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

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Disclaimer

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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.

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- 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

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

$D_g(\mathbf{r})$ = diffusion coefficient for energy group g [cm],

$\phi_g(\mathbf{r})$ = scalar neutron flux for energy group g $\left[\frac{1}{\mathrm{cm}^2\ \mathrm{s}}\right]$,

$\Sigma_{r,g}(\mathbf{r})$ = macroscopic removal cross section for energy group g $\left[\frac{1}{\mathrm{cm}}\right]$,

$\widetilde{\chi_g}(\mathbf{r})$ = effective fission spectrum for energy group g,

k_{eff} = effective neutron multiplication factor,

$\nu\Sigma_{f,g}(\mathbf{r})$ = number of fission neutrons times macroscopic fission cross section in energy group g $\left[\frac{1}{\mathrm{cm}}\right]$,

$\Sigma_{s,g'\rightarrow g}(\mathbf{r})$ = macroscopic scatter cross section from energy group g' to energy group g $\left[\frac{1}{\mathrm{cm}}\right]$,

G = total number of energy groups (typically $G = 33$).

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, $\alpha = \frac{1}{2}$.

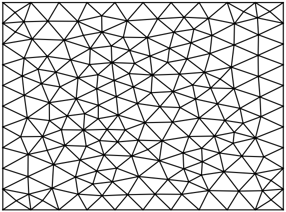
3. Zero Flux.

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

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.

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

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

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

- 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:

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

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

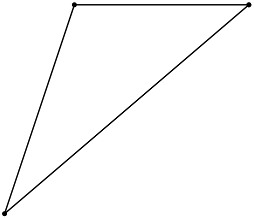
$$\int_{\Omega_e} N_i(\mathbf{r}) \; d\mathbf{r}$$

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

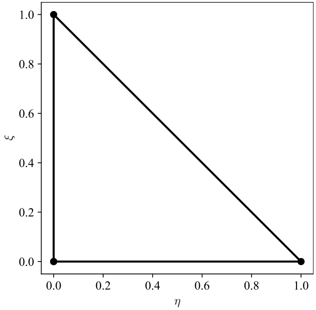
Options for integration:

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

Triangular Elements

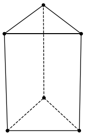


General Triangle Element.

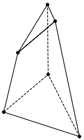


Reference Triangle.

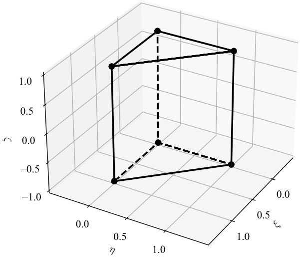
Wedge Elements



General Wedge Element.



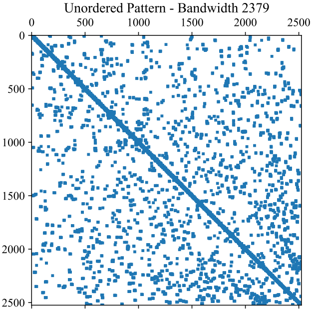
Distorted Wedge Element.

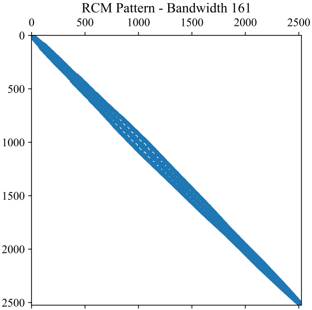


Description of Reference Wedge.

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 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 $\phi_g$ 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

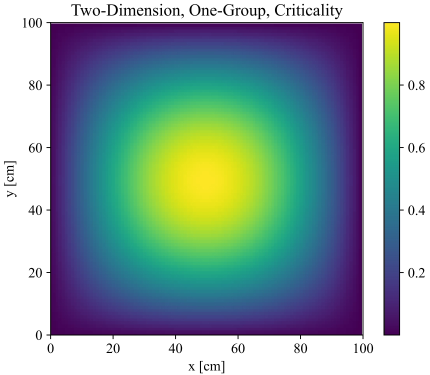
- 6 analytic multigroup neutron diffusion problems.
- Varied number of spatial dimensions, energy groups, and number of materials.

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	$\lVert\mathbf{e}\rVert_\infty$	$\lVert\mathbf{e}\rVert_\infty$ 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

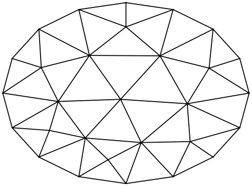


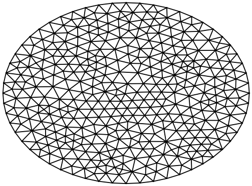
$$\phi(x,y) = \phi_0 \sin\left(\frac{\pi}{L_x}x\right)\sin\left(\frac{\pi}{L_y}y\right)$$

Three-Dimension, One-Group, Finite Cylinder

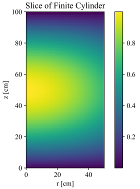
Refine	k_{eff}	k_{eff} error [pcm]	k_{eff} ratio	RMS	RMS ratio	$\|\|\mathbf{e}\|\|_\infty$	$\|\|\mathbf{e}\|\|_\infty$ ratio
0	0.895108	10160.26	4.18	5.34E-02	2.57	2.12E-01	1.62
1	0.972412	2429.90	4.16	2.07E-02	3.19	1.31E-01	4.65
2†	0.990870	584.06	3.90	6.50E-03	1.85	2.81E-02	1.79
3	0.995215	149.61	3.99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

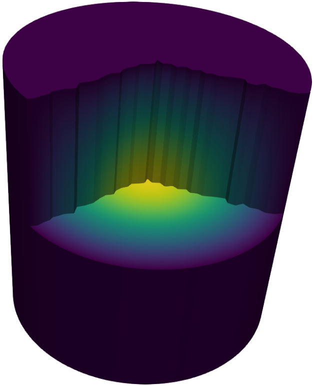
† Refinement ratio ≈ 1 but next case ≈ 8.
This is due to the movement of mesh nodes in the process of circular mesh regeneration.





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

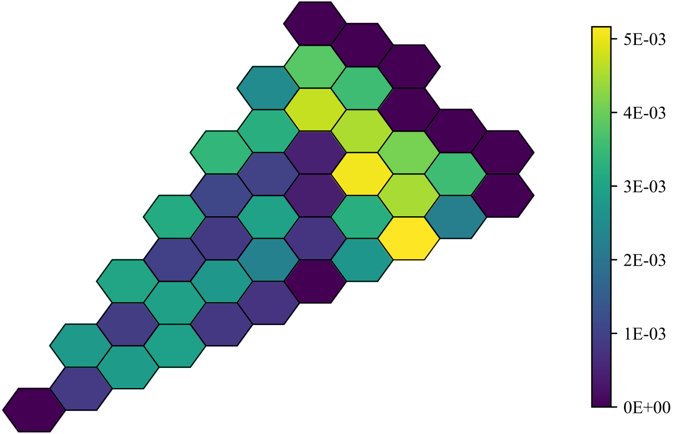
VVER440

- 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.

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 [Δk]	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

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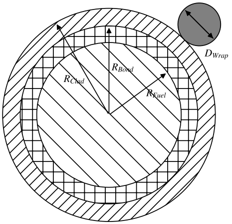
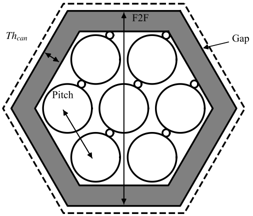
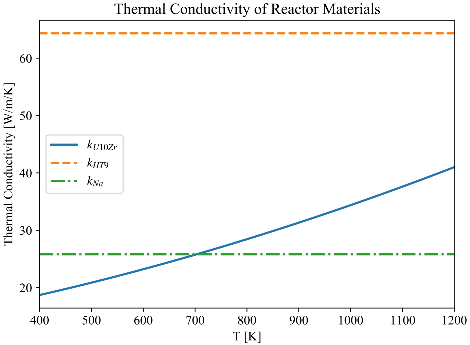
Assembly Geometry



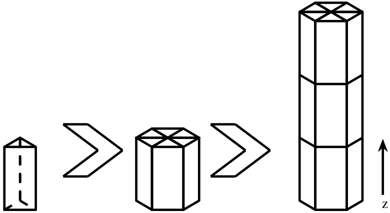


Material Properties

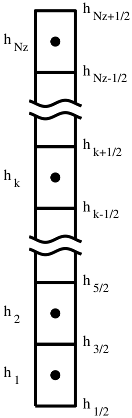
- Functional sodium properties [Fin95].
- Clad and bond thermal conductivity assumed constant [Lei88].
- Fuel thermal conductivity assumed a function of temperature [Kim14].



Axial Convection Geometric Model



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



Nodalization for channel i.

Channel Enthalpy

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

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

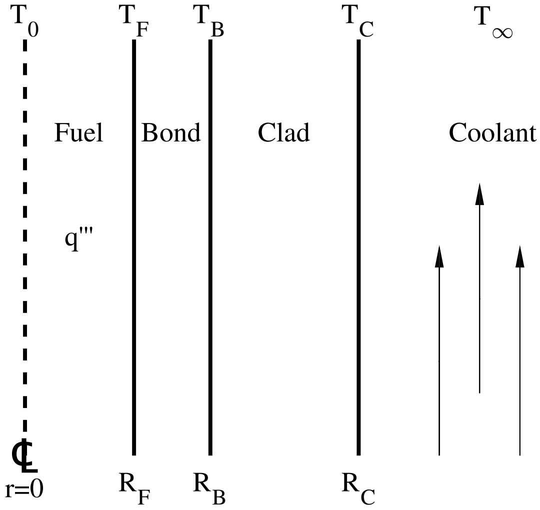
Use a first-order approximation to estimate the chunk-average enthalpy.

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

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

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

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.

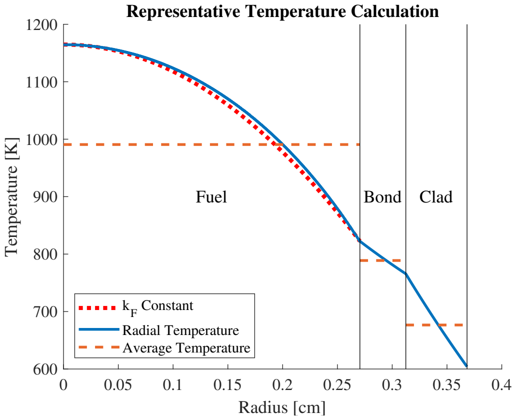
$$\overline{k_F} = \frac{q'''_{i,k} R_F^2}{4(T_0 - T_F)}$$

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).

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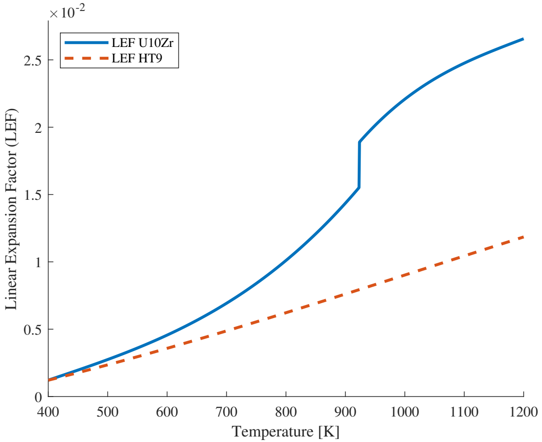
Material Properties



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.

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

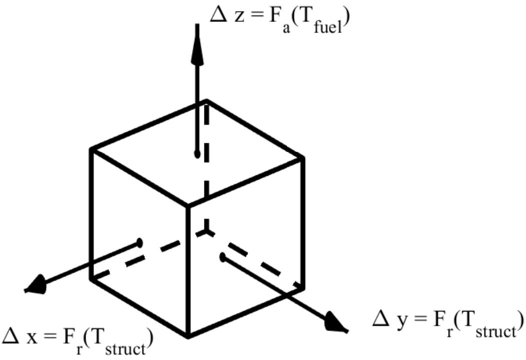
$$F_a\left(T_{exp,fuel}\right) = 1 + \left(\frac{\Delta L}{L}\right)_{\text{U10Zr}}$$

- 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.

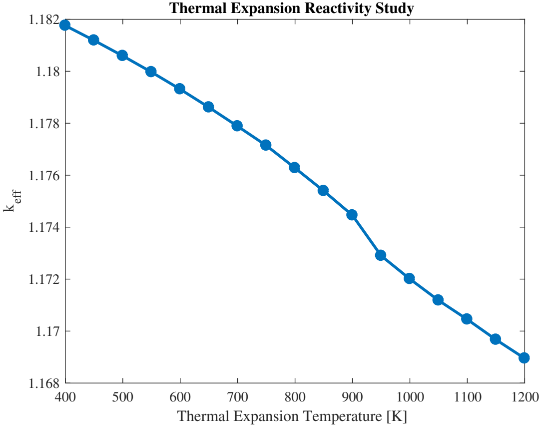
$$N_i^H = N_i^C \frac{a_j^C V_e^C}{a_j^H V_e^H}$$

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.

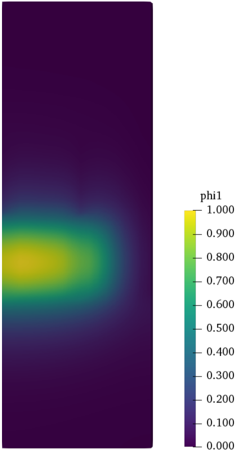
Remember why we are here.

Model a nuclear reactor.

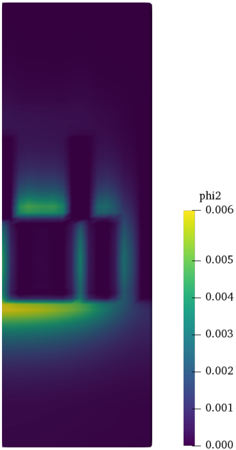
Advanced Burner Reactor (ABR) – MET-1000

- 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.

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

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.

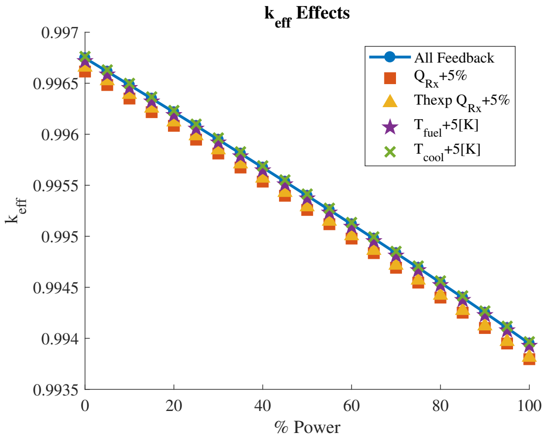
$$\alpha_{power}(Q_{Rx,i}) = \frac{\rho(Q_{Rx,i}) - \rho(Q_{Rx,i} + \Delta Q_{Rx})}{\Delta Q_{Rx}}$$

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

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

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

Eigenvalue Feedback



k_{eff} Feedback Effects.

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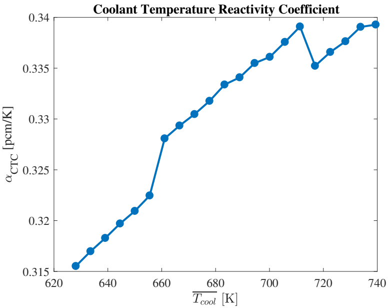
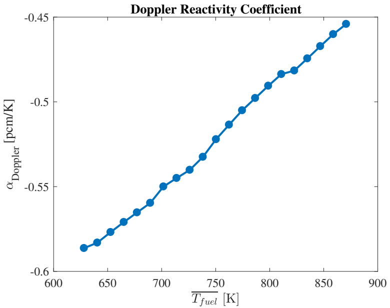
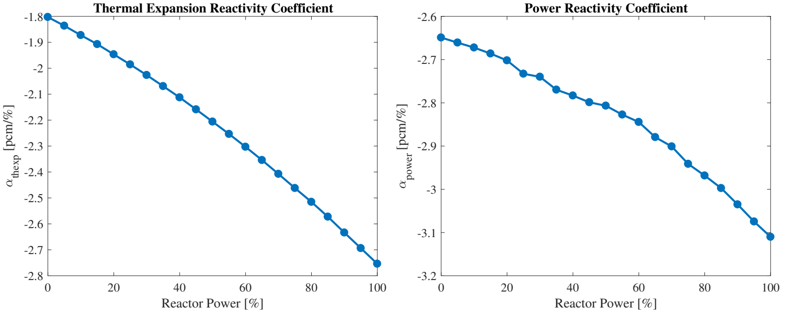
Temperature Reactivity Coefficients





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

1. Introduction
2. Finite Element Neutron Diffusion
3. Neutron Diffusion Results
4. Thermal Hydraulics
5. Thermal Expansion
6. Coupled Results
7. Conclusions

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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References I

[Cha95] Y. A. Chao and Y. A. Shatilla. "Conformal Mapping and Hexagonal Nodal Methods: Implementation in the ANC-H Code." In: *Nuclear Science and Engineering* 121.2 (1995), pp. 210–225.

[Cut69] E. Cuthill and J. McKee. "Reducing the Bandwidth of Sparse Symmetric Matrices." In: *Proceedings of the 1969 24th National Conference*. New York, NY, USA: Association for Computing Machinery, 1969, pp. 157–172.

[Fin95] J. K. Fink and L. Leibowitz. *Thermodynamic and Transport Properties of Sodium Liquid and Vapor*. Tech. rep. ANL/RE-95/2. Argonne National Laboratory, 1995.

[Hos13] S. A. Hosseini and N. Vosoughi. "Development of Two-Dimensional, Multigroup Neutron Diffusion Computer Code Based on GFEM with Unstructured Triangle Elements." In: *Annals of Nuclear Energy* 51 (2013), pp. 213–226.

[Hug87] T. J. R. Hughes. *The Finite Element Method*. Englewood Cliffs, NJ: Prentice-Hall, 1987.

[Kel95] C. T. Kelley. *Iterative Methods for Linear and Nonlinear Equations*. Society for Industrial and Applied Mathematics, 1995, p. 166.

[Kim14] Y. S. Kim et al. "Thermal Conductivities of Actinides (U, Pu, Np, Cm, Am) and Uranium-Alloys (U-Zr, U-Pu-Zr and U-Pu-TRU-Zr)." In: *Journal of Nuclear Materials* 445.1-3 (2014), pp. 272–280.

[Kom78] Y. Komano et al. *Improved Few-Group Coarse-Mesh Method for Calculating Three-Dimensional Power Distribution in Fast Breeder Reactor*. Tech. rep. NEACRP-L-204. Nuclear Energy Agency, 1978.

References II

[Lei88] L. Leibowitz and R. A. Blomquist. "Thermal Conductivity and Thermal Expansion of Stainless Steels D9 and HT9." In: *International Journal of Thermophysics* 9.5 (1988), pp. 873–883.

[Li18] Z. Li et al. *Numerical Solution of Differential Equations*. Cambridge (England): Cambridge University Press, 2018.

[OEC16] OECD Nuclear Energy Agency. *Benchmark for Neutronic Analysis of Sodium-cooled Fast Reactor Cores with Various Fuel Types and Core Sized*. Tech. rep. NEA/NSC/R(2015)9. Feb. 2016.

[Pfr07] W. Pfrang and D. Struwe. *Assessment of Correlations for Heat Transfer to the Coolant for Heavy Liquid Metal Cooled Core Designs*. Tech. rep. FZKA 7352. Karlsruhe: Forschungszentrum Karlsruhe GmbH, 2007.

[Pla87] H. Planchon et al. "Implications of the EBR-II Inherent Safety Demonstration Test." In: *Nuclear Engineering and Design* 101.1 (1987), pp. 75–90.

[Pus13] M. Pusa. "Numerical Methods for Nuclear Fuel Burnup Calculations." PhD thesis. Espoo, Finland: Aalto University, 2013.

[Ryu13] E. H. Ryu and H. G. Joo. "Finite Element Method Solution of the Simplified P3 Equations for General Geometry Applications." In: *Annals of Nuclear Energy* 56 (2013), pp. 194–207.

[Til11] C. Till and Y. Chang. *Plentiful Energy*. CreateSpace Independent Publishing Platform, 2011.

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.