Simulation of Fast Reactors with the Finite Element Method and Multiphysics Models

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March 8, 2019

Disclaimer

This material is based upon work supported under an Integrated University Program Graduate Fellowship. Any opinions, findings, conclusions, or recommendations expressed in this publication are those of the author and do not necessarily reflect the views of the Department of Energy Office of Nuclear Energy.

Table of Contents

Outline

Why are we here?

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Model a nuclear reactor.

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Model a nuclear reactor.

- Neutron distribution.
- Thermal hydraulics.
- Thermal expansion.

Current Simulation Procedure

- Heuristically estimate material temperatures.
- Manually calculate thermally expanded dimensions.
- Manually homogenize assembly number densities.
- Run DIF3D and collect k_{eff} and power distribution.

Current Simulation Procedure

- Heuristically estimate material temperatures.
- Manually calculate thermally expanded dimensions.
- Manually homogenize assembly number densities.
- Run DIF3D and collect k_{eff} and power distribution.

No thermal feedback or multiphysics simulation capability.
Modern numerical methods can be implemented.

Goals

- Easy user input with intuitive keywords.
  - Reactor geometry via VTK mesh.
  - Temperature dependent cross sections either plain-text or ISOTXS format.
  - Pin and assembly dimensions.
  - Material compositions.
- Simulate thermal expansion and thermal hydraulics internally.
- Collect k_{eff}, reactor power distribution, and average material temperatures.

Outline

Multigroup Neutron Diffusion Equation

$$
\begin{aligned}
&-\nabla \cdot \left(D_g(\mathbf{r})\nabla\phi_g(\mathbf{r})\right) + \Sigma_{r,g}(\mathbf{r})\phi_g(\mathbf{r}) = \\
&\qquad \frac{\widetilde{\chi_g}(\mathbf{r})}{k_{eff}} \sum_{g'=1}^{G} \nu\Sigma_{f,g'}(\mathbf{r})\phi_{g'}(\mathbf{r}) + \sum_{\substack{g'=1 \\ g'\neq g}}^{G} \Sigma_{s,g'\to g}(\mathbf{r})\phi_{g'}(\mathbf{r})
\end{aligned}
$$

$$
\begin{aligned}
D_g(\mathbf{r}) &= \text{diffusion coefficient for energy group } g \text{ [cm]}, \\
\phi_g(\mathbf{r}) &= \text{scalar neutron flux for energy group } g \left[\frac{1}{\text{cm}^2\ \text{s}}\right], \\
\Sigma_{r,g}(\mathbf{r}) &= \text{macroscopic removal cross section for energy group } g \left[\frac{1}{\text{cm}}\right], \\
\widetilde{\chi_g}(\mathbf{r}) &= \text{effective fission spectrum for energy group } g, \\
k_{eff} &= \text{effective neutron multiplication factor}, \\
\nu\Sigma_{f,g}(\mathbf{r}) &= \text{number of fission neutrons times macroscopic fission} \\
& \ \text{cross section in energy group } g \left[\frac{1}{\text{cm}}\right], \\
\Sigma_{s,g'\to g}(\mathbf{r}) &= \text{macroscopic scatter cross section from energy group } g' \text{ to} \\
& \ \text{energy group } g \left[\frac{1}{\text{cm}}\right], \\
G &= \text{total number of energy groups (typically } G = 33\text{)}.
\end{aligned}
$$

Boundary Conditions

For problem domain Ω and boundary $\partial\Omega$.
$\hat{\mathbf{n}}$ is the outward normal direction on the boundary.

1. Mirror.

$$\nabla \phi_g(\mathbf{r}) \cdot \hat{\mathbf{n}} = 0 \text{ for } \mathbf{r} \in \partial\Omega$$

2. Albedo.

$$D_g(\mathbf{r}) \nabla \phi_g(\mathbf{r}) \cdot \hat{\mathbf{n}} + \alpha \phi_g(\mathbf{r}) = 0 \text{ for } \mathbf{r} \in \partial\Omega$$

   $\alpha \in \mathbb{R}$ is a scalar constant specified by the user.
   For non-reentrant (vacuum) boundary condition, $\alpha = \frac{1}{2}$.

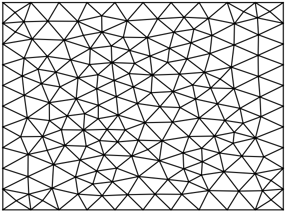
3. Zero Flux.

$$\phi_g(\mathbf{r}) = 0 \text{ for } \mathbf{r} \in \partial\Omega$$

Finite Element Method (FEM) Discretization

Divide the domain Ω into a set of unstructured, non-overlapping, finite elements (e.g. Delaunay triangulation).

$$\Omega = \Omega_1 \cup \Omega_2 \cup \Omega_3 \cup \ldots \cup \Omega_{N_E}$$
$$\Omega = \{\Omega_e\} \text{ for } e = 1, 2, \ldots, N_E$$
$$\Omega_i \cap \Omega_j = \emptyset \text{ for } i \neq j$$



Example Rectangular Mesh.

Combining Neutron Source

- Neutron sources are combined into a single term.

$$-\nabla \cdot (D_g(\mathbf{r})\nabla\phi_g(\mathbf{r})) + \Sigma_{r,g}(\mathbf{r})\phi_g(\mathbf{r}) = q_g(\mathbf{r})$$

$$q_g(\mathbf{r}) = q_{g,e} \; \forall \; \mathbf{r} \in \Omega_e$$

$$\overline{\phi}_{g,e} = \frac{1}{N_p} \sum_{i \in \Omega_e}^{N_p} \phi_{i,g}$$

- Neutron source $q_{g,e}$ is constant over an element Ω_e.
- Cross sections are constant within an element.

Finite Element Method (FEM)

Multiply the multigroup neutron diffusion equation by a testing function $v(\mathbf{r}) \in H_1(\Omega)$ and integrate over the problem domain. $H_1(\Omega)$ is a Sobolev space.

This yields the **Weak Form** of the problem.

$$-\int_{\Omega} \nabla\cdot(D_g(\mathbf{r})\nabla\phi_g(\mathbf{r}))v(\mathbf{r})\ d\mathbf{r} + \int_{\Omega} \Sigma_{r,g}(\mathbf{r})\phi_g(\mathbf{r})v(\mathbf{r})\ d\mathbf{r} = \int_{\Omega} q_g(\mathbf{r})v(\mathbf{r})\ d\mathbf{r}$$

Partition the integral into a summation of integrals over elements.

$$-\sum_{e=1}^{N_E} D_{g,e}\int_{\Omega_e} \nabla\cdot\nabla\phi_g(\mathbf{r})v(\mathbf{r})\ d\mathbf{r} + \sum_{e=1}^{N_E}\Sigma_{r,g,e}\int_{\Omega_e}\phi_g(\mathbf{r})v(\mathbf{r})\ d\mathbf{r} = \sum_{e=1}^{N_E} q_{g,e}\int_{\Omega_e} v(\mathbf{r})\ d\mathbf{r}$$

Second Green's Theorem

Use the Second Green's Theorem to rewrite the first integral [Li18].

$$-\sum_{e=1}^{N_E} D_{g,e} \int_{\partial\Omega_e} v(\mathbf{r}) \nabla \phi_g(\mathbf{r}) \cdot \hat{\mathbf{n}} \; ds + \sum_{e=1}^{N_E} D_{g,e} \int_{\Omega_e} \nabla \phi_g(\mathbf{r}) \cdot \nabla v(\mathbf{r}) \; d\mathbf{r} + \sum_{e=1}^{N_E} \Sigma_{r,g,e} \int_{\Omega_e} \phi_g(\mathbf{r}) v(\mathbf{r}) \; d\mathbf{r} = \sum_{e=1}^{N_E} q_{g,e} \int_{\Omega_e} v(\mathbf{r}) \; d\mathbf{r}$$

Galerkin Finite Element Method (FEM)

Galerkin FEM assumes the solution $\phi_g(\mathbf{r})$ is a linear combination of chosen basis functions $\{N_i\}$.

$$\phi_g(\mathbf{r}) = \sum_{i=1}^{DOF} \upsilon_{g,i} N_i(\mathbf{r})$$

$v(\mathbf{r}) \in H_1(\Omega)$ is arbitrary and is chosen to be a linear combination of the basis functions with unit magnitude.

$$v(\mathbf{r}) = \sum_{j=1}^{DOF} N_j(\mathbf{r})$$

Typically, $N(\mathbf{r})$ is a polynomial of a chosen order (e.g. linear, quadratic, cubic).

Linear System of Equations

Including albedo form of boundary condition and assumption of linear combination of basis functions.

$$\sum_{i=1}^{DOF} \upsilon_{i,g} \sum_{j=1}^{DOF} \left(\sum_{e=1}^{N_E} \alpha \int_{\partial\Omega_e} N_i(\mathbf{r}) N_j(\mathbf{r}) ds + \sum_{e=1}^{N_E} D_{g,e} \int_{\Omega_e} \nabla N_i(\mathbf{r}) \cdot \nabla N_j(\mathbf{r}) d \right.$$

$$\left. + \sum_{e=1}^{N_E} \Sigma_{r,g,e} \int_{\Omega_e} N_i(\mathbf{r}) N_j(\mathbf{r})\ d\mathbf{r} \right) = \sum_{i=1}^{DOF} \left(\sum_{e=1}^{N_E} q_{g,e} \int_{\Omega_e} N_i(\mathbf{r})\ d\mathbf{r} \right)$$

Rewriting in the form common to the FEM.

$$a_g(N_i, N_j) = f_g(N_i)$$

In the form common to linear systems.

$$\mathbf{A}_g\, \mathbf{u}_g = \mathbf{f}_g$$
$$\mathbf{u}_g = \{\upsilon_{i,g}\}$$

Properties of $\mathbf{A}_g \, \mathbf{u}_g = \mathbf{f}_g$

- Properties of the linear system include:
  - Sparse.
  - Matrix, $\mathbf{A}_g$, is Symmetric Positive Definite (SPD) [Hug87].
  - Solution, $\mathbf{u}_g$, is unique and bounded by Lax-Milgram Lemma [Li18].
- Solution via Conjugate Gradient (CG) method [Kel95].

Integration

Integrals of interest:

$$\int_{\Omega_e} \nabla N_i(\mathbf{r}) \cdot \nabla N_j(\mathbf{r}) \, d\mathbf{r}$$

$$\int_{\Omega_e} N_i(\mathbf{r}) N_j(\mathbf{r}) \, d\mathbf{r}$$

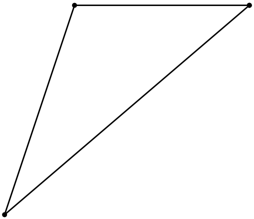
$$\int_{\Omega_e} N_i(\mathbf{r}) \, d\mathbf{r}$$

$$\int_{\partial\Omega_e} N_i(\mathbf{r}) N_j(\mathbf{r}) \, ds$$

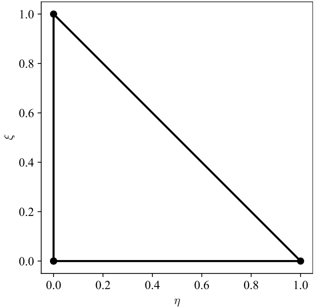
Options for integration:

- Analytic.
- Numeric (quadrature).
  - Linear (Gaussian).
  - Triangular.

Triangular Elements

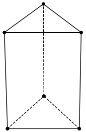


General Triangle Element.

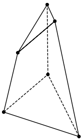


Reference Triangle.

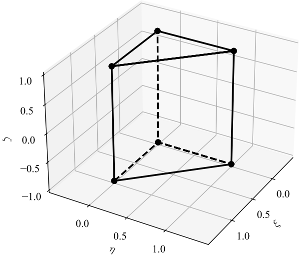
Wedge Elements



General Wedge Element.



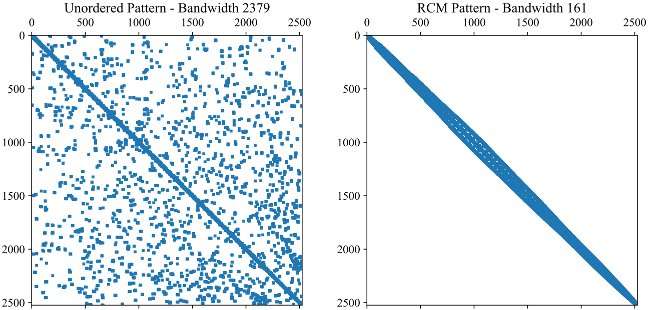
Distorted Wedge Element.



Description of Reference Wedge.

RCM Matrix Ordering

- Matrix is reordered to increase computational efficiency and compute the same solution.
- Reverse Cuthill-McKee (RCM) order is chosen [Cut69].



Power Iteration Method

- Solution for largest eigenvalue k_{eff} and associated eigenvector Φ.
- Rewrite the multigroup neutron diffusion equation.

$$\mathbf{B}(\Phi, k_{eff})\,\Phi = \frac{1}{k_{eff}}\mathbf{M}\,\Phi$$

- The solution can be written.

$$\Phi = \frac{1}{k_{eff}}\mathbf{R}\,\Phi \quad \text{where} \quad \mathbf{R} = \mathbf{B}^{-1}\,\mathbf{M}$$

- Note: the FEM is used to calculate Φ, not $\mathbf{R}$.
- The power iteration method proceeds.

$$\Phi^{(s+1)} = \frac{1}{k_{eff}^{(s)}}\mathbf{R}\,\Phi^{(s)}$$

$$k_{eff}^{(s+1)} = k_{eff}^{(s)}\frac{\langle \mathbf{w}, \Phi^{(s+1)}\rangle}{\langle \mathbf{w}, \Phi^{(s)}\rangle} \qquad s = 1, 2, \ldots, \infty$$

Power Iteration Algorithm

Algorithm 1 General Iteration Scheme

Read mesh from VTK.
Initialize $\overline{\phi}_g^{(0)}$.
Order the nodes of the mesh into RCM order.
Calculate $\Sigma_{s,g'\to g}$, $\Sigma_{r,g}$, and $\nu\Sigma_{f,g}$ for each element.
Calculate finite element matrix $\mathbf{A}_g$ for each group. Store this.
while Power Iteration **do**
    Update the iteration counter. $s = s + 1$
    Update $q_{fiss,g}$ and $q_{up,g}$ for all groups from previous data $\overline{\phi}^{(s-1)}$.
    Update $\widetilde{\chi_g}$ in each element using previous data.
    for $g = 1, G$ **do**
        Update $q_{down,g}$ from current data $\overline{\phi}_g^{(s)}$
        Calculate total source in each element.
        Update finite element Vector $\mathbf{f}_g$ with new source.
        Solve $\mathbf{A}_g \mathbf{u}_g = \mathbf{f}_g$ using an iterative technique (CG).
        Parse $\mathbf{u}_g$ for ϕ_g solution on nodes.
        Calculate element-average $\overline{\phi}_g$.
    Update k_{eff}.
    Check convergence.
    Perform non-linear update if necessary and update $\mathbf{A}_g$.

Outline

Verification and Validation

- "Code Verification"
  - Compare computational results to exact analytic or manufactured results.
  - Demonstrate the code is solving equations correctly as designed.
  - Quantified numerical errors.
- "Solution Verification"
  - Compare computational results to benchmark results for the intended application of the solver.
  - Computational results from a different method or experimental data.
  - Typically verified by others previously.

Error Analysis

FEM with linear elements is second-order convergent in space [Li18].

$$\mathbf{e} = \phi(\mathbf{r}) - \phi_{FEM}$$

$$\|\mathbf{e}\|_\infty \leq ch^2 \|\nabla^2 \phi(\mathbf{r})\|_\infty$$

Define Root-Mean-Squared (RMS), maximum, and k_{eff} errors.

$$\mathrm{RMS}(\mathbf{e}) = \sqrt{\frac{1}{N}\sum_{i=1}^{N} e_i^2}$$

$$\|\mathbf{e}\|_\infty = \max_{i=1,2,\ldots,N} |e_i|$$

$$k_{eff} \text{ error [pcm]} = (k_{ref} - k_{eff}) \times 10^5$$

The method is second-order spatially convergent.

$$4 = \frac{e^{(i-1)}}{e^{(i)}}$$

Analytic Solutions

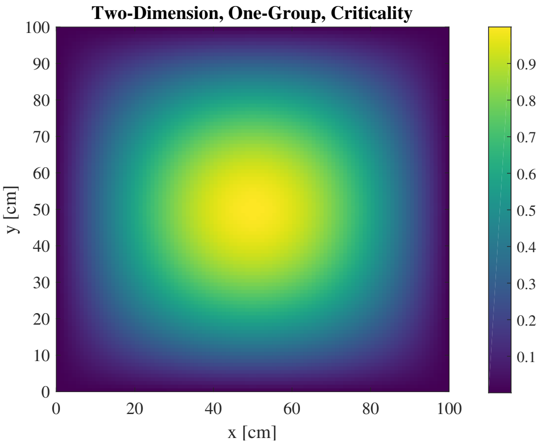
- 6 analytic multigroup neutron diffusion problems.
- Varied number of spatial dimensions, energy groups, and number of materials.

Case	Dimensions	Groups	Criticality	Materials
1	1	1		1
2	1	1	✓	1
3	2	1	✓	1
4	1	2	✓	1
5	1	1	✓	2
6	3	1	✓	1

Two-Dimension, One-Group, Criticality

Refine	k_{eff}	k_{eff} error [pcm]	k_{eff} ratio	RMS	RMS ratio	$\|\|\mathbf{e}\|\|_\infty$	$\|\|\mathbf{e}\|\|_\infty$ ratio
0	1.983243	1281.65	4.03	1.90E-02	1.66	6.63E-02	1.49
1	1.992884	317.64	3.96	1.15E-02	2.65	4.45E-02	2.59
2	1.995258	80.16	3.98	4.32E-03	3.43	1.72E-02	3.41
3	1.995858	20.15	3.99	1.26E-03	3.88	5.04E-03	3.87
4	1.996009	5.05	4.00	3.25E-04	3.96	1.30E-03	3.96
5	1.996047	1.26	4.00	8.20E-05	3.93	3.28E-04	3.93
6	1.996057	0.32		2.09E-05		8.34E-05	
Ref.	1.996060						

Two-Dimension, One-Group, Criticality

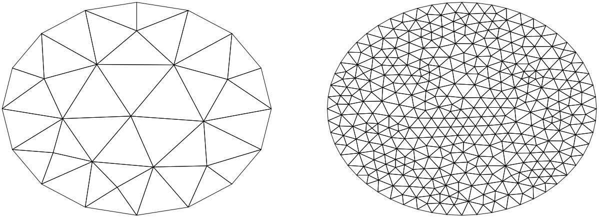


$$\phi(x,y) = \phi_0 \sin\left(\frac{\pi}{L_x}x\right)\sin\left(\frac{\pi}{L_y}y\right)$$

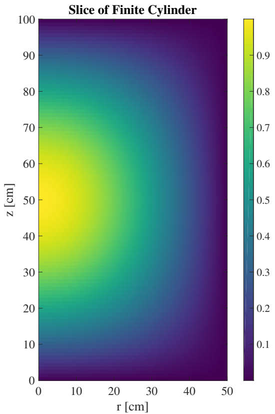
Three-Dimension, One-Group, Finite Cylinder

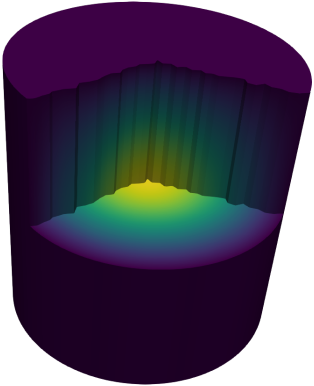
Refine	k_{eff}	k_{eff} error [pcm]	k_{eff} ratio	RMS	RMS ratio	$\lVert\mathbf{e}\rVert_\infty$	$\lVert\mathbf{e}\rVert_\infty$ ratio
0	0.895108	10160.26	4.18	5.34E-02	2.57	2.12E-01	1.62
1	0.972412	2429.90	4.16	2.07E-02	3.19	1.31E-01	4.65
2†	0.990870	584.06	3.90	6.50E-03	1.85	2.81E-02	1.79
3	0.995215	149.61	3.99	3.51E-03	9.22	1.57E-02	8.28
4	0.996336	37.48		3.81E-04		1.90E-03	
Ref.	0.996711						

† Refinement ratio $\approx$ 1 but next case $\approx$ 8.
This is due to the movement of mesh nodes in the process of circular mesh regeneration.



Three-Dimension, One-Group, Finite Cylinder





$$\phi(r,z) = \phi_0 \, J_0\left(\frac{\alpha_0}{T} r\right) \sin\left(\frac{\pi}{H} z\right)$$

Benchmark Solutions

- 9 benchmark problems.
- Two and three dimensional geometry.
- Varied energy group structure and neutron spectrum.

Benchmark	Dimensions	Groups	Reactor Type	Neutron Spectrum
VVER440	2	2	LWR	Thermal
SNR	2	4	SFR	Fast
HWR	2	2	HWR	Thermal
IAEA (×4)	2	2	PWR	Thermal
MONJU	3	3	SFR	Fast
KNK	3	4	SFR	Fast

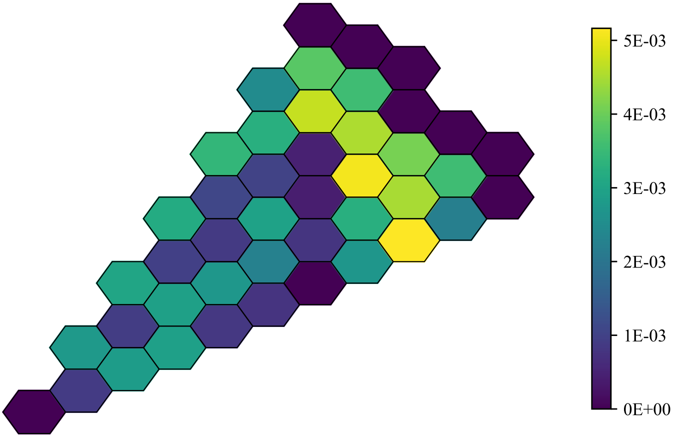
VVER440

- Two-dimensional.
- Light Water Reactor (LWR).
- Two-group.

Refine	k_{eff}	k_{eff} error [pcm]
0	1.005932	376.80
1	1.008980	72.00
2	1.009572	12.82
3	1.009666	3.35
4	1.009692	0.76
5	1.009698	0.22
Ref.†	1.009700	

† See [Cha95].

VVER440 Benchmark Power Comparison



VVER440 Benchmark Power Comparison for Most Refined Mesh.

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MONJU

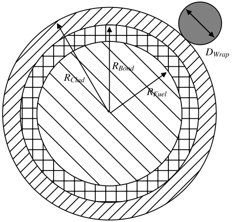
- Three-dimensional.
- Sodium-cooled Fast Reactor (SFR).
- Three-group.
- Case A. Control rods fully removed.
- Case B. Control rods partially inserted.
- Case C. Control rods fully inserted.

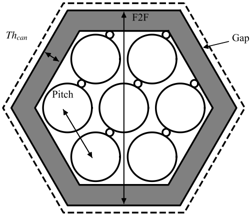
Pattern	k_{eff}	Rod Worth $[\Delta k]$	Rod Difference $[\%\Delta k]$
A	1.056816		
B	1.031623	0.023 (2.51E-5) †	2.52 (-0.07)
C	1.006519	0.047 (1.77E-3)	5.03 (0.04)

† Value in parentheses is difference to reference value [Kom78].

Outline

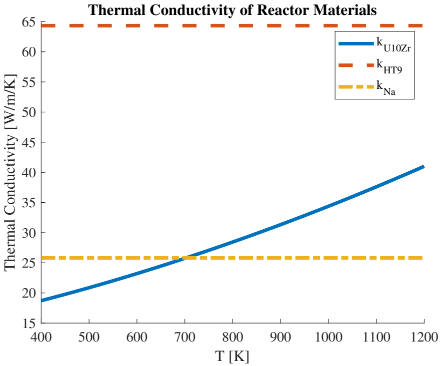
Assembly Geometry



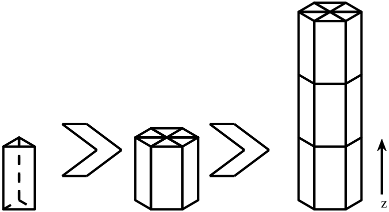


Material Properties

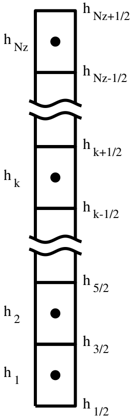
- Functional sodium properties [Fin95].
- Clad and bond thermal conductivity assumed constant [Lei88].
- Fuel thermal conductivity assumed a function of temperature [Kim14].



Axial Convection Geometric Model



Progression of Element (left), to Chunk (center), to Channel (right).



Nodalization for channel i.

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Channel Enthalpy

Steady-state coolant enthalpy within the channel is given by an energy balance.

$$h_{i,k+1/2} = h_{in} + \frac{1}{\dot{m}_i} \sum_{k'=1}^{k} q_{i,k'}$$

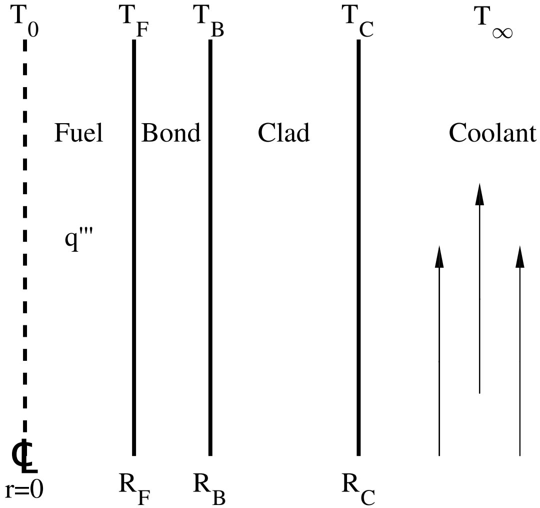
Use a first-order approximation to estimate the chunk-average enthalpy.

$$h_{i,k} = \frac{1}{2}\left(h_{i,k-1/2} + h_{i,k+1/2}\right)$$

$T_{\infty,i,k}$ is then given by a state relationship [Fin95].

$$T_{\infty,i,k} = T\left(h_{i,k}\right)$$

Radial Conduction Geometric Model



Clad Surface Temperature – Subbotin-Ushakov

Using Newton's Law of Cooling.

$$q''_{clad} = H_c (T_C - T_\infty)$$

H_c is given by the Subbotin-Ushakov correlation [Pfr07] which relates the Nusselt and Péclet numbers for $1 < Pe < 4,000$ and $1.2 \leq S/D \leq 2.0$.

$$Pe = Re\,Pr$$

$$Nu = 7.55\frac{S}{D} - 20\left(\frac{S}{D}\right)^{-13} + \frac{3.67}{90\left(\frac{S}{D}\right)^2} Pe^{\left(0.56+0.19\frac{S}{D}\right)}$$

$$H_c = \frac{Nu\,k}{D_e}$$

Then, the clad surface temperature, T_C follows.

Fuel Centerline Temperature

Define a conductivity integral.

$$K_F(T) = \int_0^T k_F(T')\, dT'$$

The value of the conductivity integral is given by the heat conduction equation.

$$K_F(T_0) = K_F(T_F) + \frac{q'''_{i,k}}{4} R_F^2$$

Then, a bisection method search is used to calculate T_0 given a functional form of $K_F(T)$.

Average Material Temperatures

Average temperatures in the clad and bond are calculated analytically.

$$\overline{T_C} = T_B - \frac{q'''_{i,k}}{4k_C} R_F^2 \left(\frac{2\, R_C^2 \ln\left(\frac{R_C}{R_B}\right)}{R_C^2 - R_B^2} - 1 \right)$$

$$\overline{T_B} = T_F - \frac{q'''_{i,k}}{4k_B} R_F^2 \left(\frac{R_F^2 - R_B^2 + 2\, R_B^2 \ln\left(\frac{R_B}{R_F}\right)}{R_B^2 - R_F^2} \right)$$

Average Fuel Temperature

Calculate an effective thermal conductivity in the fuel.

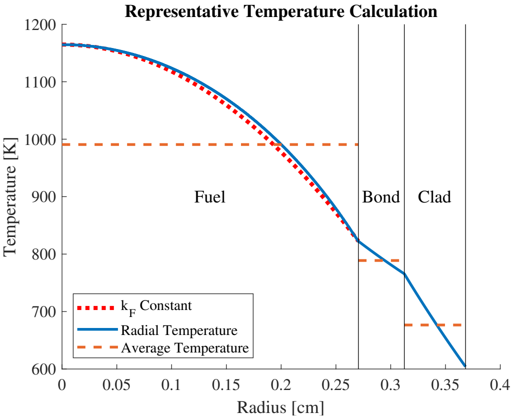
$$\overline{k_F} = \frac{q'''_{i,k} R_F^2}{4(T_0 - T_F)}$$

Assume thermal conductivity is constant $\overline{k_F}$.
Calculate an analytic value for the average fuel temperature.

$$\overline{T_F} = T_0 - \frac{q'''_{i,k}}{8\overline{k_F}} R_F^2$$

$\overline{T_F}$ is used to calculate fuel cross sections.
Due to self-shielding, an effective fuel temperature would weight the surface temperature more.

Radial Temperatures for Typical Fuel Rod



Difference less than 15 [K].

Cross Section Treatment – Coolant & Bond

- Number density and microscopic cross sections are functionalized and updated based on $T_{\infty,i,k}$.
- Linear interpolation for microscopic cross sections.

Number density functionalization.

$$M_{Na} = 22.989769 \left[\frac{\text{gram}}{\text{mol}}\right]$$

$$N_{Na}(T) = \frac{\rho_{Na}(T)\, N_A}{M_{Na}}$$

Microscopic cross section functionalization for $T_n < T_{\infty,i,k} < T_{n+1}$.

$$\Sigma_{x,i,k,g} = N_{Na}(T_{\infty,i,k}) \left(\frac{T_{\infty,i,k} - T_n}{T_{n+1} - T_n} (\sigma_{x,Na,g,n+1} - \sigma_{x,Na,g,n}) + \sigma_{x,Na,g,n} \right)$$

Bond is assumed to have the same macroscopic cross section as coolant. Consistent with homogenization approximation.

Cross Section Treatment – Clad

- Macroscopic cross section updated based on $\overline{T_{C,i,k}}$.
- Linear interpolation.

Macroscopic cross section functionalization for $T_n < \overline{T_{C,i,k}} < T_{n+1}$.

$$\Sigma_{x,i,k,g} = \frac{\overline{T_{C,i,k}} - T_n}{T_{n+1} - T_n} \left(\Sigma_{x,g,n+1} - \Sigma_{x,g,n}\right) + \Sigma_{x,g,n}$$

Cross Section Treatment – Fuel

- Macroscopic cross section update based on $\overline{T_{F,i,k}}$.
- Square-root interpolation due to Doppler effect.

Macroscopic cross section functionalization for $T_n < \overline{T_{F,i,k}} < T_{n+1}$.

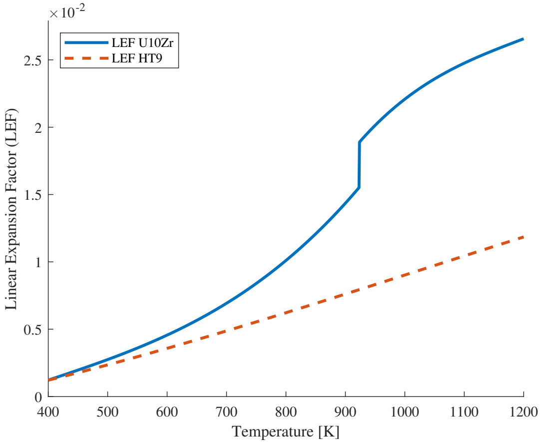
$$\Sigma_{x,i,k,g} = \frac{\sqrt{\overline{T_{F,i,k}}} - \sqrt{T_n}}{\sqrt{T_{n+1}} - \sqrt{T_n}} \left(\Sigma_{x,g,n+1} - \Sigma_{x,g,n}\right) + \Sigma_{x,g,n}$$

Outline

Thermal Expansion Motivation

- Strong feedback.
- Metallic fuels.
- Small active fuel region with high leakage ($\mathcal{L} \approx 20\%$).
- Experimental Breeder Reactor II (EBR-II) designed and built by Argonne National Laboratory (ANL) [Til11].
  - Full-power demonstrations from April 1986 [Pla87].
  - Unprotected Loss-Of-Flow (ULOF).
  - Unprotected Loss-Of-Heat-Sink (ULOHS).

Material Properties



Linear Expansion Factor for HT9 Steel and U10Zr Fuel.

Simplified Thermal Expansion Model

- User input expansion temperatures $T_{exp,fuel}$ and $T_{exp,struct}$.
- Leakage effects.
  - Finite Elements.
    - Radial (x and y) directions expanded as structural material, HT9 stainless steel.
    - Axial (z) direction expanded as fuel material, U10Zr.
  - Area fractions.
    - Fuel radius expanded as U10Zr.
    - All other material expanded as HT9 stainless steel.
- Density Effects.
  - Material densities decreased to conserve quantity of material.
  - Cross sections decrease proportionally according to $\Sigma = N\sigma$.

Finite Element Expansion

- Define radial and axial expansion factors.

$$F_r\left(T_{exp,struct}\right) = 1 + \left(\frac{\Delta L}{L}\right)_{\text{HT9}}$$

$$F_a\left(T_{exp,fuel}\right) = 1 + \left(\frac{\Delta L}{L}\right)_{\text{U10Zr}}$$

- Expand all coordinates in the finite element mesh.

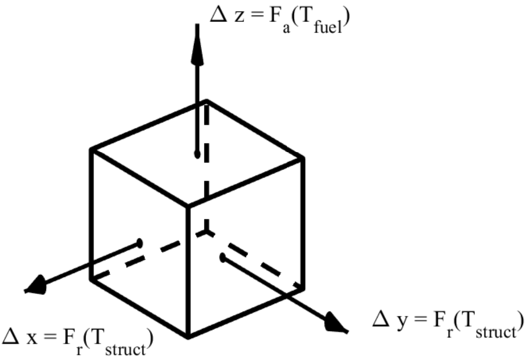
$$x^H = x^C \, F_r\left(T_{exp,struct}\right)$$

$$y^H = y^C \, F_r\left(T_{exp,struct}\right)$$

$$z^H = z^C \, F_a\left(T_{exp,fuel}\right)$$

- Elements will not overlap or intersect due to uniform expansion assumptions.

Arbitrary Volume Expansion



$$\frac{V^C}{V^H} = \frac{1}{(F_r(T_{exp,struct}))^2(F_a(T_{exp,fuel}))}$$

Area Fraction Expansion

- Dimensions within a hexagonal assembly are expanded.
- Area fractions are used for cross section homogenization.
- Fuel radius, R_F, expanded as U10Zr.
- All other dimensions expanded as HT9 stainless steel.
- No general formula for expansion of area fractions, calculated directly.

Conservation of Material & Cross Section Effects

Conservation of number of atoms of species i.

$$n_i^H = n_i^C$$

Rewrite the number of atoms using number density and volume.

$$N_i^H V_i^H = N_i^C V_i^C$$

Volume V_i can be expressed using element volume and area fraction.

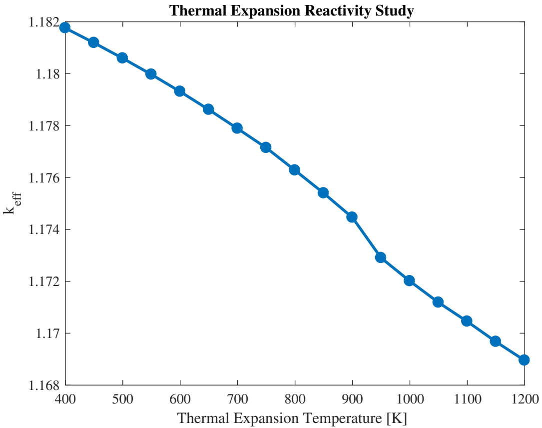
$$N_i^H = N_i^C \frac{a_j^C V_e^C}{a_j^H V_e^H}$$

Recall the volume ratio.

$$N_i^H = N_i^C \frac{a_j^C}{a_j^H} \frac{1}{(F_r(T_{exp,struct}))^2 F_a(T_{exp,fuel})}$$

Macroscopic cross sections can be updated directly.

Demonstration of Reactor Thermal Expansion



Effective Neutron Multiplication Factor as a Function of Thermal Expansion Temperature.

Outline

Remember why we are here.

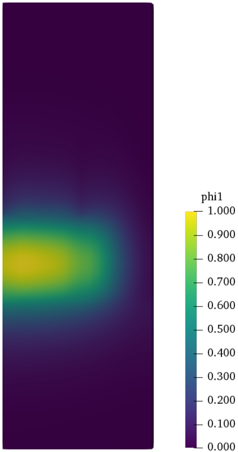
Remember why we are here.

Model a nuclear reactor.

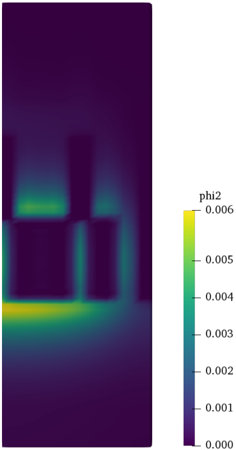
Advanced Burner Reactor (ABR) – MET-1000

- Benchmark published February 2016 [OEC16].
- Four designs including MET-1000.
- 31 independent solutions submitted so far including DIF3D.
- Cross sections generated independently.

Benchmark Results



ϕ_1



ϕ_2

$$k_{eff} = 1.006694 \quad \text{(DIF3D} -700 \text{ [pcm])}$$

Reactivity Coefficients

The reactivity of a reactor can be defined.

$$\rho_i = \frac{k_{\mathit{eff},i} - 1}{k_{\mathit{eff},i}}$$

Reactivity coefficient is a derivative with respect to a variable of interest.

$$\alpha_x(x_i) = \left.\frac{\partial \rho}{\partial x}\right|_{x=x_i}$$

$$\Delta\rho \approx \alpha_x(x_i)\,\Delta x$$

Reactivity Coefficient Formulae

Consider a series of reactor powers $Q_{Rx,i} = \{0\%, \ldots, 100\%\}$. Define the following reactivity coefficients.

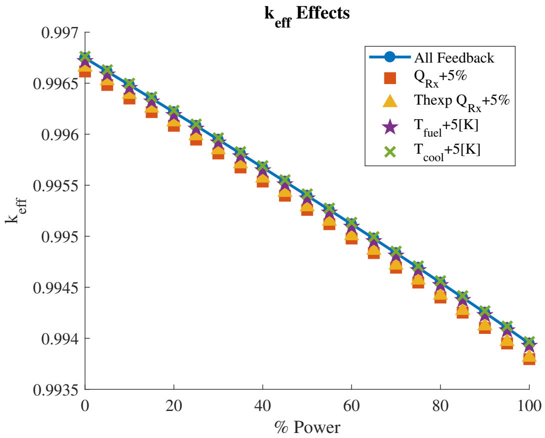
$$\alpha_{power}(Q_{Rx,i}) = \frac{\rho(Q_{Rx,i}) - \rho(Q_{Rx,i} + \Delta Q_{Rx})}{\Delta Q_{Rx}}$$

$$\alpha_{thexp}(Q_{Rx,i}) = \frac{\rho(T_{exp}(Q_{Rx,i})) - \rho(T_{exp}(Q_{Rx,i} + \Delta Q_{Rx}))}{\Delta Q_{Rx}}$$

$$\alpha_{CTC}(Q_{Rx,i}) = \frac{\rho(Q_{Rx,i}) - \rho(T_{cool} + \Delta T_{cool})}{\Delta T_{cool}}$$

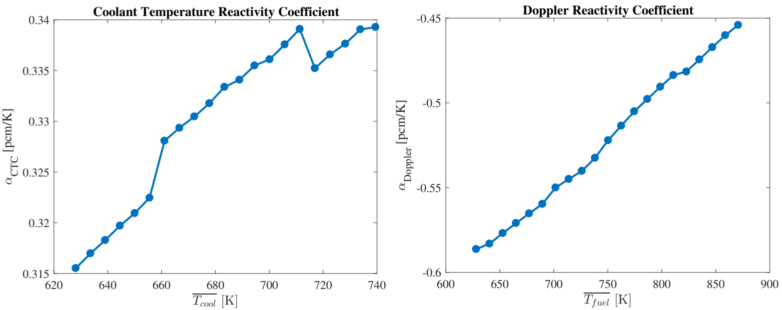
$$\alpha_{Doppler}(Q_{Rx,i}) = \frac{\rho(Q_{Rx,i}) - \rho_i(T_{fuel} + \Delta T_{fuel})}{\Delta T_{fuel}}$$

Eigenvalue Feedback

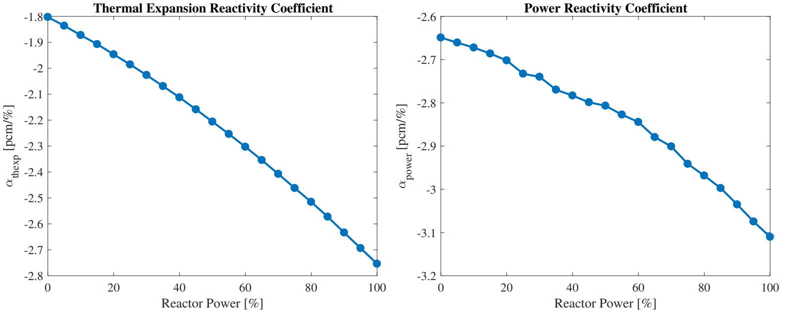


k_{eff} Feedback Effects.

Temperature Reactivity Coefficients



Power Reactivity Coefficients



Multiphysics Contributions to Total Power Defect

- -559.64 [pcm] due to thermal expansion effects.
- -29.85 [pcm] due to thermal hydraulics effects.
- Cancellation of error due to $\alpha_{Doppler}$ and α_{CTC}.

Case	Thermal Expansion Power	Thermal Hydraulic Power	k_{eff}	Reactivity [pcm]
1	0%	0%	0.999808	
2	100%	0%	0.994246	-559.64
3	100%	100%	0.993950	-589.49

Outline

Summary

Summary

Modeled a nuclear reactor.

Summary

- Solved multigroup neutron diffusion equation via FEM.
- Developed thermal hydraulics models.
- Developed thermal expansion model.
- Demonstrated multiphysics simulation based on ABR.
- Estimated multiphysics reactivity coefficients.

Future Improvements

- Code Enhancements and New Features.
  - Depletion with Chebyshev Rational Approximation Method (CRAM) [Pus13].
  - Higher order finite elements (e.g. quadratic) [Hos13].
  - Simplified P_N ($\mathrm{SP_N}$) [Ryu13].
- Encouraging Code Usage.
  - Should be a tool for core design optimization.
  - More users encourage more feedback.
  - Unique reactor designs encourage feature additions.

Thank You!

Thank you all for coming this morning!

I would like to thank my advisor, Dr. Scott Palmtag, and my committee, Dr. J. Michael Doster and Dr. Ralph Smith.

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Acronyms I

ABR	Advanced Burner Reactor.
ANL	Argonne National Laboratory.
CG	Conjugate Gradient.
CRAM	Chebyshev Rational Approximation Method.
EBR-II	Experimental Breeder Reactor II.
FEM	Finite Element Method.
LWR	Light Water Reactor.
RCM	Reverse Cuthill-McKee.
RMS	Root-Mean-Squared.
SFR	Sodium-cooled Fast Reactor.
SPD	Symmetric Positive Definite.

Source Codes

Defense Slides & Thesis.
`https://github.com/wcdawn/WilliamDawn-thesis`

Thesis Code.
`https://github.ncsu.edu/wcdawn/masters_thesis`
Note: Not currently open-source. Contact the author for access.