PennState
College of Engineering

NucE 497: Reactor Fuel Performance

Lecture 15: 1D Numerical solutions of Thermomechanics

February 13, 2017

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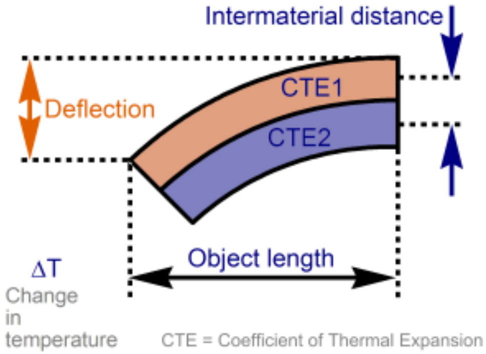
Material is taken from Dr. Motta's book, chapter 6

Today we will finish talking about the coupling of temperature and stress and start numerical solutions

- Module 1: Fuel basics
- Module 2: Heat transport
- Module 3: Mechanical behavior
  - Introduction to solid mechanics
  - Analytical solutions of the mechanics equations
  - **Thermomechanics, thermal expansion**
  - **Solving equations in 1D numerically**
  - Solving in multiple dimensions with FEM
  - Summary of fuel performance codes
- Module 4: Materials issues in the fuel
- Module 5: Materials issues in the cladding
- Module 6: Accidents, used fuel, and fuel cycle

Here is some review from last time

- Consider this metal strip (see picture). Which material has the larger thermal expansion coefficient?
    a) CTE1
    b) CTE2



a) Why do fuel pellets fracture during reactor startup?
    a) Due to mechanical interaction between cladding and pellet
    b) Due to expansion of fission gas
    c) Due to thermal expansion and the temperature gradient
    d) Due to expansion of gas in the gap and plenum

Quiz question: Fuel pellets crack due to

a) Compressive stresses once the pellet expands and pushes on the cladding
b) Tensile stresses that result from thermal expansion and the temperature gradient
c) Compressive stresses that result from thermal expansion and the temperature gradient
d) Earthquakes

Attempts: 39 out of 39

+0.65

Discrimination Index

Fuel pellets crack due to

Compressive stresses once the pellet expands and pushes on the cladding		0 %
Tensile stresses that result from thermal expansion and the temperature gradient	33 respondents	**85 %** ✓
Compressive stresses that result from thermal expansion and the temperature gradient	6 respondents	15 %
Earthquakes		0 %

Thermal expansion causes a decrease in the gap

- Both the pellet and the cladding swell

$$\Delta\delta_{gap} = \delta_{gap} - \delta_{gap}^0$$

$$\Delta\delta_{gap} = \Delta\bar{R}_C - \Delta R_f$$

$$\frac{\Delta R_f}{R_f} = \alpha_f(\bar{T}_f - T_{fab})$$

$$\frac{\Delta R_C}{\bar{R}_C} = \alpha_C\left(\bar{T}_C - T_{fab}\right)$$

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

- 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.

We need to calculate the steady state temperature profile in the rod, including thermal expansion

- LHR = 200 W/cm, δ^0_{gap} = 30 μm, R_f = 0.5, T_{cool} = 580 K, T_0 = 373 K, k_{gap} = 0.0026 W/cm-K, δ_C= 0.06 cm, α_f = 11.0e-6 1/K, α_C = 7.1e-6 1/K

$$\Delta\delta_{gap} = \bar{R}_c \alpha_C \left(\bar{T}_C - T_{fab}\right) - \bar{R}_f \alpha_f \left(\bar{T}_f - T_{fab}\right) \quad \Delta T_{gap} = \frac{LHR}{2\pi R_f k_{gap}/\delta_{gap}}$$

- ΔT_{cool} = 25.5 K, ΔT_{clad} = 22.5 K, ΔT_{fuel} = 530.5 K
- So, T_{IC} = 580 + 25.5 + 22.5 = 628.0 K, T_s = 701.5 K, T_0 = 1232.0 K
- First, we will deal with expansion in the cladding
  - Av(R_c) = 0.5 + 30e-4 + 0.06/2 = 0.533 cm, Av(T_C) = 580 + 25.5 + 22.5/2 = 616.75 K
  - ΔR_c = 0.533*7.1e-6*(616.75 – 373) = 9.22e-4 cm
- Second, we deal with the fuel
  - Av(Tf) = (1232 + 701.5)/2 = 966.7 K
  - ΔR_f = 0.5*11e-6*(966.7 – 373) = 0.0033 cm
- The total change in the gap is 9.22e-4 – 0.0033 = -0.0023
- 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 effect 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

i = 0; chng = 1;

While chng > 1e-6

$i = i+1;$

$\Delta R_f = \alpha_f R_f*((T_s + T_0)/2 - T_{fab})$

$Old\_\Delta\delta_{gap} = \Delta\delta_{gap}$

$\Delta\delta_{gap} = \Delta R_C - \Delta R_f$

$\delta_{gap} = \delta_{gap} + \Delta\delta_{gap}$

$h_{gap} = k_{gap}/\delta_{gap}$

$T_s = T_{Cl} + LHR/(2\,\pi\,(R_f + \Delta R_f)\,h_{gap})$

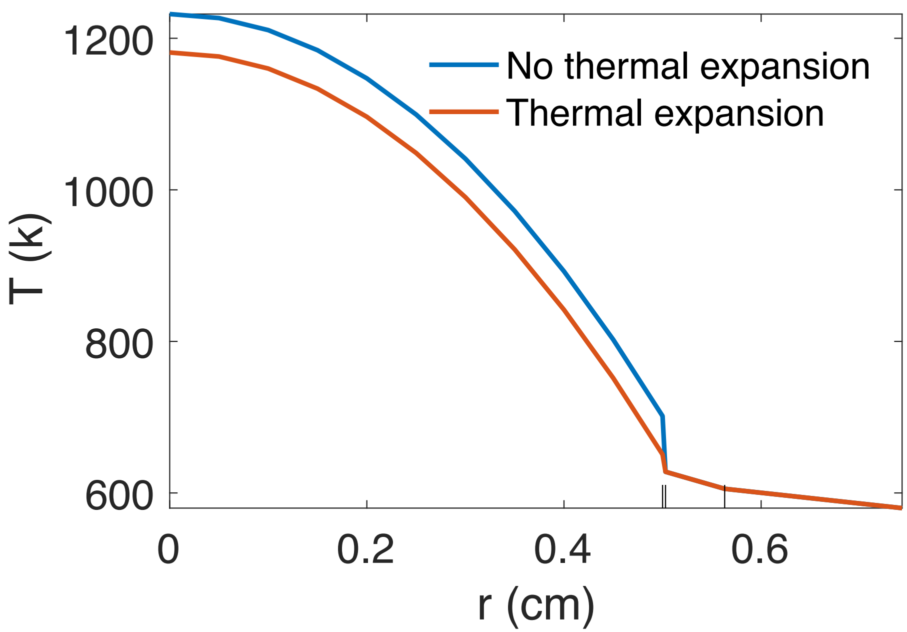
$T_0 = T_s + LHR/(4\,\pi\,k)$

$chng = |\Delta\delta_{gap} - Old\_\Delta\delta_{gap}|/Old\_\Delta\delta_{gap}$

end

Here are the iterations required for the previous problem

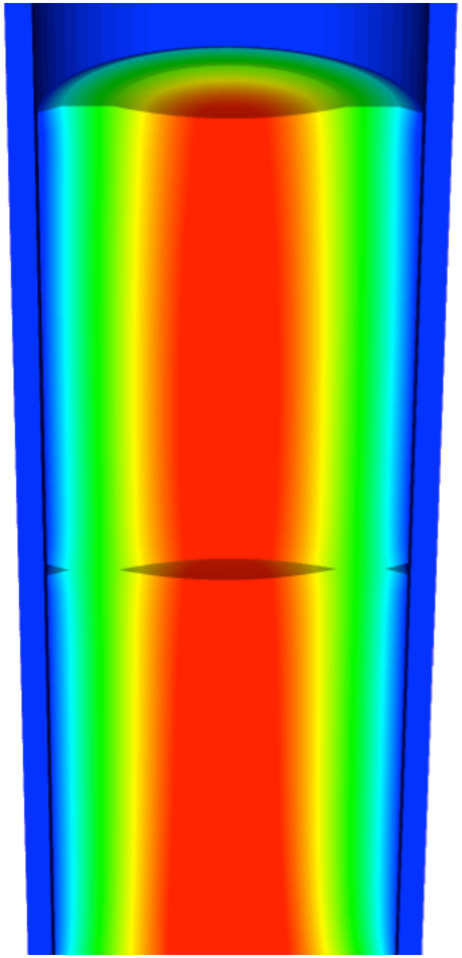
Iteration	δ_{gap} (cm)	T_s (K)	T_0 (K)
0	0.003	701	1232
1	0.00066	644	1174
2	0.00097	652	1182
3	0.00094	651	1181
4	0.00094	651	1181



The temperature and the displacement vector are solved for with the full thermomechanical problem

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

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



- 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 thermomechanical problem becomes 2D when we assume axisymmetry

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

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

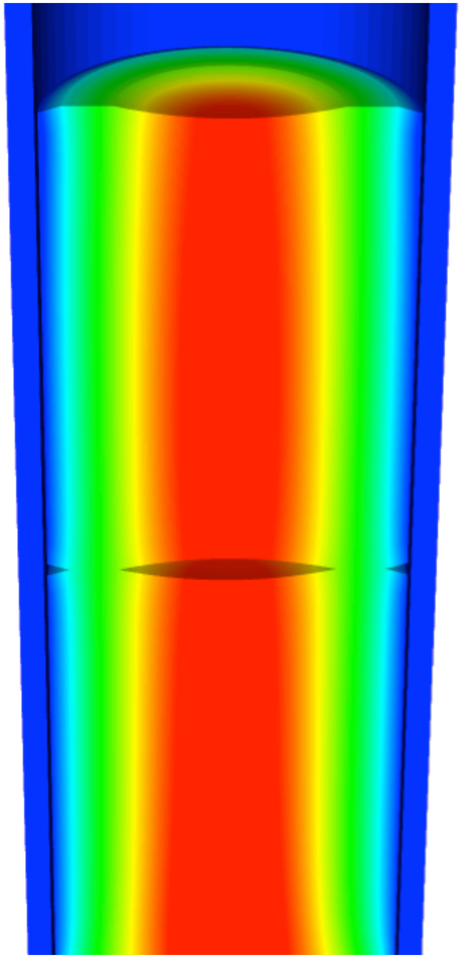
- Assumption 1: Problem is axisymmetric

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

$$\frac{\partial \sigma_{rr}}{\partial r} + \frac{\sigma_{rr} - \sigma_{\theta\theta}}{r} + \frac{\partial \sigma_{rz}}{\partial z} = 0$$

$$\frac{1}{r}\frac{\partial (r\sigma_{rz})}{\partial r} + \frac{\partial \sigma_{zz}}{\partial z} = 0 \qquad \boldsymbol{\sigma} = \boldsymbol{\mathcal{C}}(\boldsymbol{\epsilon} - \alpha(T - T_{fab})\mathbf{I})$$

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



If we assume isotropy, we can solve for the stress from the strain

- The hoop strain is included in the calculation of the stress

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

We can further simplify the problem to be 1D

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

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

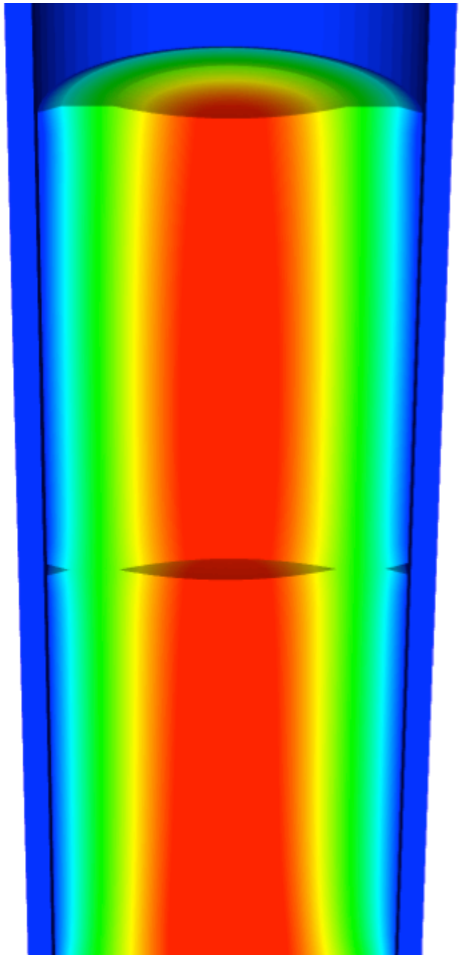
- Assumption 2: The solution does not change with z

$$\rho c_p \frac{\partial T}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(r k(T) \frac{\partial T}{\partial r}\right)$$

$$\frac{\partial \sigma_{rr}}{\partial r} + \frac{\sigma_{rr} - \sigma_{\theta\theta}}{r} = 0$$

$$\boldsymbol{\sigma} = \boldsymbol{\mathcal{C}}(\boldsymbol{\epsilon} - \alpha(T - T_{fab})\mathbf{I}) \qquad \boldsymbol{\epsilon} = \begin{bmatrix} u_{r,r} & 0 \\ 0 & u_r/r \end{bmatrix}$$

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



For a given 1D displacement function, we can now define the strain and stress in the pellet

- Assume the radial displacement in the fuel pellet is ur(r) = 0.05r cm.
- What is the strain tensor at the center and at the outer edge?

$$\boldsymbol{\epsilon} = \begin{bmatrix} u_{r,r} & 0 \\ 0 & u_r/r \end{bmatrix} \qquad \boldsymbol{\epsilon} = \begin{bmatrix} 0.05 & 0 \\ 0 & 0.05 \end{bmatrix}$$

- We are dealing with UO_2, so E = 200 GPa and ν = 0.345
  - C_{11} = E (1 – ν)/((1+ν)(1–2 ν)) = 200*(1–0.345)/(1.345*(1–2*.345)) = 314.2 Gpa
  - C_{12} = E ν/((1+ν)(1–2 ν)) = 200*0.345/(1.345*(1–2*.345)) = 165.5 Gpa

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

- Now we can calculate the stresses
  - σ_{rr} = 0.05*314.2 + 0.05*165.5 = 23.98 GPa
  - $\sigma_{\theta\theta}$ = 0.05*314.2 + 0.05*165.5 = 23.98 GPa

$$\boldsymbol{\sigma} = \begin{bmatrix} 23.98 & 0 \\ 0 & 23.98 \end{bmatrix} \text{GPa}$$

Now here is a problem for you to try

- 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.

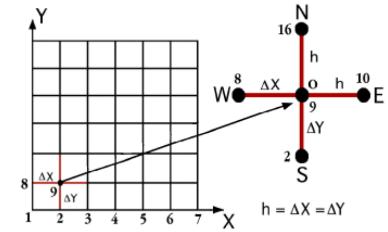
$$\epsilon = \begin{bmatrix} u_{r,r} & 0 \\ 0 & u_r/r \end{bmatrix}$$

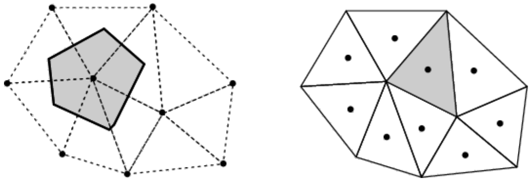
- First, calculate the strain tensor
- $\varepsilon_{rr} = u_{r,r} = 2r/5$
- $\varepsilon_{\theta\theta} = u_r/4 = r/5$
- At the center there is no strain, and at the outer edge $\epsilon = \begin{bmatrix} 0.2 & 0 \\ 0 & 0.1 \end{bmatrix}$

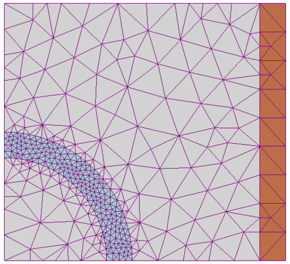
- To calculate the stress, convert to a strain vector and multiply by C matrix
- The stress in the center is zero
- On the outer edge
    - $\sigma_{rr} = 0.2*314.2 + 0.1*165.5 = 79.4$ GPa
    - $\sigma_{\theta\theta} = 0.1*314.2 + 0.2*165.5 = 64.52$ GPa

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







Quiz question: Which numerical method is most often used to solve the mechanics equations?

a) Finite Difference
b) Finite Element
c) Finite Volume
d) Spectral methods

Attempts: 39 out of 39

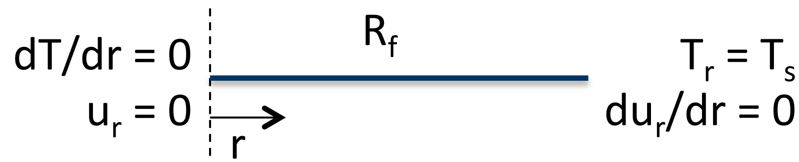
+0.48

Discrimination Index

Which numerical method is most often used to solve the mechanics equations?

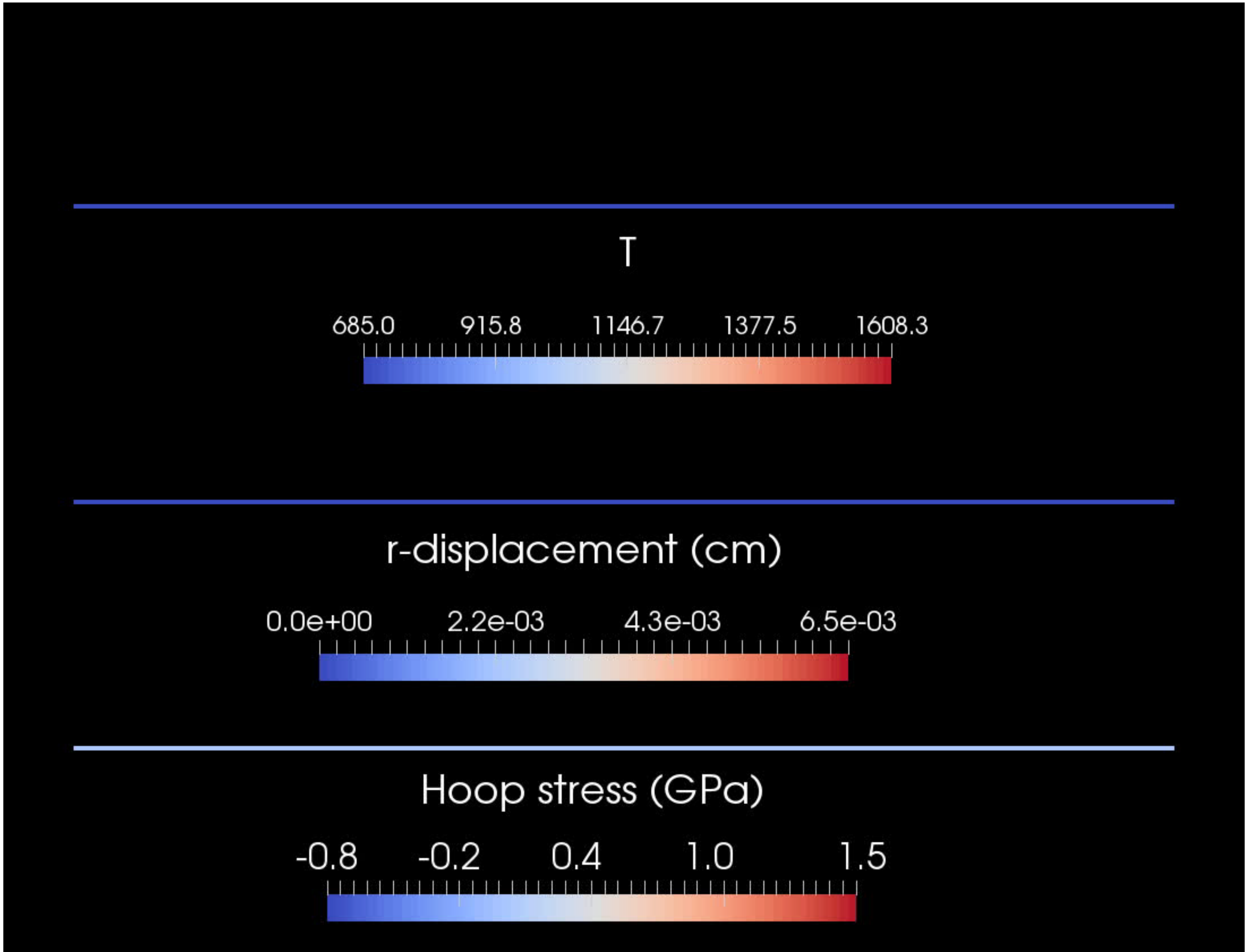
Finite Difference	6 respondents	15 %
Finite Element	32 respondents	82 % ✓
Finite Volume	1 respondents	3 %
Spectral methods		0 %

The 1D thermomechanics problem definition

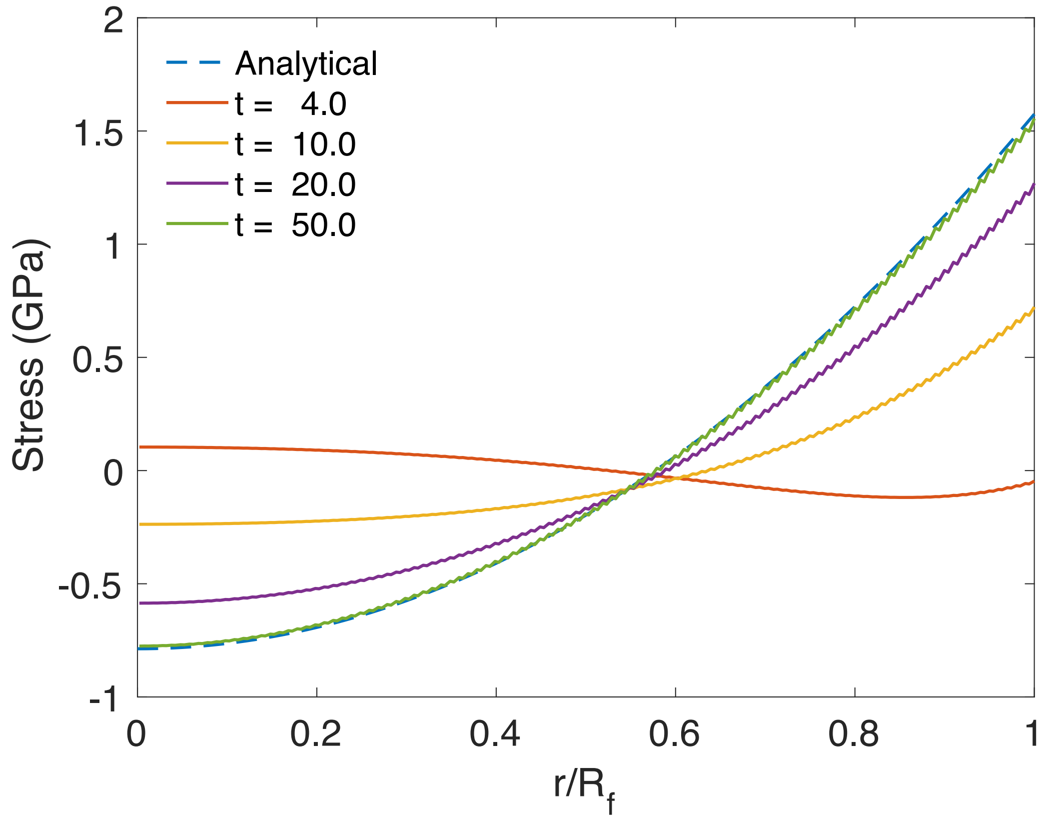


- The initial temperature is set to 273 K
- We will take 50 time steps of 0.5 s
- The full power of Q = 450 begins at time t = 0.
- UO_2 material properties are used for both the thermal and mechanics equations

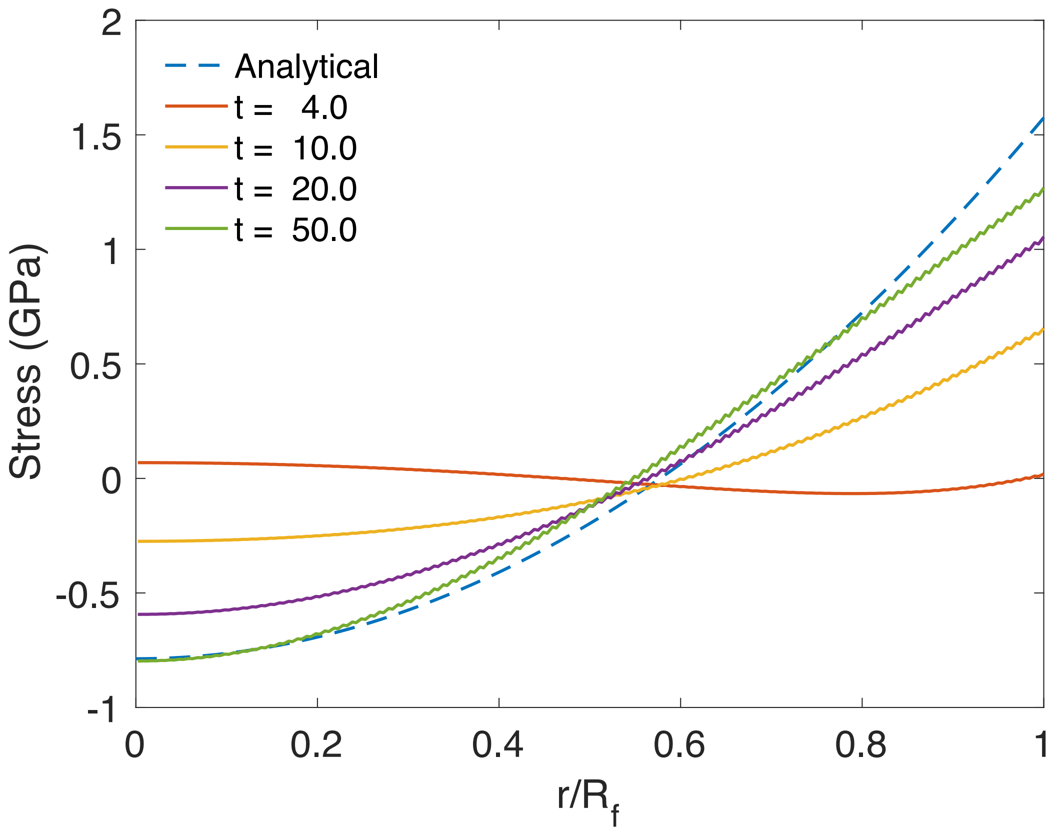
1D thermomechanics simulation of the fuel rod radius



When we use a constant k, the analytical theory matches very well



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



Summary

- The impact of thermal expansion on the gap can be accounted for using the analytical equations, but it requires an iterative solution
- With axisymmetry, the hoop stress is still calculated even in a 2D or 1D solution
- The thermomechanics equations are typically solved using FEM
- The analytical solution for the stress in a fuel pellet is exact in 1D when k is constant

Life Lessons: What do you do with different degrees

- This is a bit of review to start and is a large generalization
- Bachelors degrees get the basic work done
  - Plant operators
  - Part designers/drafters
- Masters degrees improve and inspect things
  - Reactor physics analysts
  - Finite element analyst
  - Design or improve an assembly
  - Inspectors
  - Team leaders/low level managers
- Ph.D.s primarily focus on research and development (R&D)

So, what is R&D?

- As I have said, a Ph.D. enables you to do R&D work
- R&D stands for research and development
- You will also see
  - R&D&C – research, development, and commercialization
  - R&D&I – research, development, and innovation

What is research?

- The process of finding out something we (everyone) don't already know
- A process, not an end state – that's why we keep doing it
- Finding out something – research results in **new knowledge**
- Examples:
    - Discovering a new type of material
    - Learning a new way to cut material
    - Learning how to run programs faster on a supercomputer

What is development?

- Taking knowledge we possess (obtained by research) and making it useful
- Developing an artifact—a device, a product, a system, a process, an algorithm, etc
- Examples include:
  - Optimizing how we make a material
  - Creating an algorithm to solve a given model
  - Reducing the cost to fabricate a fuel cell

Who funds R&D?

- National Science Foundation (NSF) – Funds research but cannot fund development
- Industry – Funds development and more rarely funds research
- Other government programs – Funds research and some development
  - Small business grants
  - Basic energy science
  - Office of nuclear energy
  - NRC
  - EPRI

Where do you have to work to do R&D?

- Industry
  - Development and some research funded by your company
  - R&D funded by the government (small business grants)
- National laboratory
  - Research funded by office of basic energy science (BES)
  - R&D funded by other government programs
- Universities
  - Research funded by NSF
  - Research funded by BES
  - R&D funded by government programs
  - R&D funded by industry