Nuclear Fuel Performance

NE 533: Spring 2025

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

- $T_0 - T_{fuel} = \frac{Q}{4k} R_{fuel}^2$ $\quad T_0 - T_{fuel} = \frac{LHR}{4\pi k}$
- $T_{fuel} - T_{gap} = \frac{Q}{2h_{gap}} R_{fuel}$ $\quad T_{fuel} - T_{gap} = \frac{LHR}{2\pi R_{fuel} h_{gap}}$ $\quad h_{gap} = \frac{k_{gap}}{t_{gap}}$
- $T_{gap} - T_{clad} = \frac{Qt_{clad}}{2k_{clad}} R_{fuel}$ $\quad T_{gap} - T_{clad} = \frac{LHRt_{clad}}{2\pi R_{fuel} k_{clad}}$
- $T_{clad} - T_{cool} = \frac{Q}{2h_{cool}} R_{fuel}$ $\quad T_{clad} - T_{cool} = \frac{LHR}{2\pi R_{fuel} h_{cool}}$

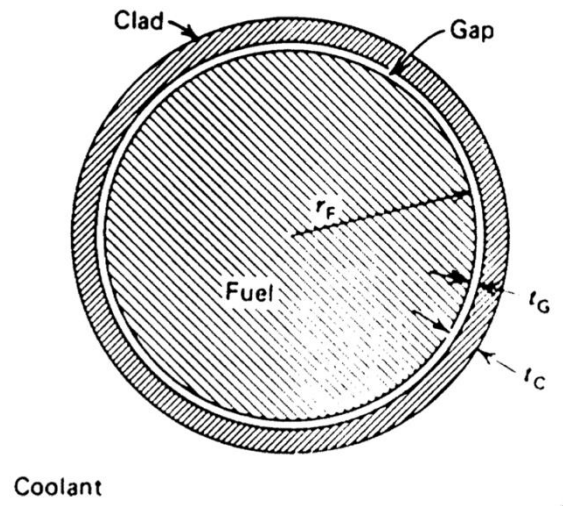
Review of Assumptions

- 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

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

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

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



THERMAL OPERATIONAL LIMITS

Thermal Operational Limits

- Thermal limits are prescribed for normal operation and accident conditions, with the goal of avoiding fuel damage
- Operational limits provide an envelope under which fuel failure will not occur
- LHR limits
- Centerline temperature limits
- Critical Heat Flux (CHF)
- The CHF is the heat flux at which boiling ceases to be an effective form of transferring heat from a solid surface to a liquid
- As the coolant temperature increases, the mode of heat transfer changes
- A boiling curve can be determined experimentally by increasing the temperature and measuring heat flux to the liquid
- Nucleate boiling is a type of boiling that takes place when the surface temperature is hotter than the saturated fluid temperature

Critical Heat Flux

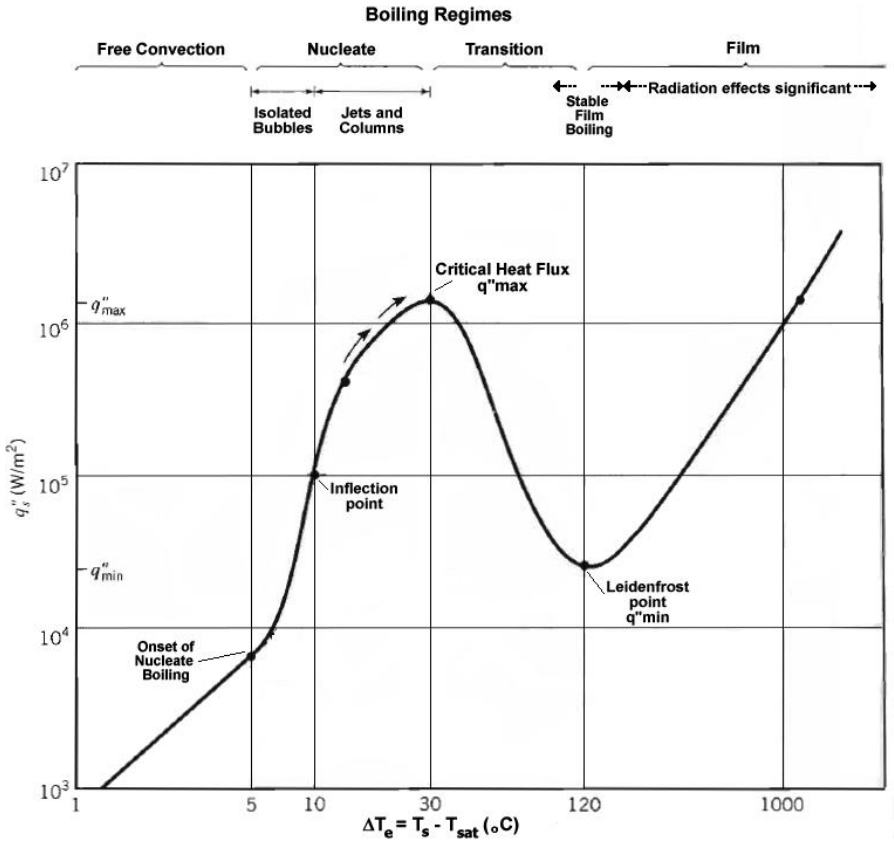
- In the single-phase mode (region I), flux is driven by temperature difference between the outer cladding surface and the coolant

$$q = h(T_{CO} - T_{cool})$$

- The heat transfer coefficient can be determined by the Dittus-Boelter equation:

$$\frac{hd_{eq}}{k_{cool}} = 0.023Re^{0.8}Pr^{0.4}$$

- Re is the Reynolds number and Pr is the Prandtl number, d_{eq} is the equivalent diameter of the flow channel, k_{cool} is the coolant thermal cond.
- We typically assuming a nominal value for h, but in reality, it is temperature dependent



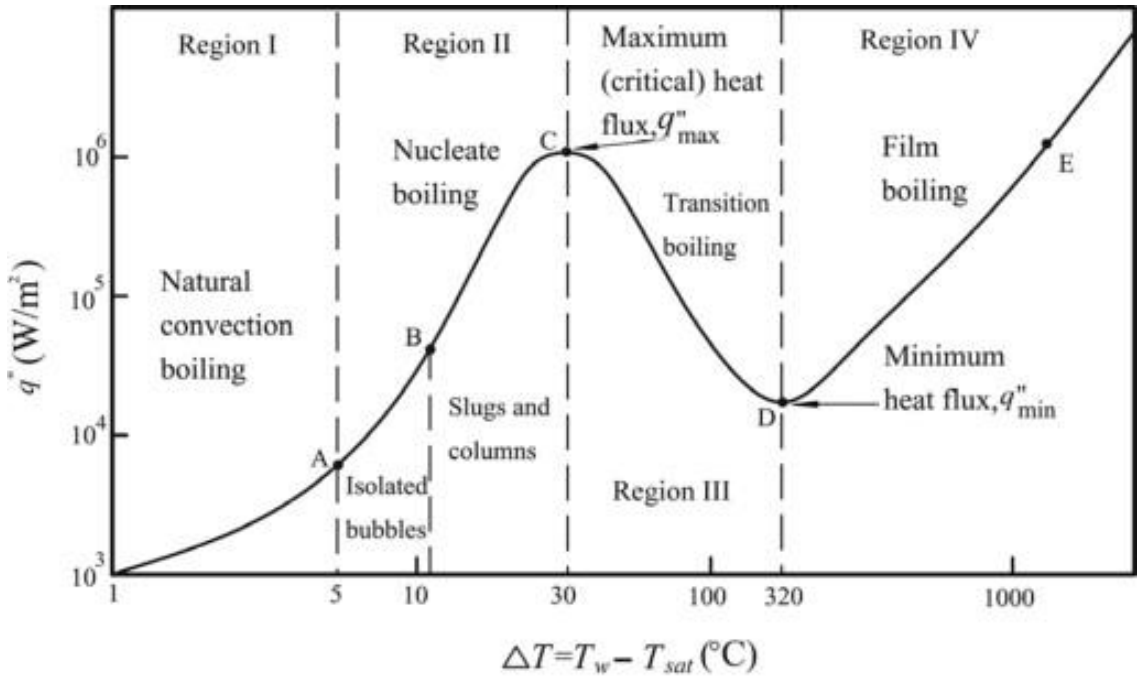
Boiling Curve for water at 1 atm.
Surface heat flux q" as a function of excess temperature $\Delta T_e = T_s - T_{sat}$

Critical Heat Flux

- At point A, the onset of nucleate boiling provides greater heat transfer to the coolant
- Typical nucleate boiling correlation relating heat flux and temperature is:

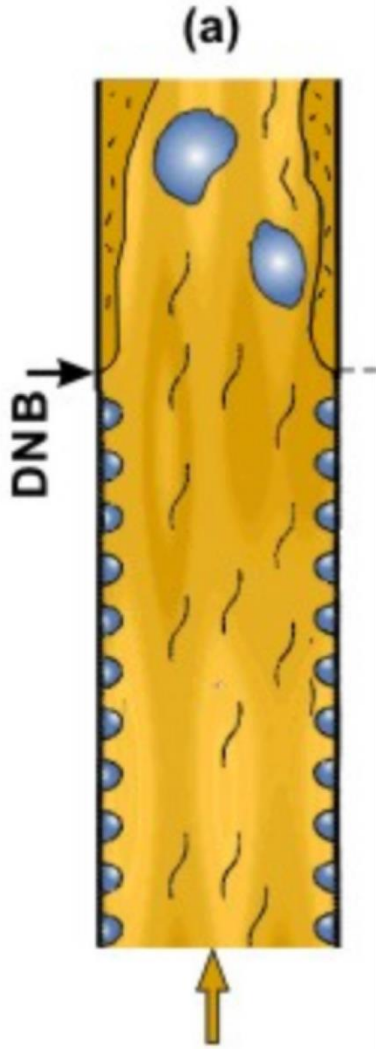
$$q\left(\frac{W}{m^2}\right) = 6(T_{CO} - T_{cool})^4$$

- Heat transfer mechanism is more complex in this region with two distinct phases
- At a critical point, C, the bubbles coalesce, and a continuous film of steam starts to form
- Point C is known as the critical heat flux



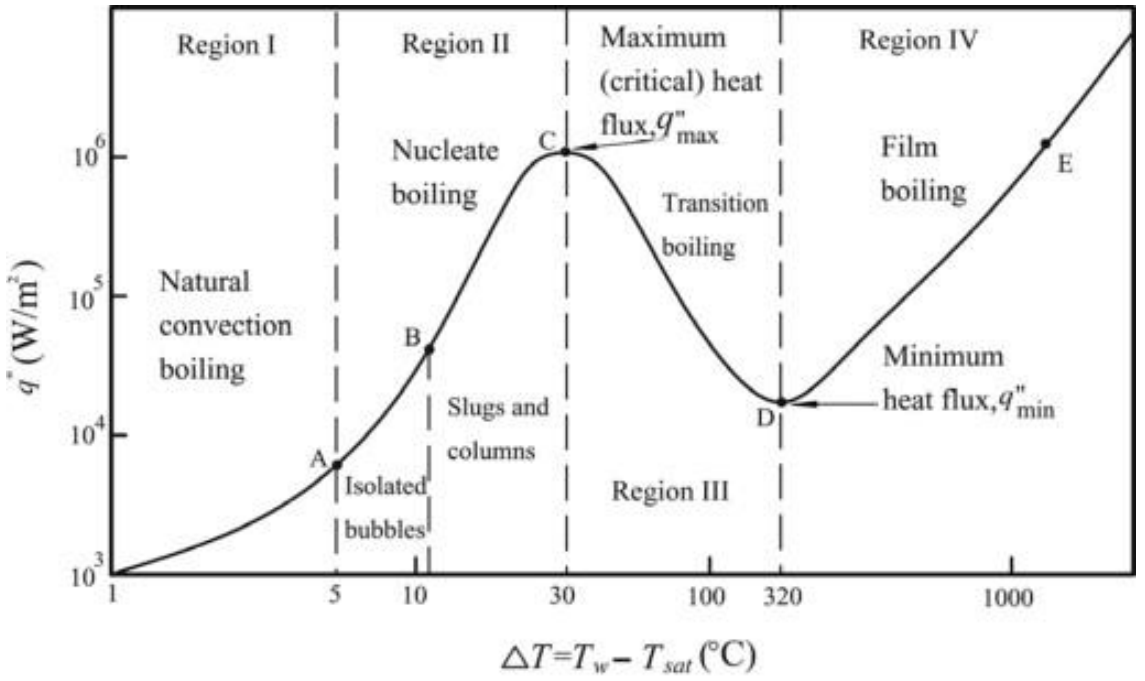
Departure from Nucleate Boiling

- If the heat flux of a boiling system is higher than the critical heat flux (CHF) of the system, the bulk fluid may boil, or in some cases, regions of the bulk fluid may boil where the fluid travels in small channels
- Large bubbles form, sometimes blocking the passage of the fluid
- This results in a departure from nucleate boiling (DNB) in which steam bubbles no longer break away from the solid surface of the channel, bubbles dominate the channel or surface, and the heat flux dramatically decreases
- Vapor essentially insulates the bulk liquid from the hot surface, increasing surface temperatures



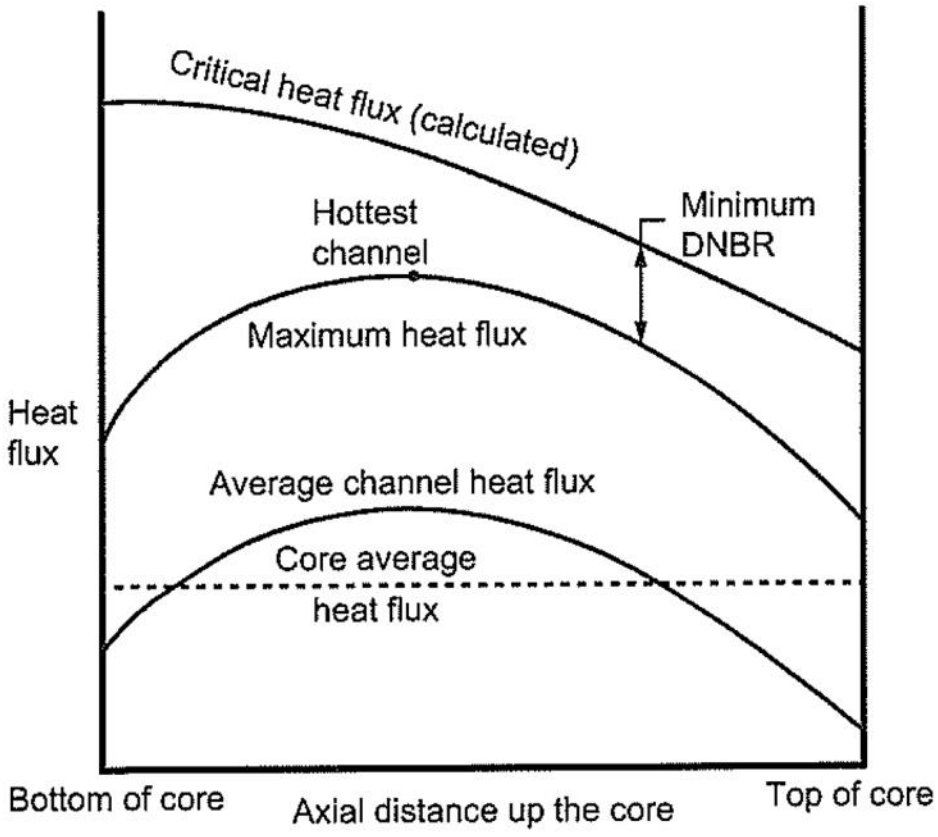
Critical Heat Flux

- Transition boiling is an oscillating mixture of nucleate and film boiling
- Beyond point D the rod is ”coated” in steam and the heat flux is dramatically reduced
- The heat transfer coefficient from cladding to steam is much lower than from cladding to water
- T_{sat} is the saturation temperature, which is fixed for a given pressure, whereas the coolant temperature (T_{cool}) increases
- Beyond point D, film boiling can occur



DNBR

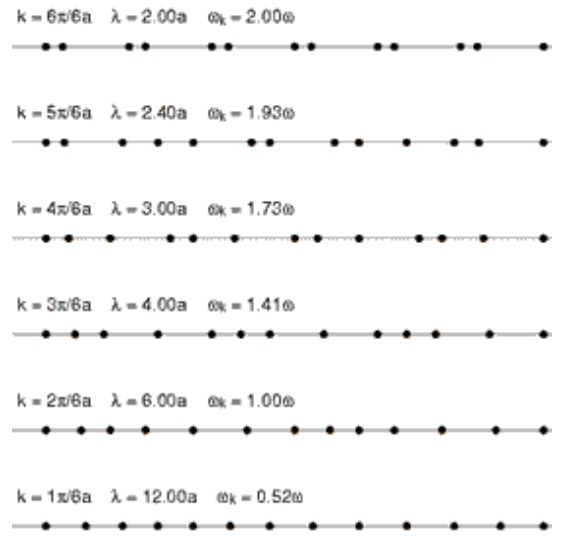
- The departure from nucleate boiling ratio (DNBR) is the ratio of the heat flux that causes dryout (the critical heat flux) to the actual heat flux
- The limits on the DNBR in the hottest channel is 1.15 to 1.3, or a margin of 15-30 percent
- The DNBR is determined by identifying the hottest channel, and the location where the heat flux most closely approaches the CHF
- When CHF is surpassed, cladding temperature can increase to above 1100 K



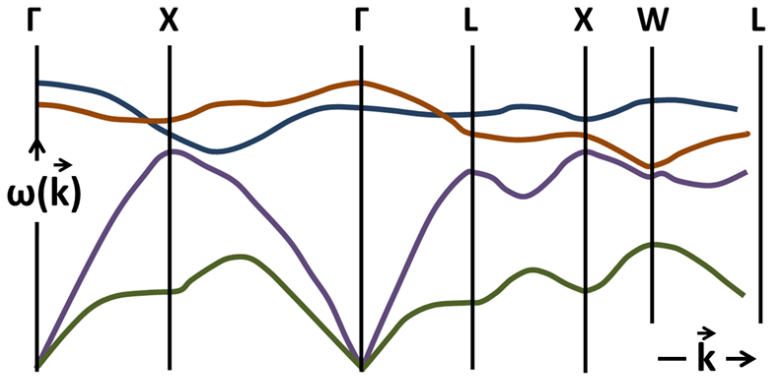
THERMAL CONDUCTIVITY

Phonons

- A phonon is a collective excitation in a periodic, elastic arrangement of atoms or molecules in condensed matter, specifically in solids and some liquids
- Phonons can be thought of as quantized sound waves, or quantized modes of vibrations for elastic structures of interacting particles
- The thermodynamic properties of a solid are directly related to its phonon structure
- Heat capacity is dominated by high frequency phonons while thermal conductivity is dominated by low frequency phonons

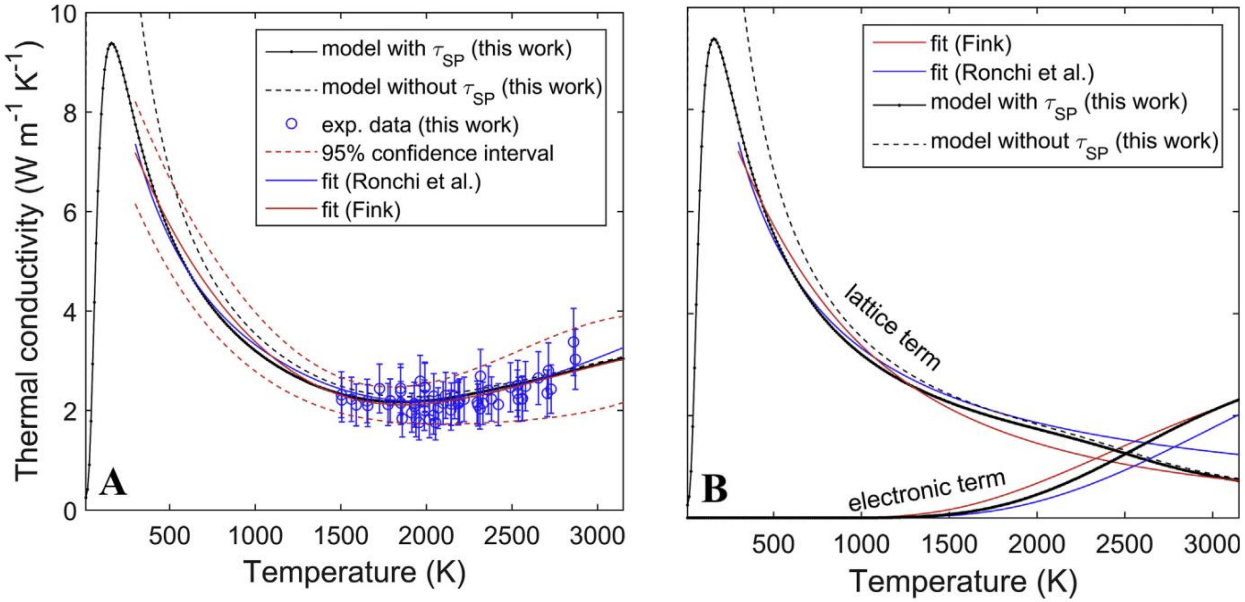


Animation showing 6 normal modes of a one-dimensional lattice



Phonon Scattering

- Phonons can scatter through several mechanisms as they travel through the material:
  - phonon-phonon; phonon-impurity; phonon-electron; phonon-boundary
- Temperature increases thermal fluctuations, and thus increases phonon scattering
- Electronic contributions in UO2 become much more prevalent at higher temperatures, with an increases kth as T increases



https://doi.org/10.1016/j.actamat.2017.07.060

Thermal Conductivity with Porosity

- Sintering creates a porous oxide with about 95% theoretical density
- The pores provide space to accommodate fission gases, and thus reduce swelling, but diminish the thermal conductivity
- Additional porosity develops from fission gas accumulation
- Porosity will degrade thermal conductivity by creating scattering centers
- Approximations for that degradation can be developed based upon a parallel thermal resistance framework

- This framework accounts for porosity volume, assuming that the pores are approximately cubic
- If we assume that the thermal conductivity of the oxide is much larger than the k_{th} of the pore, then:

$$\frac{k_{eff}}{k_{ox}} = 1 - P^{2}/_{3}$$

- where k_{eff} is the effective therm. cond. of the fuel, k_{ox} is the therm. cond. of the oxide, and P is the porosity

Thermal Conductivity with Burnup

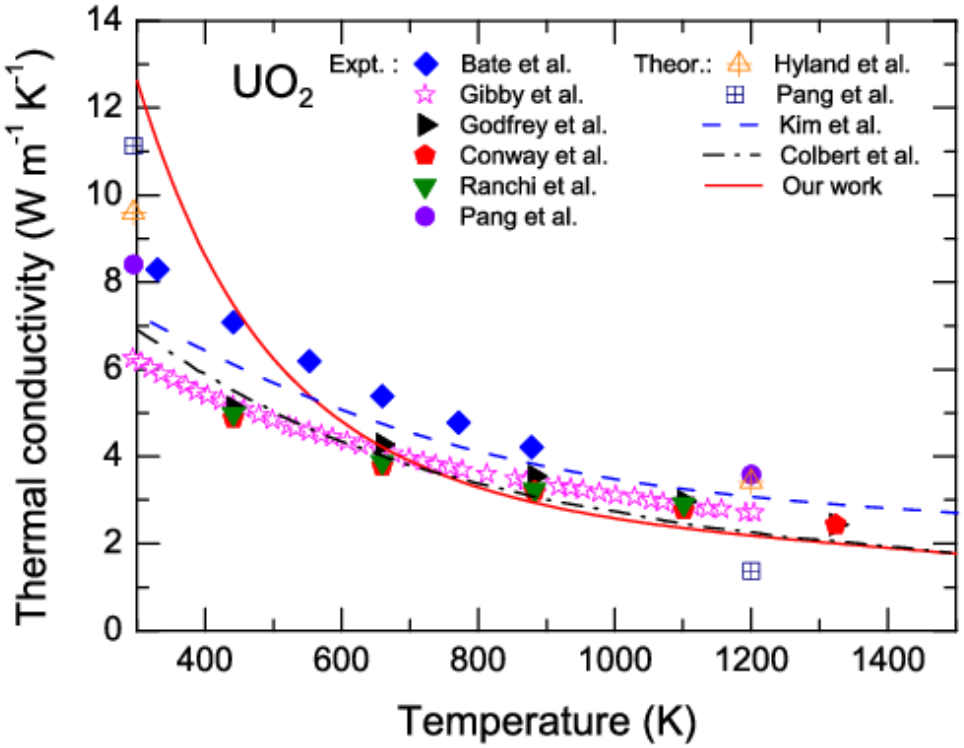
- An empirical relation for the thermal conductivity of UO2:

$$k_{ox} = \frac{1}{A + BT}$$

- A=3.8+200xFIMA (cmK/W)
- B=0.0217 (cm/W)
- The temperature at the fuel centerline and fuel surface are related by:

$$\frac{1}{B}\ln\left(\frac{A + BT_0}{A + BT_s}\right) = \frac{LHR}{4\pi}$$

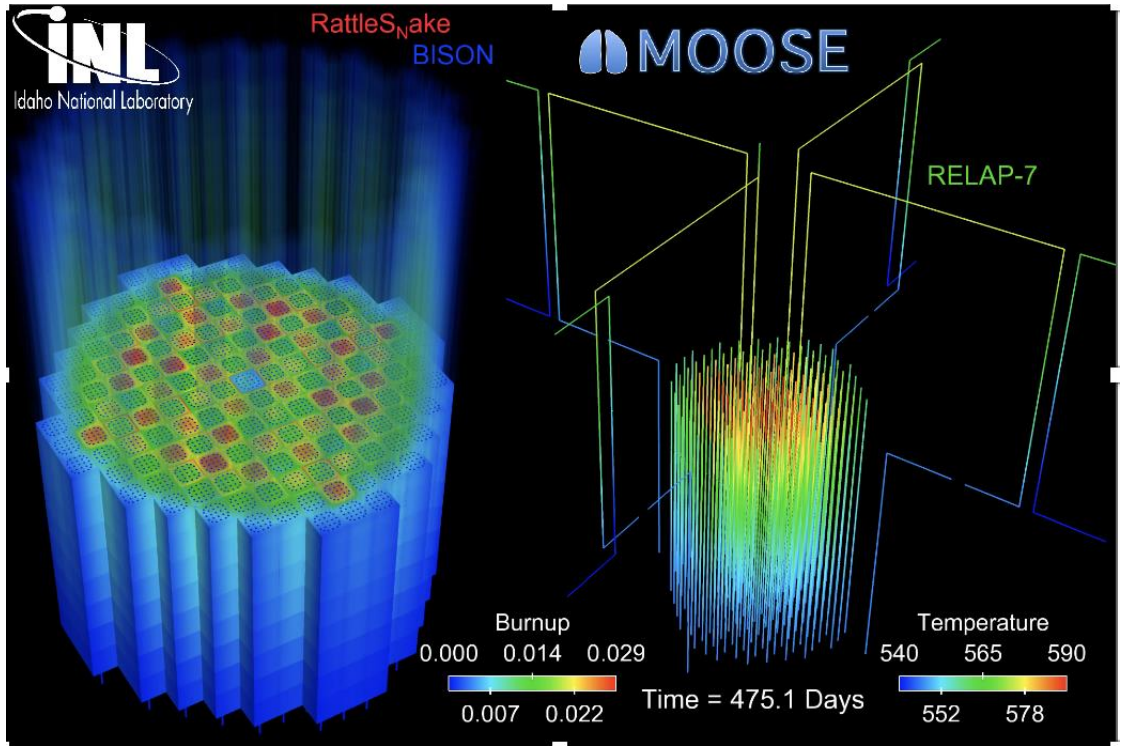
- Solving the heat conduction equation with temperature-dependent k_{th} requires numerical methods



NUMERICAL SOLVE

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



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

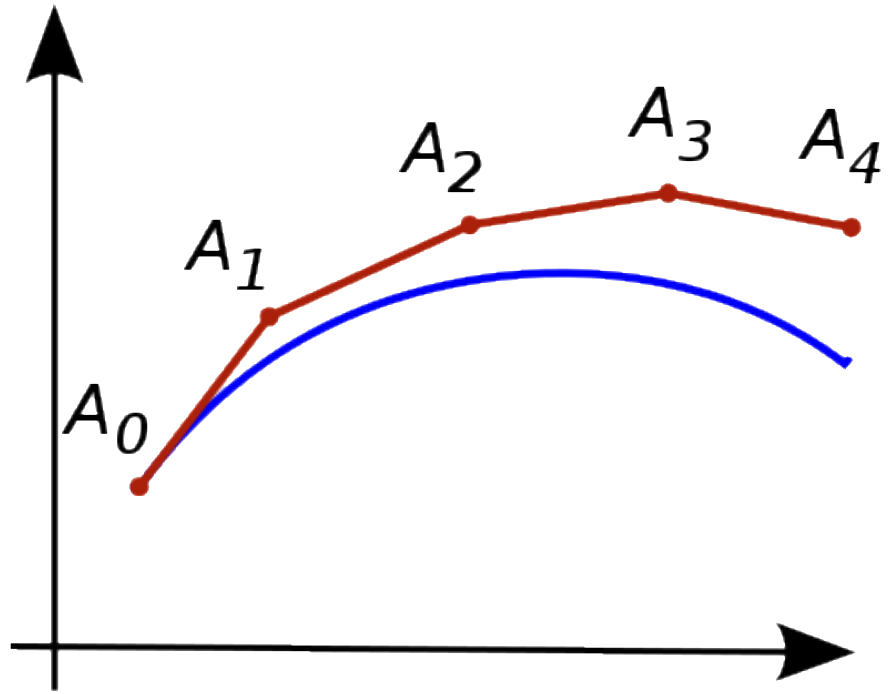
$$\rho c_p \frac{\partial T}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(rk\frac{\partial T}{\partial r}\right) + Q$$

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

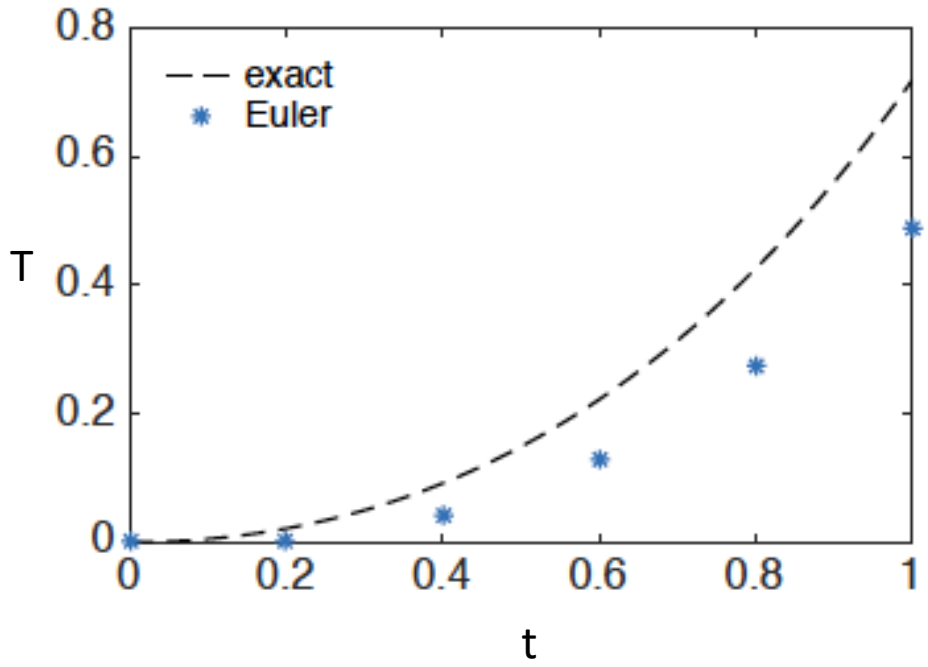
$$T(r, t + dt) = T(r, t) + dt\frac{\partial T(r,t)}{\partial t}$$

- 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

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



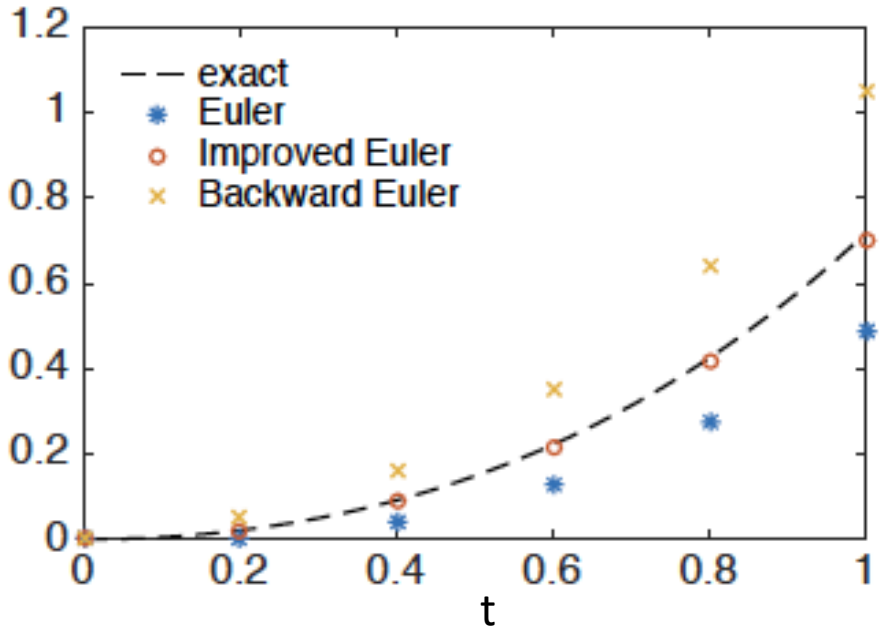
Backwards Euler

- 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

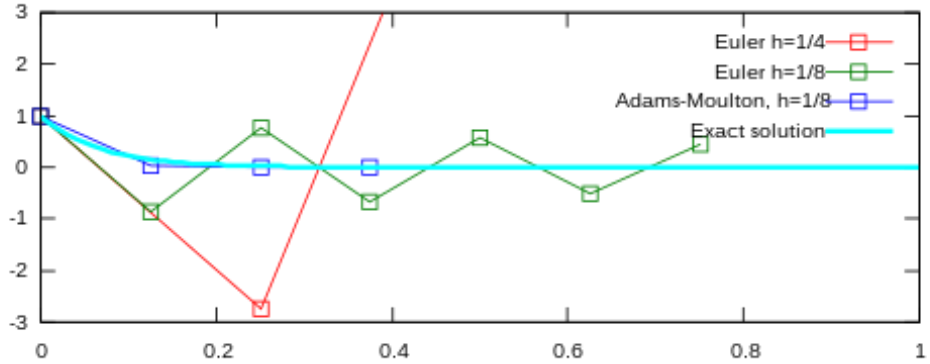
Stiff Equations

- 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:

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



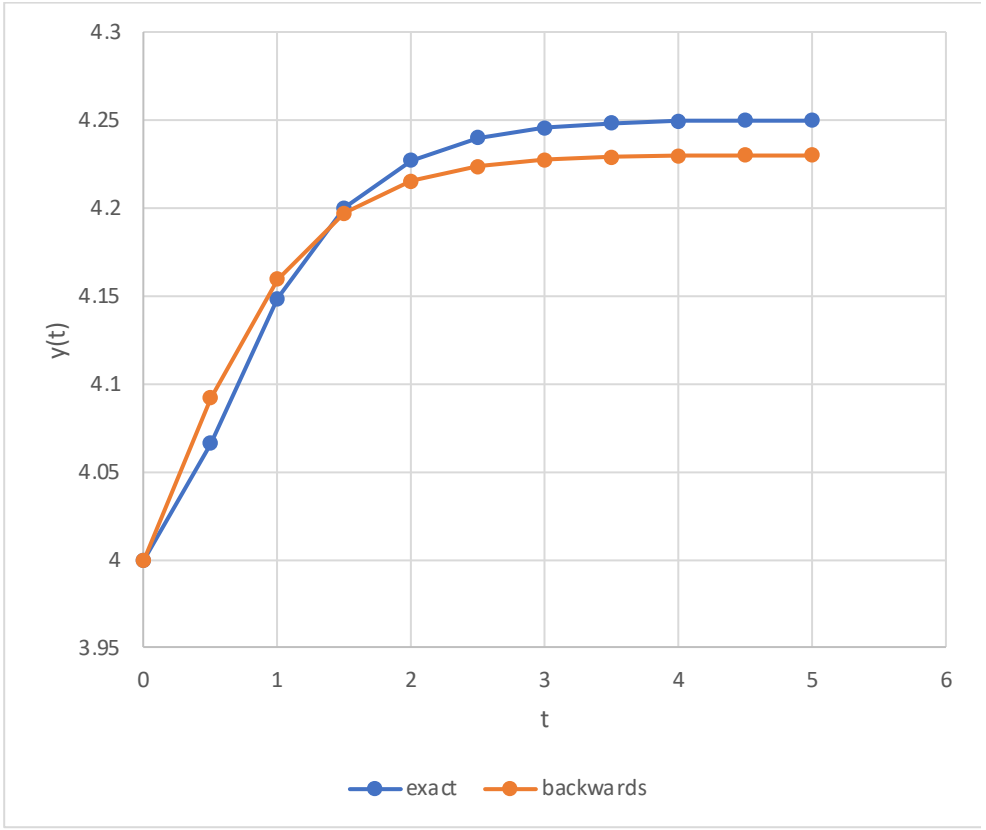
- Euler's method with a step size of h=1/4 oscillates wildly
- Euler's method with half the step size, h=/18, produces a solution within the graph boundaries, but oscillates about zero
- The trapezoidal method (similar to backwards Euler) is implicit, and converges to the correct solution

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

Example Problem

Example Problem

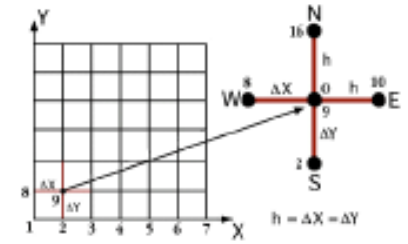
- y'=t*exp(-2t)
- y0=4
- dt=0.5
- Backwards Euler

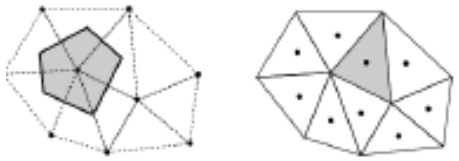


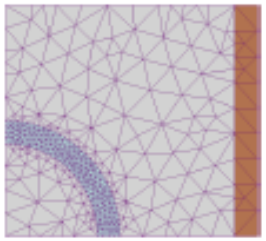
SPATIAL DISCRETIZATION

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



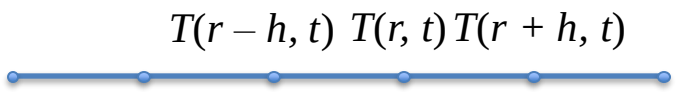




Finite Difference

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

- 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

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

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

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

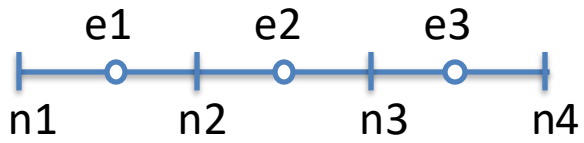
$$\frac{T_{i+1} - T_i}{h_2} - \frac{T_i - T_{i-1}}{h_1} + q\frac{h_2}{k} = 0$$

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

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



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

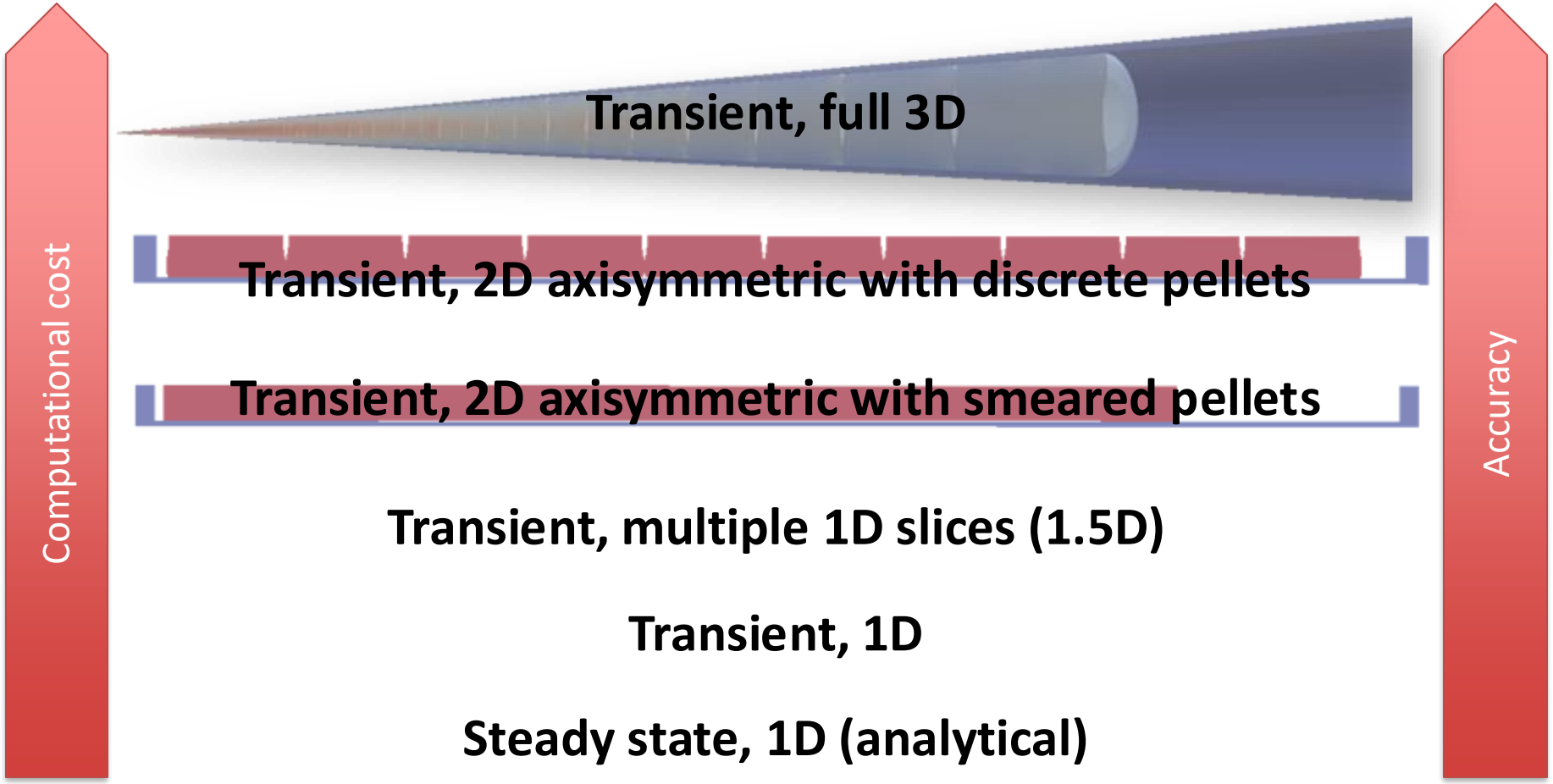
$$-\nabla \cdot \frac{\mathbf{K}}{\mu}\nabla p = 0 \in \Omega$$

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

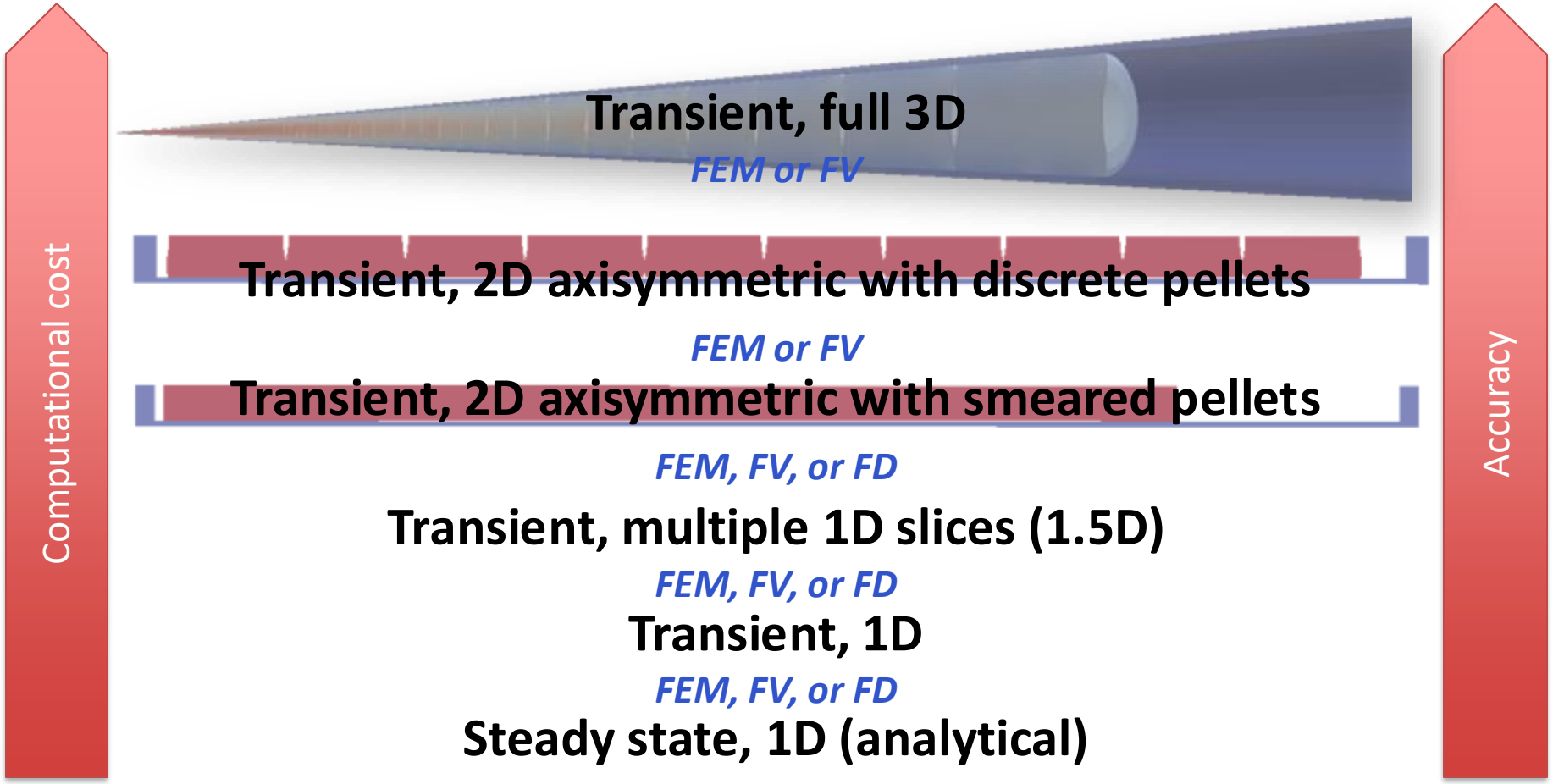
Spatial resolution

- 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



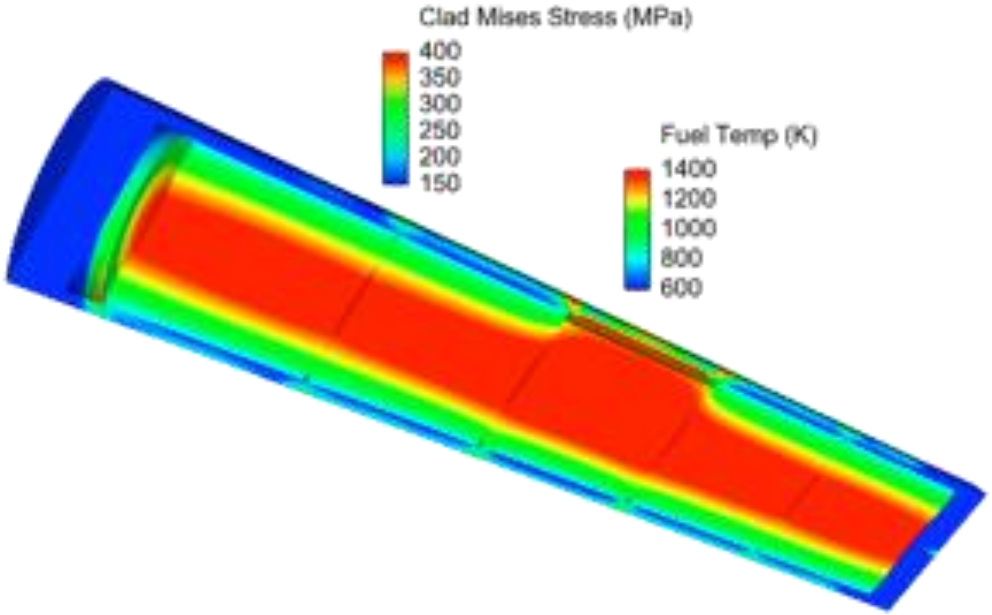
Heat equation solution approach summary

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 becoming an option



Summary

- The heat equation can be solved using numerical methods
- Explicit or implicit time integration can be used
- 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

End of Module 1

- Problem session on Tuesday 21st
- Exam on 23rd
- Exam to be completed during class period
  - bring calculators, can use your own paper or what I provide
- Reminder of office hours on Wednesdays at 9am
- Reminder of slack channel for rapid communication
- Will schedule exams with distance students

- Cheat sheet for exam: one page, one sided, turned in with exam