Fuel Performance

NE 533: Spring 2023

Last Time

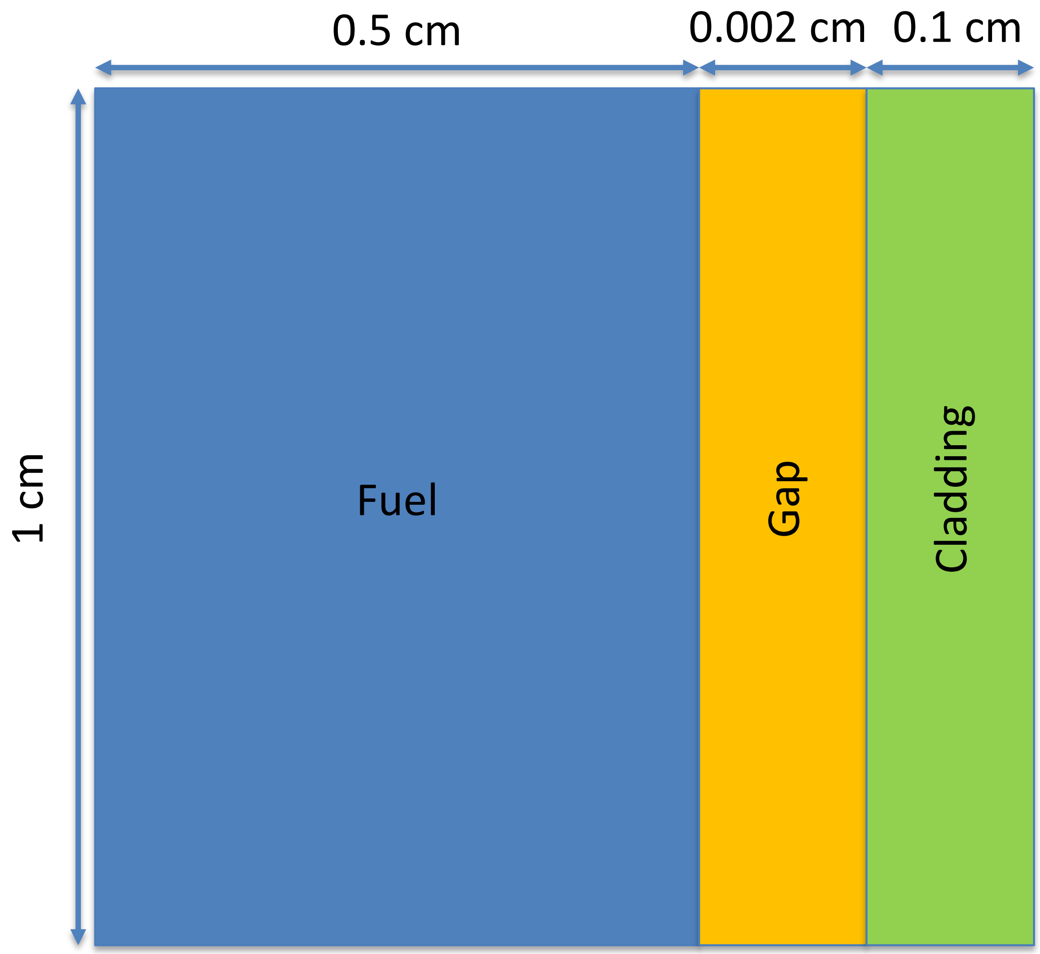
- Had an exam…
- Any feedback?

MOOSE Project

- Three-part project
- Will upload input and output files to Moodle
- Will upload a final written report, 5-10 pages (including figures), times new roman, 12pt, 1.5 space, pdf
- Final report is due April 21 – Friday last week of classes
- This is an individual project, but some collaboration is encouraged
- Part 1 is due Feb 24
  - just input/output submitted to moodle; 1 page report outlining results
  - don’t wait until the last minute to do this! ask questions

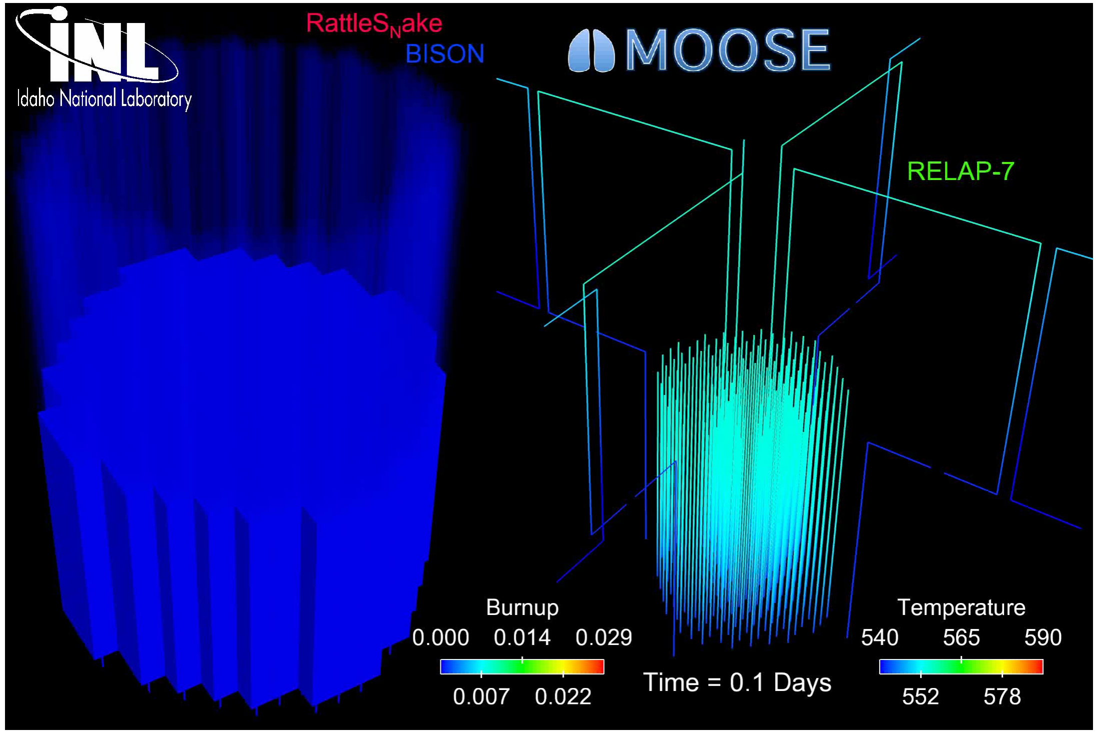
MOOSE Project Part 1

- Fuel pellet dimensions listed
- This is a 1-D problem, but I want your geometry to be set up in 2-D RZ
- Assume reasonable values for material properties
- Can assume constant k
- Outer cladding temperature: 600 K
- Mesh: something sufficiently converged
- Solve temperature profile for:
    - Steady-state: LHR = 350 W/cm^2
    - Compare against analytical solution
- Solve for centerline temperature vs time
    - Transient: LHR = 500*[(t/100)^0.5]*[(1-(t/100))^4] + 150
    - for up to t=100



The most accurate solution is numerical, in 3D, requires modeling the entire core, and is multi-physics

- Solution is 3D and changes in time
- All the properties are functions of temperature
- The boundary conditions comes from information about the coolant flow
- The heat generation rate comes from information about the neutronics in the reactor
- No analytical solution is possible



NUMERICAL TIME INTEGRATION

For numerical solutions, deal with discretization in space/time

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

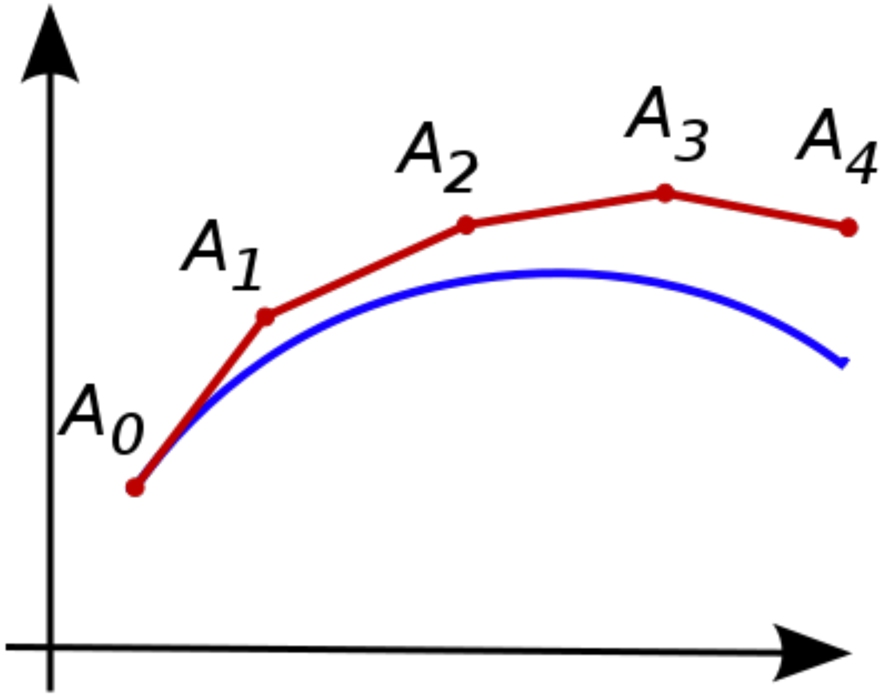
$$\rho c_p \frac{\partial T}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(rk\frac{\partial T}{\partial r}\right) + Q$$

Forward Euler

- Step forward through time in increments, dt
- The Euler method is a first-order method, which means that the local error (error per step) is proportional to the square of the step size
- Expand a function y(t), with a timestep size, h

$$y(t_0 + h) = y(t_0) + h\, y'(t_0) + \frac{1}{2}h^2 y''(t_0) + \cdots$$

- Euler takes only the first derivative
- $y_{n+1} = y_n + hy'(t)$
- Value y_n is an approximation of the solution to the ODE at time t_n



Forward Euler

- Applying to our temperature system

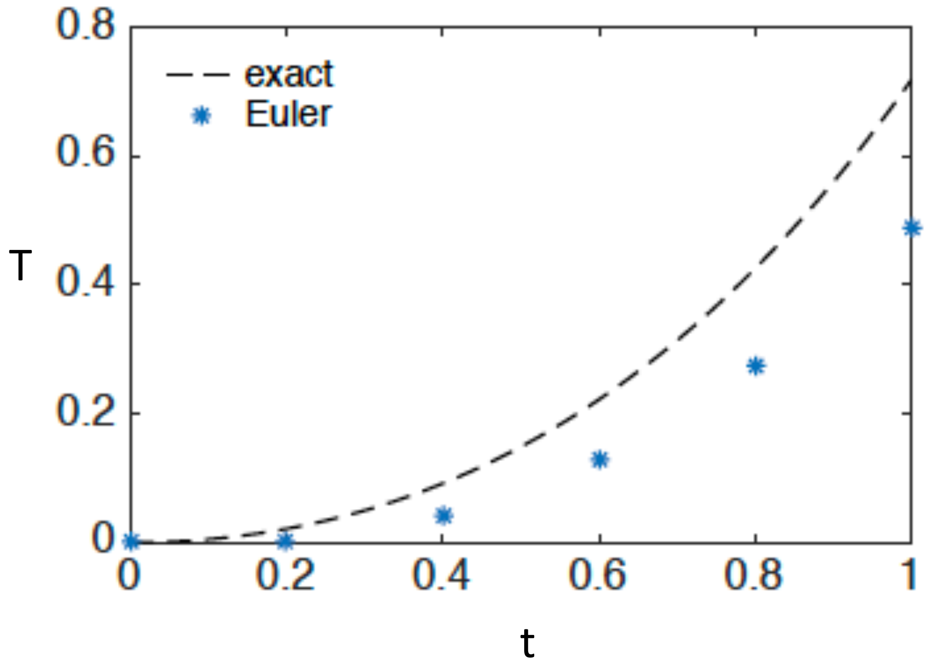
$$T(r, t + dt) = T(r, t) + dt\,\frac{\partial T(r,t)}{\partial t}$$

- Using the heat conduction equation:

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

- We input T_0, which here is T @ t=0, step size dt

$$T_{n+1} = T_n + dt{*}T'; \; t_{n+1} = t_n + dt$$



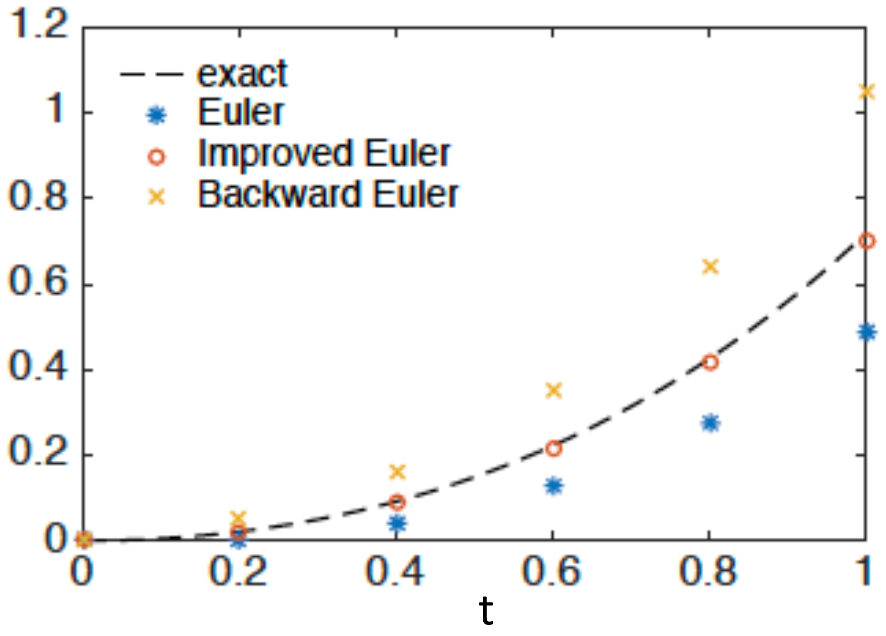
Backwards Euler

- Backwards Euler for a function T(r,t)

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

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

- This differs from Forward Euler in that here we use (r,t+dt), instead of (r,t)
- $T_{n+1} = T_n + dt\, T'(r,t+dt)$, $t_{n+1} = t_n + dt$
- The new approximation appears on both sides of the equation, thus this method needs to solve an algebraic equation for the unknown future state
- This can be done with fixed-point iteration or non-linear solvers
- Improved Euler is a form of explicit Euler (explicit trapezoidal rule), which takes the derivative at the midpoint



Explicit vs Implicit

- Forward Euler is explicit
  - Explicit methods calculate the state of a system at a later time from the state of the system at the current time
  - Can be unstable if step size is too much
- Backwards Euler is implicit
  - Implicit methods find a solution by solving an equation involving both the current state of the system and a later state
  - Implicit require an extra computation and they can be much harder to implement
  - Implicit methods are used because many problems arising in practice are stiff, for which the use of an explicit method requires very small timesteps

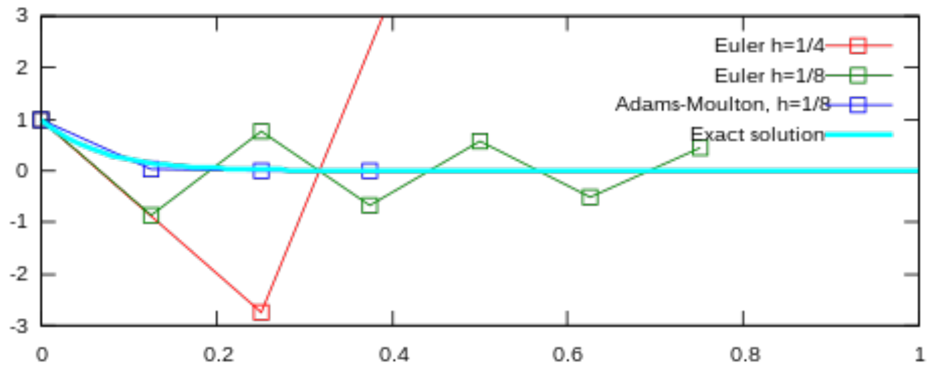
Stiff Equations

- A stiff equation is a differential equation for which certain numerical methods for solving the equation are numerically unstable, unless the step size is taken to be extremely small
- Consider the problem:

$$y'(t) = -15y(t), \quad t \geq 0, \quad y(0) = 1.$$

- Where the exact solution is:

$$y(t) = e^{-15t}, \quad y(t) \to 0 \text{ as } t \to \infty.$$



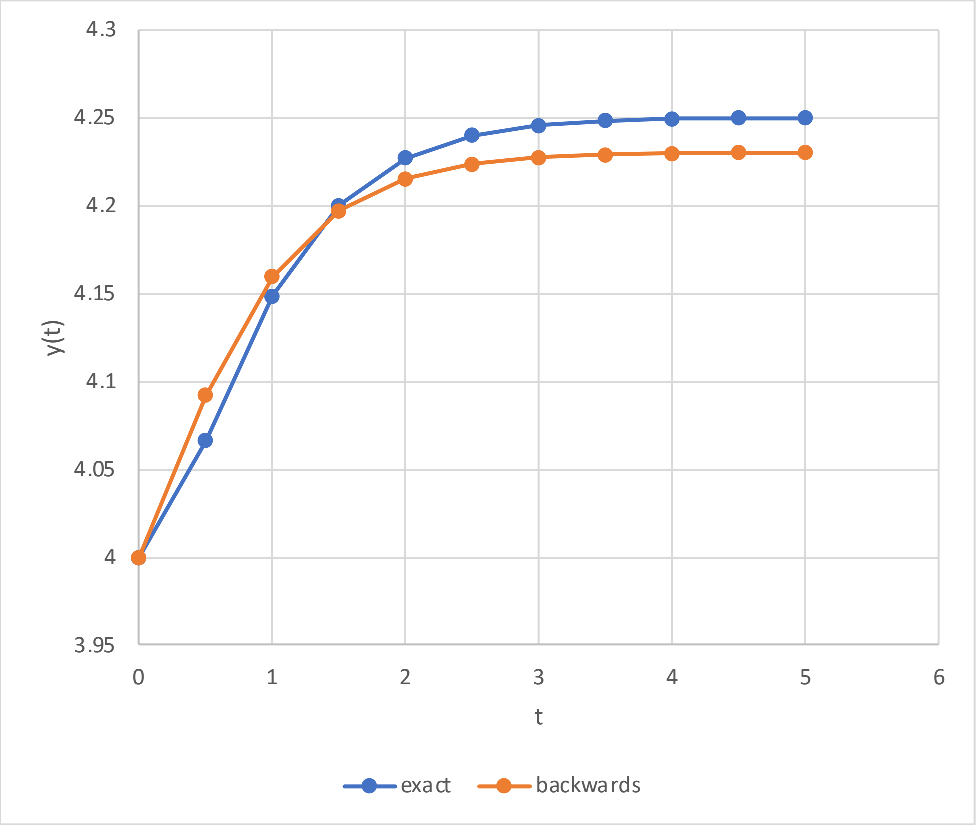
- Euler's method with a step size of h=1/4 oscillates wildly
- Euler's method with half the step size, h=/18, produces a solution within the graph boundaries, but oscillates about zero
- The trapezoidal method (similar to backwards Euler) is implicit, and converges to the correct solution

$$y_{n+1} = y_n + \tfrac{1}{2}h\big(f(t_n, y_n) + f(t_{n+1}, y_{n+1})\big),$$

Example Problem

Example Problem

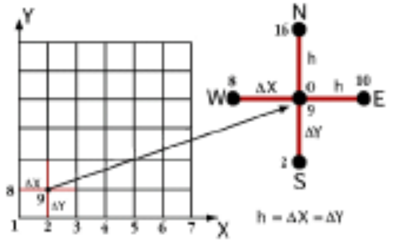
- y'=t*exp(-2t)
- y0=4
- dt=0.5
- Backwards Euler

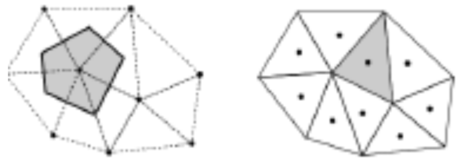


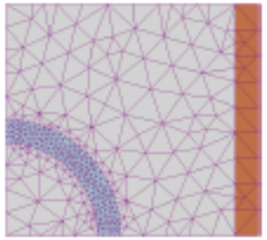
SPATIAL DISCRETIZATION

Spatial resolution

- To numerically solve in space, we need to discretize
  - Finite difference
    - convert differential equations into a system of equations that can be solved by matrix algebra techniques
  - Finite volume
    - volume integrals in a partial differential equation that contain a divergence term are converted to surface integrals, using the divergence theorem. These terms are then evaluated as fluxes at the surfaces of each finite volume
  - Finite element
    - subdivides a large system into smaller, simpler parts that are called finite elements, the equations that model these finite elements are then assembled into a larger system of equations that models the entire problem



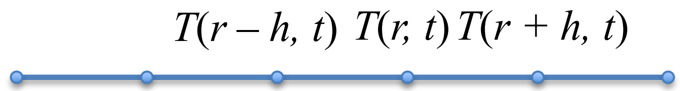




Finite Difference

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

- The finite difference method solves on a grid and uses numerical derivatives
- Derivatives are approximated by differences
- Boundary conditions must have either a fixed T or dT/dr
- Typically restricted to handle rectangular shapes
- Once you compute the time derivative, you can use either forward or backward Euler to march through time



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

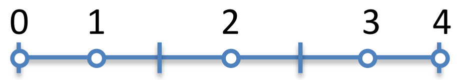
$$q = rk(T)\frac{\partial T(r,t)}{\partial r} = \frac{rk(T(r,t))}{2h}\left(T(r+h,t) - T(r-h,t)\right)$$

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

Finite Volume

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

- Discretize the domain by subdomains
  - Domain size h
  - We place points in the subdomain centers and on either boundary
- The finite volume method balances fluxes across the boundaries of your divided subdomains
- Integrate our PDE across the subdomain
- Evaluate the integral using a linear approximation of the variable
- Restricted to flux boundary conditions, often used in flow-type problems



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

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

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

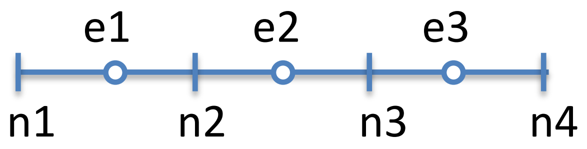
$$\frac{T_{i+1} - T_i}{h_2} - \frac{T_i - T_{i-1}}{h_1} + q\frac{h_2}{k} = 0$$

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

Finite Element

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

- In the finite element method, we interpolate the variable using nodal values and integrate over elements
- Systematically recombine all sets of element equations into a global system of equations for the final calculation
- Write the strong form of the equation, rearrange to get zero on the right-hand side, multiply by the test function, integrate over the domain, yielding weak form
- The **strong form** states conditions that must be met at every material point, whereas **weak form** states conditions that must be met only in an average sense
- Finite element works for any geometry and any boundary condition



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

$$-\nabla \cdot \frac{\mathbf{K}}{\mu}\nabla p = 0 \in \Omega$$

$$\left(\nabla\psi, \frac{\mathbf{K}}{\mu}\nabla p\right) - \left\langle \psi, \frac{\mathbf{K}}{\mu}\nabla p \cdot \hat{n}\right\rangle = 0$$

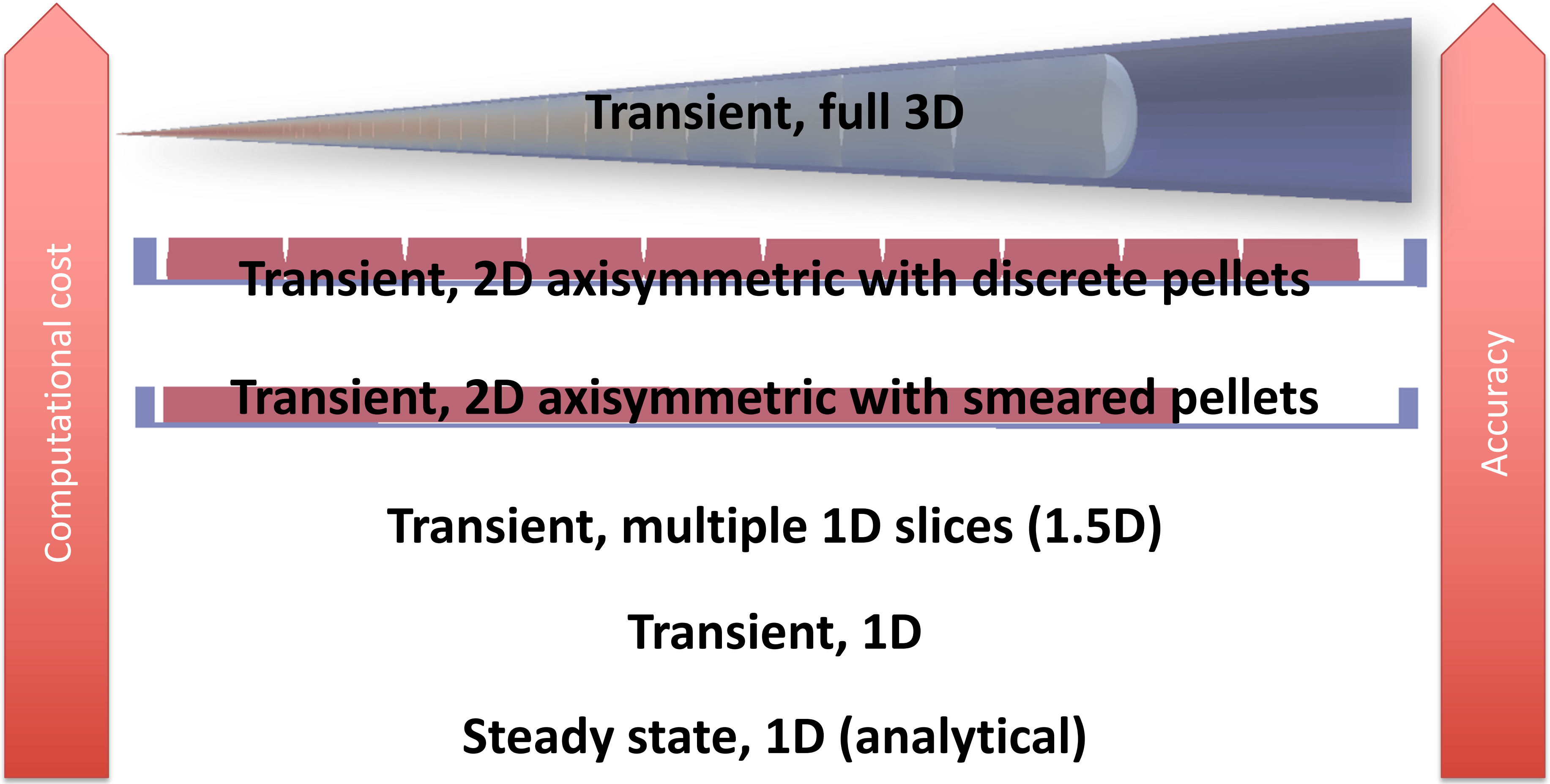
Spatial resolution

- Finite difference
  - Advantages
    - Simple
    - Easy to code
    - Fast
  - Disadvantages
    - Difficult to model complex geometries
    - Difficult to model complex BCs
    - Only represents solution at points
    - Difficult to represent heterogeneous properties

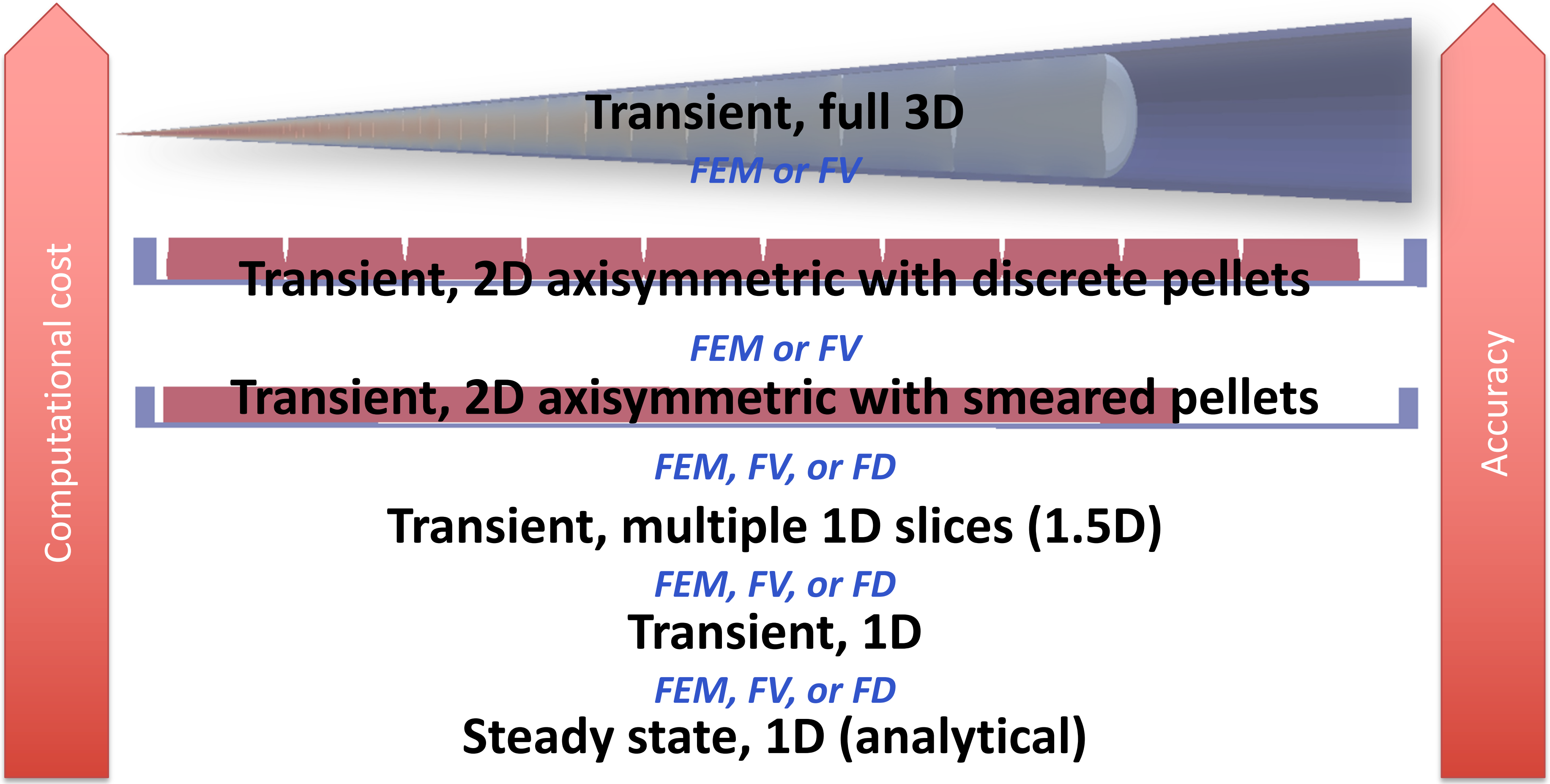
- Finite Volume
  - Advantages
    - Can model any geometry
    - Naturally conservative
    - Heterogeneous properties
  - Disadvantages
    - Boundary conditions add complexity
    - More complicated than finite difference

- Finite Element
  - Advantages
    - Can model any geometry
    - Can model any BC
    - Continuous representation
    - Heterogeneous properties
  - Disadvantages
    - Complicated
    - Somewhat more expensive

Different Fuel Performance Problems



Numerical Approaches to Different Fuel Performance Problems



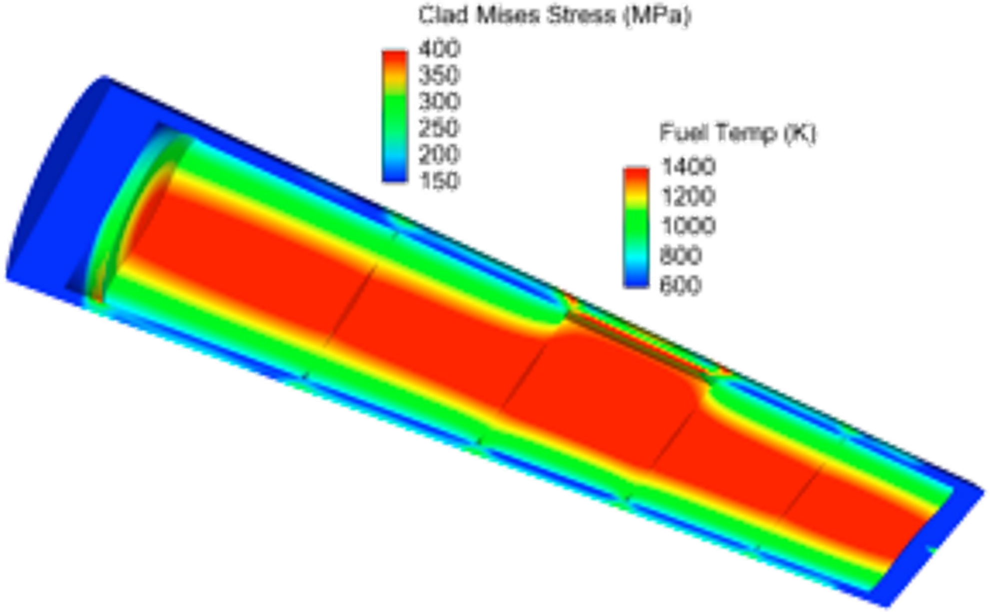
Heat equation solution approach summary

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

Each numerical solution can be solved explicitly or implicitly

Solving with fuel performance codes

- 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 becoming an option



Summary

- The heat equation can be solved using numerical methods.
- Spatial derivative solution methods divide the domain up into smaller pieces
  - Finite difference
  - Finite volume
  - Finite element
- Each discretization has strengths/weaknesses
- Finite element is primary method for high fidelity fuel performance codes

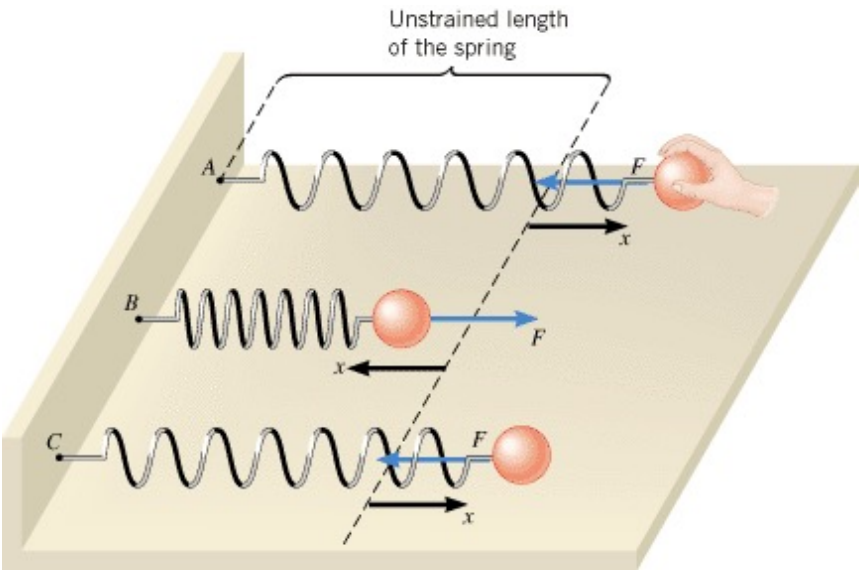
MECHANICS

Solid mechanics

- When a load is applied to a body, it changes shape and perhaps size
- Motions throughout a body are called **displacements**
  - $\mathbf{u}(\mathbf{r}, t)$
- Rigid body displacements do not change the shape and/or size
  - the rigid body is translated
- Changes in shape and/or size are call **deformations**
- The objective of **Solid Mechanics** is to relate loads (applied force) to deformation

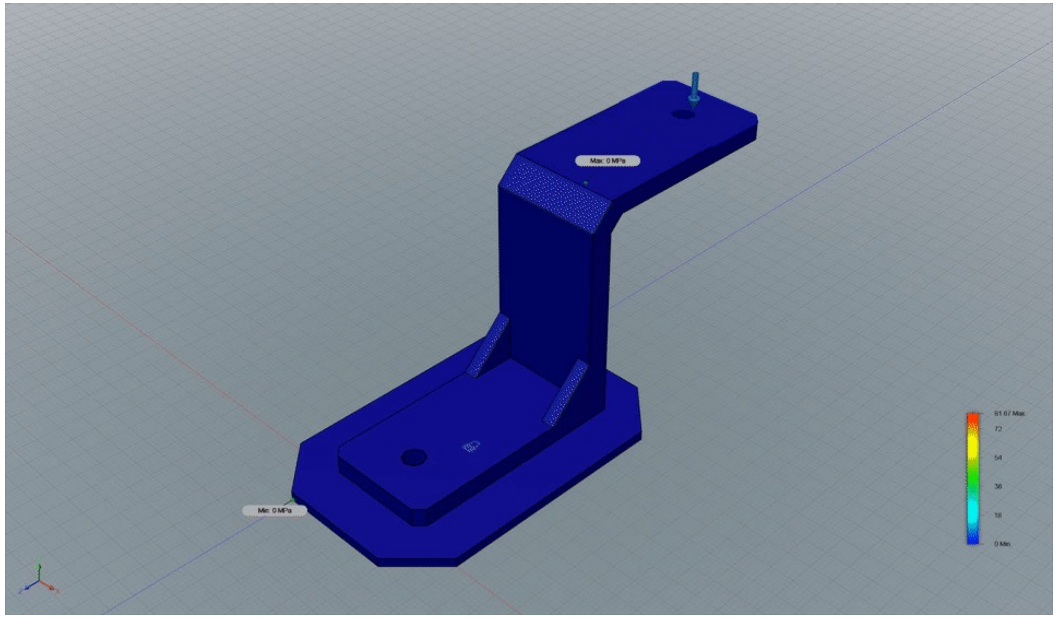
Ideal springs

- It can be instructive to view solids as a spring
- When we apply some force F, we get some displacement x
  - $F = k\,x$
- When the spring is displaced by x, there is force that responds in the opposite direction equal to kx
- Due to the displacement, there is a stored energy $E = ½\,k\,x^2$



Observed deformation due to a force

- Solid mechanics is similar to the behavior of an ideal spring but throughout a body
- An applied load results results in deformation.
- The internal **strain** is like the displacements x
- The internal **stress** is like the internal force F



Elasticity

- Elasticity is the ability of a body to resist a distorting influence and to return to its original size and shape when that influence or force is removed
- In elastic deformation, we are stretching the atomic bonds
- The more we stretch the bonds, the more force it takes to stretch
- When we release the load, the atoms spring back into their lattice sites