Using the Application Builder for Neutron Transport in Discrete Ordinates

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(This material is based upon work supported under a Department of Energy Nuclear Energy University Programs Graduate Fellowship.)

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Presented at: COMSOL CONFERENCE 2015 BOSTON

NEUP Nuclear Energy University Programs
U.S. Department of Energy

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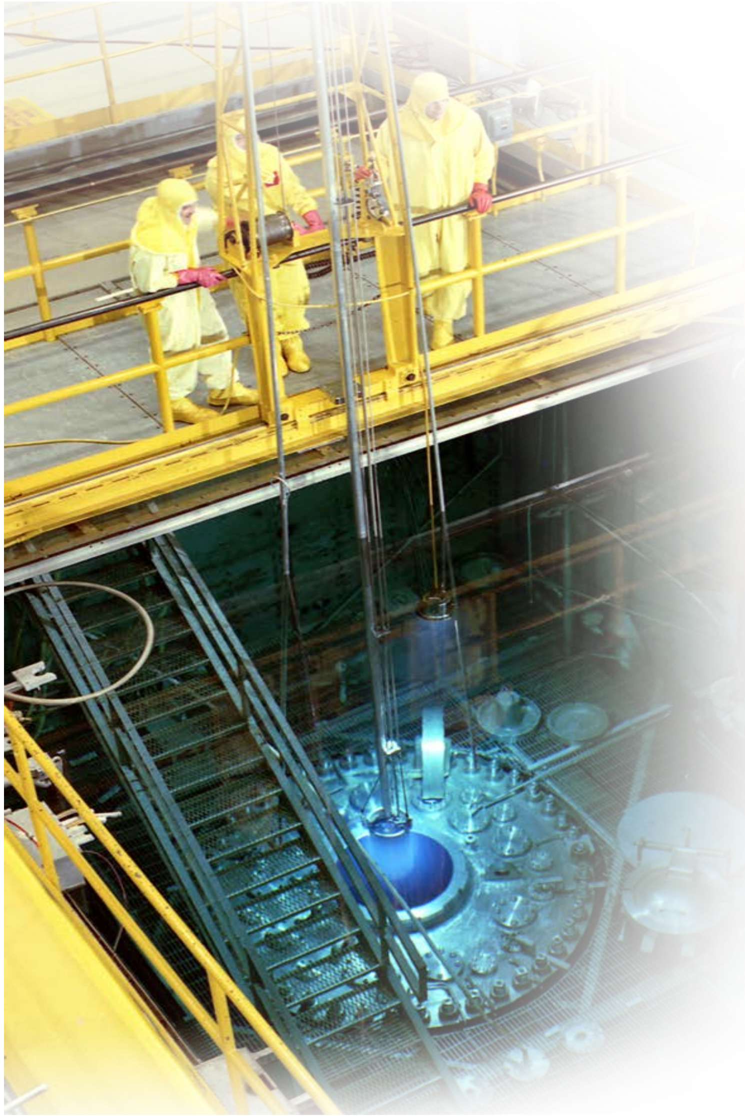
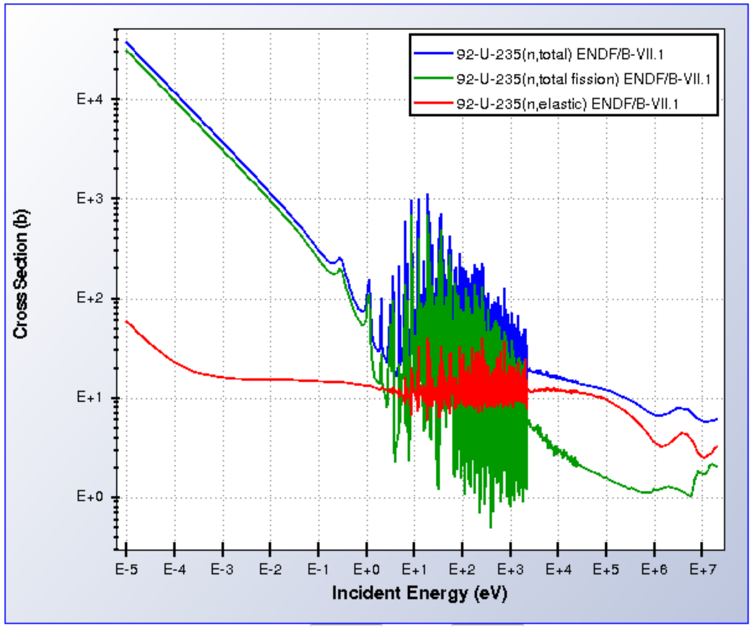
Presentation Outline

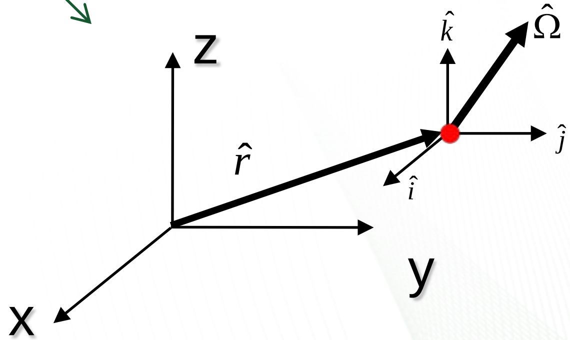


- Brief review of neutron transport
- Discrete ordinates methodology
- (Mis-)Use of the App. Builder
- Transport Benchmarks
  - Kobayashi benchmarks
  - Simple eigenvalue problems
- Results
- Conclusions

Neutron Transport

- Solve **7** independent variables:
  - Energy (1) – E
  - Angle (2) – Ω (ξ,ω)
  - Space (3) – r (x,y,z)
  - Time (1) – t

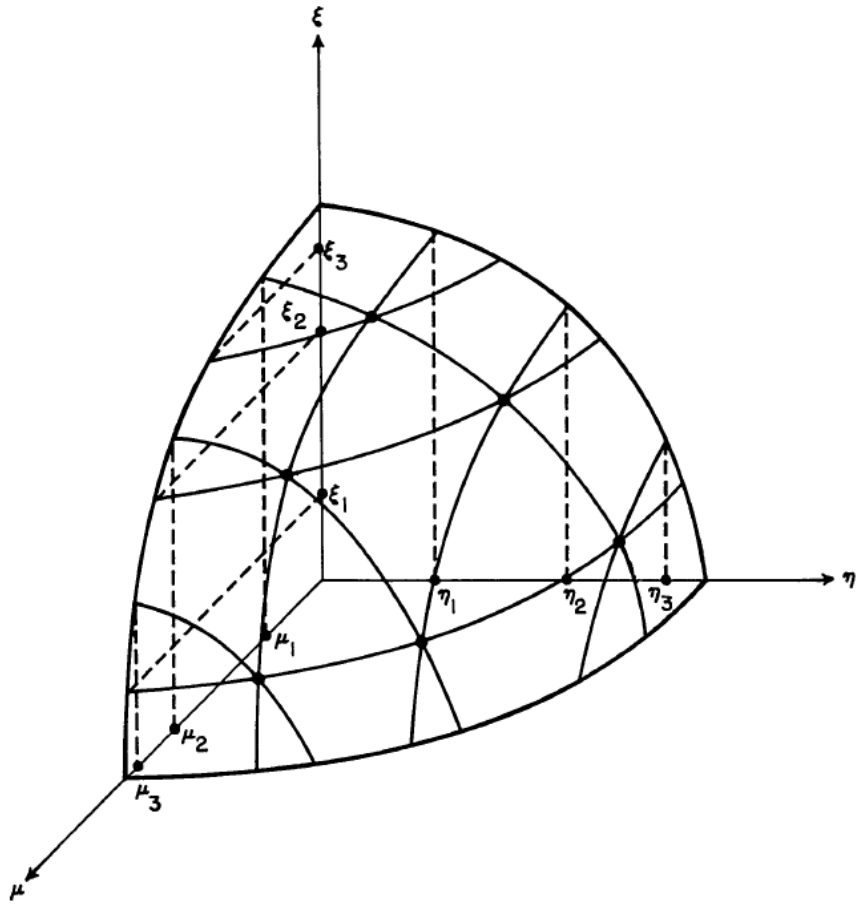




- Two primary methods:
  - *Stochastic* (MCNP5, SCALE's KENO, Serpent)
  - *Deterministic* (PARTISN, DORT, Attila)
- Nuclear Data

Discrete Ordinates Method

- **Spatial variables** – finite difference, nodal, FEM
- **Energy variables** – multigroup method, split problem into energy groups
- **Angular variables** – <u>discrete directions</u> and quadrature approximation
- Gauss-Legendre quadrature for numerical integration over the angular domain:



$$\phi_l^m(r,E) = \int_{4\pi} Y_{lm}(\hat{\Omega}')\psi(r,E,\hat{\Omega}')d\Omega' = \sum_{n=1}^{N} Y_{lm}(\hat{\Omega}_n)\psi(r,E,\hat{\Omega}_n)$$

Flux moments

Weak form application mode.

Multi-Group Neutron Transport Equation for Discrete Ordinates

$$[\hat{\Omega}_n \cdot \nabla + \Sigma_t^g(r)]\psi_n^g(r,\hat{\Omega}_n) = q_{ext}^g(r)$$
$$+ \chi^g \sum_{g'=1}^{G} \nu\Sigma_f^{g'}(r)\phi^{g'}(r) + \sum_{l=0}^{SCT}\sum_{m=-l}^{l} Y_{lm}^*(\hat{\Omega}_n)\sum_{g'=1}^{G}\Sigma_{sl}^{g'\to g}(r)\phi_l^{g'}(r)$$

ψ_n^g	angular neutron flux(neutrons/m^2-s)
ϕ_l^g	neutron flux moment (neutrons/m^2-s)
$\hat{\Omega}_n$	discrete ordinate direction, n
r	spatial coordinates
Σ_t^g	total cross section (1/m)
χ^g	probability of neutron born in group g
ν	average # of neutrons emitted per fission
Σ_f^g	fission cross section (1/m)
$\Sigma_{sl}^{g\to g'}$	scattering moment cross sec. g→g' (1/m)
Y_{lm}^*	conjugate spherical harmonic functions

q_{ext}^g	external scattering source (neutrons/m^3-s)
n	discrete ordinate index
g	energy group index
l, m	scattering order index
SCT	maximum scattering order (0 = isotropic)

Scattering Moment

$$\Sigma_{sl}^{g\to g'} = \int_{-1}^{1} d\mu_0 \Sigma_s^{g\to g'}(\mu_0)P_l(\mu_0)$$

μ_0	cosine of scattering angle, $\Omega \cdot \Omega'$
P_l	Legendre polynomials
$\Sigma_s^{g\to g'}$	scattering cross section g→g' (1/m)

Neutron Transport Equation – Streaming

- Neutron transport equation (simplified):

$$\Omega \cdot \nabla\psi + \sigma\psi = q$$

- "Streaming" terms:

Dimension	Spatial Var.	Angular Var.	$\Omega \cdot \nabla\psi$
1D Cartesian	x	μ	$\mu \frac{\partial}{\partial x}$
2D Cartesian	x,y	μ, η	$\mu \frac{\partial}{\partial x} + \eta \frac{\partial}{\partial y}$
3D Cartesian	x,y,z	μ, η, ξ	$\mu \frac{\partial}{\partial x} + \eta \frac{\partial}{\partial y} + \xi \frac{\partial}{\partial z}$
2D Cylindrical	ρ,z	$\mu,\ \xi$	$\frac{\mu}{\rho} \frac{\partial}{\partial \rho} \rho - \frac{1}{\rho} \frac{\partial}{\partial \omega} \eta + \xi \frac{\partial}{\partial z}$

- Curvilinear geometry: The variation of the angular coordinate system with position introduces a troublesome angular derivative or "directional transfer" term

Use of Application Builder to “streamline” physics building of G-by-N interfaces

SCALE:
Material Processing

↓

Working Xs directory text file

→

COMSOL Application Builder

1. Create model equations, BC’s, variables
2. Mix Xs
3. Save Intermediary App. File

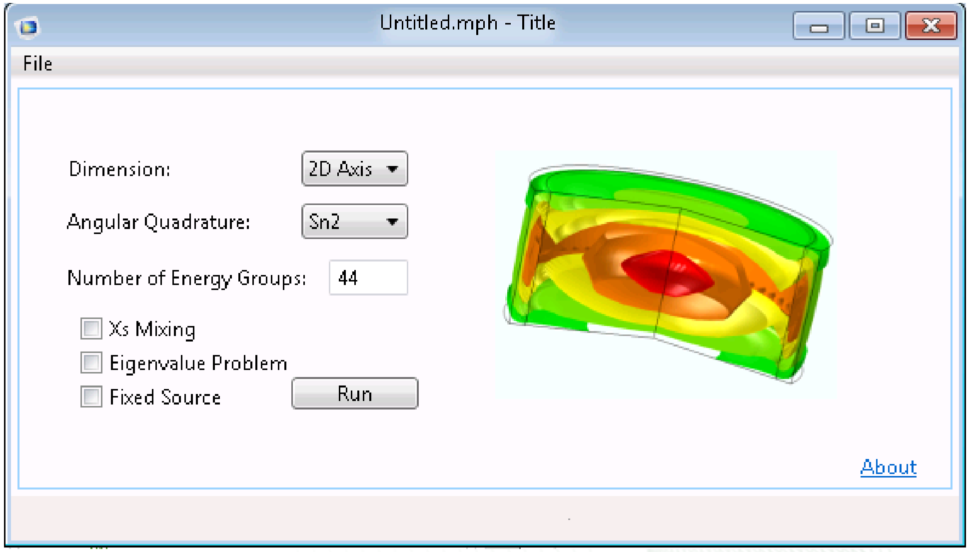
↓

COMSOL App:

1. Develop geometry, solver, parameters, etc.
2. Run edits
3. Save as model file

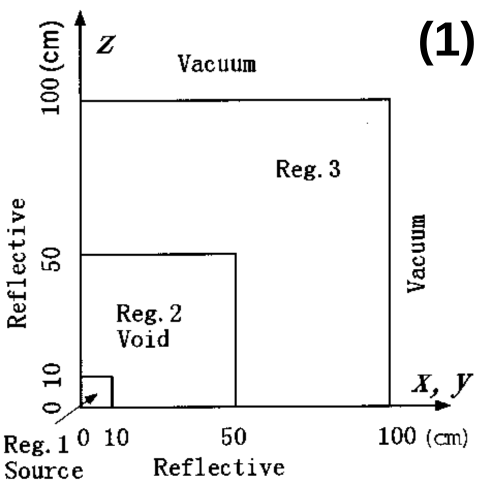
↓

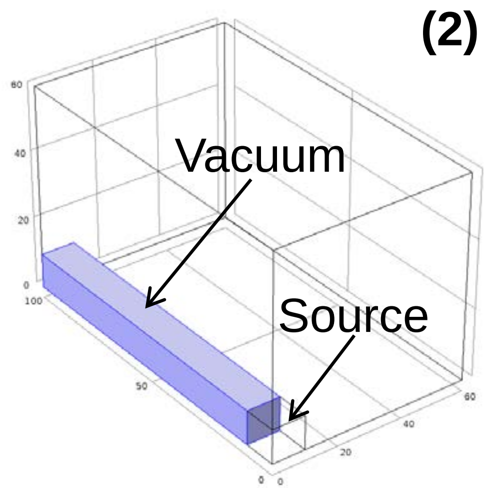
COMSOL Model:
Run simulations

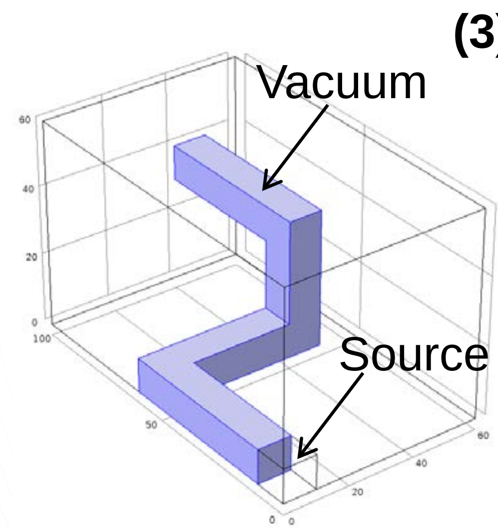


Kobayashi Benchmark Problems 1 – 3

- **Difficult problems to assess:**
  - ***"…the accuracy of the flux distribution for systems which have void regions in a highly absorbing medium."***
- **3 problems in two cases:**
  - **i. Pure absorber**
  - **ii. 50% scattering**
- **Expected "ray effects" allowed unmitigated**







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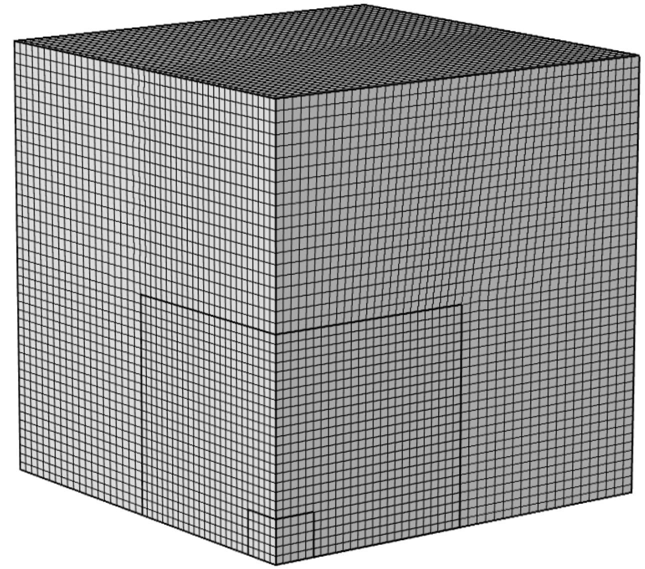
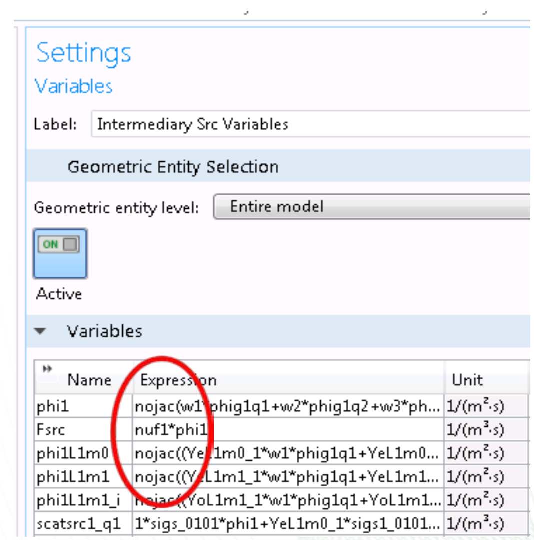
Meshing, Solver and Problem Parameters

- Swept, mapped mesh everywhere
  - 2 cm mesh intervals, uniform
  - Mesh control domains utilized
- Each model set up with ~45-125k elements
  - ~14-28 million DOF → 1-2 hr solution time
  - 1+ compute nodes, dual quad core processors, 128 GB RAM
- PARDISO for single node batch runs, MUMPS for batch runs across multiple nodes
- Fully-coupled or segregated solvers both used
  - Segregated slower convergence, offers "lower limit" feature and minimal memory savings
- Sn16 Level-Symmetric Quadrature
- Pn0 Scattering Order





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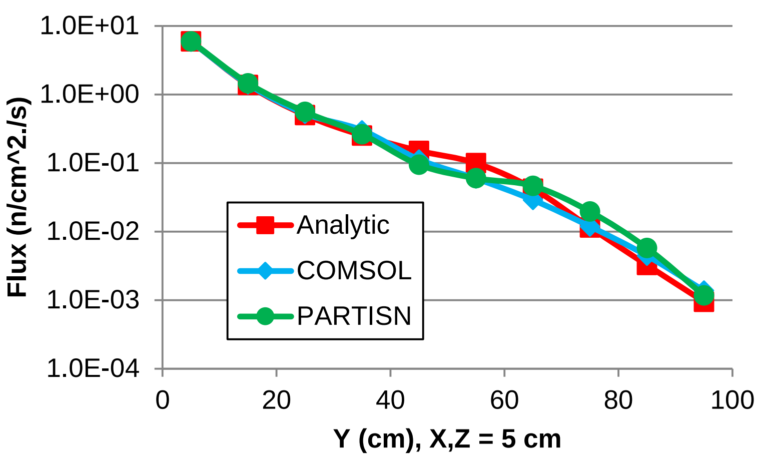
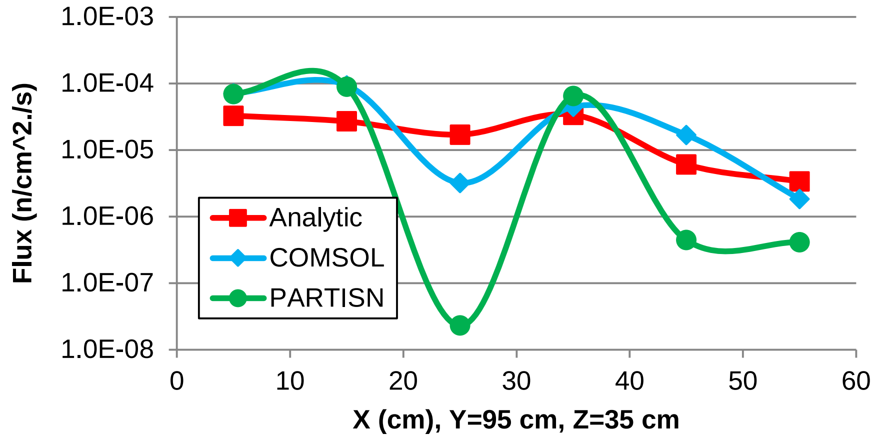
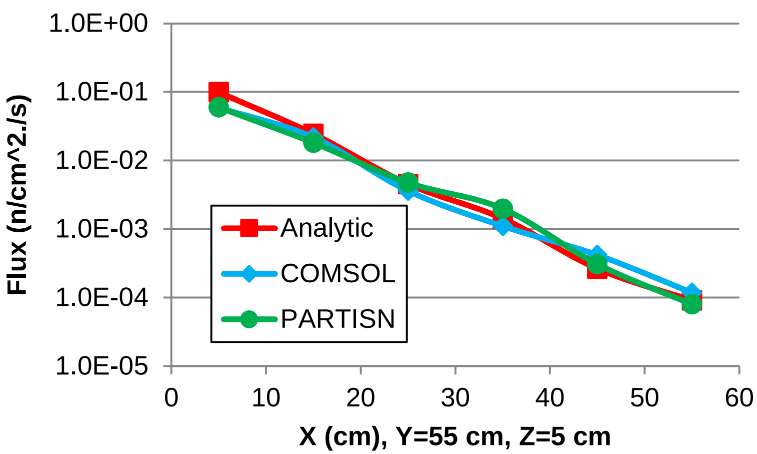
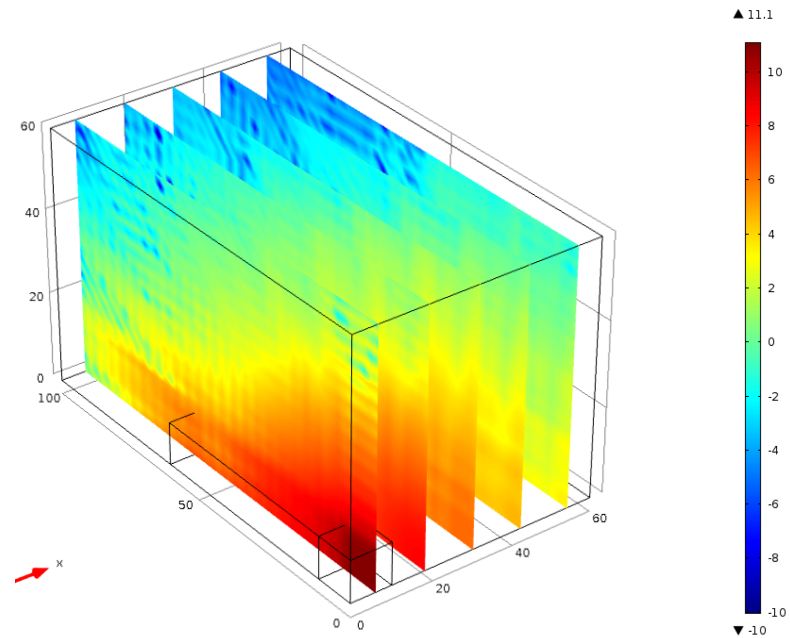
Kobayashi Benchmark 3 Fluxes (w/o scattering)









Log plot of flux

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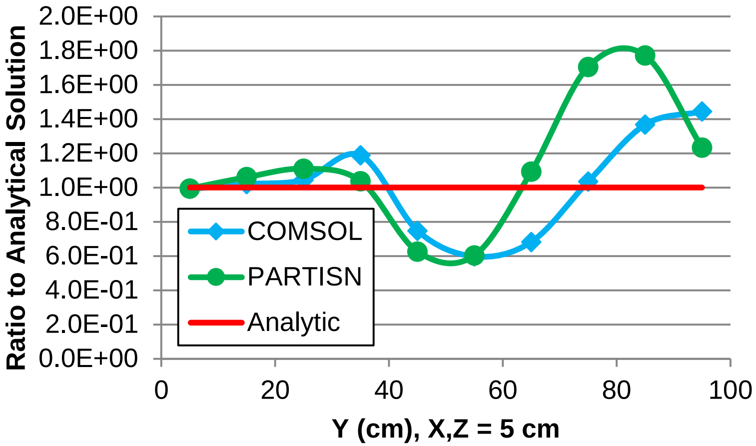
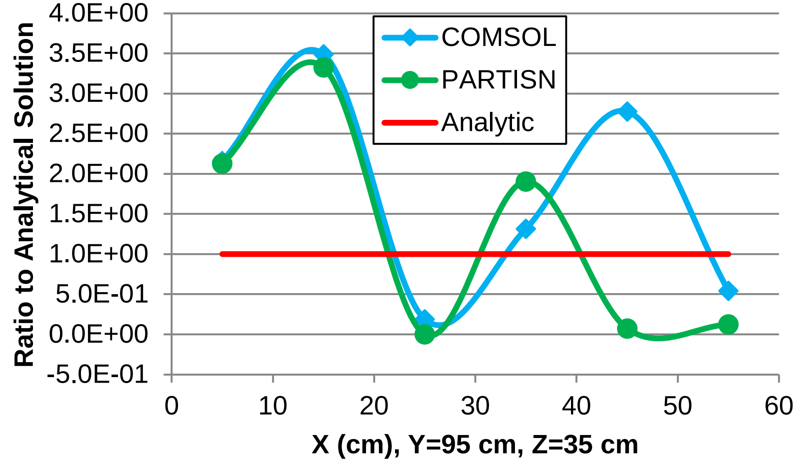
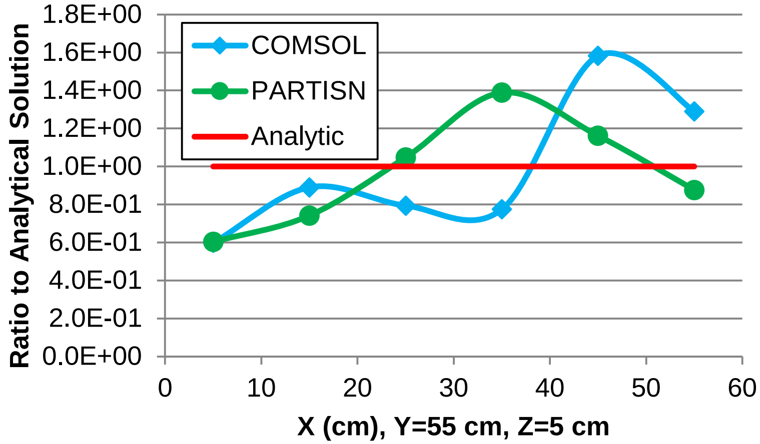
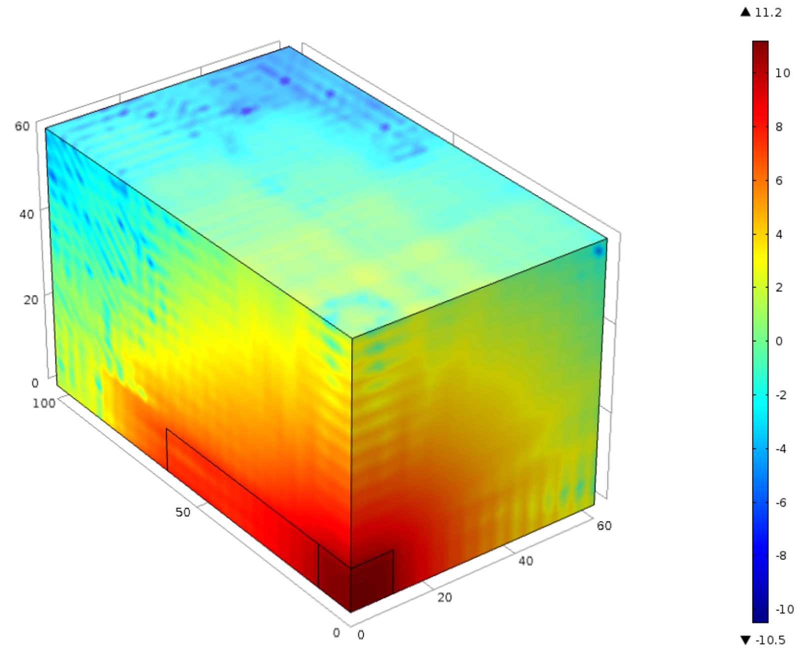
Kobayashi Benchmark 3 Fluxes (w/o scattering)









Log plot of flux

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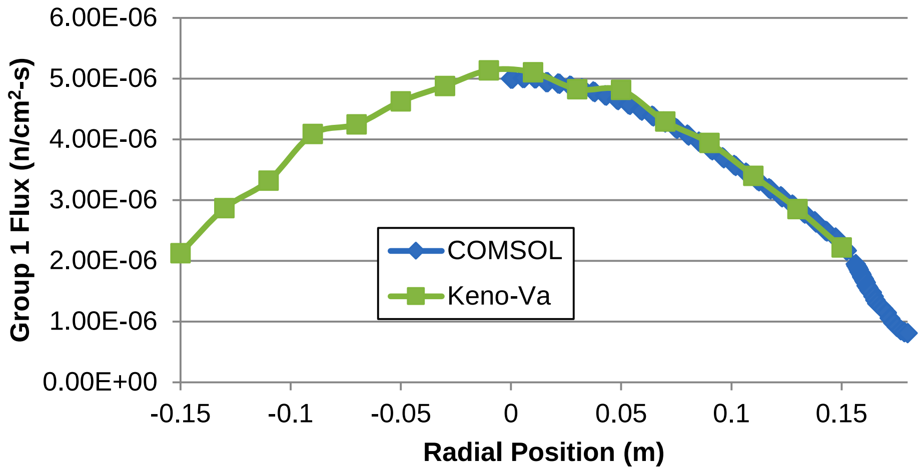
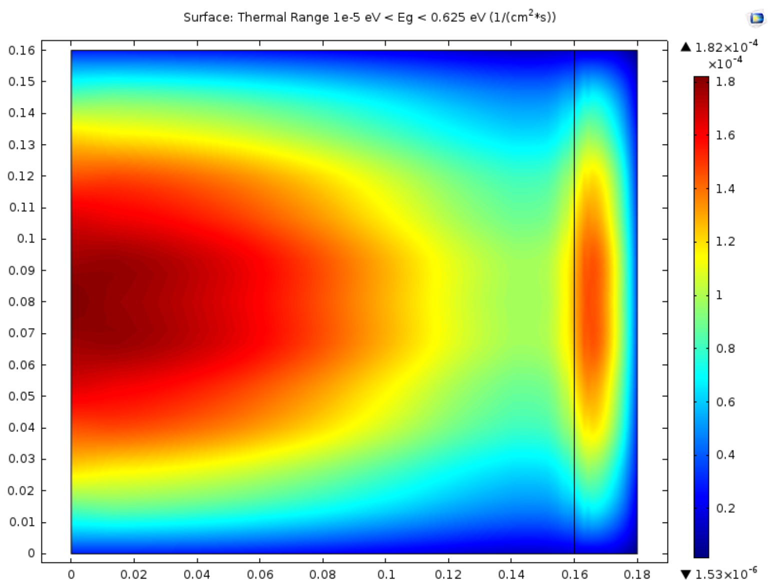
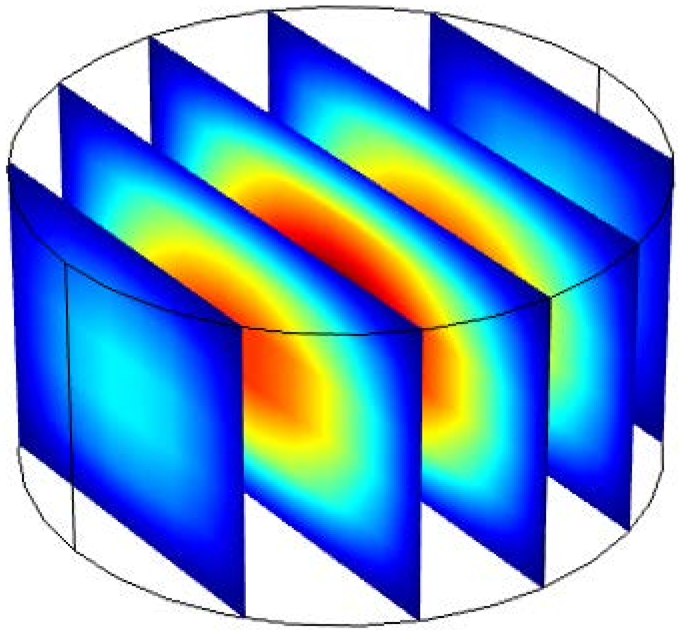
Simple Eigenvalue Problems



HEU metal and water configurations, Sn2-4

k_{eff}		
KENOVa MG	0.2834	--
COMSOL Sn2	0.2600	8.24%
COMSOL Sn4	0.2705	4.56%
COMSOL Sn6	0.2713	4.27%
MCNP CE	0.2748	--





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Summary and Conclusions

- COMSOL-based neutron transport physics were developed for the discrete ordinates method
  - Variable dimension (1-D, 2-D, 2-D Axisymmetric, 3-D)
  - Variable energy group, angular quadrature
  - Neutron cross sections from SCALE, mixed in COMSOL
- New use of the COMSOL Application Builder for streamlining physics and model building in the weak form interface
- Results from compared benchmarks promising, primary limitation is computation time
- Future HFIR applications for neutron transport approaches in COMSOL has a variety of avenues