

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

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William  
Christopher Dawn

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Finite Element  
Neutron Diffusion

Neutron Diffusion  
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Thermal  
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# 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.

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



- 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.

- 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.

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# Multigroup Neutron Diffusion Equation

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

$$\frac{\widetilde{\chi}_g(\mathbf{r})}{k_{eff}} \sum_{g'=1}^G \nu \Sigma_{f,g'}(\mathbf{r}) \phi_{g'}(\mathbf{r}) + \sum_{\substack{g'=1 \\ g' \neq g}}^G \Sigma_{s,g' \rightarrow g}(\mathbf{r}) \phi_{g'}(\mathbf{r})$$

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

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

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

$\widetilde{\chi}_g(\mathbf{r})$  = 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  $g$   $\left[ \frac{1}{\text{cm}} \right]$ ,

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

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

For problem domain  $\Omega$  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.

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

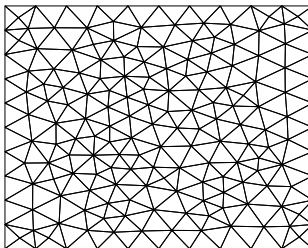
# Finite Element Method (FEM) Discretization

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

$$\Omega = \Omega_1 \cup \Omega_2 \cup \Omega_3 \cup \dots \cup \Omega_{N_E}$$

$$\Omega = \{\Omega_e\} \text{ for } e = 1, 2, \dots, N_E$$

$$\Omega_i \cap \Omega_j = \emptyset \text{ for } i \neq j$$



Example Rectangular Mesh.

- Neutron sources are combined into a single term.

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

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

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

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

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.

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



# Second Green's Theorem

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

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

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

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

$v(\mathbf{r}) \in H_1(\Omega)$  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.

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

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.

$$\mathbf{A}_g \mathbf{u}_g = \mathbf{f}_g$$

$$\mathbf{u}_g = \{v_{i,g}\}$$

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

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- 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].

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.

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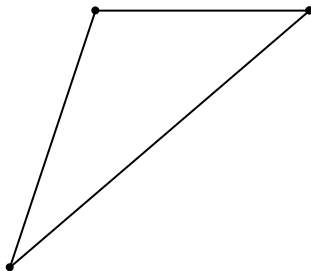
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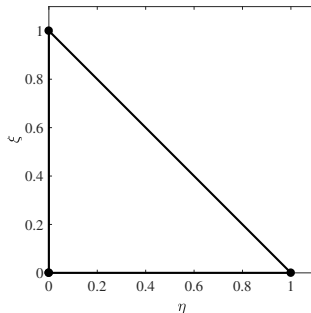
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General Triangle Element.



Reference Triangle.

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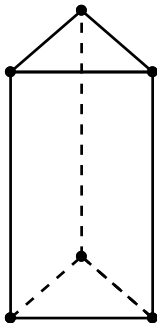
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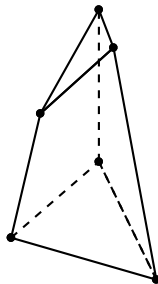
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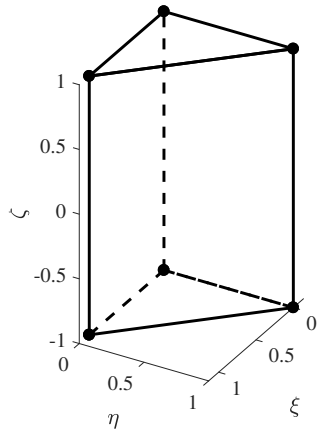
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General Wedge  
Element.

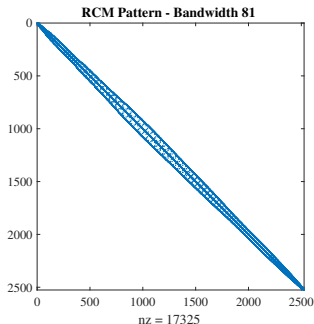
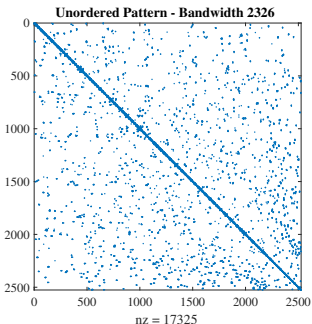


Distorted Wedge  
Element.



Description of Reference Wedge.

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





- Solution for largest eigenvalue  $k_{eff}$  and associated eigenvector  $\Phi$ .
- 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  $\Phi$ , not  $\mathbf{R}$ .
- The power iteration method proceeds.

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

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

# Power Iteration Algorithm

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## Algorithm 1 General Iteration Scheme

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- 1: Read mesh from VTK.
  - 2: Initialize  $\bar{\phi}_g^{(0)}$ .
  - 3: Order the nodes of the mesh into RCM order.
  - 4: Calculate  $\Sigma_{s,g' \rightarrow g}$ ,  $\Sigma_{r,g}$ , and  $\nu \Sigma_{f,g}$  for each element.
  - 5: Calculate finite element matrix  $\mathbf{A}_g$  for each group. Store this.
  - 6: **while** Power Iteration **do**
  - 7:     Update the iteration counter.  $s = s + 1$
  - 8:     Update  $q_{fiss,g}$  and  $q_{up,g}$  for all groups from previous data  $\bar{\phi}^{(s-1)}$ .
  - 9:     Update  $\chi_g$  in each element using previous data.
  - 10:    **for**  $g = 1, G$  **do**
  - 11:       Update  $q_{down,g}$  from current data  $\bar{\phi}_g^{(s)}$
  - 12:       Calculate total source in each element.
  - 13:       Update finite element Vector  $\mathbf{f}_g$  with new source.
  - 14:       Solve  $\mathbf{A}_g \mathbf{u}_g = \mathbf{f}_g$  using an iterative technique (CG).
  - 15:       Parse  $\mathbf{u}_g$  for  $\phi_g$  solution on nodes.
  - 16:       Calculate element-average  $\bar{\phi}_g$ .
  - 17:    Update  $k_{eff}$ .
  - 18:    Check convergence.
  - 19:    Perform non-linear update if necessary and update  $\mathbf{A}_g$ .
-

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- “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.

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.

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

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

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

The method is second-order spatially convergent.

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

- 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

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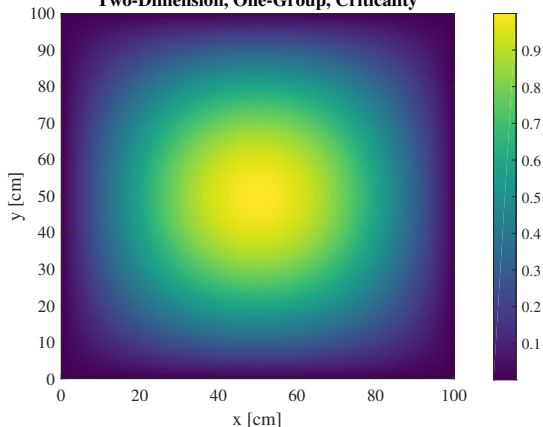
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Refine	$k_{eff}$	$k_{eff}$ error [pcm]	$k_{eff}$ ratio	RMS	RMS ratio	$\ e\ _{\infty}$	$\ e\ _{\infty}$ ratio
0	1.983243	1281.65	4.03	1.90E-02	1.66	6.63E-02	1.49
1	1.992884	317.64	3.96	1.15E-02	2.65	4.45E-02	2.59
2	1.995258	80.16	3.98	4.32E-03	3.43	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

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

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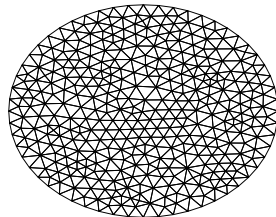
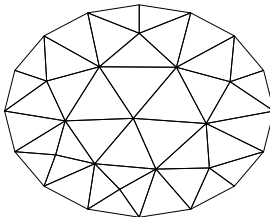
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Refine	$k_{eff}$	$k_{eff}$ error [pcm]	$k_{eff}$ ratio	RMS	RMS ratio	$\ e\ _{\infty}$	$\ e\ _{\infty}$ ratio
0	0.895108	10160.26	4.18	5.34E-02	2.57	2.12E-01	1.62
1	0.972412	2429.90	4.16	2.07E-02	3.19	1.31E-01	4.65
2 <sup>†</sup>	0.990870	584.06	3.90	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						

<sup>†</sup> 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.



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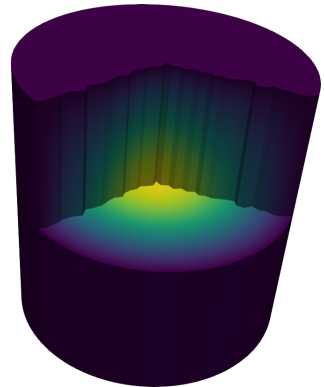
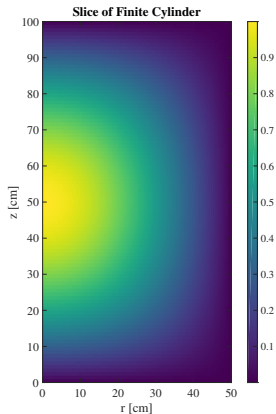
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$$\phi(r, z) = \phi_0 J_0 \left( \frac{\alpha_0}{T} r \right) \sin \left( \frac{\pi}{H} z \right)$$

- 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 ( $\times 4$ )	2	2	PWR	Thermal
MONJU	3	3	SFR	Fast
KNK	3	4	SFR	Fast

- 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. <sup>†</sup>	1.009700	

<sup>†</sup> See [Cha95].

# VVER440 Benchmark Power Comparison

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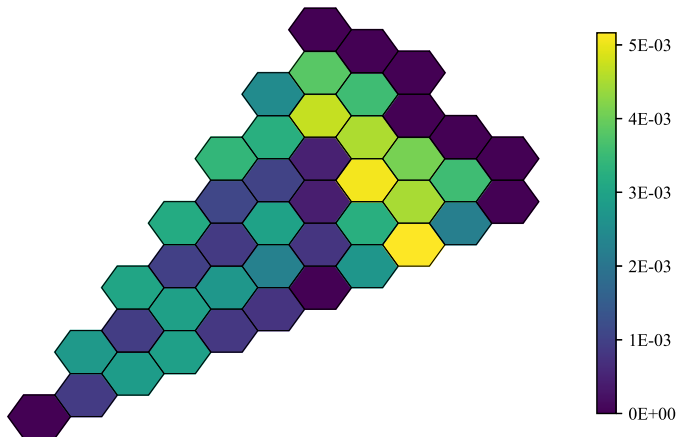
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VVER440 Benchmark Power Comparison for Most Refined Mesh.

- 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) <sup>†</sup>	2.52 (-0.07)
C	1.006519	0.047 (1.77E-3)	5.03 (0.04)

<sup>†</sup> Value in parentheses is difference to reference value [Kom78].

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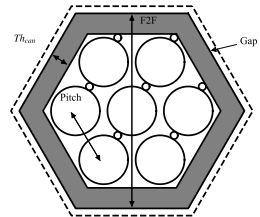
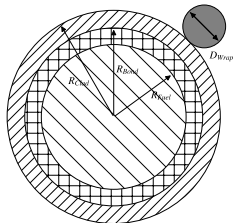
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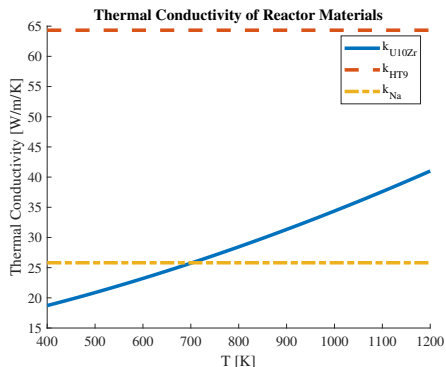
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- Functional sodium properties [Fin95].
- Clad and bond thermal conductivity assumed constant [Lei88].
- Fuel thermal conductivity assumed a function of temperature [Kim14].



# Axial Convection Geometric Model

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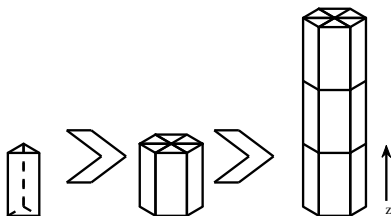
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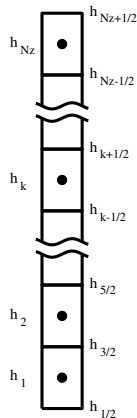
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Progression of Element (left), to Chunk (center), to  
Channel (right).



Nodalization for channel  $i$ .

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

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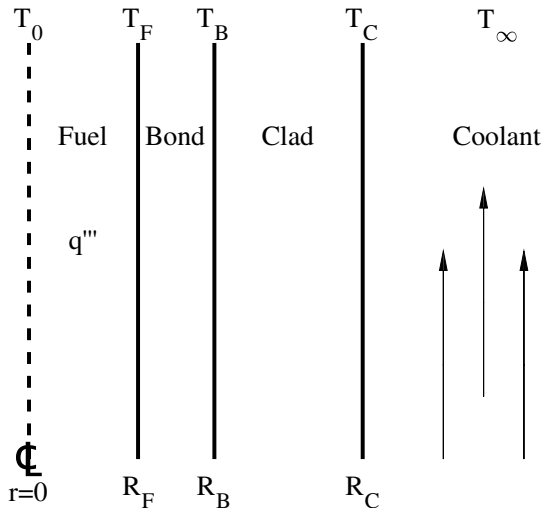
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Using Newton's Law of Cooling.

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

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

$$Pe = Re Pr$$

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

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

Then, the clad surface temperature,  $T_C$  follows.

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 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

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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

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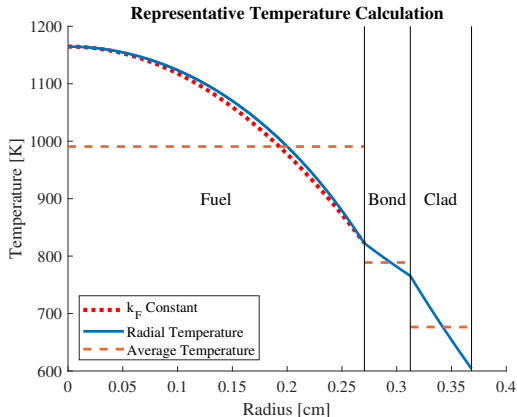
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Difference less than 15 [K].

- 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.

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

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

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

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

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

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

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- 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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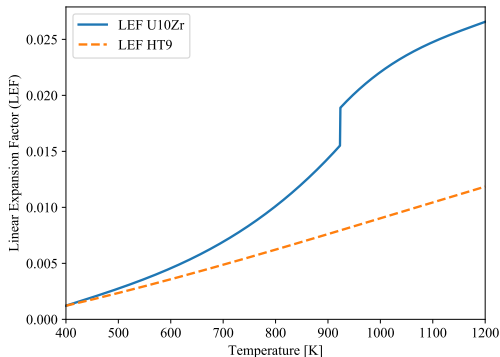
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Linear Expansion Factor for HT9 Steel and U10Zr Fuel.

# Simplified Thermal Expansion Model

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- 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  $\Sigma = N \sigma$ .



- Define radial and axial expansion factors.

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

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

- Expand all coordinates in the finite element mesh.

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

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

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

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

# Arbitrary Volume Expansion

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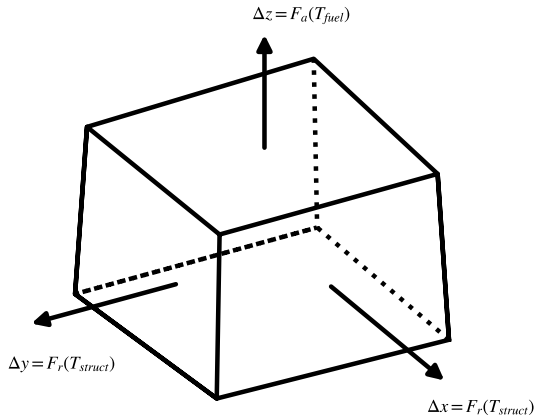
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$$\frac{V^C}{V^H} = \frac{1}{(F_r(T_{exp,struct}))^2 (F_a(T_{exp,fuel}))}$$

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- 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 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

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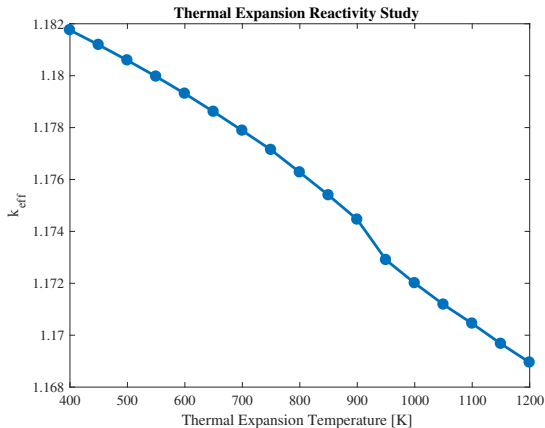
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Effective Neutron Multiplication Factor as a Function of Thermal Expansion Temperature.

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# Model a nuclear reactor.



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

# Benchmark Results

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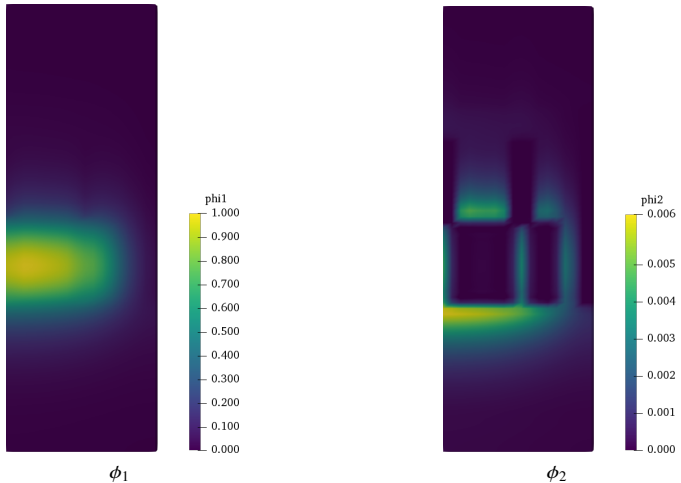
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$$k_{eff} = 1.006694 \quad (\text{DIF3D -700 [pcm]})$$

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

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Consider a series of reactor powers  $Q_{Rx,i} = \{0\%, \dots, 100\%\}$ . 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

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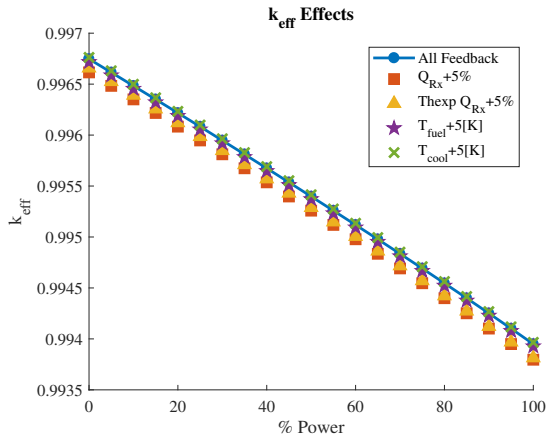
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$k_{eff}$  Feedback Effects.

# Temperature Reactivity Coefficients

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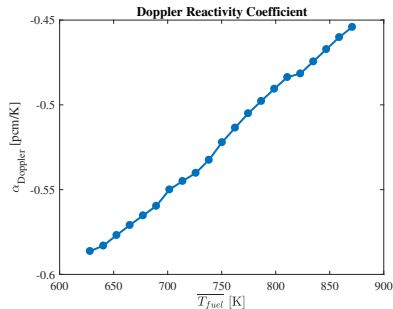
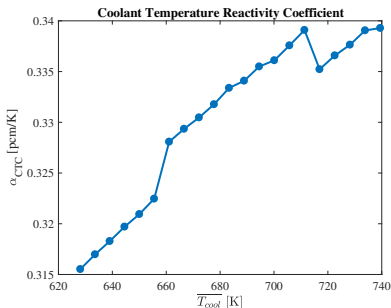
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# Power Reactivity Coefficients

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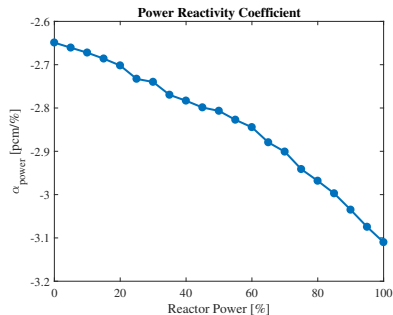
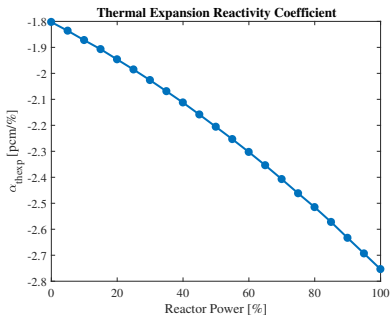
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- $-559.64$  [pcm] due to thermal expansion effects.
- $-29.85$  [pcm] due to thermal hydraulics effects.
- Cancellation of error due to  $\alpha_{Doppler}$  and  $\alpha_{CTC}$ .

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



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## Modeled a nuclear reactor.

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- 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.

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

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

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Defense Slides & Thesis.

<https://github.com/wcdawn/WilliamDawn-thesis>

Thesis Code.

[https://github.ncsu.edu/wcdawn/masters\\_thesis](https://github.ncsu.edu/wcdawn/masters_thesis)

Note: Not currently open-source. Contact the author for access.