

Fuel Performance

NE 591

Last Time

- Developed analytical solutions for temperature profile
- This time, we move from the analytical into the numerical framework
- Parabolic profile of temperature in fuel
- Cosine profile of LHR as a function of z on fuel rod

$$\bullet \quad T_0 - T_{fuel} = \frac{Q}{4k} R_{fuel}^2 \quad T_0 - T_{fuel} = \frac{LHR}{4\pi k}$$

$$\bullet \quad T_{fuel} - T_{gap} = \frac{Q}{2h_{gap}} R_{fuel} \quad T_{fuel} - T_{gap} = \frac{LHR}{2\pi R_{fuel} h_{gap}} \quad h_{gap} = \frac{k_{gap}}{t_{gap}}$$

$$\bullet \quad T_{gap} - T_{clad} = \frac{Q t_{clad}}{2k_{clad}} R_{fuel} \quad T_{gap} - T_{clad} = \frac{LHR t_{clad}}{2\pi R_{fuel} k_{clad}}$$

$$\bullet \quad T_{clad} - T_{cool} = \frac{Q}{2h_{cool}} R_{fuel} \quad T_{clad} - T_{cool} = \frac{LHR}{2\pi R_{fuel} h_{cool}}$$

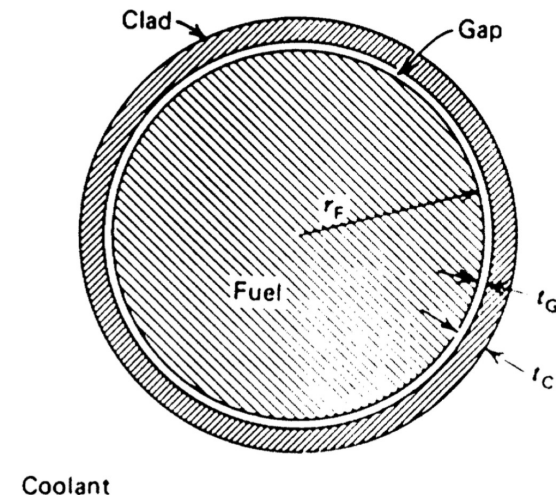
Review of Assumptions

- Analytical solution requires:
 - Steady-state solution
 - Temperature is axisymmetric
 - T is constant in Z
 - Thermal conductivity is independent of temperature
 - Temperature profile in the fuel is parabolic, linear profiles in gap, clad and coolant

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

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

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



Clarifications

- Heat flux is a conserved quantity, described by Fourier's first and second laws:

$$\vec{q} = -\lambda \nabla T,$$

λ = thermal cond.

$$\rho c \frac{\partial T}{\partial t} = \nabla(\lambda \nabla T) + q^*,$$

- If there are no sources of heat, as if the case in the cladding and gap, the temperature field is constant with time and heat flux is unidirectional

$$q = -\lambda \frac{dT(x)}{dx},$$

Clarifications

- For boundary conditions T_1 and T_2 and a thickness d :

$$q = \frac{T_1 - T_2}{\frac{d}{\lambda}} \quad T(x) = T_1 - \frac{T_1 - T_2}{d} x$$

- This assumes a spatially constant thermal conductivity
- Our thin slab assumption sets the thermal conductivity to a single value in the gap and cladding
- We know that thermal conductivity is a function of temperature

$$q = \frac{T_1 - T_2}{R_{eff}^*} \quad R_{eff}^* = \frac{d}{\lambda_{eff}^*}, \quad \lambda_{eff}^* = \lambda(T_{eff}^*) = \frac{\lambda(T_1) + \lambda(T_2)}{2}$$

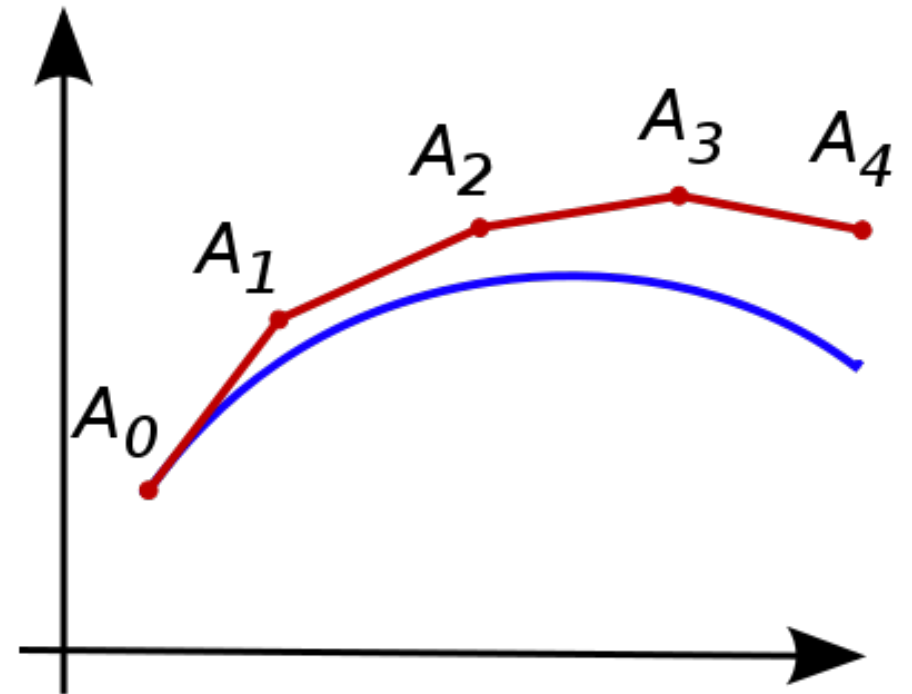
NUMERICAL TIME INTEGRATION

For numerical solutions, deal with derivatives in space/time

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

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
$$y(t_0 + h) = y(t_0) + h y'(t_0) + \frac{1}{2}h^2 y''(t_0) + \dots$$
- Euler takes only the first derivative
- $y_{n+1} = y_n + h y'(t)$
- Value y_n is an approximation of the solution to the ODE at time t_n



Forward Euler

- Applying to our temperature system

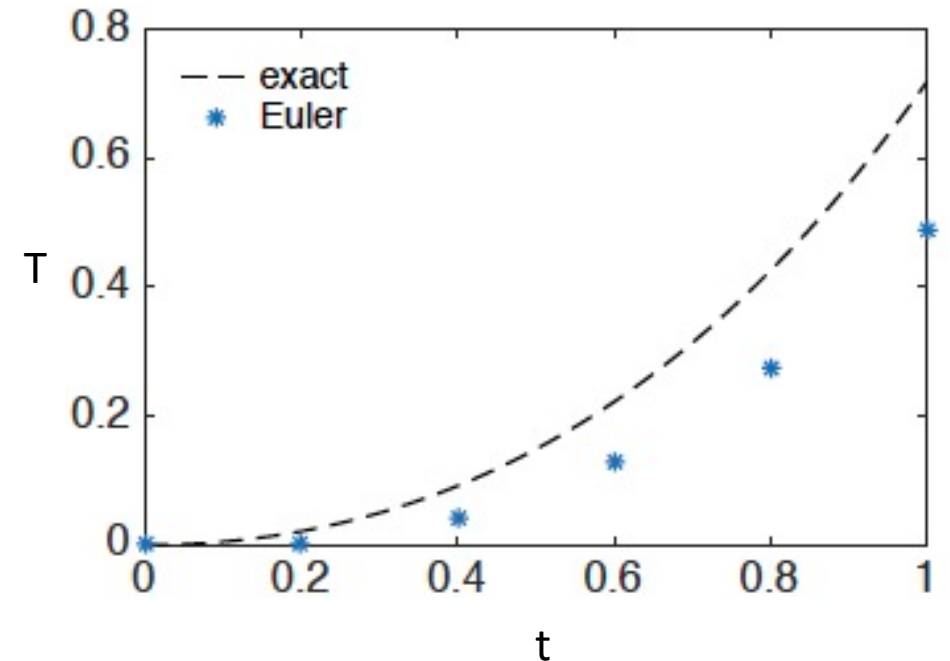
$$T(r, t + dt) = T(r, t) + dt \frac{\partial T(r, t)}{\partial t}$$

- Using the heat conduction equation:

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

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

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

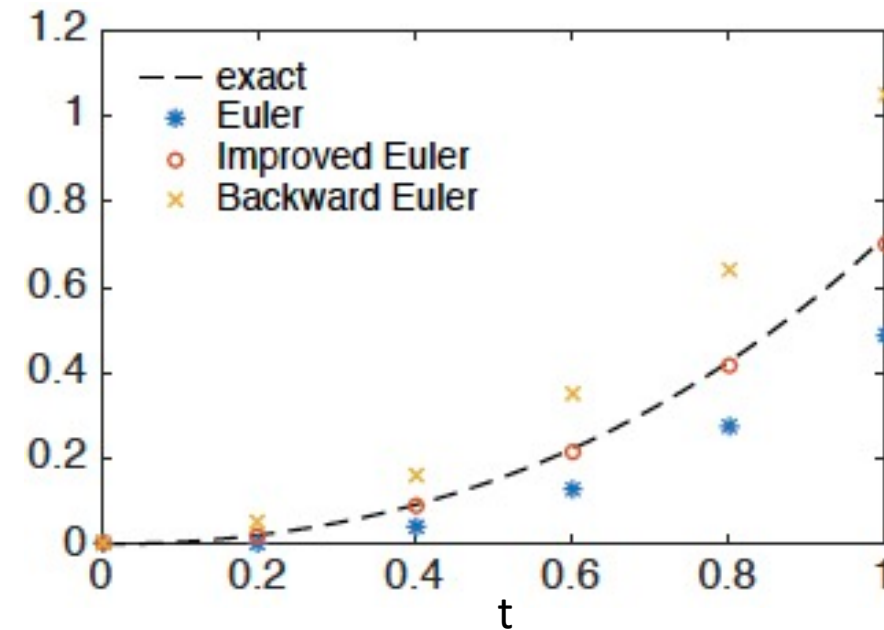


Backwards Euler

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

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

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

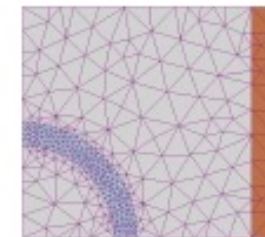
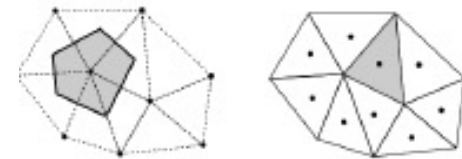
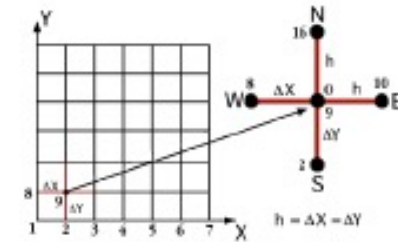
- Forward Euler is explicit
 - Explicit methods calculate the state of a system at a later time from the state of the system at the current time
 - Can be unstable if step size is too much
- Backwards Euler is implicit
 - Implicit methods find a solution by solving an equation involving both the current 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

Example Problem

SPATIAL DISCRETIZATION

Spatial resolution

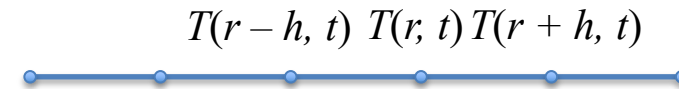
- To numerically solve in space, we need to discretize
 - Finite difference
 - convert differential equations into a system of equations that can be solved by matrix algebra techniques
 - Finite volume
 - volume integrals in a partial differential equation that contain a divergence term are converted 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

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

- 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



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

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

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

Finite Volume

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

- 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



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

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

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

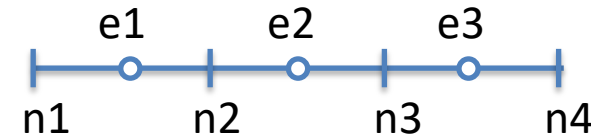
$$\frac{T_{i+1} - T_i}{h_2} - \frac{T_i - T_{i-1}}{h_1} + q \frac{h_2}{k} = 0$$

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

Finite Element

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

- 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



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

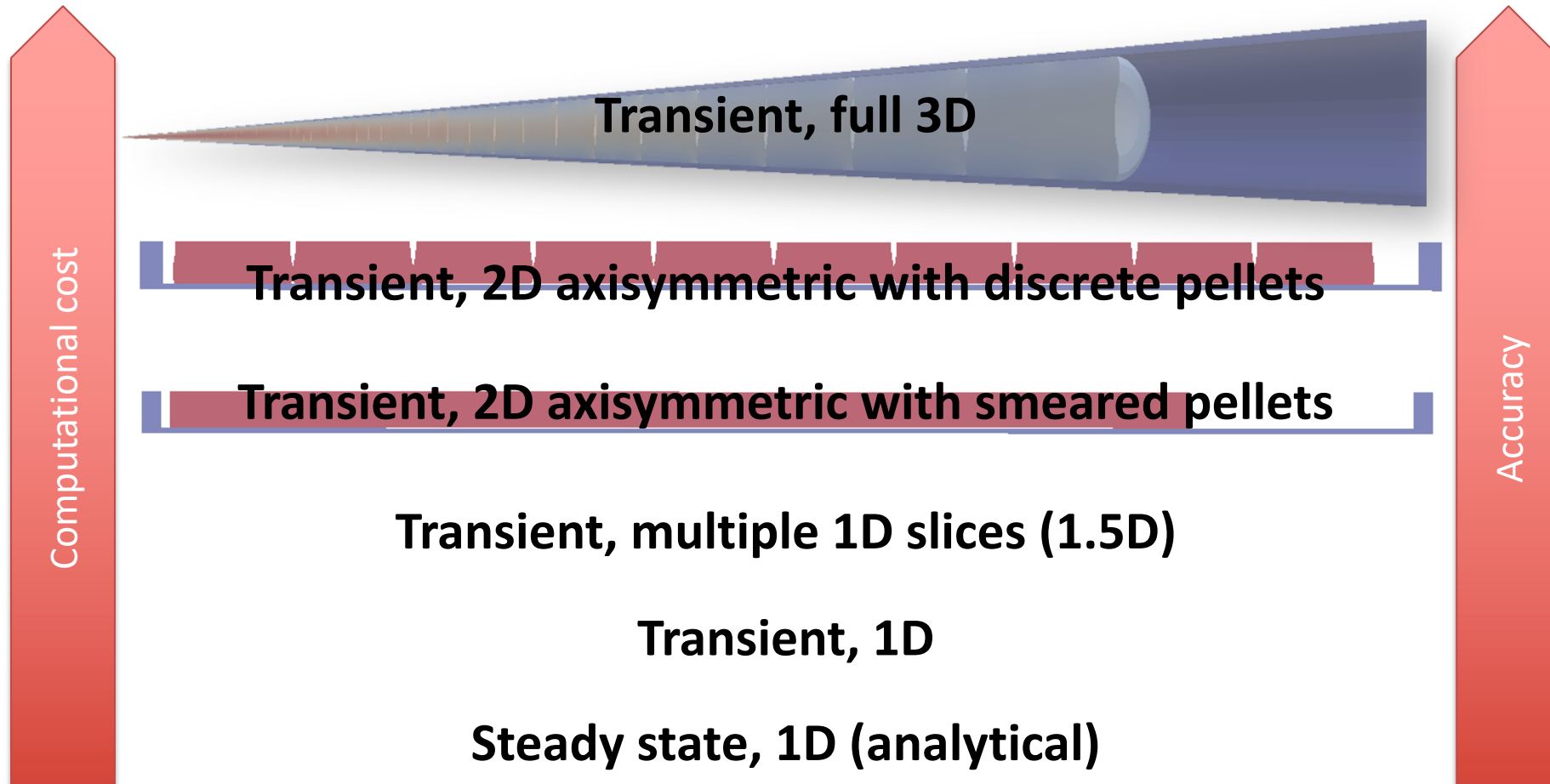
$$-\nabla \cdot \frac{\mathbf{K}}{\mu} \nabla p = 0 \in \Omega$$

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

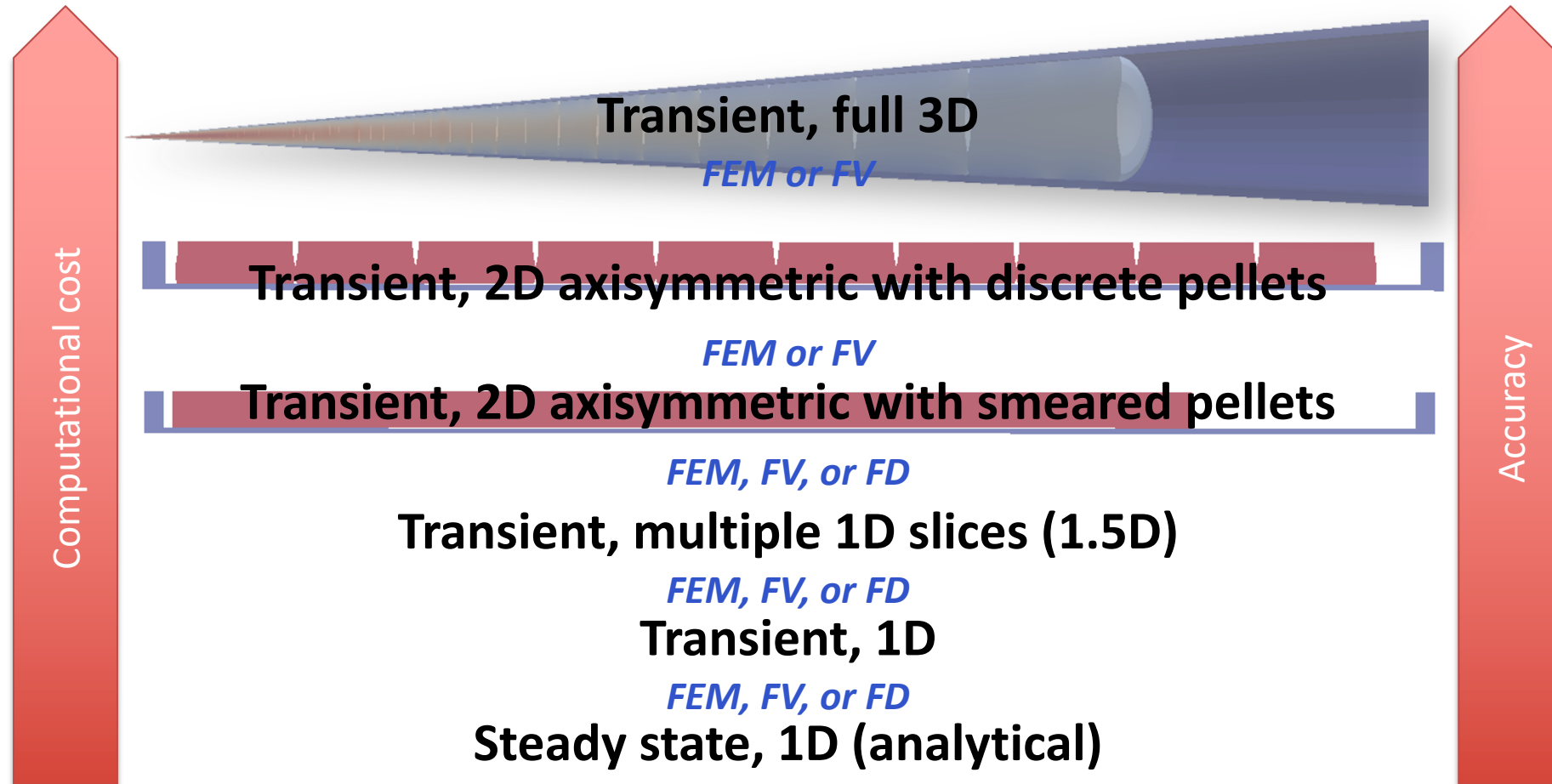
Spatial resolution

- 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



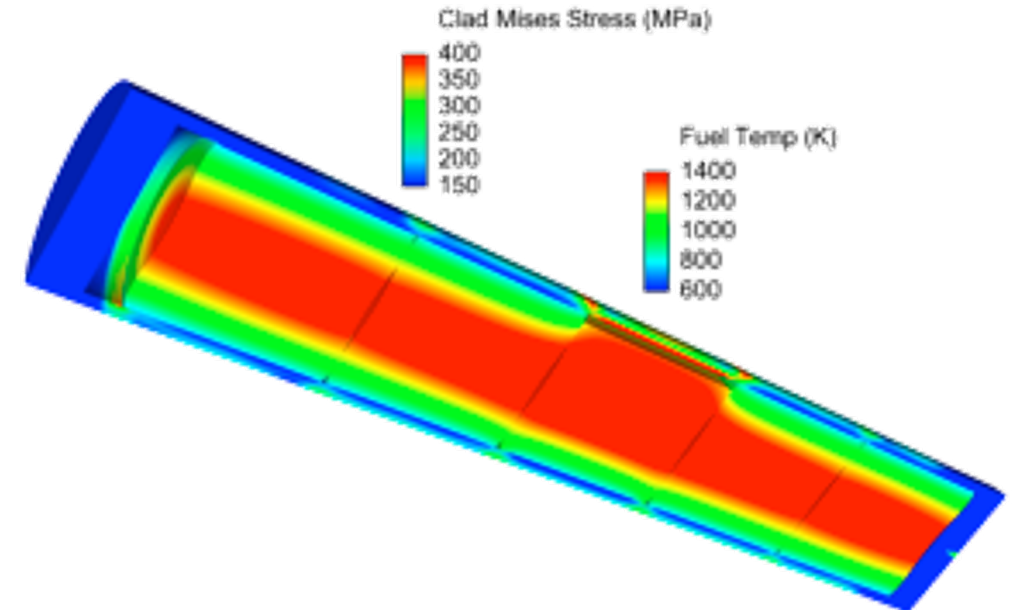
Heat equation solution approach summary

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 not used because it can't solve for the stress



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

Notes

- Exam on Feb. 3
- Will cover all classes through this Thursday
- Will contain both conceptual and work-through problems
- Major topics covered:
 - Fuel types; Heat generation; Reactor Systems; Fuel fabrication; Heat transfer; Analytical solution to heat transfer; Numerical solution to heat transfer; Thermal conductivity; Operational Limits
- In-person: during class time
- Online: total of 1.5 hours to complete the exam (class period plus 15-minute buffer)
- Distance students: please schedule your exam with me, otherwise it will be assumed you will be completing it during class time
- In person students: Option to complete in person during class, or online during the class period
- Next time will be partial lecture and partial problem session

Time Integration From Class

t	y'		forward	backward		function
1	1		6	6		6
1.333333	1.3333E-06		6.333333	6.00000044		6.18518519
1.666666	-1.6666627		6.33333344	5.44444678		5.92592704
1.999999	-3.999992		5.77777978	4.11111744		5.000004
2.333332	-6.9999867		4.44445044	1.77779089		3.18519452
2.666665	-10.666647		2.11112389	-1.7777544		0.25927704
2.999998	-14.999972		-1.4444214	-6.7777401		-3.99997
3.333331	-19.999963		-6.4444071	-13.444388		-9.8147681
3.666664	-25.666619		-13.111055	-21.999919		-17.407339

