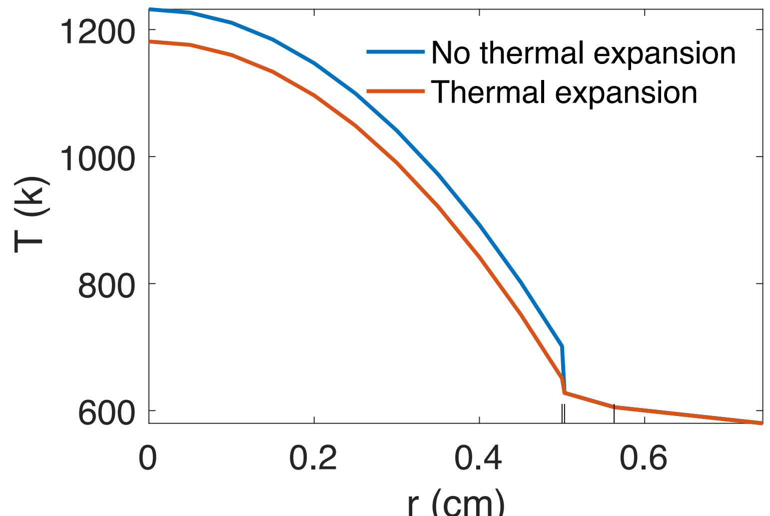
$$\Delta\delta_{gap} = \bar{R}_c\alpha_C\left(\bar{T}_C - T_{fab}\right) - \bar{R}_f\alpha_f\left(\bar{T}_f - T_{fab}\right)$$

- The total change in the gap is 0.001 – 0.0037 = -0.0027
- However, that means the gap is smaller and so our temperatures were wrong!

This calculation is repeated until the gap width stops changing significantly

- The change in the gap does NOT affect the coolant or cladding temperatures, just the gap and fuel temperatures
- We only need to repeat the calculation of the fuel and cladding temperatures and the change in the gap

Iteration	δ_{gap} (cm)	T_s (K)	T_0 (K)
0	0.003	701	1232
1	0.00066	644	1174
2	0.00097	652	1182
3	0.00094	651	1181
4	0.00094	651	1181

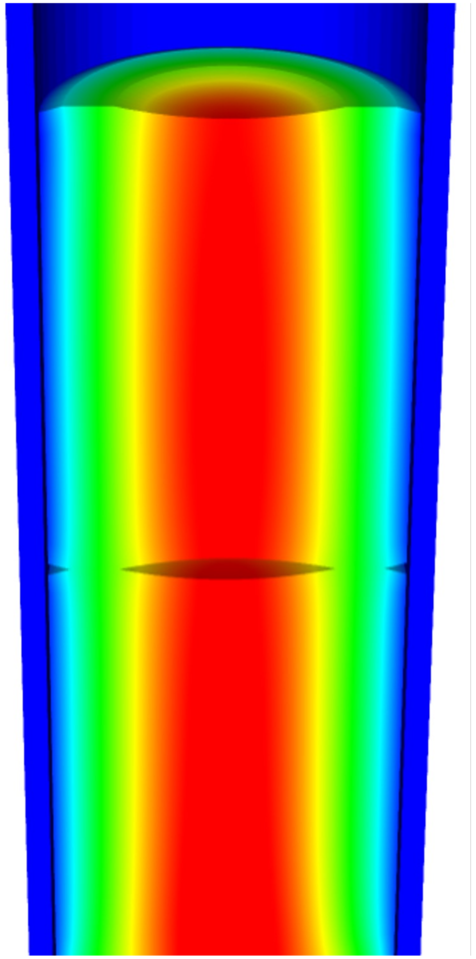


THERMO-MECHANICS

Relating Displacements to Stress

- We have been determining the stress due to some internal pressure (or temperature)
- Often, the information more readily obtainable are the displacements
- Utilizing the previous equations, can develop displacement to stress relationships for our geometry

$$\frac{\partial \sigma_{rr}}{\partial r} + \frac{\sigma_{rr} - \sigma_{\theta\theta}}{r} + \frac{\partial \sigma_{rz}}{\partial z} = 0 \qquad \frac{1}{r}\frac{\partial (r\sigma_{rz})}{\partial r} + \frac{\partial \sigma_{zz}}{\partial z} = 0$$



Assuming problem is axisymmetric

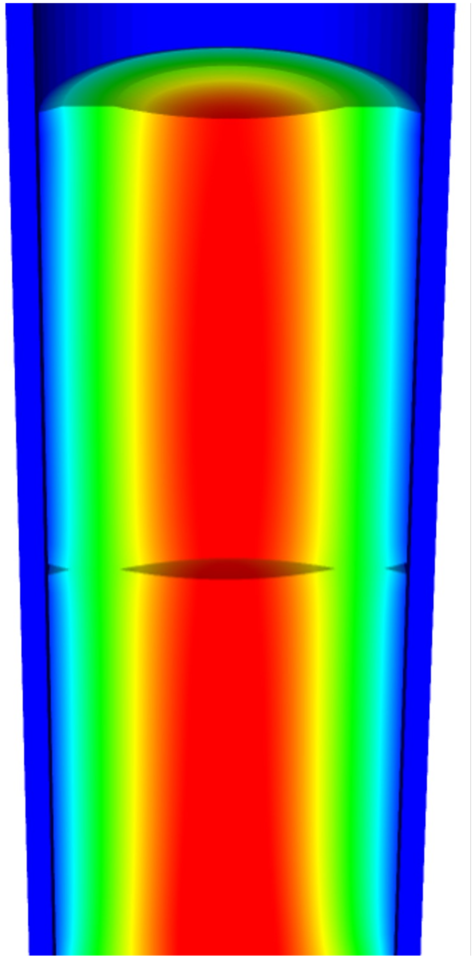
$$\rho c_p \frac{\partial T}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(rk(T)\frac{\partial T}{\partial r}\right) + \frac{\partial}{\partial z}\left(k(T)\frac{\partial T}{\partial z}\right) + Q(r,z)$$

$$\frac{\partial \sigma_{rr}}{\partial r} + \frac{\sigma_{rr} - \sigma_{\theta\theta}}{r} + \frac{\partial \sigma_{rz}}{\partial z} = 0 \qquad \frac{1}{r}\frac{\partial (r\sigma_{rz})}{\partial r} + \frac{\partial \sigma_{zz}}{\partial z} = 0$$

$$\boldsymbol{\sigma} = \boldsymbol{\mathcal{C}}(\boldsymbol{\epsilon} - \alpha(T - T_{fab})\mathbf{I}) \qquad \epsilon_{rr} = \frac{1}{E}(\sigma_{rr} - \nu(\sigma_{\theta\theta} + \sigma_{zz})) + \alpha\Delta T$$

$$\epsilon_{rr} = \frac{\partial u_r}{\partial r},\ \epsilon_{\theta\theta} = \frac{u_r}{r}, \epsilon_{zz} = \frac{\partial u_z}{\partial z}, \epsilon_{rz} = \frac{1}{2}\left(\frac{\partial u_r}{\partial z} + \frac{\partial u_z}{\partial r}\right)$$

$$\boldsymbol{\epsilon} = \begin{bmatrix} u_{r,r} & (u_{r,z} + u_{z,r})/2 & 0 \\ (u_{r,z} + u_{z,r})/2 & u_{z,z} & 0 \\ 0 & 0 & u_r/r \end{bmatrix}$$



Solve for the stress from the strain

- Assume isotropic materials
- Can perform matrix multiplication for the calculation of the stress, given the displacements

$$\begin{bmatrix}\sigma_{rr}\\ \sigma_{zz}\\ \sigma_{\theta\theta}\\ \sigma_{rz}\end{bmatrix} = \frac{E}{(1+\nu)(1-2\nu)}\begin{bmatrix}1-\nu & \nu & \nu & 0\\ \nu & 1-\nu & \nu & 0\\ \nu & \nu & 1-\nu & 0\\ 0 & 0 & 0 & \frac{1-2\nu}{2}\end{bmatrix}\begin{bmatrix}u_{r,r}\\ u_{z,z}\\ u_r/r\\ (u_{r,z}+u_{z,r})/2\end{bmatrix}$$

Further simplify the problem to be 1D

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + Q \qquad \boldsymbol{\sigma} = \boldsymbol{\mathcal{C}}(\boldsymbol{\epsilon} - \alpha(T - T_{fab})\mathbf{I})$$

$$0 = \nabla \cdot \boldsymbol{\sigma} \qquad \boldsymbol{\epsilon} = \tfrac{1}{2}\left(\nabla \mathbf{u} + \nabla \mathbf{u}^T\right)$$

- No change in Z:

$$\rho c_p \frac{\partial T}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(r k(T) \frac{\partial T}{\partial r}\right) \qquad \frac{\partial \sigma_{rr}}{\partial r} + \frac{\sigma_{rr} - \sigma_{\theta\theta}}{r} = 0$$

$$\boldsymbol{\epsilon} = \begin{bmatrix} u_{r,r} & 0 \\ 0 & u_r/r \end{bmatrix} \qquad \begin{bmatrix} \sigma_{rr} \\ \sigma_{\theta\theta} \end{bmatrix} = \frac{E}{(1+\nu)(1-2\nu)} \begin{bmatrix} 1-\nu & \nu \\ \nu & 1-\nu \end{bmatrix} \begin{bmatrix} u_{r,r} \\ u_r/r \end{bmatrix}$$

Determine the strain and stress in the pellet for 1D case

- Assume the radial displacement in the fuel pellet is $u_r(r) = 0.05r$ cm.
- What is the strain tensor? $\epsilon = \begin{bmatrix} u_{r,r} & 0 \\ 0 & u_r/r \end{bmatrix}$ At the outer edge: $\epsilon = \begin{bmatrix} 0.05 & 0 \\ 0 & 0.05 \end{bmatrix}$

- We are dealing with UO_2, so E = 200 GPa and v = 0.345

$$\begin{bmatrix} \sigma_{rr} \\ \sigma_{\theta\theta} \end{bmatrix} = \frac{E}{(1+\nu)(1-2\nu)} \begin{bmatrix} 1-\nu & \nu \\ \nu & 1-\nu \end{bmatrix} \begin{bmatrix} u_{r,r} \\ u_r/r \end{bmatrix}$$

  - C_{11} = E (1 – v)/((1+v)(1–2 v)) = 200*(1–0.345)/(1.345*(1–2*.345)) = 314.2 Gpa
  - C_{12} = E v/((1+v)(1–2 v)) = 200*0.345/(1.345*(1–2*.345)) = 165.5 Gpa
- Now we can calculate the stresses
  - σ_{rr} = 0.05*314.2 + 0.05*165.5 = 23.98 GPa
  - $\sigma_{\theta\theta}$ = 0.05*165.5 + 0.05*314.2 = 23.98 GPa

$$\sigma = \begin{bmatrix} 23.98 \\ 23.98 \end{bmatrix}$$

Example problem

- Compute the stress and strain tensors in the center and at the outer edge (r = 0.5 cm) in 1D axisymmetric coordinates in a fuel pellet with $u_r(r) = r^2/5$. C_{11} = 314.2 Gpa, C_{12} = 165.5 Gpa. $\epsilon = \begin{bmatrix} u_{r,r} & 0 \\ 0 & u_r/r \end{bmatrix}$

- First, calculate the strain tensor
- $\varepsilon_{rr} = u_{r,r} = 2r/5$
- $\varepsilon_{\theta\theta} = u_r/r = r/5$
- At the center there is no strain; at the outer edge $\epsilon = \begin{bmatrix} 0.2 & 0 \\ 0 & 0.1 \end{bmatrix}$

- To calculate the stress, convert to a strain vector and multiply by elastic constant matrix
- The stress in the center is zero
- On the outer edge
  - σ_{rr} = 0.2*314.2 + 0.1*165.5 = 79.4 GPa
  - $\sigma_{\theta\theta}$ = 0.1*314.2 + 0.2*165.5 = 64.52 GPa

NUMERICAL THERMO-MECHANICS

Now we can solve the temperature and the displacement vector for the full thermomechanical problem

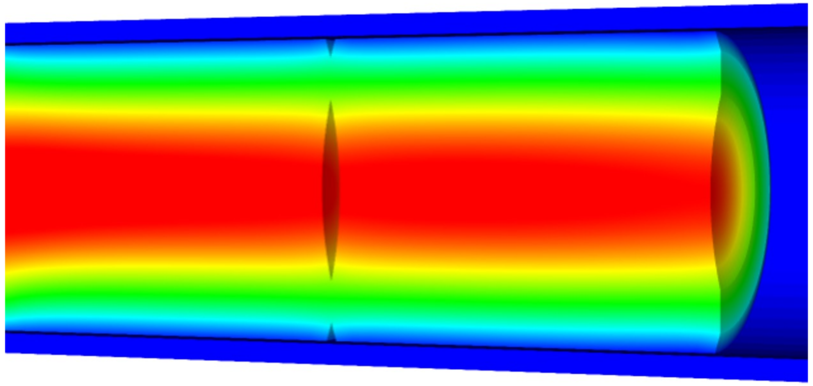
$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + Q$$

$$\boldsymbol{\sigma} = \boldsymbol{\mathcal{C}}(\boldsymbol{\epsilon} - \alpha(T - T_{fab})\mathbf{I})$$

$$0 = \nabla \cdot \boldsymbol{\sigma}$$

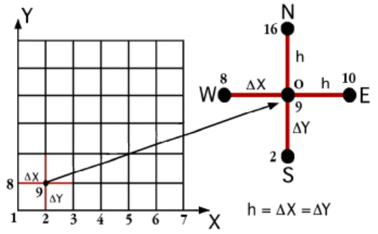
$$\boldsymbol{\epsilon} = \tfrac{1}{2}\left(\nabla \mathbf{u} + \nabla \mathbf{u}^T\right)$$

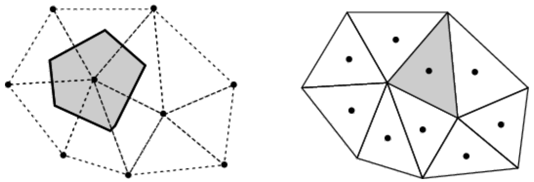
- T impacts the value of **u** through thermal expansion
- **u** impacts the value of T through changes in the thickness of the gap
- The value for T evolves with time
- The value for **u** also evolves with time, even though there is not time in its PDE

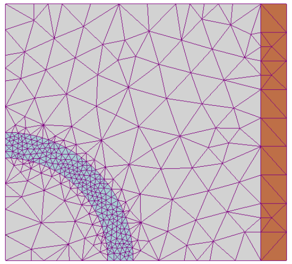


The primary tool for solving all thermomechanics problems is the finite element method

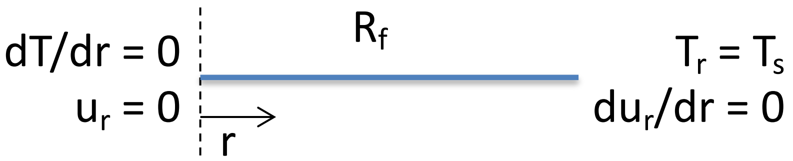
- **Finite difference**
  - Can solve the heat conduction equation
  - Can't easily solve the mechanics equations
- **Finite Volume**
  - Can solve the heat conduction equation
  - Can't easily solve the mechanics equations
- **Finite Element**
  - Can solve the heat conduction equation
  - Can solve the mechanics equations
  - Can handle any geometry
  - Can handle any boundary condition







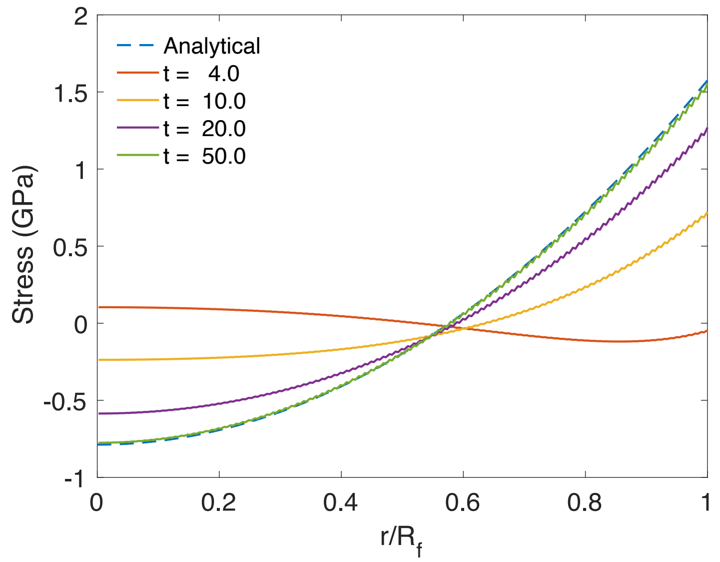
The 1D thermomechanics problem definition



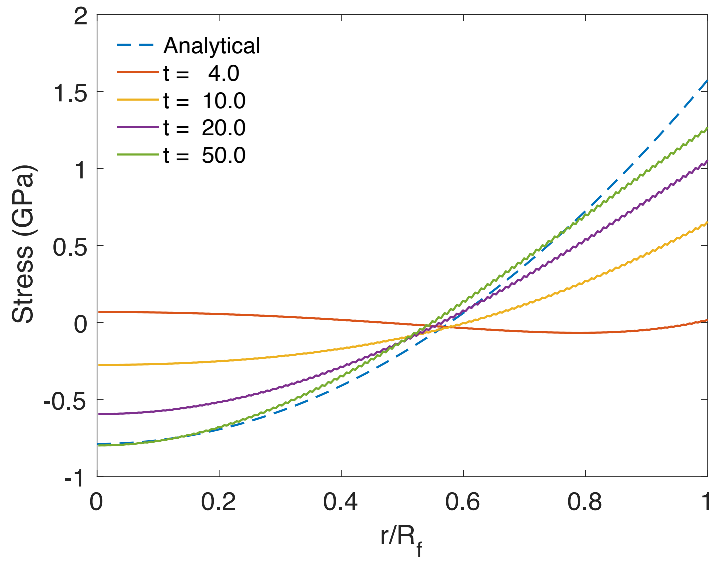
- The initial temperature is set to 273 K
- We will take 50 time steps of 0.5 s
- The full power of Q = 450 begins at time t = 0.
- UO_2 material properties are used for both the thermal and mechanics equations

Comparison to analytical theory

- If we use a constant thermal conductivity, analytical 1D model matches very well



- When k is a function of temperature, there is a difference between the FEM and analytical stress



There are various available tools for solving coupled thermomechanical problems with FEM

- Commercial tools
  - ABAQUS
  - ANSYS
  - COMSOL
- Open source
  - MOOSE
- NRC-based
  - FRAPCON/FRAPTRAN

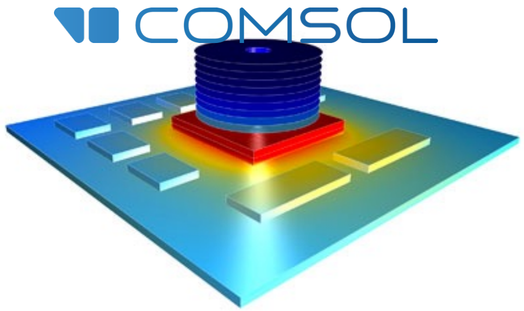
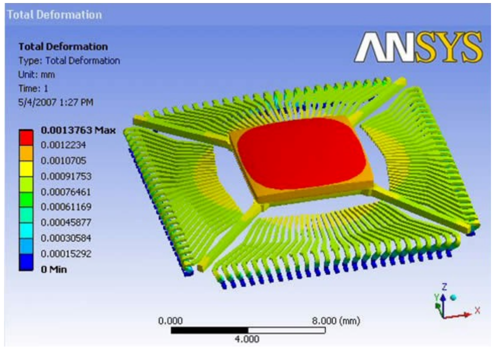


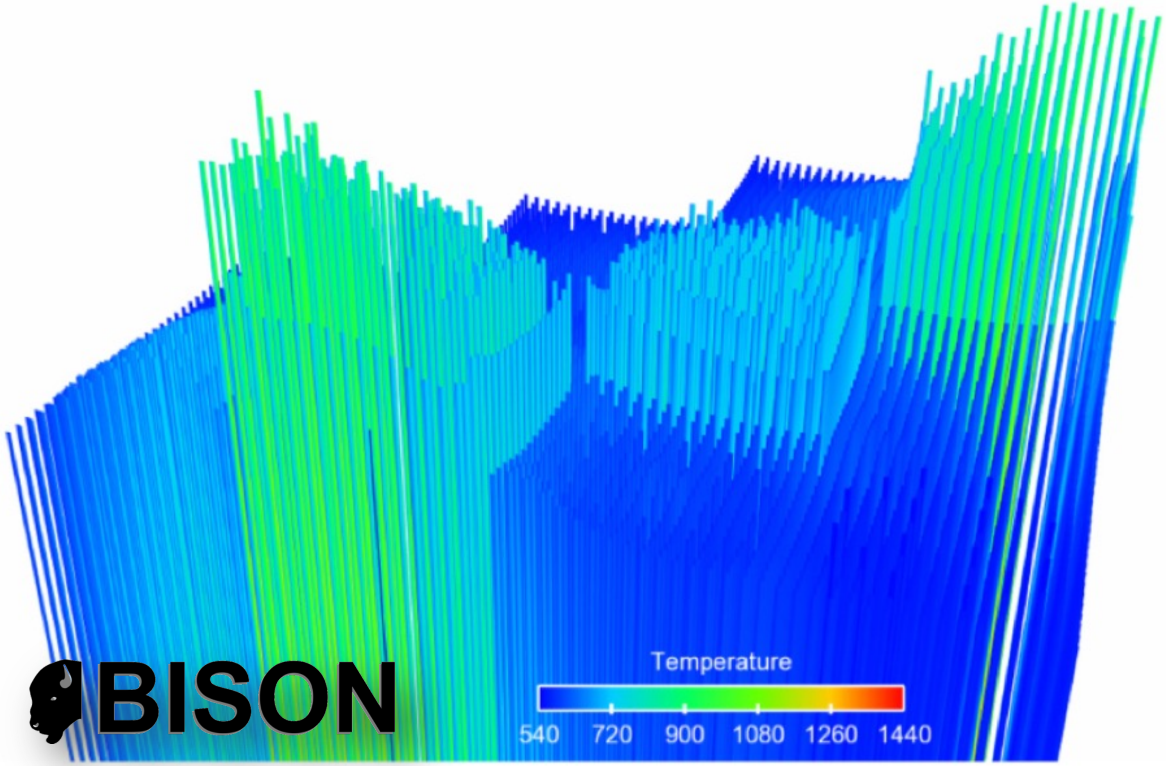
Figure 4. Temperature contour plot of exhaust manifold.

MOOSE



The purpose of a fuel performance code is to simulate and evaluate fuel rod behavior

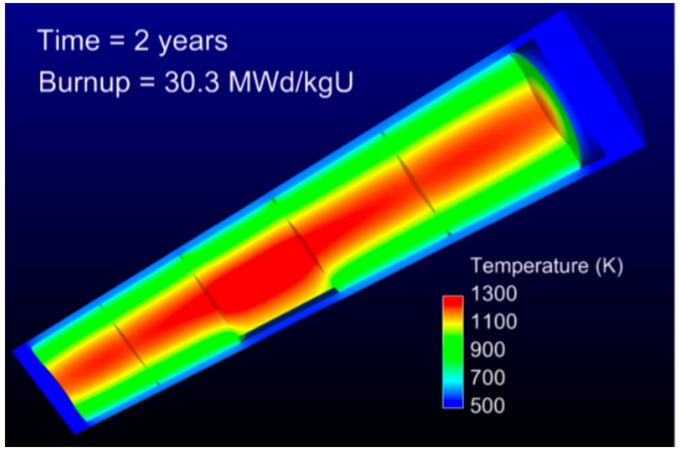
- The first fuel performance codes were developed in the mid seventies
- Advanced fuel performance codes are still under development today

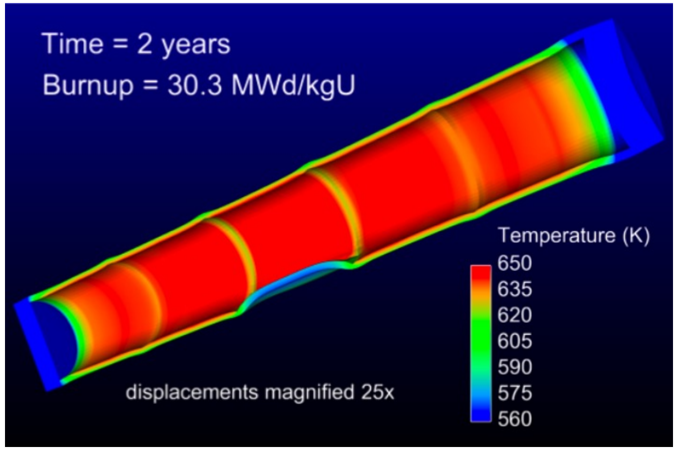


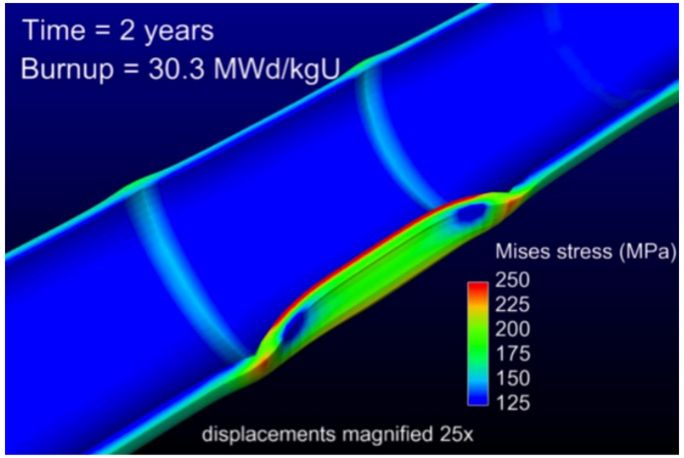
KAIST-3A benchmark results, showing displacement of 3432 rods, from Gaston et al. 2014

How are fuel performance codes used?

- The primary goals are to predict the fuel centerline temperature and the stress in the cladding
- Fuel performance codes aren't focused on predicting power production, but rather to predict safety margins, provide coupling to other codes



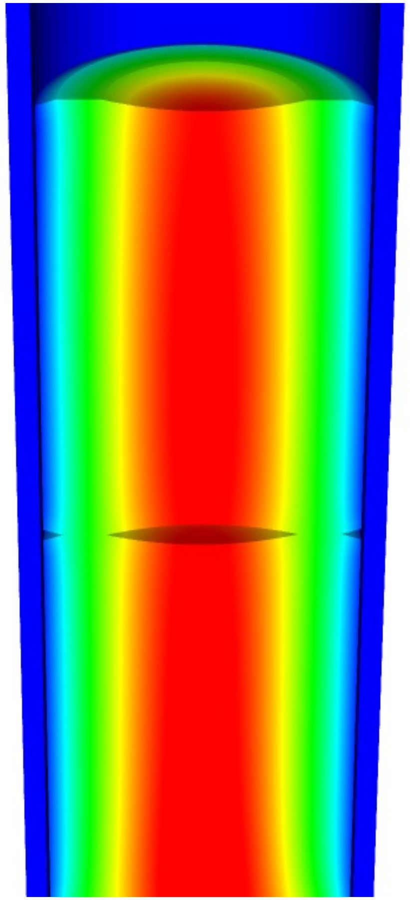




A fuel performance code must be able to predict:

Fuel
- Temperature profile
- Volumetric change

Cladding
- Temperature profile
- Stress



Gap
- Gap heat transport
- Mechanical interaction between fuel and cladding
- Gap pressure

The primary focus is solving the thermomechanical problem

Fuel

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + Q$$

Solved Numerically

$$0 = \nabla \cdot \boldsymbol{\sigma}$$

Solved Numerically or analytically

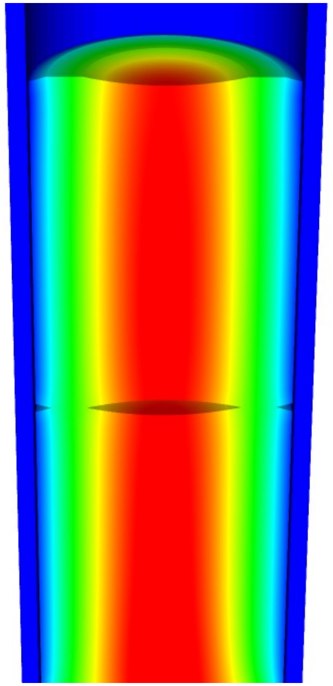
Cladding

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + Q$$

Solved Numerically or analytically

$$0 = \nabla \cdot \boldsymbol{\sigma}$$

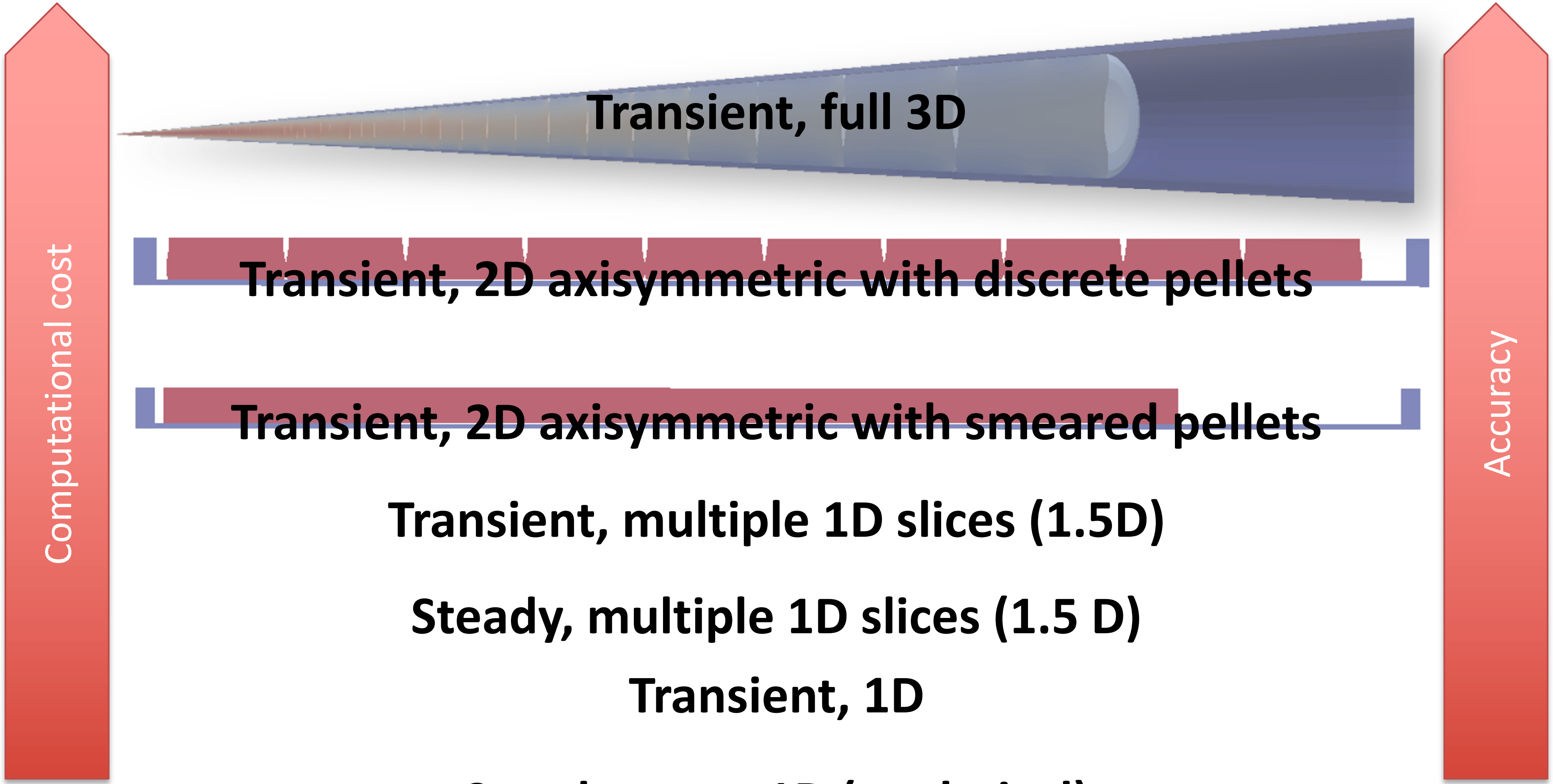
Solved Numerically



Gap

- The handling of the gap changes the most between different codes

Various approaches to model the fuel rod



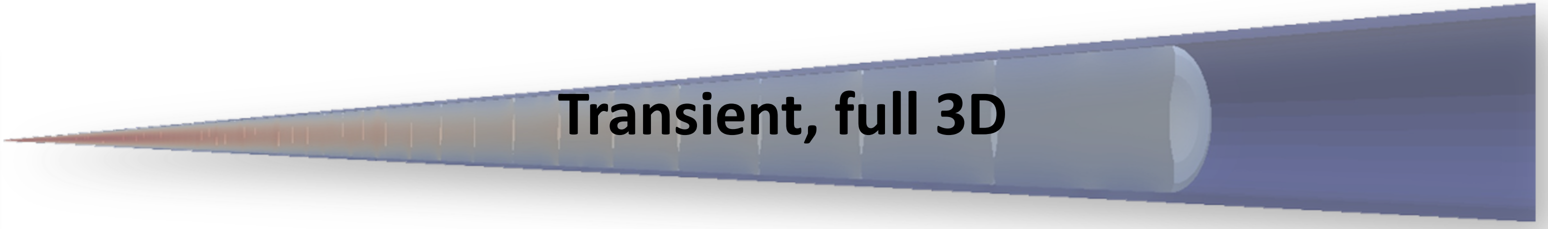
Steady state, 1D (analytical)

Early fuel performance codes were made for either steady state or transient operation

- Steady state codes
  - Leave off the time derivative part of the heat equation $\nabla \cdot (k \nabla T) + Q = 0$
  - The material properties still evolve with time as a function of burnup
  - The volumetric changes in the fuel are also a function of burnup
  - Creep of fuel and cladding change with time
- Transient codes
  - Include the time derivative $\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + Q$
  - Have similar burnup dependent models like steady state codes, but don't include creep
  - Have additional models for rapid transients

Start with FRAPCON

Computational cost



Transient, full 3D

Transient, 2D axisymmetric with discrete pellets

Transient, 2D axisymmetric with smeared pellets

Transient, multiple 1D slices (1.5D)

Steady, multiple 1D slices (1.5 D)

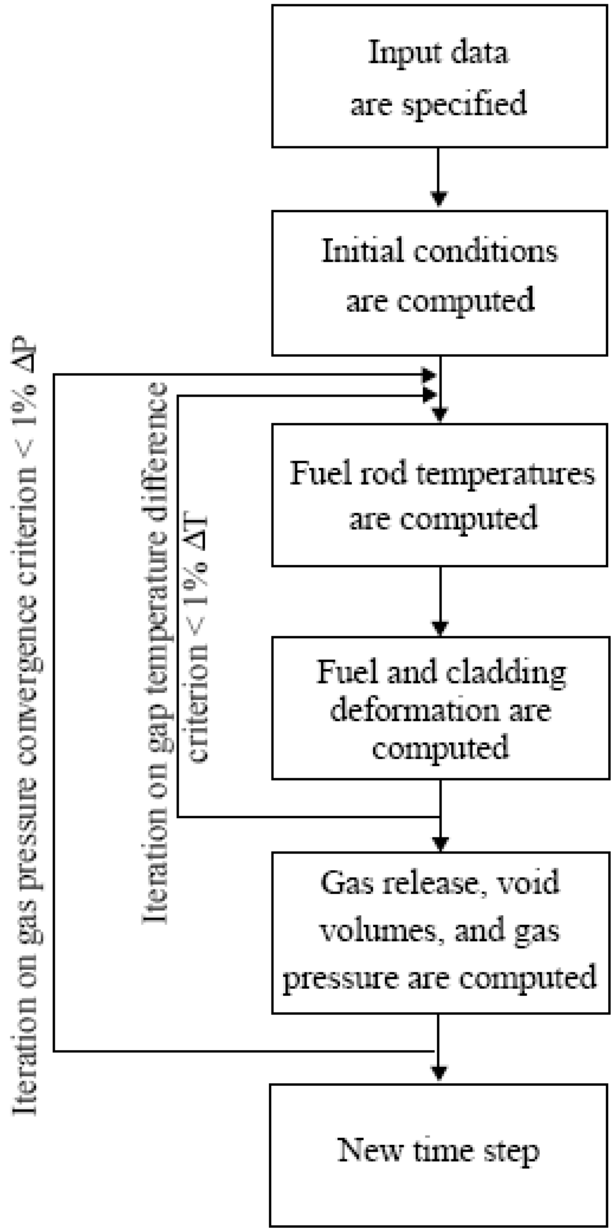
Transient, 1D

Steady state, 1D (analytical)

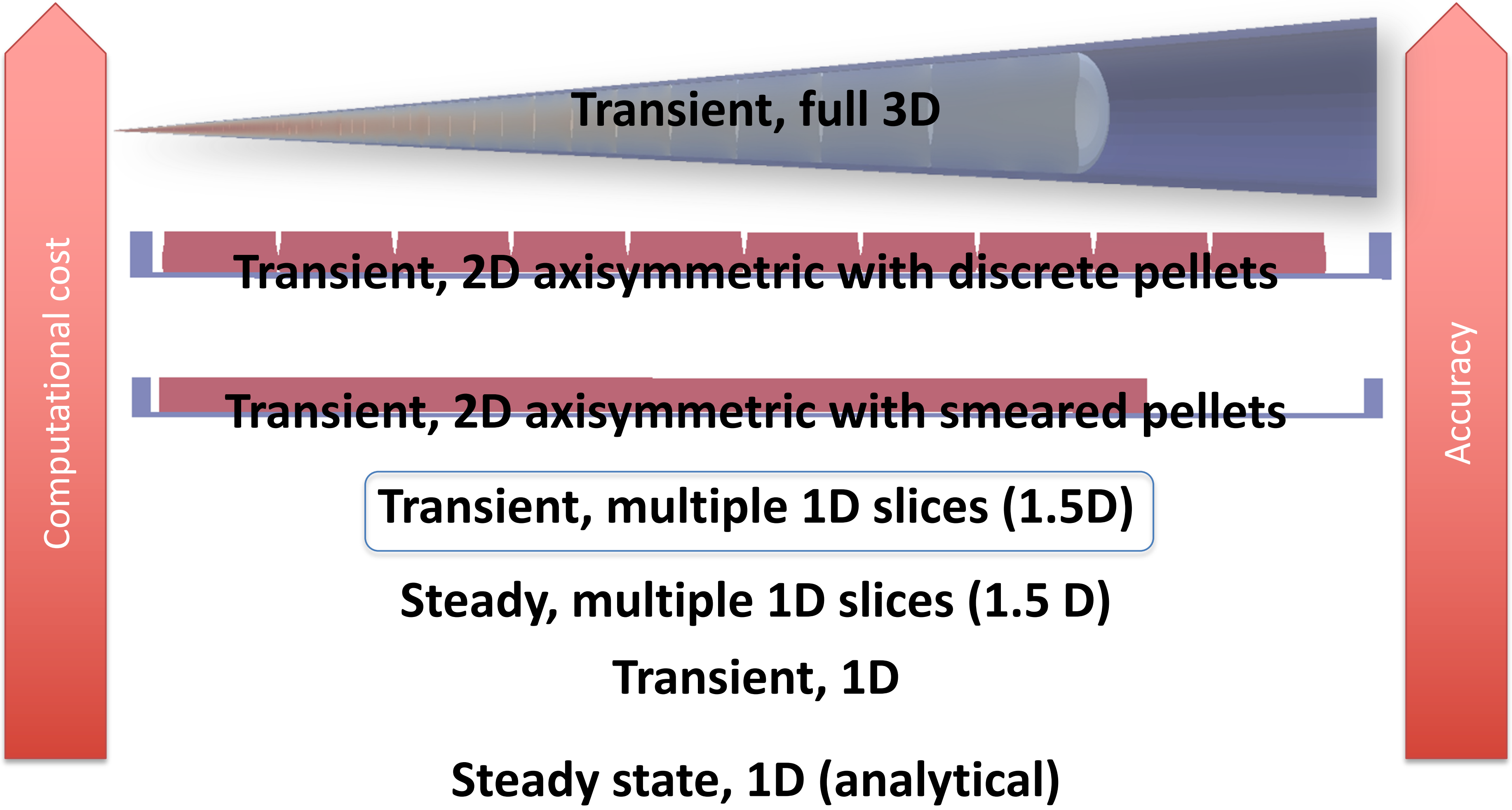
Accuracy

FRAPCON Flow Chart

- FRAPCON is the NRC's steady-state fuel performance code
- FRAPCON has the ability to accurately calculate the high-burnup response of light-water reactor fuel rods
- FRAPCON iterates to determine fuel rod temperatures, fuel and cladding deformation
- This converged data is iterated to produce gas release, void volumes and plenum pressure
- Then marches forward in time



FRAPTRAN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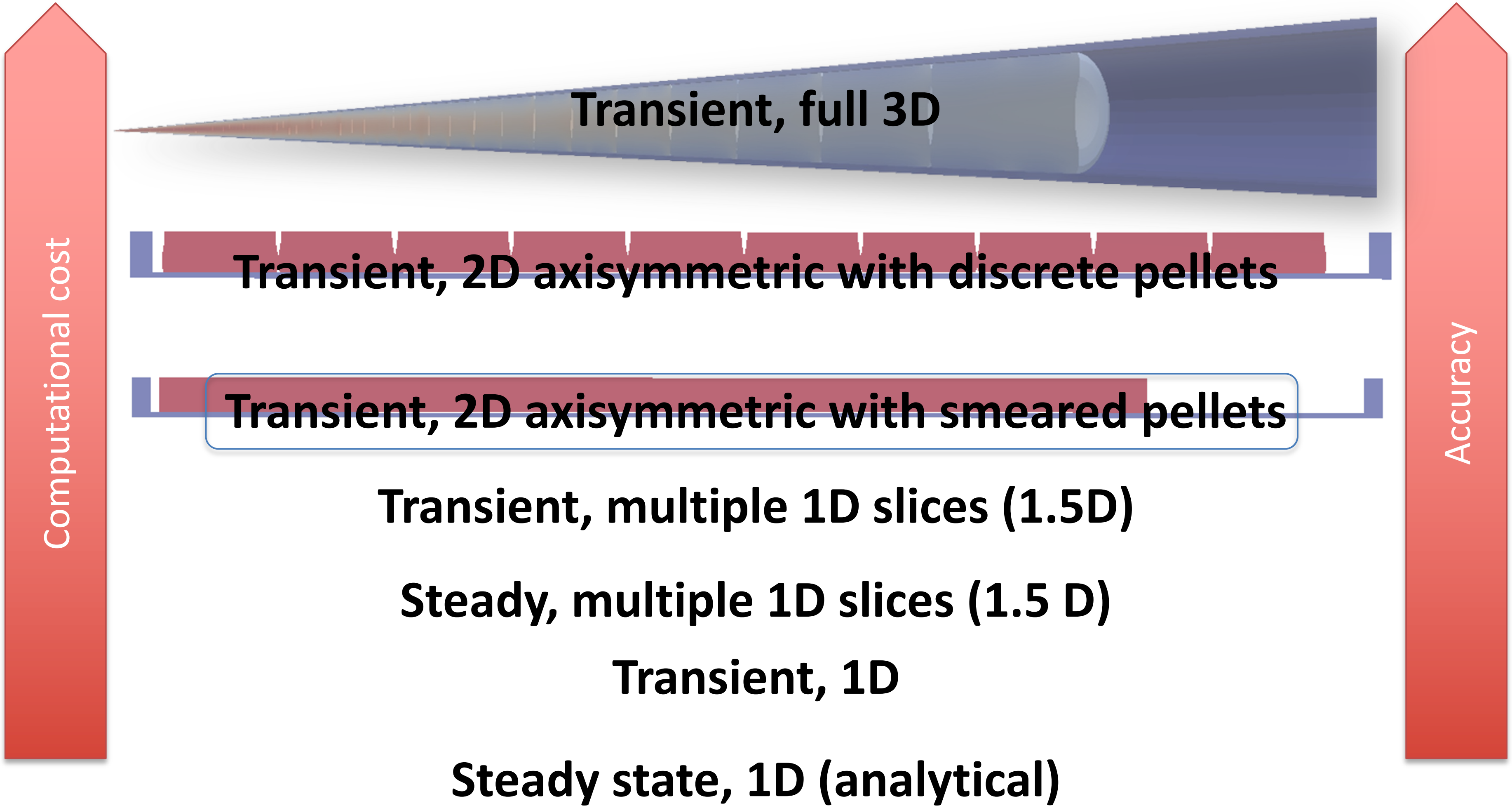
Steady, multiple 1D slices (1.5 D)
Transient, 1D
Steady state, 1D (analytical)
Accuracy

FALCON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Steady, multiple 1D slices (1.5 D)
Transient, 1D
Steady state, 1D (analytical)
Accuracy

FALCON

- FALCON is a 2D fuel performance code developed by EPRI
- Development of FALCON started in 1996
- The beta version was released in 2003
- It was developed by ANATECH for EPRI
- FALCON is proprietary, owned by EPRI
- It is no longer under active development in the US

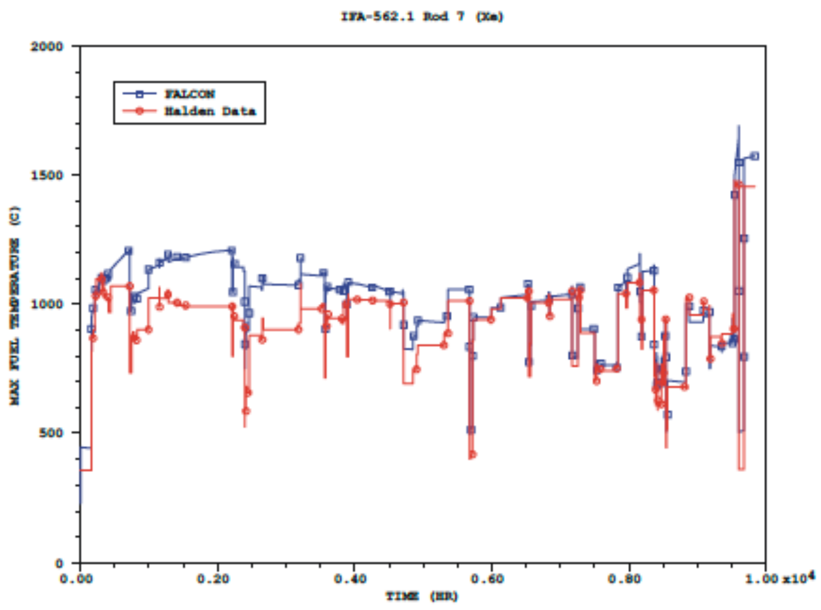


Figure 3-6
Calculated Fuel Temperatures Versus Measured Data for IFA-562.1 Rod 7 (Xe-filled)

FALCON is a 2D transient and steady state code

Fuel

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + Q$$

Solved with FEM

$$0 = \nabla \cdot \boldsymbol{\sigma}$$

Solved with FEM

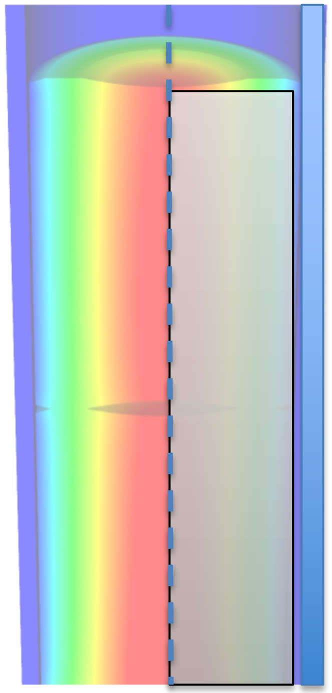
Cladding

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + Q$$

Solved with FEM

$$0 = \nabla \cdot \boldsymbol{\sigma}$$

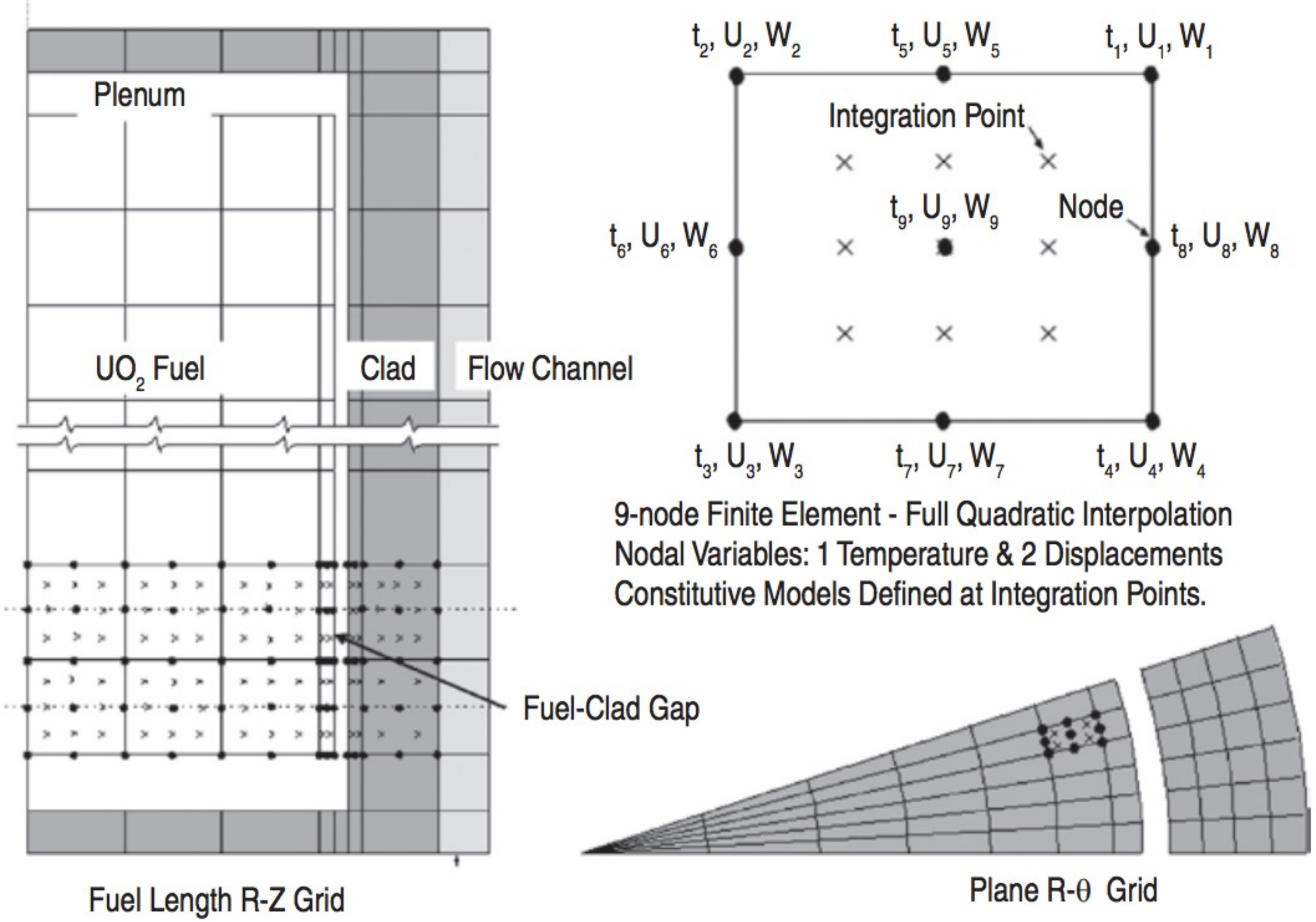
Solved with FEM



Gap

- Pressure is calculated using equation of state
- Simplified contact model is used for gap closure
- Gap heat transfer model is used

FALCON can predict the fuel performance in axisymmetric RZ space or in Rθ space



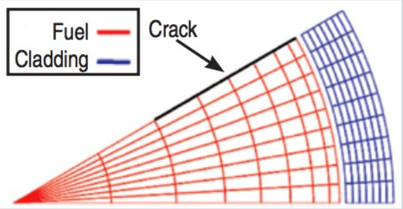


Figure 3. Standard PCI model.

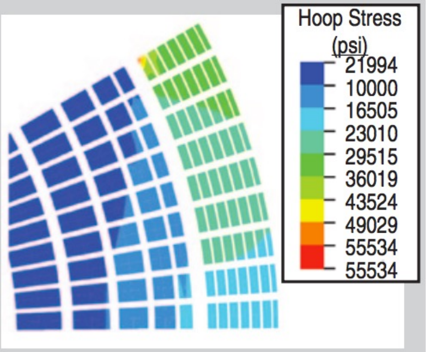


Figure 4. Calculated cladding hoop stress distribution (psi) using the standard PCI model.

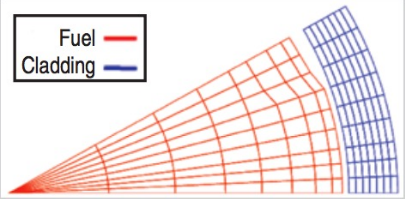
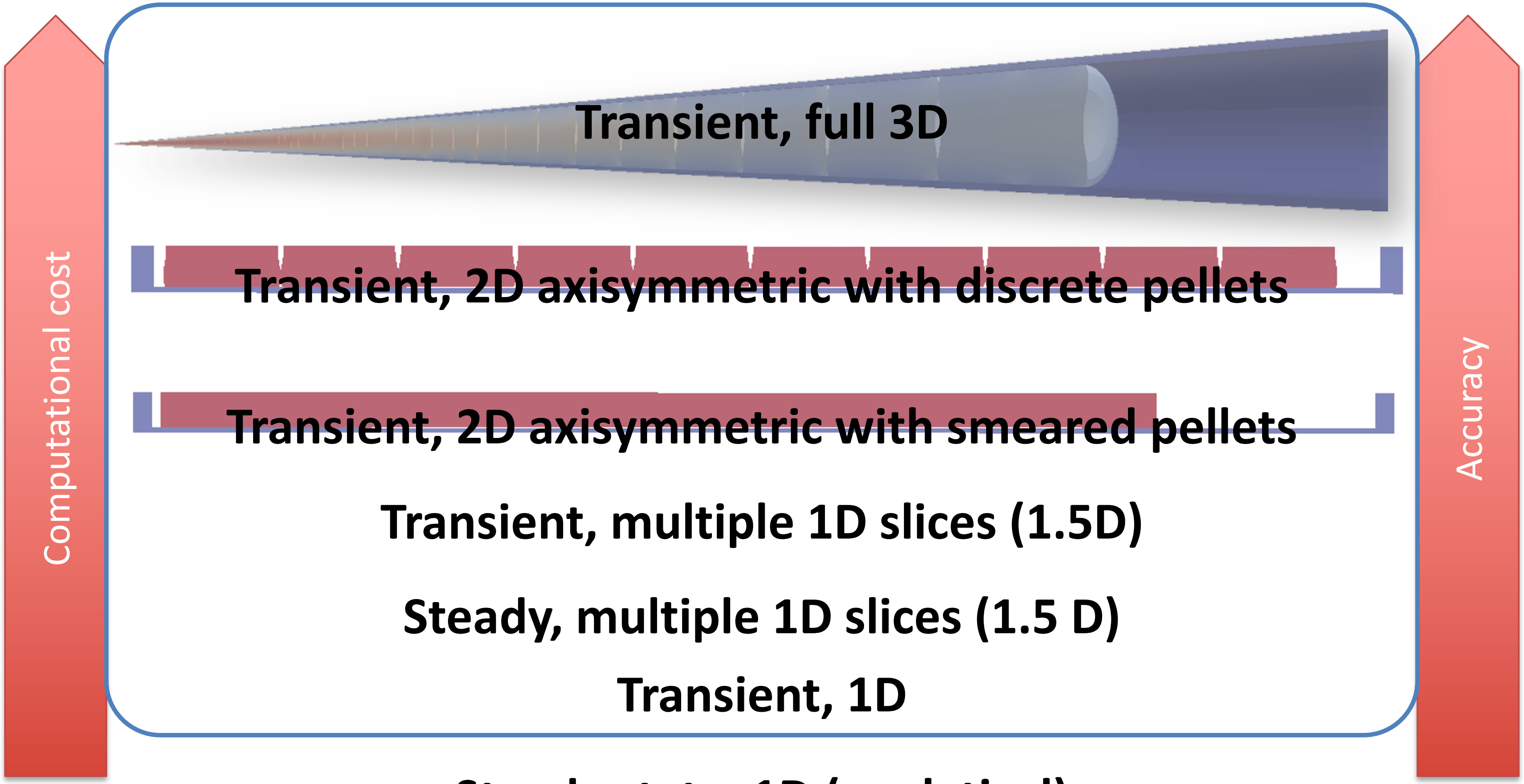


Figure 5. Missing pellet surface (MPS) PCI model.

BISON



Steady state, 1D (analytical)

BISON

- The next generation fuel performance code under development in the US
- It uses the MOOSE framework
- Development was begun in 2008
- The first paper using BISON was published in 2009 and the paper summarizing its full capabilities was published in 2012
- It was developed at Idaho National Laboratory, with some support by ANATECH
- BISON is available for free, but it is export controlled and requires a license agreement be signed

BISON models the fuel behavior ranging from 1D to full 3D and uses FEM

Fuel

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + Q$$

Solved with FEM

$$0 = \nabla \cdot \boldsymbol{\sigma}$$

Solved with FEM

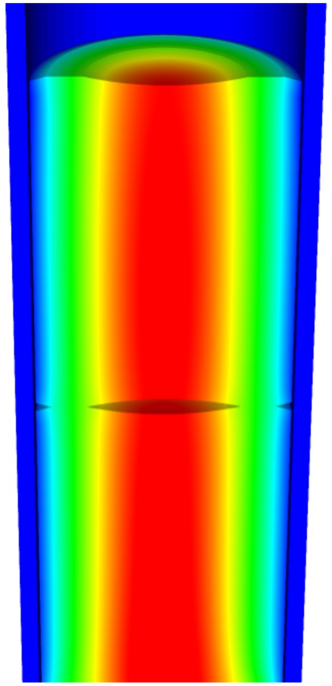
Cladding

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + Q$$

Solved with FEM

$$0 = \nabla \cdot \boldsymbol{\sigma}$$

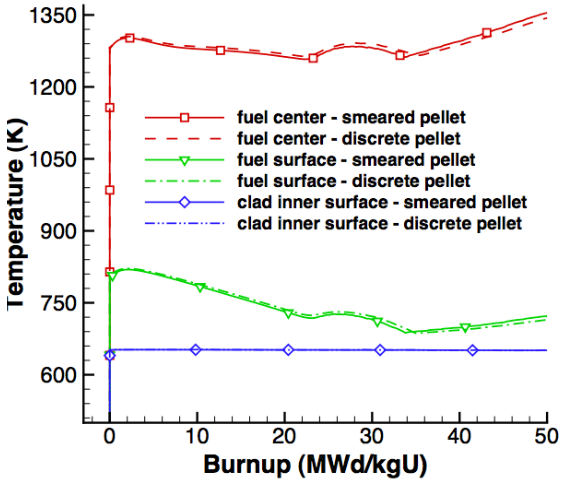
Solved with FEM

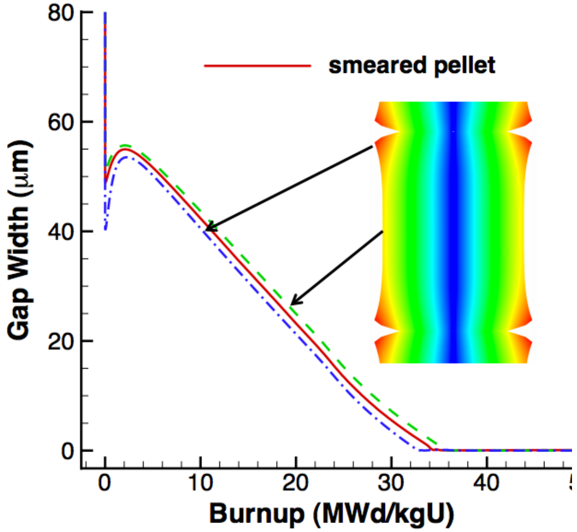


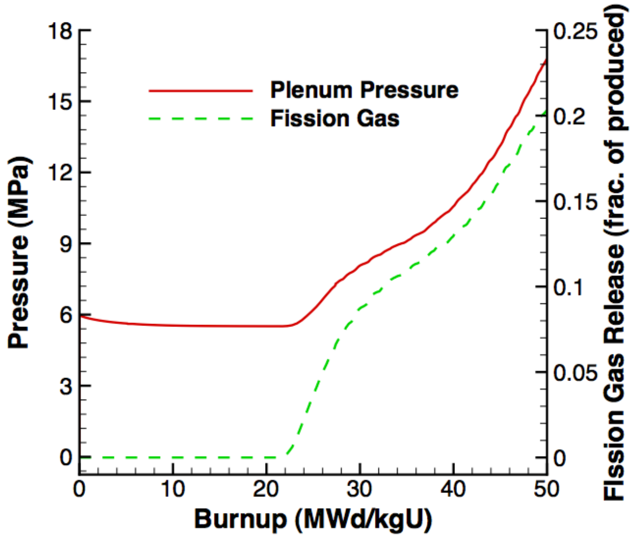
Gap

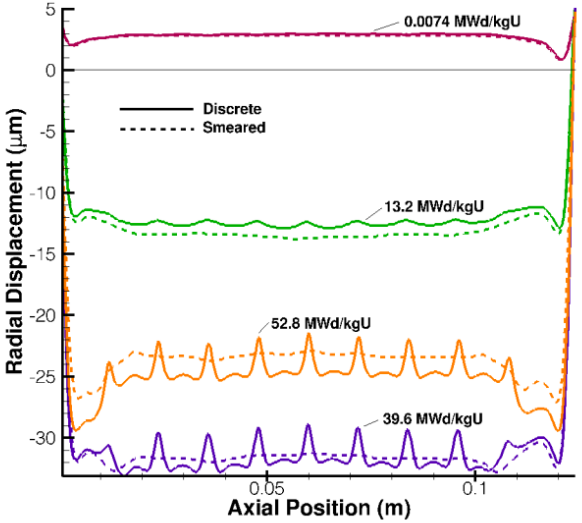
- Pressure is calculated using equation of state
- Fully implemented implicit contact algorithm
- Gap heat transfer model is used

Can handle smeared or discrete pellets, asymmetric pellet geometry and deformation

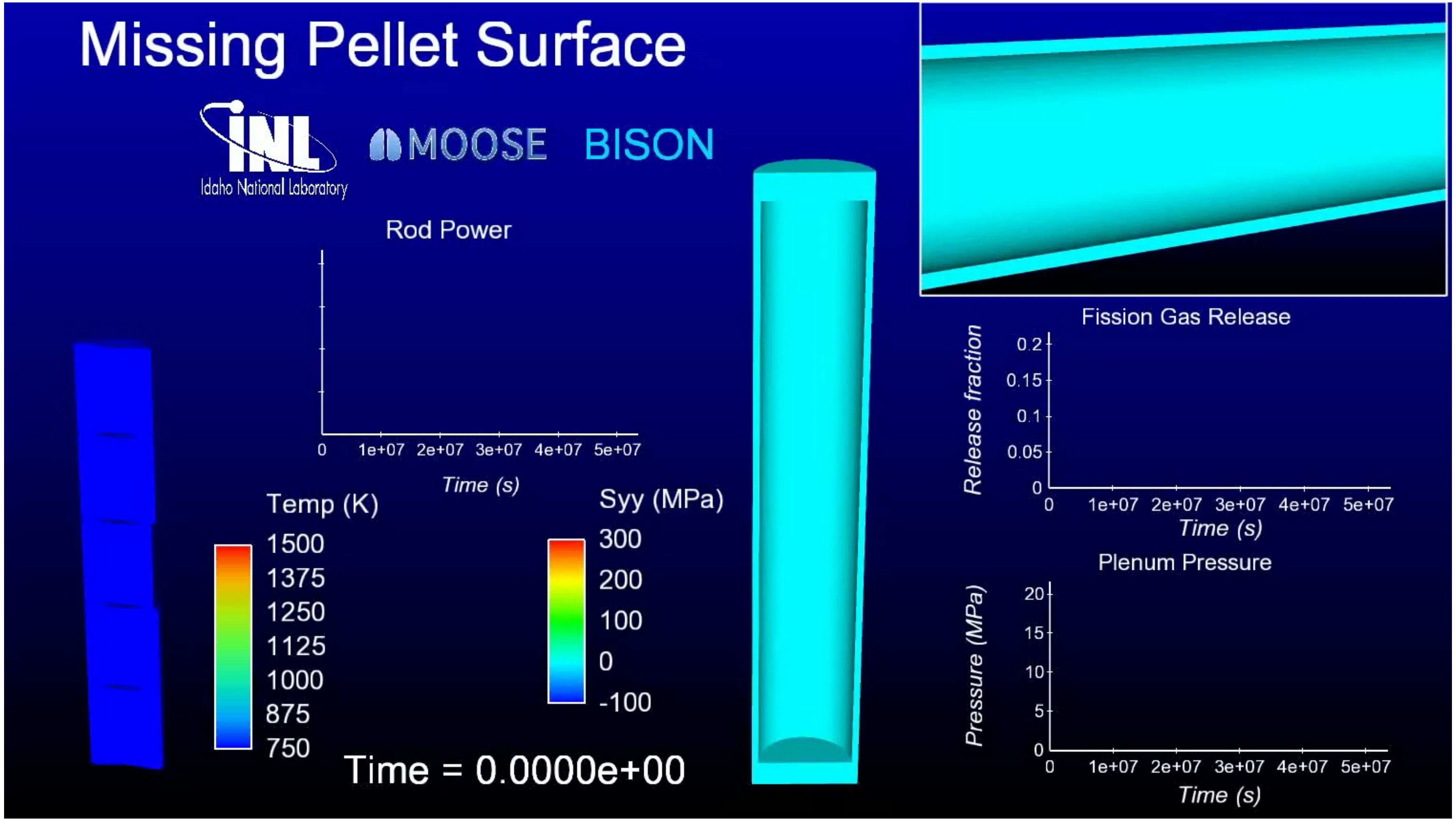








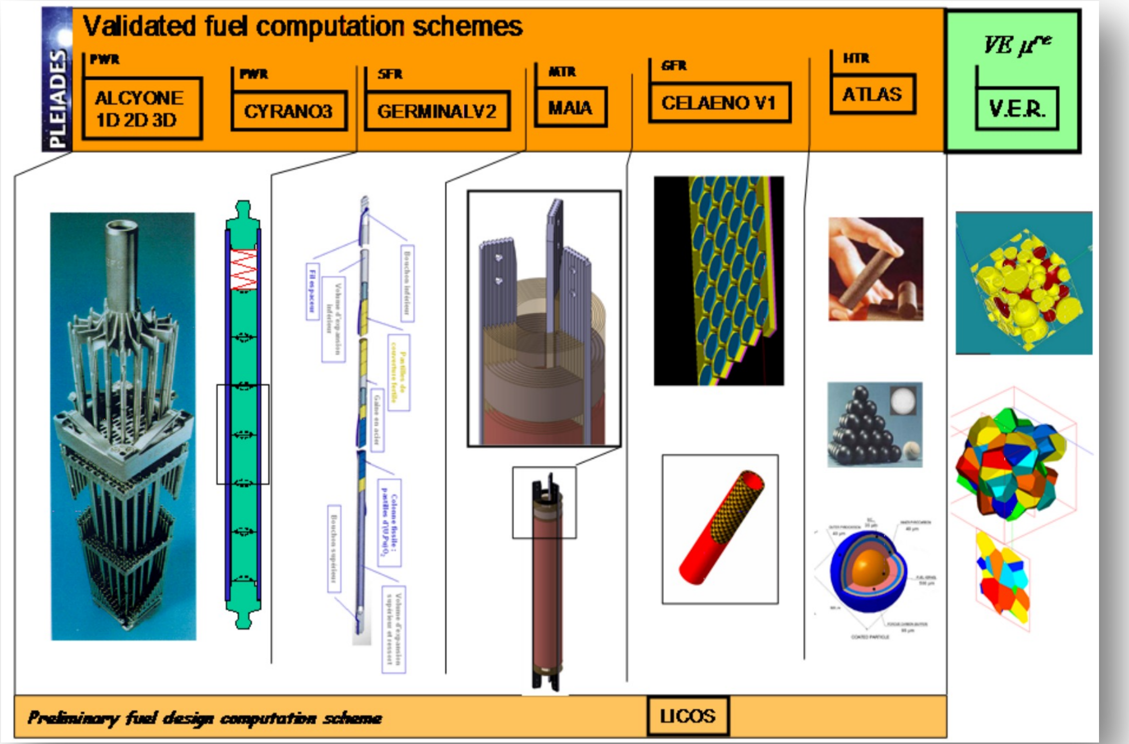
Because of its unique 3D capability, BISON can model truly 3D fuel performance problems



Other countries have other fuel performance codes

Table 1
List of fuel rod performance codes developed in different parts of the world for light water reactor fuel. More information is provided in Appendix: Overview of main fuel rod performance code developments across the globe.

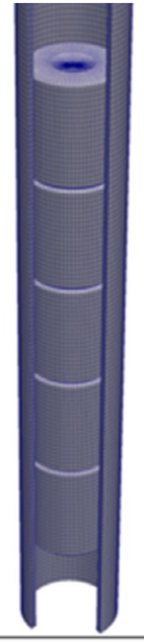
Country	Organization	Code name (precursor codes)
Argentina	CNEA	BACO, DIONISIO
Belgium	Belgonucleaire	COMETHE
	SCK-CEN	MACROS (ASFAD)
China	Xi'an Xiaotong Univeristy	FROBA
	CIAE	FTPAC
	NPIC	FUPAC
	CGNPC	JASMINE
Czech Republic	UJV	PIN-MICRO (GAPCON-THERMAL2)
France	CEA	ALCYONE (METEOR-TRANSURANUS)
	Framatome	COPERNIC (TRANSURANUS), GALILEO (COPERNIC/RODEX/CARO)
	EdF	CYRANO
	IRSN	SCANAIR
Germany	Siemens	CARO
	Framatome	GALILEO (COPERNIC/RODEX/CARO)
	GRS	TESPA-ROD (TESPA)
	JRC	TRANSURANUS (URANUS)
Hungary	MTA EK	FUROM (PIN-MICRO)
India	BARC	FAIR, PROFESS
	PNC	FUDA
Japan	CRIEPI	EIMUS (FEMAXI-III)
	JAEA	FEMAXI, RANNS
	SEPC	IRON (FEMAXI-III)
	NFD	TRUST
Korea	KAERI	COSMOS, INFRA
Russian Federation	VNIINM	START, RAPTA
	TRINITI	RTOP
	IBRAE	SFPR (MFPR)
Sweden	Westinghouse Sweden Electric	STAV
United Kingdom	NNL, EDF Energy	ENIGMA (MINIPAT, SLEUTH, HOTROD)
USA	USNRC	FRAPCON, FRAPTRAN (FRAP), FAST
	Siemens	RODEX
	EPRI	FALCON (FREY, ESCORE)
	INL	BISON
	Framatome	GALILEO (COPERNIC/RODEX/CARO)
	Westinghouse	PAD



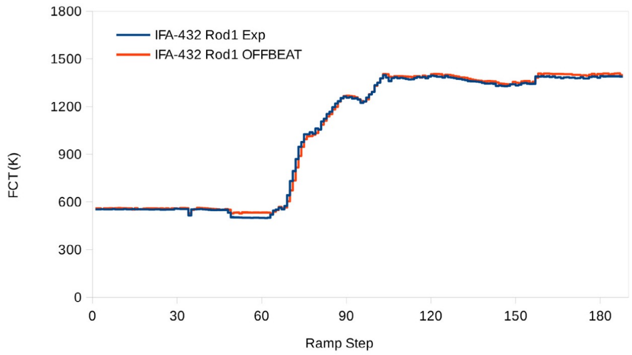
http://www.materials.cea.fr/en/PDF/PLEIADES-Platform.pdf

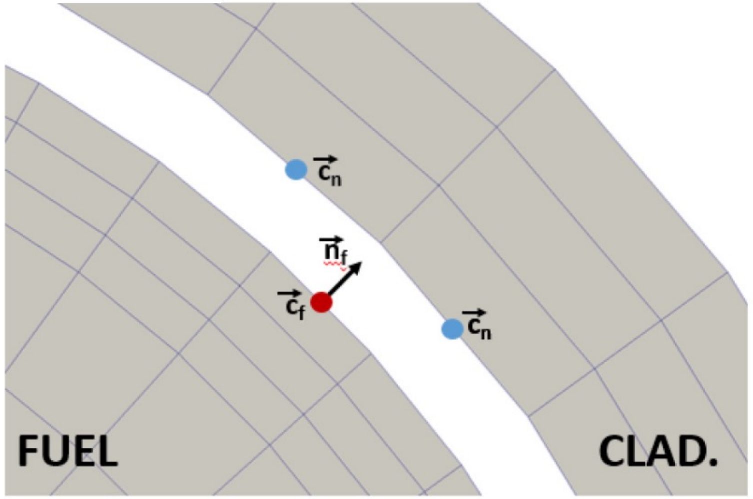
OFFBEAT – new tool

- The OpenFOAM Fuel BEhavior Analysis Tool (OFFBEAT) is a multi-dimensional fuel performance code developed in Switzerland
- The code can be used both for studying complex 2D or 3D local effects and for more traditional 1.5D base irradiation analyses
- OFFBEAT is based on the open-source C++ library OpenFOAM, thus the governing equations are discretized with modern finite volume techniques



3D Model





Summary

- Gap size changes due to thermal expansion
- Often have displacements instead of strains, and can solve for stress via displacements
- Fuel performance codes are focused on predicting the center temperature of the pellet and the stress in the cladding
- All fuel performance codes
  - Numerically model the temperature in the fuel
  - Numerically model the stress in the cladding
  - And consider gap pressure, closure, and heat transfer in some way
- The primary US codes are
  - FRAPCON – Steady state 1.5D, uses finite difference
  - FRAPTRAN – Transient 1.5D, uses finite difference
  - FALCON – Steady or transient 2D, uses finite element
  - BISON – Steady or transient, 1D – 3D, uses finite element