PennState
College of Engineering

NucE 497: Reactor Fuel Performance

Lecture 8: Numerical solution of the fuel temperature profile

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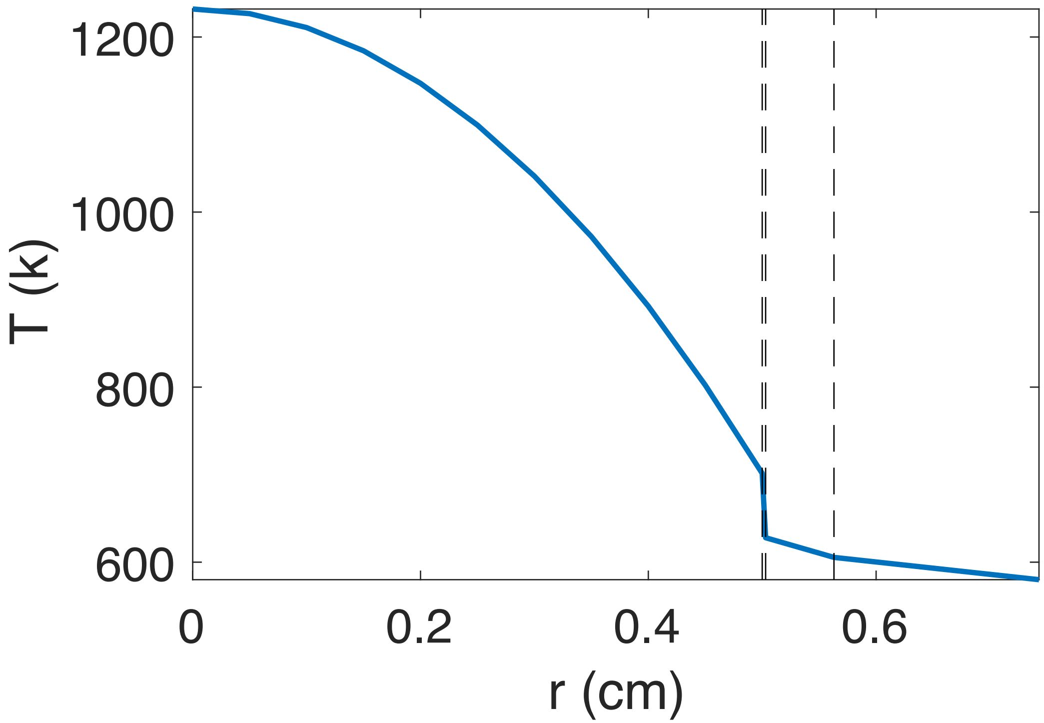
Today we will begin our discussion of heat transport in the fuel

- Module 1: Fuel basics
- Module 2: Heat transport
  - Intro to heat transport and the heat equation
  - Analytical solution of the heat equation
  - **Numerical solution of the heat equation**
  - 1D solution of the heat equation using Matlab
  - 2D solution of the heat equation using Matlab
  - Coolant temperature change, power generation, and melting
- Module 3: Mechanical behavior
- Module 4: Materials issues in the fuel
- Module 5: Materials issues in the cladding
- Module 6: Accidents, used fuel, and fuel cycle

Let’s review some from last time:

- What is NOT an assumption we made to allow for an analytical model of the temperature profile?
  - The geometry is axisymmetric
  - The thermal conductivity is constant
  - There is no axial variation in the temperature
  - The solution is steady state
  - None of the above
- Which statement is true
  - The temperature in the fuel pellet varies linearly with radius
  - The temperature in the cladding is quadratic with radius
  - The temperature changes more across the gap than across the cladding
  - The temperature in the gap is quadratic with the radius

And here is a little more review



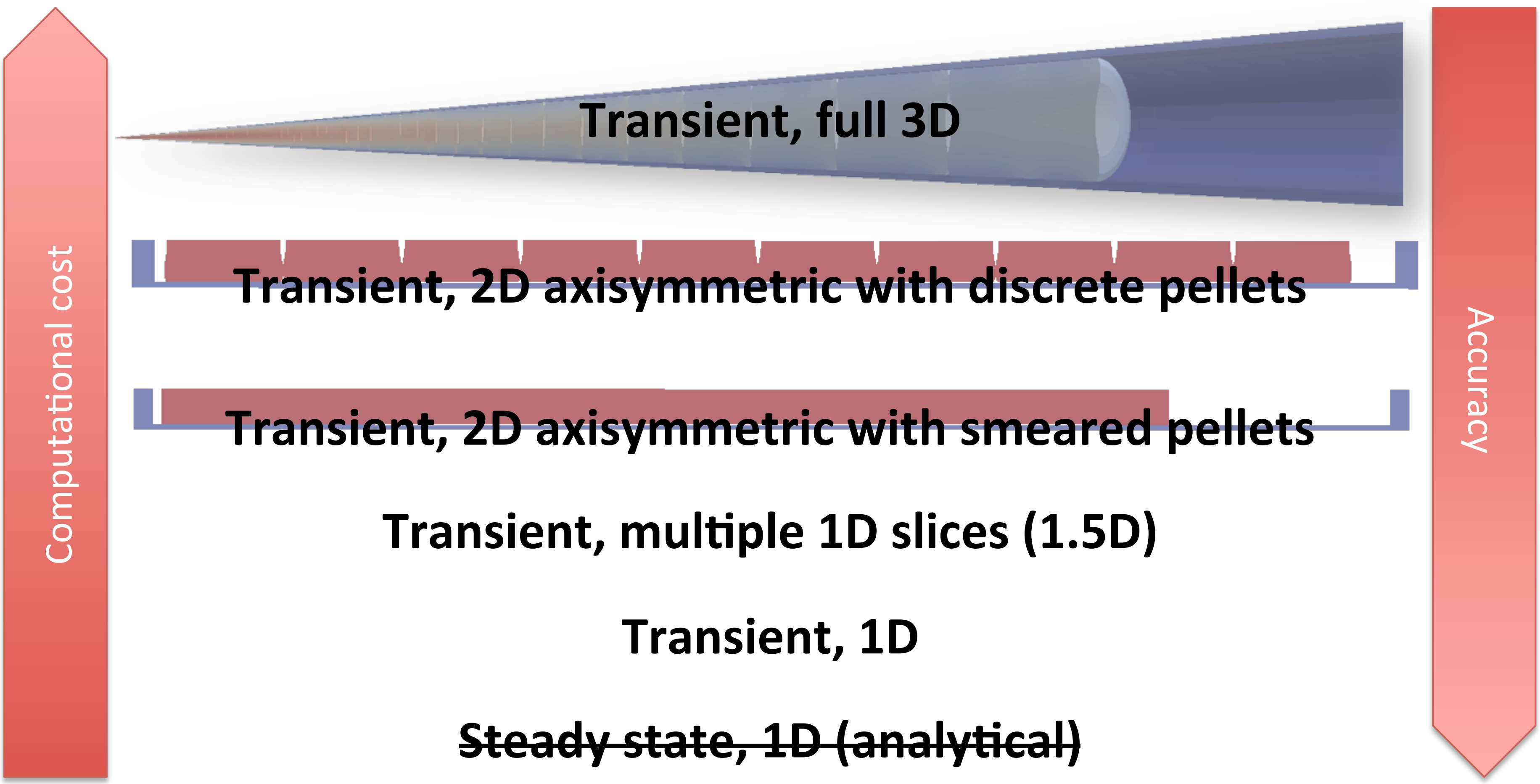
$$T_0 - T_s = \frac{LHR}{4\pi k}$$

$$T_s - T_{IC} = \frac{LHR}{2\pi R_f h_{gap}}$$

$$T_{IC} - T_{OC} = \frac{LHR\, t_C}{2\pi R_f k_C}$$

$$T_{CO} - T_{cool} = \frac{LHR}{2\pi R_f h_{cool}}$$

We’ve talked about the analytical solution, today we will learn how to do the other solutions



We will begin by making two assumptions

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

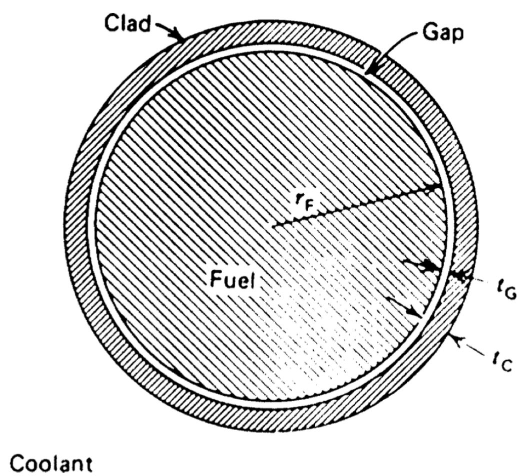
- *Assumption 1:* The behavior is axisymmetric

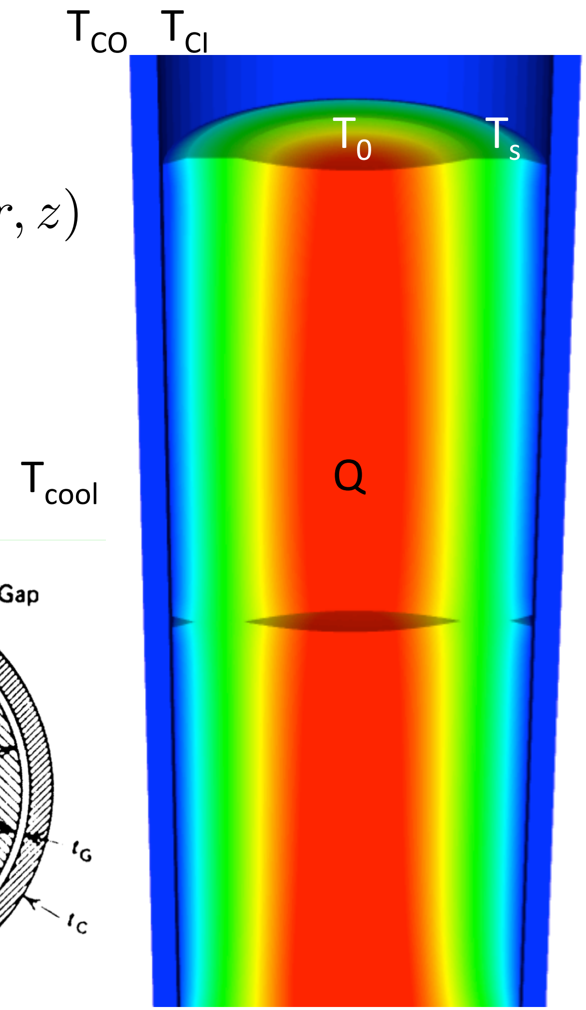
$$\rho c_p \frac{\partial T}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(r k(T) \frac{\partial T}{\partial r}\right) + \frac{\partial}{\partial z}\left(k(T) \frac{\partial T}{\partial z}\right) + Q(r,z)$$

- *Assumption 2: T is constant in z*

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

- **This equation cannot be solved analytically**



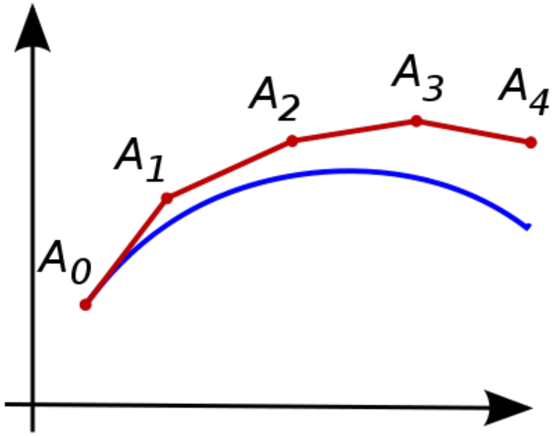


For the numerical solution, we have to handle the derivatives in time and space

- Derivatives in time
  - Forward Euler's method (explicit)
  - Backward Euler's method (implicit)
- Derivatives in space
  - Finite difference
  - Finite volume
  - Finite element

We can compute numerical time derivatives using forward Euler's method

- We march through time, dividing the total time into steps of size dt



- The equation to approximate the derivative comes from a Taylor expansion

$$y(x_0 + h) = y(x_0) + hy'(x_0) + \frac{1}{2}h^2 y''(x_0) + O(h^3) + \ldots$$

- This leads to the equation

$$\frac{\partial T(r,t)}{\partial t} = \dot{T}(r,t) = \frac{T(r,t+dt) - T(r,t)}{dt}$$

We can compute numerical derivatives using forward Euler's method

- We solve for T(r,t + dt) to get

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

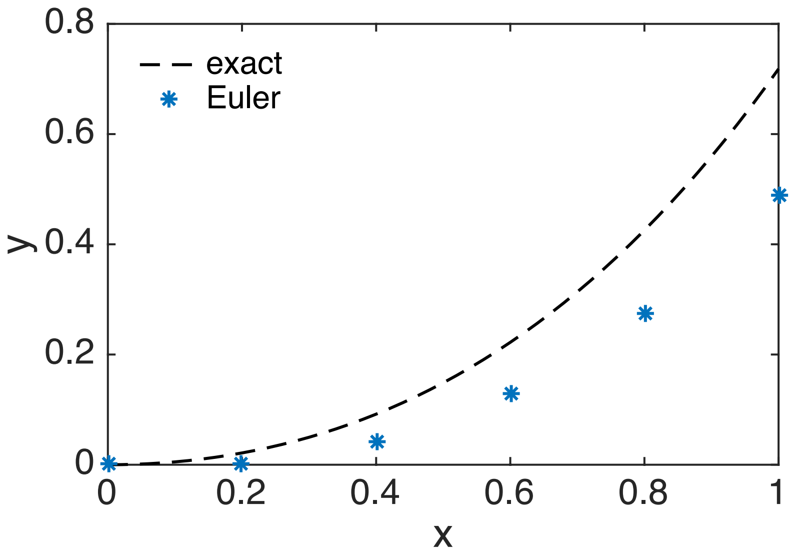
- This is the forward Euler's method and it is **explicit**.

INPUT: Initial values x_0, y_0, step size dx, number of steps N

```
y(0) = y0 #initialize y
x_1 = x_0 + dx

For n = 0, …, N - 1
    y' = f(x_n, y_n) #Calculate derivative at previous step
    y_{n+1} = y_n + dx y' #Find y value at this step
    x_{n+1} = x_n + dx #take next step
end
```

$$y' = y + x$$

$$y_{n+1} = y_n + dx(y + x)$$



Explicit Methods vs Implicit Methods

- Forward Euler's method is **explicit**

Explicit methods calculate the state of a system at a later time from the state of the system at the current time

- Explicit methods can be unstable if the step size is too big.
- This can make explicit methods EXPENSIVE

Implicit methods find a solution by solving an equation involving both the current state of the system and the later one

We can also solve the heat equation using backward Euler's method, which is implicit

- The backward Euler equation is

$$T(r,t+dt) = T(r,t) + dt\,\dot{T}(r,t+dt)$$

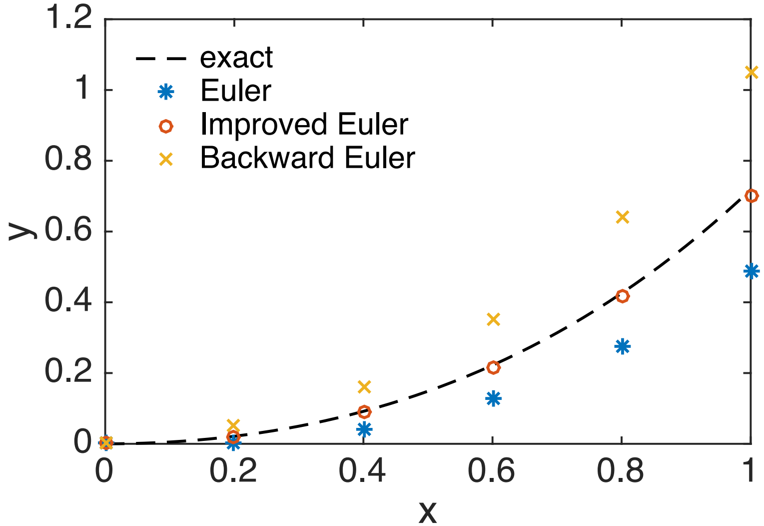
$$\dot{T}(r,t+dt) = \frac{1}{\rho c_p}\frac{1}{r}\frac{\partial}{\partial r}\left(r\,k(T)\frac{\partial T(r,t+dt)}{\partial r}\right) + \frac{1}{\rho c_p}Q(r)$$

INPUT: Initial values x_0, y_0, step size dx, number of steps N

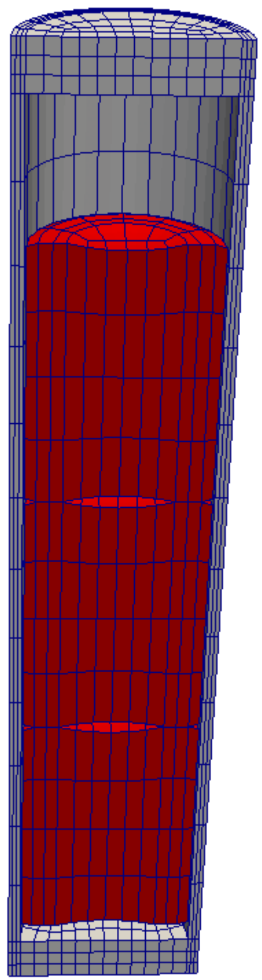
```
y(0) = y0 #initialize y
x_1 = x_0 + dx

For n = 0, …, N – 1
    #Find y at this step
    Solve: R = -y_{n+1} + y_n + dx f(x_{n+1}, y_{n+1}) = 0

    x_{n+1} = x_n + dx #take next step
end
```

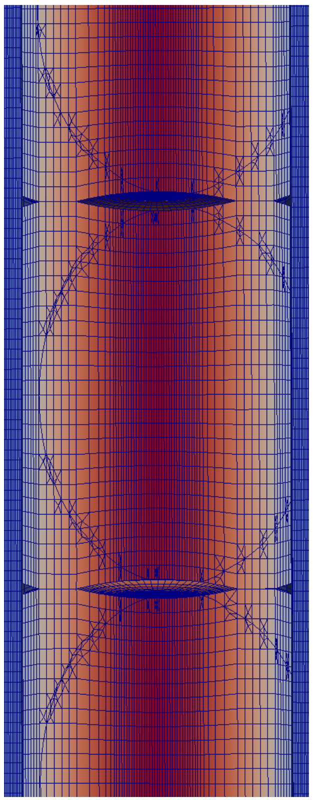
$$y' = y + x$$

$$y_{n+1} = y_n + dx(y + x)$$



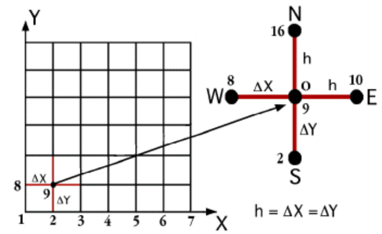
To numerically solve the derivatives in space, we divide up the domain into small sections



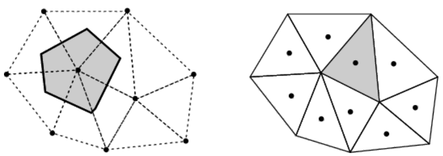


There are three primary numerical methods for obtaining the spatial derivatives in our problem

Finite Difference Method

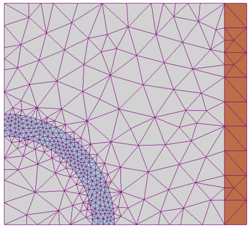


Finite Volume Method



Each of these methods are regularly used to solve the heat equation

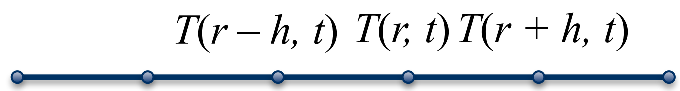
Finite Element Method



Each method has advantages and disadvantages

- Finite Difference
  - Advantages
    - Simple
    - Easy to code
  - Disadvantages
    - Difficult to model complex geometries
    - Difficult to model complex BCs
    - Only represents solution at points
    - Difficult to represent heterogeneous properties
    - No guarantee of convergence
- Finite Element
  - Advantages
    - Can model any geometry
    - Can model any BC
    - Continuous representation
    - Heterogeneous properties
  - Disadvantages
    - Complicated
    - Somewhat more expensive
- Finite Volume
  - Advantages
    - Can model any geometry
    - Naturally conservative
    - Heterogeneous properties
  - Disadvantages
    - Boundary conditions add complexity
    - More complicated than finite difference

The finite difference method solves on a grid and uses numerical derivatives



$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{1}{6}h^2 f'''(x) + \ldots$$

$$f''(x) = \frac{1}{h^2}\left(f(x+h) + f(x-h) - 2f(x)\right) + \ldots$$

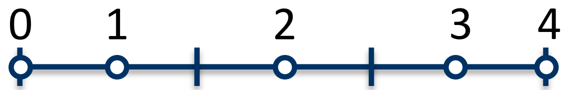
$$\dot{T}(r,T) = \frac{1}{\rho\, c_p}\frac{1}{r}\frac{\partial}{\partial r}\left(rk(T)\frac{\partial T(r,T)}{\partial r}\right) + \frac{1}{\rho\, c_p}Q(r)$$

$$q = rk(T)\frac{\partial T(r,t)}{\partial r} = \frac{rk(T(r,t))}{2h}\left(T(r+h,t) - T(r-h,t)\right)$$

$$\dot{T}(r,t) = \frac{1}{\rho c_p}\frac{1}{r}\frac{\partial q}{\partial r} + \frac{1}{\rho c_p}Q(r) = \frac{1}{\rho c_p}\frac{1}{2h\, r}\left(q(r+h,t) - q(r-h,t)\right) + \frac{1}{\rho c_p}Q(r)$$

- Once you compute the time derivative, you can use either forward or backward Euler to march through time
- Boundary conditions must have either a fixed T or dT/dr

The finite volume method balances fluxes across the boundaries of your divided subdomains



$$\frac{d}{dx}k\frac{dT}{dx} + q = 0$$

1. Discretize the domain by subdomains
   - Domain size h = 1
   - We place points in the subdomain centers and on either boundary
2. Integrate our PDE across the subdomain

$$\int_a^{a+h} \frac{d}{dx}k\frac{dT}{dx} + q\ dx = 0$$

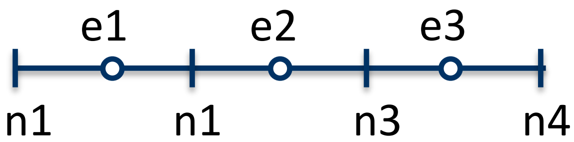
$$k\frac{dT}{dx}\bigg|_{a+h} - k\frac{dT}{dx}\bigg|_{a} + qh = 0$$

3. Evaluate the integral using a linear approximation of the variable

$$\frac{T_{i+1} - T_i}{h_2} - \frac{T_i - T_{i-1}}{h_1} + q\frac{h_2}{k} = 0$$

$$T_i = \frac{h_1 h_2}{h_1 + h_2}\left(\frac{T_{i+1}}{h_2} + \frac{T_{i-1}}{h_1} + q\frac{h_2}{k}\right)$$

In the finite element method, we interpolate the variable using nodal values and integrate over elements



$$T(r,t) = \sum_n T_n(t)\phi_n(r)$$

Where ϕ_n are basis functions

- The equation is put in residual form

$$0 = \rho c_p \dot{T}(r,t) - \frac{1}{r}\frac{\partial}{\partial r}\left(rk(T)\frac{\partial T(r,t)}{r}\right) - Q(r)$$

- Then, we effectively average the equation over the volume (using integration), and only force it to be true for the entire body. This is called the **weak form**.
- The volume integral is carried out using numerical integration (Gaussian quadrature) in each element
- Finite element works for any geometry and any boundary condition

These numerical approaches can also be used with less assumptions

Computational cost

Accuracy

Transient, full 3D

FEM or FV

Transient, 2D axisymmetric with discrete pellets

FEM or FV

Transient, 2D axisymmetric with smeared pellets

FEM, FV, or FD

Transient, multiple 1D slices (1.5D)

FEM, FV, or FD

Transient, 1D

FEM, FV, or FD

~~Steady state, 1D (analytical)~~

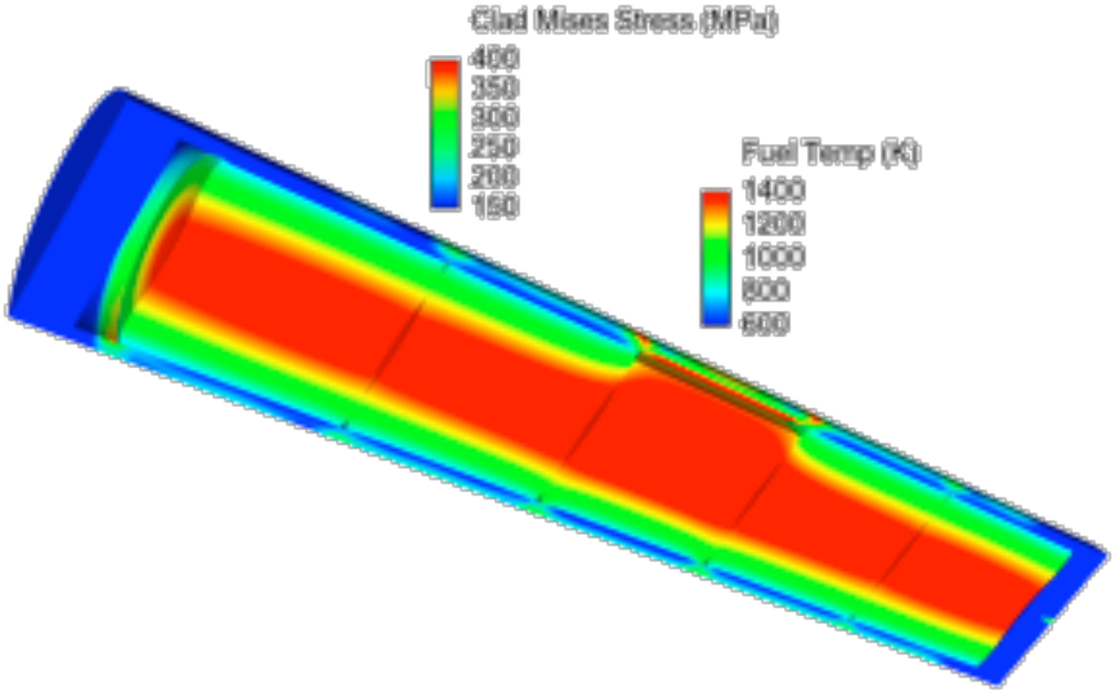
Heat equation solution approach summary

Approach	Solution	Assumptions
1D steady state	Analytical	Steady state, axisymmetric, no axial variation, constant k
1D transient	FEM, FD, FV	Axisymmetric, no axial variation
1.5D transient	FEM, FD, FV with multiple slices	Axisymmetric, no axial variation
2D transient, smeared pellets	FEM, FD, FV	Axisymmetric, fuel pellets act as one body, fuel pellets are perfect cylinders
2D transient, discrete pellets	FEM, FV	Axisymmetric
3D transient	FEM, FV	You have a big computer

Note that each numerical solution could be done implicit or explicit

Fuel performance codes primarily use either finite difference or finite element

- The earliest fuel performance codes solved the heat equation in 1.5D using finite difference (with multiple axial slices)
- More modern codes have switched to finite element, due to more flexibility with geometry and boundary conditions
- Finite volume is not used because it can't solve for the stress



For the next two class periods, I will show you how to solve the heat equation with finite element in Matlab

Summary

- The heat equation can be solved using numerical methods.
- Numerical solution methods are needed for time derivative and gradients.
- Time derivative solution methods march through time in steps and can be
  - Implicit
  - Explicit
- Spatial derivative solution methods divide the domain up into smaller pieces
  - Finite difference
  - Finite volume
  - Finite element