

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

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December 8, 2011

Outline

1 Introduction

1 Governing Equations

1 Solvers

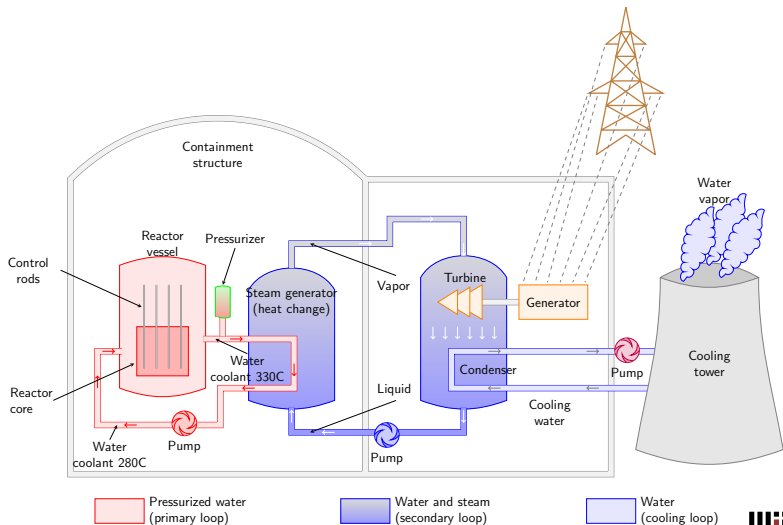
1 Results

1 Conclusions

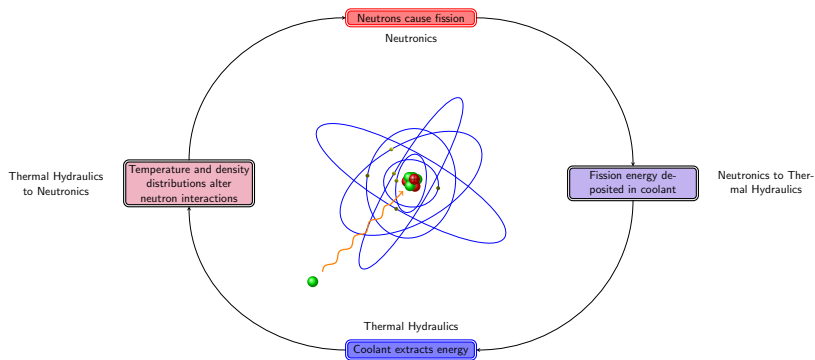
Motivation

- 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



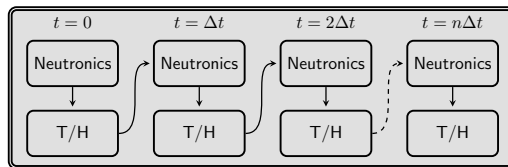
Nuclear Feedback



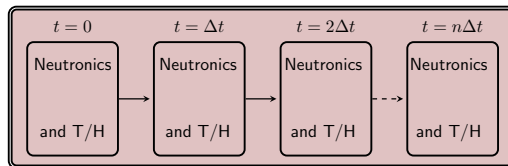
- Fuel Temperature Feedback - $T_f \uparrow$, U-238 Capture \uparrow , Fission Rate \downarrow , Power \downarrow
- Coolant Density Feedback - $\rho \downarrow$, $E_n \uparrow$, Fission Rate \downarrow , Power \downarrow

Common Approach to Coupling: Operator Splitting

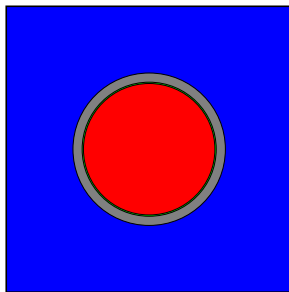
- Solve physics independently and iterate between them



- Fully coupled approach solves the nonlinear physics together

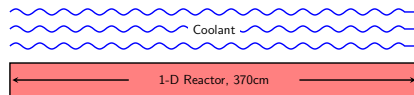


1-D Slab Reactor Geometry



■ Coolant ■ Clad ■ Gas Gap ■ Fuel

Top-view
Fuel Rod Unit-Cell



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

Neutronics

■ Basic Neutron Conservation:

$$\textit{Change} + \textit{Leakage} + \textit{Interactions} = \textit{Scattering} + \textit{Fission}$$

■ Neutron Transport Equation:

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

■ Neutron Diffusion Equation (1-D Energy Integrated)

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

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

Discretization of Neutronics Equations

Assumptions:

- 1 One-dimensional finite volume spatial discretization
- 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

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

- Matrix-form of precursors

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

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 volumetric heat source in 1-D

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

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

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

Discretization of Energy Equation

Assumptions:

- 1 One-dimensional finite volume spatial discretization
- 2 Upwind difference scheme for flux
- 3 Specify inlet conditions and mass flow rate
- 4 Implicit Euler time discretization

- spatial discretization

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

- Matrix-form with time discretization

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

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

Physics Coupling

Neutronics-Thermal Hydraulics

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

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

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

Thermal Hydraulics-Neutronics

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

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

The Steady-State Eigenvalue Problem

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

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

- Eigenvalue, λ , and eigenvector, Φ , must be determined
- Flux-power normalization constant determined from reactor power

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

- λ and \tilde{c} are input as constants for time-dependent calculations

Newton's Method

Procedure:

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

Three major tasks:

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

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

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

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

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

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

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

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

[‡]Yousef 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.

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, η , is used

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

- At initial Newton iterations, GMRES will not be converged very tightly
- For the last couple of Newton iterations, convergence may be too tight - Limit how small linear tolerance is

Jacobian-Free Approximation

- Recall a Krylov subspace: $\mathcal{K}_n(\mathbb{A}, \mathbf{v}) = \text{span} \{ \mathbf{v}, \mathbb{A}\mathbf{v}, \mathbb{A}^2\mathbf{v}, \dots, \mathbb{A}^{n-1}\mathbf{v} \}$
- The matrix \mathbb{A} is always multiplying a vector, so why create \mathbb{A} when it is only used to multiply a vector?
- Option 1: Preform Jacobian-vector analytically

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

- Analytic method can get very complex, but can be done!
- 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: 2 Function calls, saves memory and possibly computational time to form Jacobian
- ϵ is the perturbation parameter and is somewhat arbitrary - Mousseau[§] recommends:

$$\epsilon = \frac{\sum_{i=1}^N bx_i}{N \|\mathbf{y}\|_2}$$

[§]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.

Preconditioning

- Want to limit number of GMRES iterations - computational time and memory
- An approx. preconditioner is formed from the Jacobian
- 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:

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

Steady State - Neutronics

- Residual Equations

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

- 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 (dominance ratio)
- Use a few power iterations to get gross flux shape

Conclusions