# Jacobian-Free Newton-Krylov (JFNK) Methods for Nonlinear Neutronics/Thermal-Hydraulic Equations

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December 10, 2011

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# Outline



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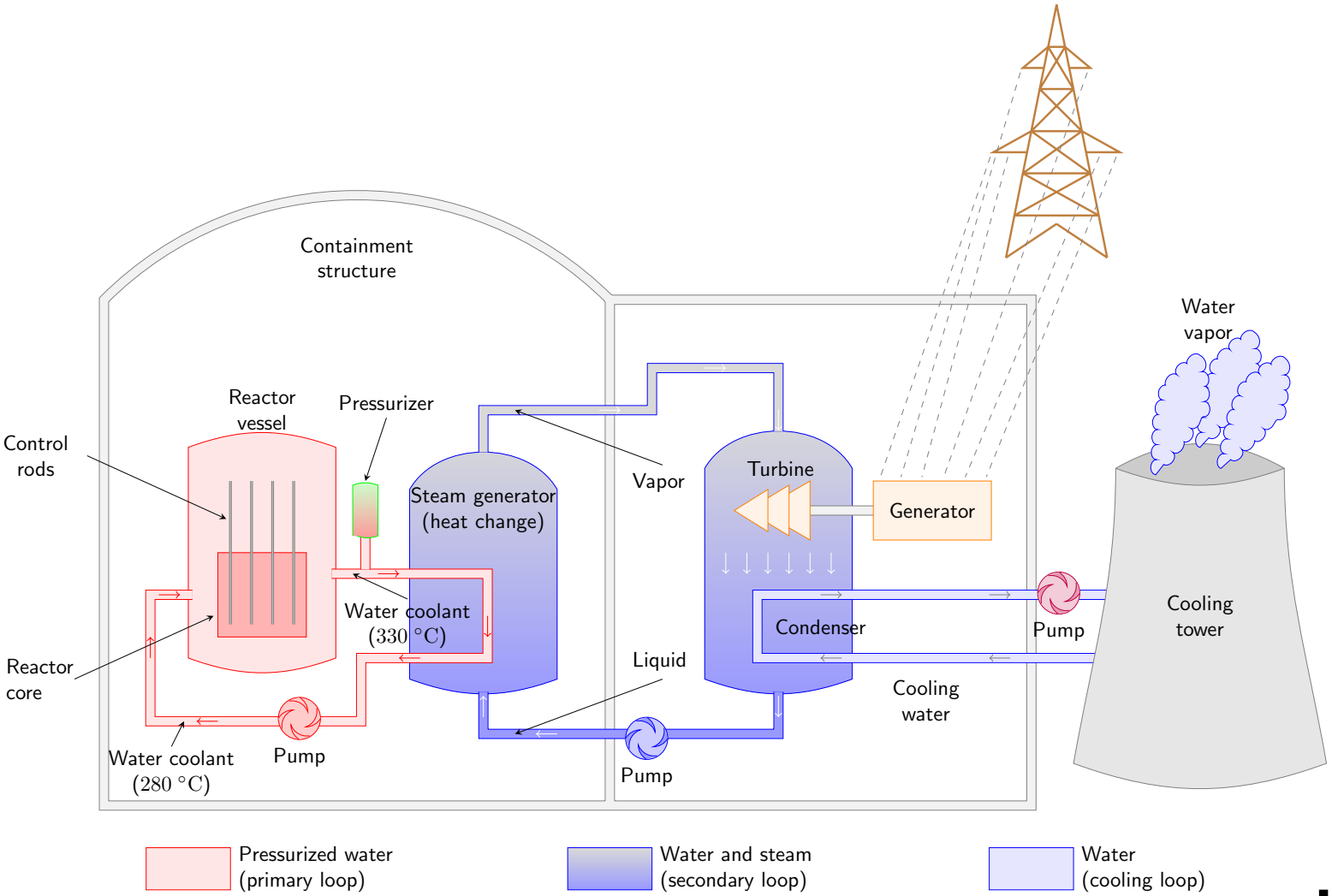
# Motivation

- Eventually will be part of thesis work
- JFNK method not currently used in nuclear reactor analysis
- Incorporates a lot of ideas from 2.29 class
- Coupled physics is fun!

# Nuclear Reactor Plant

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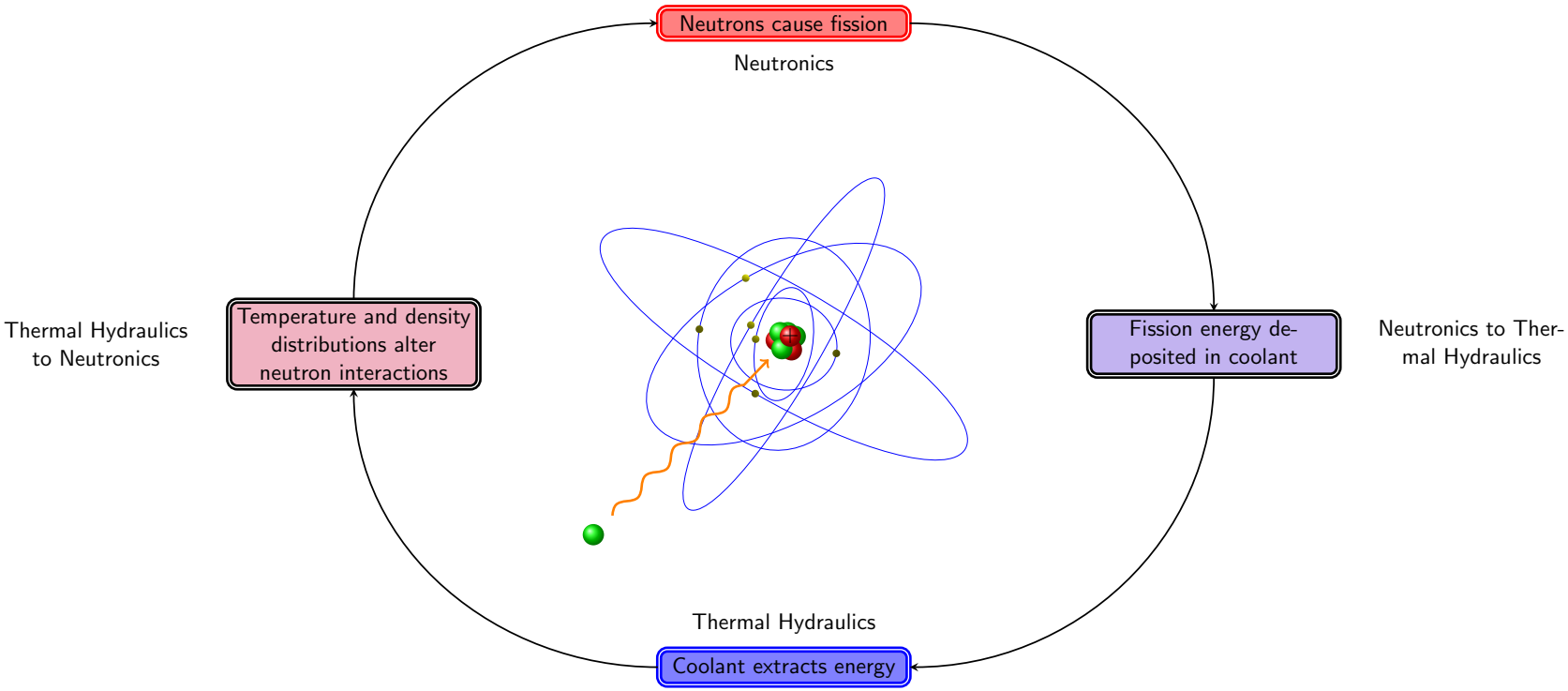
# Nuclear Feedback




- Fuel Temperature Feedback - $T_f \uparrow$, U-238 Capture $\uparrow$, Fission Rate $\downarrow$, Power $\downarrow$
- Coolant Density Feedback - $\rho \downarrow$, $E_n \uparrow$, Fission Rate $\downarrow$, Power $\downarrow$

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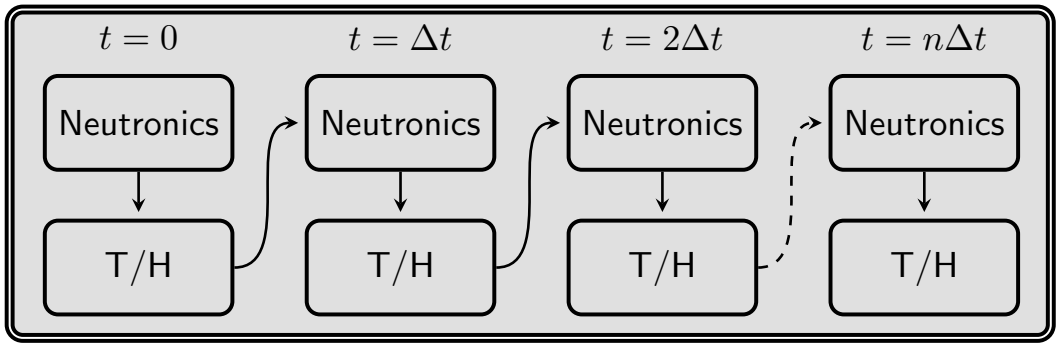
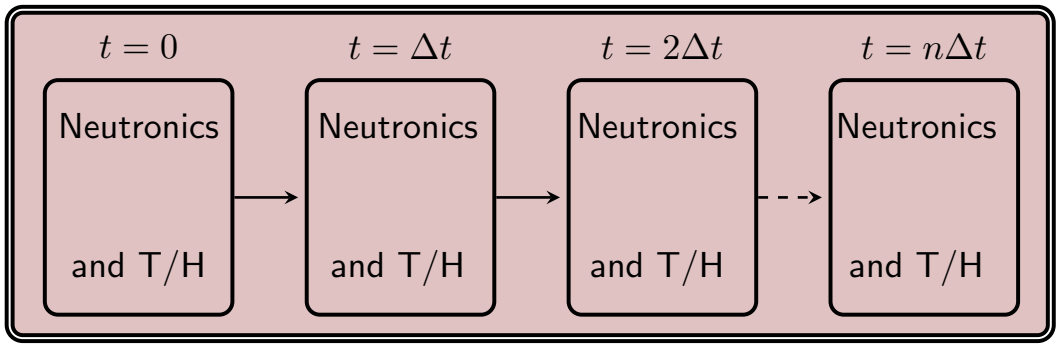
# Common Approach to Coupling: Operator Splitting

- Solve physics independently and iterate between them




- Fully coupled approach solves the nonlinear physics together

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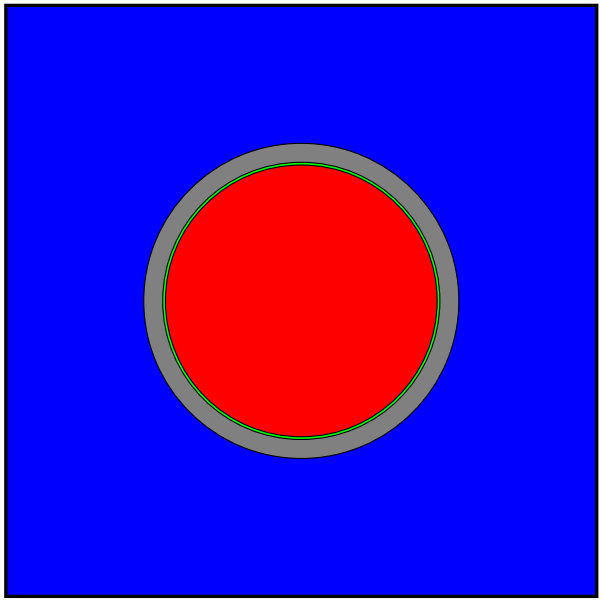
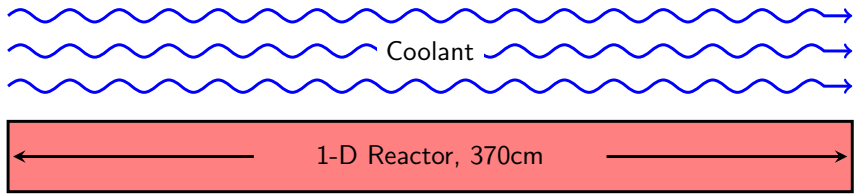
# 1-D Slab Reactor Geometry




Top-view
Fuel Rod Unit-Cell




Side-view (vertical)
1-D Model of Reactor

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# Neutronics

- Basic Neutron Conservation:

$$Change + Leakage + Interactions = Scattering + Fission$$

- Neutron Transport Equation:

$$\underbrace{\frac{1}{v}\frac{\partial \varphi}{\partial t}}_{\text{time-dependent}} + \underbrace{\boldsymbol{\Omega}\cdot\nabla\varphi\left(\mathbf{r},E,\boldsymbol{\Omega},t\right)}_{\text{neutron leakage}} + \underbrace{\Sigma_t\left(\mathbf{r},E,t\right)\varphi\left(\mathbf{r},E,\boldsymbol{\Omega},t\right)}_{\text{interaction of neutrons with medium}} = \underbrace{Q\left(\mathbf{r},E,\boldsymbol{\Omega},t\right)}_{\text{neutron source}}$$

- Neutron Diffusion Equation (1-D Energy Integrated)

$$\frac{1}{v}\frac{\partial \phi}{\partial t} - D\left(x,t\right)\frac{\partial^2 \phi}{\partial^2 x} + \Sigma_a\left(x,t\right)\phi\left(x,t\right) = \frac{1-\beta}{k_{eff}}\nu\Sigma_f\left(x,t\right)\phi\left(x,t\right) + \lambda_d c\left(x,t\right)$$

$$\frac{\partial c}{\partial t} = \frac{\beta}{k_{eff}}\nu\Sigma_f\left(x,t\right)\phi\left(x,t\right) - \lambda_d c\left(x,t\right)$$

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# Discretization of Neutronics Equations

**Assumptions:**

1. One-dimensional finite volume spatial discretization, uniform $\Delta x$
2. Central difference scheme for diffusion term
3. No incoming current of neutrons at boundaries
4. Implicit Euler time discretization

- Discretized neutronics equation for interior cell

$$\frac{1}{v}\frac{d\bar{\phi}_i}{dt} - \frac{2}{\Delta x^2}\frac{D_i D_{i-1}}{D_i + D_{i-1}}\bar{\phi}_{i-1} + \left(\frac{2}{\Delta x^2}\frac{D_{i+1}D_i}{D_{i+1}+D_i} + \frac{2}{\Delta x^2}\frac{D_i D_{i-1}}{D_i + D_{i-1}} + \Sigma_{a,i}\right)\bar{\phi}_i - \frac{2}{\Delta x^2}\frac{D_{i+1}D_i}{D_{i+1}+D_i}\bar{\phi}_{i+1} = \frac{1-\beta}{k_{eff}}\nu\Sigma_{f,i}\bar{\phi}_i + \lambda_d \bar{c}_i$$

- Matrix-form of neutronics equations

$$\bar{\mathbf{\Phi}}^{n+1} - \bar{\mathbf{\Phi}}^{n} + v\Delta t\left(\mathbb{M}\bar{\mathbf{\Phi}}^{n+1} - (1-\beta)\lambda\mathbb{F}\bar{\mathbf{\Phi}}^{n+1} - \lambda_d \bar{\mathbf{c}}^{n+1}\right) = 0$$

- Matrix-form of precursors

$$\bar{\mathbf{c}}^{n+1} - \bar{\mathbf{c}}^{n} + \Delta t\left(\lambda_d \bar{\mathbf{c}}^{n+1} - \beta\lambda\mathbb{F}\bar{\mathbf{\Phi}}^{n+1}\right) = 0$$

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# Thermal Hydraulics

- Energy Equation - single phase fluid and inviscid fluid

$$\frac{\partial (\rho h)}{\partial t} + \nabla \cdot (\rho h \mathbf{u}) = -\nabla \cdot \mathbf{q}'' + q'''$$

- Assuming fissions are a volumetic heat source in 1-D

$$\rho A \frac{\partial h}{\partial t} + \dot{m} \frac{\partial h}{\partial x} = q'$$

- For an incompress2cmible fluid, $dh = c_p dT$

$$\rho A c_p \frac{\partial T}{\partial t} + \dot{m} c_p \frac{\partial T}{\partial x} = q'$$

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# Discretization of Energy Equation

**Assumptions:**

1. One-dimensional finite volume spatial discretization, uniform $\Delta x$
2. Upwind difference scheme for flux
3. Specify inlet conditions and mass flow rate
4. Implicit Euler time discretization

- Spatial discretization

$$\frac{\rho A \Delta x}{\dot{m}} \frac{d\bar{T}_i}{dt} + \bar{T}_i - \bar{T}_{i-1} = \frac{1}{2\dot{m}c_p} \left(Q_{i-1} + Q_i\right)$$

- Matrix-form with time discretization

$$\bar{\mathbf{T}}^{n+1} - \bar{\mathbf{T}}^{n} + \frac{\dot{m}\Delta t}{\mathcal{P}^{n+1} A \Delta x} \left(\mathbb{S}\bar{\mathbf{T}}^{n+1} - \mathbb{R}\mathbf{Q}^{n+1}\right) = 0$$

Note: $\mathcal{P}$ is a vector of cell-averaged coolant densities

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# Physics Coupling

## Neutronics-Thermal Hydraulics

- Neutrons cause fission
- Large portion of fission energy deposited in coolant
- This is represented by

$$\mathbf{Q} = \tilde{c}\mathbb{E}\bar{\mathbf{\Phi}}\Delta x$$

where $\mathbb{E} = \text{diag}\left\{\kappa\Sigma_f\right\}$ characterizes energy per fission and $\tilde{c}$ is the flux-to-power normalization constant

## Thermal Hydraulics-Neutronics

- Diffusion theory parameters depend on coolant density
- This dependence is determined with a transport theory code
- $D$, $\Sigma_a$, $\nu\Sigma_f$, $\kappa\Sigma_f$ are all affected by coolant density variations
- Data is correlated with a linear regression of the form:

$$\mathbf{\Sigma} = \mathbf{\Sigma}^{ref} + \frac{\partial\Sigma}{\partial\rho}\left(\mathcal{P} - \rho^{ref}\right)$$

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# The Steady State Eigenvalue Problem

- The steady state equations must be solved first
- Reducing the neutronics equation to steady state form:

$$\mathbb{M}\bar{\mathbf{\Phi}} = \lambda \mathbb{F}\bar{\mathbf{\Phi}}, \qquad \lambda = \frac{1}{k_{eff}}$$

- Eigenvalue, $\lambda$, and eigenvector, $\bar{\mathbf{\Phi}}$, must be determined
- Flux-to-power normalization constant determined from reactor power:

$$Q_R = \tilde{c}\int_0^L dx \kappa\Sigma_f(x)\phi(x) = \tilde{c}\sum_i \kappa\Sigma_{f,i}\bar{\phi}_i\Delta x = \tilde{c}\kappa\mathbf{\Sigma}_f^{\mathrm{T}}\bar{\mathbf{\Phi}}\Delta x$$

- $\lambda$ and $\tilde{c}$ are specified as constants for time-dependent calculations

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# Newton's Method

**Procedure:**

1: Goal:$\mathbf{F}(\mathbf{x}) = \mathbf{0}$
2: Guess $\mathbf{x}$
3: **for** $n = 1, 2, 3, \ldots$ **do**
4: $\quad \mathbf{r} = \mathbf{F}(\mathbf{x})$
5: $\quad$ **if** $\|\mathbf{r}\| < ntol$ **then**
6: $\quad\quad$ DONE!
7: $\quad$ **end if**
8: $\quad \mathbf{dx} = -\mathbb{J}^{-1}(\mathbf{x})\,\mathbf{F}(\mathbf{x})$
9: $\quad \mathbf{x} = \mathbf{x} + \mathbf{dx}$
10: **end for**

Three major tasks:

1. Evaluate residual vector in external function
2. Evalue Jacobian in external function (Do we have to?)
3. Calculate $\mathbf{dx}$ - Direct or Iterative Solvers?

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# Krylov Subspace Methods

- A class of iterative methods for sparse systems
- Solves $\mathbb{A}\mathbf{x} = \mathbf{b}$ by projecting a $m$ dimensional problem into a lower dimensional Krylov subspace

$$\mathcal{K}_n\left(\mathbb{A}, \mathbf{v}\right) = \text{span}\left\{\mathbf{v}, \mathbb{A}\mathbf{v}, \mathbb{A}^2\mathbf{v}, ..., \mathbb{A}^{n-1}\mathbf{v}\right\}$$

- Here $\mathbb{A}$ is nonhermitian and we use the GMRES method
- GMRES uses the Arnoldi method to reduce the system to Hessenberg form

$$\mathbb{A}\mathbb{Q} = \mathbb{Q}\mathbb{H}$$

$$\mathbb{H} = \begin{bmatrix} h_{11} & & \cdots & h_{1n} \\ h_{21} & h_{22} & & \\ & \ddots & \ddots & \vdots \\ & & h_{n,n-1} & h_{n,n} \end{bmatrix}$$

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# Generalized Minimal RESidual Method

- Goal: $\mathbf{x}_* = \mathbb{A}^{-1}\mathbf{b}$
- A step $n$, $\mathbf{x}_*$ is approximated by $\mathbf{x}_n \in \mathcal{K}_n$ that minimizes the norm of the residual $\mathbf{r}_n = \mathbf{b} - \mathbb{A}\mathbf{x}_n$

**Procedure:**

1: $q_1 = b/\|b\|$
2: **for** $n = 1, 2, 3, \ldots$ **do**
3: Perform step $n$ of Arnoldi (Creates Hessenberg matrix)
4: Find $y$ to minimize $\left\|\widetilde{\mathbb{H}}_n\mathbf{y} - \|\mathbf{b}\|\,\mathbf{e}_1\right\|$
5: **if** $\|\mathbf{r}\| < ltol$ **then**
6: DONE!
7: **end if**
8: **end for**
9: $\mathbf{x} = \mathbb{Q}_n\mathbf{y}$

- Saad et al.[‡] defines a novel method to compute $\widetilde{\mathbb{H}}_n$ from $\widetilde{\mathbb{H}}_{n-1}$ from Givens rotations

[‡] Youcef Saad and Martin H. Schultz. GMRES: A generalized minimal residual algorithm for solving nonsymmetric linear systems. Society for Industrial and Applied Mathematics, 7:856-859, 1986.

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# Inexact Newton's Method

- Newton-Krylov is an inexact Newton method since the linear step is not determined *exactly*
- In Newton-Krylov framework, two tolerances were defined:
  1. Nonlinear tolerance for Newton iteration
  2. Linear tolerance for GMRES iteration
- Why have tight linear convergence when nonlinear residual is large?
- Instead, a relative residual tolerance, $\eta$, is used

$$\left\| \mathbb{J}\left(\mathbf{x}^n\right) \mathbf{dx}_m^n + \mathbf{F}\left(\mathbf{x}^n\right) \right\| < \eta \left\| \mathbf{F}\left(\mathbf{x}^n\right) \right\|$$

- At initial Newton iterations, GMRES will not be converged very tightly
- For the last couple of Newton iterations, convergence may be too tight
  $\therefore$ limit how small linear tolerance can get

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# Jacobian-Free Approximation

- Recall a Krylov subspace: $\mathcal{K}_n(\mathbb{A}, \mathbf{v}) = \text{span}\left\{\mathbf{v}, \mathbb{A}\mathbf{v}, \mathbb{A}^2\mathbf{v}, ..., \mathbb{A}^{n-1}\mathbf{v}\right\}$
- Why create $\mathbb{A}$ when it is only used to multiply a vector?
- Option 1: Perform Jacobian-vector product analytically

$$\mathbb{J}\mathbf{y} = \begin{bmatrix} \mathbb{M} - \lambda\mathbb{F} & -\mathbb{F}\bar{\mathbf{\Phi}} \\ -\bar{\mathbf{\Phi}}^\top & 0 \end{bmatrix} \begin{bmatrix} y_\phi \\ y_\lambda \end{bmatrix} = \begin{bmatrix} (\mathbb{M} - \lambda\mathbb{F})\, y_\phi - \mathbb{F}\bar{\mathbf{\Phi}} y_\lambda \\ -\bar{\mathbf{\Phi}}^\top y_\phi \end{bmatrix}$$

- Option 2: Approximate Jacobian-vector product with finite difference

$$\mathbb{J}\mathbf{y} \approx \frac{\mathbf{F}(\mathbf{x} + \epsilon\mathbf{y}) - \mathbf{F}(\mathbf{x})}{\epsilon}$$

- Advantages: Saves memory and possibly computational time to form Jacobian
- $\epsilon$ is the perturbation parameter and is somewhat arbitrary - Mousseau[§] recommends:

$$\epsilon = \frac{\sum_{i=1}^{N} b x_i}{N \|\mathbf{y}\|_2} \qquad b = 1 \times 10^{-8}$$

[§] V.A. Mousseau. Implicitly balanced solution of the two-phase flow equations couple to nonlinear heat conduction. Journal of Computational Physics, 200:104-132, 2004.

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# Preconditioning

- Want to limit number of GMRES iterations
- Before a calculation, a Jacobian matrix is formed analytically and a zero-fill Incomplete LU (ILU) is performed:

$$\mathbb{R} = \mathbb{L}\mathbb{U} - \mathbb{A}$$

- In ILU, residual matrix $\mathbb{R}$ is constrained to certain conditions
- Zero-fill implies that the number and location of nonzeros is preserved
- Left preconditioning is used in this project:

$$\mathbb{U}^{-1}\mathbb{L}^{-1}\mathbb{A}\mathbf{x} = \mathbb{U}^{-1}\mathbb{L}^{-1}\mathbf{b}$$

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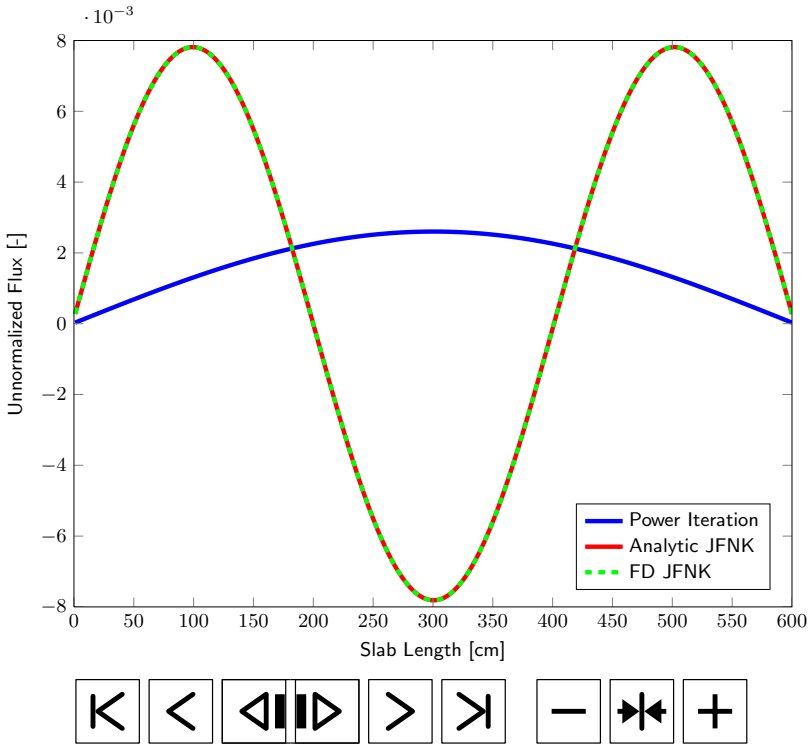
# Steady State - Neutronics

- Residual Equations

$$\mathbf{F} = \begin{bmatrix} \mathbb{M}\bar{\mathbf{\Phi}} - \lambda \mathbb{F}\bar{\mathbf{\Phi}} \\ -\frac{1}{2}\bar{\mathbf{\Phi}}^{\top}\bar{\mathbf{\Phi}} + \frac{1}{2} \end{bmatrix}$$

- Resulting neutron flux distribution:




- A Newton method cannot guarantee that the fundamental eigenmode is calculated
- Any mode satisfies the nonlinear set of equations
- Here the ratio of the first two eigenvalues is close to unity (dominance ratio)
- Use a few power iterations to get gross flux shape

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# Steady State - Coupled Neutronics/Thermal Hydraulics [1/2]

## Residual Equations

$$\mathbf{F} = \begin{bmatrix} \mathbb{M}\mathbf{\Phi} - \lambda\mathbb{F}\mathbf{\Phi} \\ Q_R - \tilde{c}\kappa\mathbf{\Sigma}_f^{\mathrm{T}}\mathbf{\Phi}\Delta x. \\ \mathbf{Q} - \tilde{c}\mathbb{E}\mathbf{\Phi}\Delta x \\ \mathbb{S}\mathbf{T} - \mathbb{R}\mathbf{Q} \\ \mathcal{P} - \rho\left(\mathbf{T}, p\right) \\ \mathbf{\Sigma}_a - \Sigma_a^{ref} - \frac{\partial \Sigma_a}{\partial \rho}\left[\mathcal{P} - \rho^{ref}\right] \\ \nu\mathbf{\Sigma}_f - \nu\Sigma_f^{ref} - \frac{\partial \nu\Sigma_f}{\partial \rho}\left[\mathcal{P} - \rho^{ref}\right] \\ \mathbf{D} - D^{ref} - \frac{\partial D}{\partial \rho}\left[\mathcal{P} - \rho^{ref}\right], \\ \kappa\mathbf{\Sigma}_f - \kappa\Sigma_f^{ref} - \frac{\partial \kappa\Sigma_f}{\partial \rho}\left[\mathcal{P} - \rho^{ref}\right] \\ -\frac{1}{2}\mathbf{\Phi}^{\mathrm{T}}\mathbf{\Phi} + \frac{1}{2} \end{bmatrix}$$

- Neutronics
- Flux normalization
- Energy deposition
- Temperature distribution
- Density distribution
- Absorption xs
- Fission xs
- Diffusion
- Energy deposition xs
- Eigenvalue

- X-Steam MATLAB tables were used to look up density as a function of temperature
- An analytical Jacobian-vector product can be formed for everything except $\frac{\partial \rho}{\partial T}$
- For this block a finite difference approximation must be used

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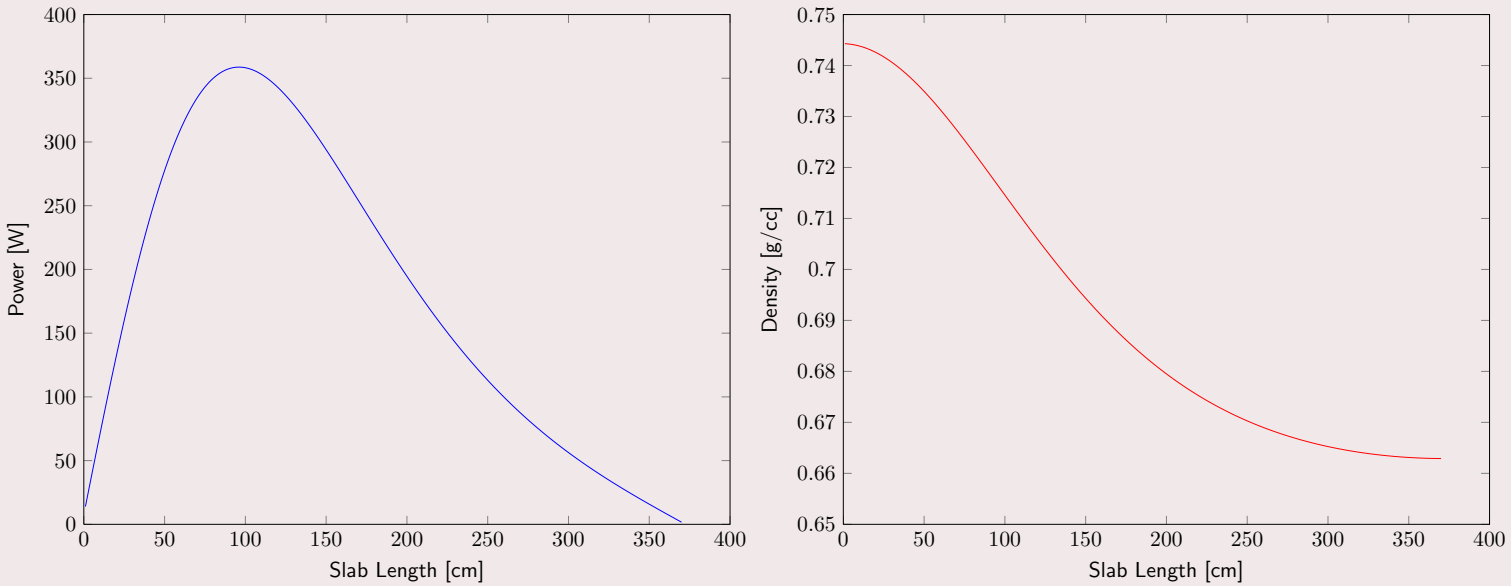
# Steady State - Coupled Neutronics/Thermal Hydraulics [2/2]

## Results




- Timing results using MATLAB profiler:
  - 7 seconds to converged overall
  - 6+ out of 7 seconds in X-Steam!
  - Solution: fit density range with polynomial - with linear fit $< 0.5$ seconds

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# Transient - Coupled Neutronics/Thermal Hydraulics [1/2]

## Residual Equations

$$\mathbf{F} = \begin{bmatrix} \boldsymbol{\Phi}^{n+1} - \boldsymbol{\Phi}^{n} + v\Delta t \left[\mathbb{M}\boldsymbol{\Phi}^{n+1} - (1-\beta)\,\lambda\mathbb{F}\boldsymbol{\Phi}^{n+1} - \lambda_d \mathbf{c}^{n+1}\right] \\ \mathbf{c}^{n+1} - \mathbf{c}^{n} + \Delta t \left(\lambda_d \mathbf{c}^{n+1} - \beta\lambda\mathbb{F}\boldsymbol{\Phi}^{n+1}\right) \\ \mathbf{Q} - \tilde{c}\mathbb{E}\boldsymbol{\Phi}\Delta x \\ \mathbf{T}^{n+1} - \mathbf{T}^{n} + \frac{\dot{m}\Delta t}{\mathcal{P}^{n+1} A \Delta x}\left(\mathbb{S}\mathbf{T}^{n+1} - \mathbb{R}\mathbf{Q}^{n+1}\right) \\ \mathcal{P} - \rho^{ref} - \frac{\partial \rho}{\partial T}\left(\mathbf{T} - T^{ref}\right) \\ \boldsymbol{\Sigma}_a - \Sigma_a^{ref} - \frac{\partial \Sigma_a}{\partial \rho}\left[\mathcal{P} - \rho^{ref}\right] \\ \nu\boldsymbol{\Sigma}_f - \nu\Sigma_f^{ref} - \frac{\partial \nu\Sigma_f}{\partial \rho}\left[\mathcal{P} - \rho^{ref}\right] \\ \mathbf{D} - D^{ref} - \frac{\partial D}{\partial \rho}\left[\mathcal{P} - \rho^{ref}\right], \\ \kappa\boldsymbol{\Sigma}_f - \kappa\Sigma_f^{ref} - \frac{\partial \kappa\Sigma_f}{\partial \rho}\left[\mathcal{P} - \rho^{ref}\right] \end{bmatrix}$$

- Code time per loop
- Number of GMRES and Newton

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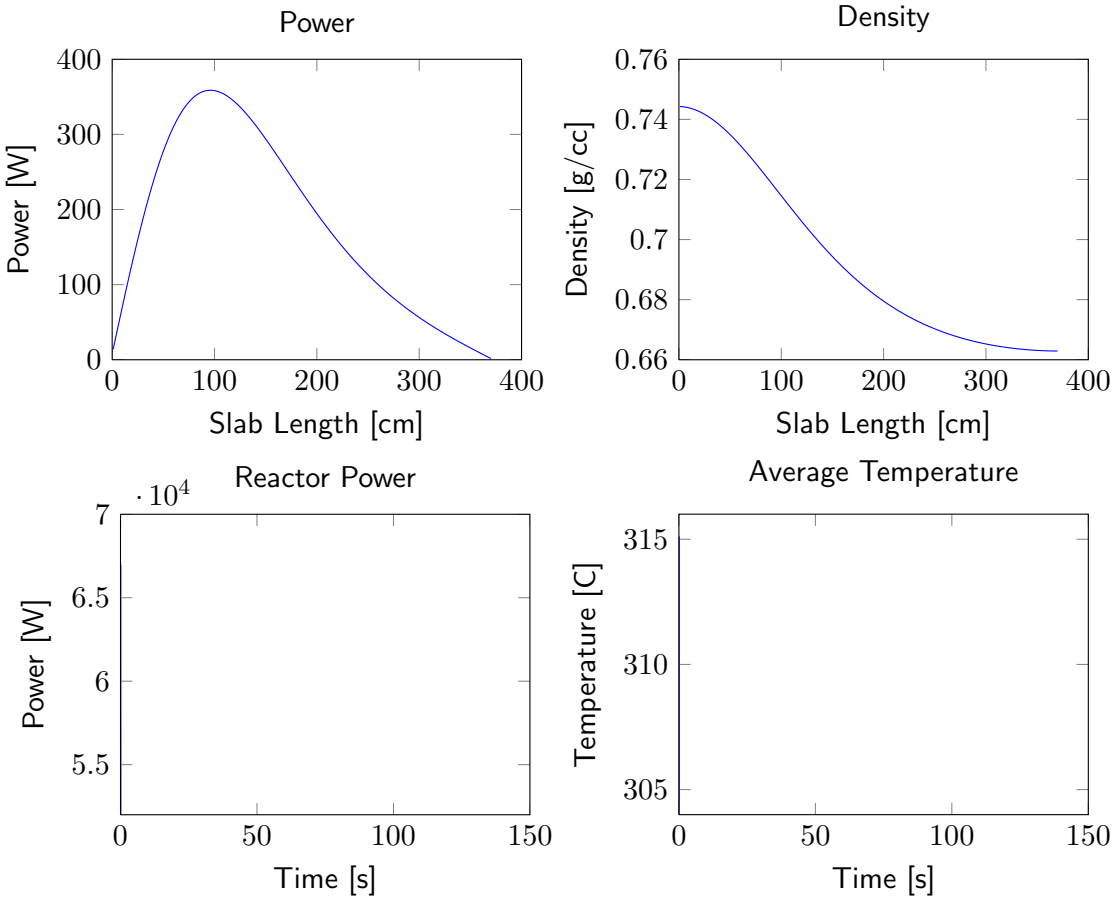
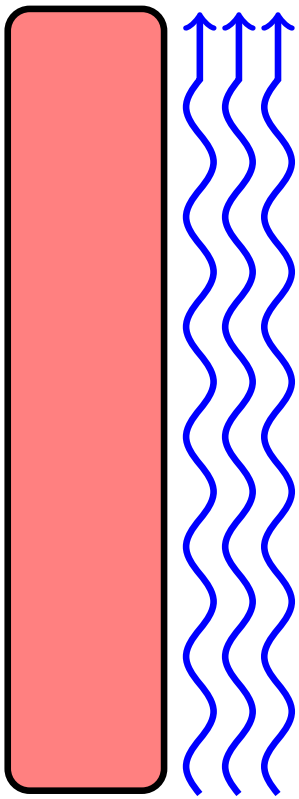
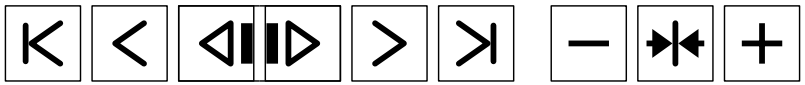
# Transient - Coupled Neutronics/Thermal Hydraulics [2/2]





# Conclusions

- JFNK methods are well suited for solving coupled systems
- Finite difference method for Jacobian-vector product works well
- Write your own steam tables or fit data with polynomial
- Watch out for scaling issues when coupling physics

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# Future Work

- Rewrite code in a compiled language (Fortran)
- Use PETSc Nonlinear solvers
- Model other important nuclear feedback mechanisms
- Compare JFNK to Operator-splitting methods
- This project can be downloaded from GitHub:

```
www.github.com/bhermanmit/JFNK
git clone git@github.com:bhermanmit/JFNK
```

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