A Generalized Framework for In-Line Energy Deposition during Steady-State Monte Carlo Radiation Transport

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Framework Overview

- Energy deposition calculations by explicit neutron/photon transport is expensive for large models (e.g., 3D reactor core model)
- Generalized energy deposition modeling framework allows control over the accuracy, and expense, of calculations at run time
  - Framework supports coupled transport along with three approximate energy deposition treatments
  - Approximate treatments neglect transport of secondary radiation(s) while still preserving energy
  - All treatments can easily be implemented in a single code, giving users the flexibility to select a treatment based on need and resource availability.

Framework Overview

- Framework separates energy deposition into three basic categories.
  - Common mathematical framework, but each energy deposition treatment uses different models for calculating deposition in each category.
  - Energy deposition for each category is based on standard nuclear data such as: reaction Q-value, KERMA (h), photon yield (γ), and energy release per fission (ENDF MT 458) data (f)

Framework Overview

Neutron Transport

$$\int_{4\pi} \hat{\Omega} \cdot \nabla \psi_{\mathrm{n}}(E, \hat{\Omega}) d\hat{\Omega} + \Sigma_{\mathrm{a}}\, \phi_{\mathrm{n}}(E) = \int_0^\infty \Sigma_{\mathrm{s},E' \to E}\, \phi_{\mathrm{n}}(E')\, dE' + S_{\mathrm{n}}(E)$$

$$S_{\mathrm{n}}(E) = \frac{1}{k_{\mathrm{eff}}} \chi_{\mathrm{n,f}}(E) \int_0^\infty \bar{\nu} \Sigma_{\mathrm{f}}\ \phi_{\mathrm{n}}(E')\, dE'$$

Photon Transport

$$\int_{4\pi} \hat{\Omega} \cdot \nabla \psi_{\gamma}(E, \hat{\Omega}) d\hat{\Omega} + \mu_{\mathrm{t}} \phi_{\gamma}(E) = \int_0^\infty \mu_{\mathrm{s},E' \to E}\, \phi_{\gamma}(E')\, dE' + S_{\gamma}(E)$$

$$S_{\mathrm{n}}(E) = \frac{1}{k_{\mathrm{eff}}} \chi_{\gamma,\mathrm{f}}(E) \int_0^\infty \bar{y}_{\gamma,\mathrm{f}} \Sigma_{\mathrm{f}}\ \phi_{\mathrm{n}}(E')\, dE' + \chi_{\gamma,\mathrm{nf}}(E) \int_0^\infty \bar{y}_{\gamma,\mathrm{nf}}\, (\Sigma_{\mathrm{t}} - \Sigma_{\mathrm{f}})\, \phi_{\mathrm{n}}(E')\, dE'$$

Energy Deposition

$$H = H_{\mathrm{f}} + H_{\mathrm{nf}} + H_{\gamma}$$

Terms give energy deposition due to:

H_{f} – Direct fission heating

H_{nf} – Neutron slowing-down heating

H_{γ} – Photon heating

Energy Deposition Treatments

- #1: Constant Energy Per Fission
  - Constant (user-defined) energy release per fission (C_1)
  - All energy deposited at fission site

$$H_{\mathrm{f}} = \int_0^{\infty} C_1 \, \Sigma_{\mathrm{f}} \, \phi_{\mathrm{n}}(E') \, dE'$$

$$H_{\mathrm{nf}} = 0$$

$$H_{\gamma} = 0$$

Energy Deposition Treatments

- #2: Constant Indirect Energy Per Fission
  - Energy and nuclide-dependent energy release per fission (ENDF MT 458 data)
    - Constant (user-defined) indirect energy release per fission (C_2) to account for exothermic reactions during neutron slowing down.
  - All energy deposited at fission site

$$H_{\mathrm{f}} = \int_0^\infty \left[\sum_i \left(f_{\mathrm{fpke},i} + f_{\mathrm{beta},i}\right)\bar{Q}_{\mathrm{f},i}(E)\Sigma_{\mathrm{f},i}\right] \phi_{\mathrm{n}}(E)\, dE = \int_0^\infty \bar{h}_{\mathrm{f}}\, \phi_{\mathrm{n}}(E)\, dE$$

$$H_{\mathrm{nf}} = \int_0^\infty \left[\sum_i \left(\left(f_{\mathrm{prompt\ n},i} + f_{\mathrm{delayed\ n},i}\right)\bar{Q}_{\mathrm{f},i}(E) + C_2\right)\Sigma_{\mathrm{f},i}\right] \phi_{\mathrm{n}}(E)\, dE$$

$$H_{\gamma} = \int_0^\infty \left[\sum_i \left(f_{\mathrm{prompt}\ \gamma,i} + f_{\mathrm{delayed}\ \gamma,i}\right)\bar{Q}_{\mathrm{f},i}(E) + C_2\Sigma_{\mathrm{f},i}\right] \phi_{\mathrm{n}}(E)\, dE$$

Energy Deposition Treatments

- #3: Local Photon Energy Deposition
  - Energy and nuclide-dependent energy release per fission (ENDF MT458 data)
  - Fission fragment and beta particle energy is deposited at fission site (direct fission heating)
  - Neutrons carry energy during transport and deposit energy at each collision
    - Energy and nuclide specific KERMA data for energy release in all non-fission neutron/nucleus interactions
    - Must normalize by k_{eff} to preserve total energy of neutron population between batches in eigenvalue calculations
  - Photon energy is deposited where created (fission or collision site)

$$H_{\mathrm{f}} = \int_0^\infty \bar{h}_{\mathrm{f}}\, \phi_{\mathrm{n}}(E)\, dE \qquad H_{\mathrm{nf}} = \int_0^\infty \bar{h}_{\mathrm{nf}}\, \phi_{\mathrm{n}}(E)\, dE$$

$$H_\gamma = \int_0^\infty C_3 \left[\sum_i \left(f_{\mathrm{prompt}\,\gamma,i} + f_{\mathrm{delayed}\,\gamma,i}\right)\bar{Q}_{\mathrm{f},i}(E)\Sigma_{\mathrm{f},i} + E\chi_{\gamma,\mathrm{nf},i}(E)\bar{y}_{\gamma,\mathrm{nf}}(E)\,(\Sigma_{\mathrm{t}} - \Sigma_{\mathrm{f}})\right] \phi_{\mathrm{n}}(E)\, dE$$

Energy Deposition Treatments

- #4: Coupled Neutron/Photon Transport
  - Energy release the same as treatment #3
  - Photons are samples at neutron collision and fission events and banked for transport in separate simulation

$$H_{\mathrm{f}} = \int_0^\infty \bar{h}_{\mathrm{f}}\, \phi_{\mathrm{n}}(E)\, dE$$

$$H_{\mathrm{nf}} = \int_0^\infty \bar{h}_{\mathrm{nf}}\, \phi_{\mathrm{n}}(E)\, dE$$

$$H_{\gamma} = \int_0^\infty \bar{h}_{\gamma}\, \phi_{\gamma}(E)\, dE$$

Energy Deposition Treatments

- #4: Coupled Neutron/Photon Transport
  - Photon energy deposition throughout problem is normalized by total energy of source photons emitted, creating a **photon redistribution function (PRF)**

$$\omega = \frac{\int_0^\infty \bar{h}_\gamma \, \phi_\gamma(E) \, dE}{\int_V \int_0^\infty E \, S_\gamma(E) \, dE \, d\vec{r}}$$

  - PRF can be used to estimate photon energy distribution for subsequent neutron calculations without additional photon transport simulations
    - PRF only needs to be recalculated when the shape and/or spectrum of the photon distribution has changed significantly.

$$H_\gamma = \omega \int_V \int_0^\infty \left[\sum_i \left(f_{\mathrm{prompt}\,\gamma,i} + f_{\mathrm{delayed}\,\gamma,i} \right) \bar{Q}_{\mathrm{f},i}(E) \Sigma_{\mathrm{f},i} + E \chi_{\gamma,\mathrm{nf},i}(E) \bar{y}_{\gamma,\mathrm{nf}}(E) \left(\Sigma_{\mathrm{t},i} - \Sigma_{\mathrm{f,i}} \right) \right] \phi_\mathrm{n}(E) \, dE \, d\vec{r}$$

Energy Deposition Treatments

Energy Deposition Treatment

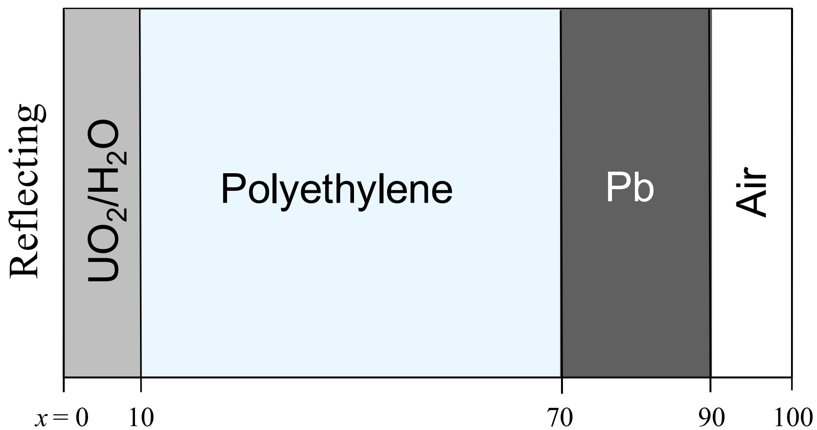
Energy Release Interactions			Constant Energy Release per Fission	Constant Indirect Energy Release per Fission	Local Photon Energy Deposition	Fully Coupled Neutron-Photon Transport
		User input constant energy per fission	at fission site	-	-	-
	fission	Kinetic energy of fission fragments	-	at fission site	at fission site	at fission site
	fission	Delayed β^- emission from fission product decay	-	at fission site	at fission site	at fission site
	fission	Prompt and delayed neutron emission	-	at fission site	*detailed neutron transport*	*detailed neutron transport*
	fission	Prompt and delayed photon emission	-	at fission site	fixed % at fission site	*detailed photon transport*
		User input indirect energy release	-	at fission site	-	-
	non-fission	Non-fission neutron-nucleus interactions	-	-	at neutron collision site	at neutron collision site
	non-fission	Capture photons from neutron interactions	-	-	fixed % at neutron collision site	at photon collision site

Energy Deposition Tally Categories

Dark blue	Local fission energy deposition
Light blue	Neutron slowing-down energy deposition
Grey	Photon energy deposition

Comparison of In-Line Heating Treatments

1-D Core / Composite Shield
100 cm, reflecting at center

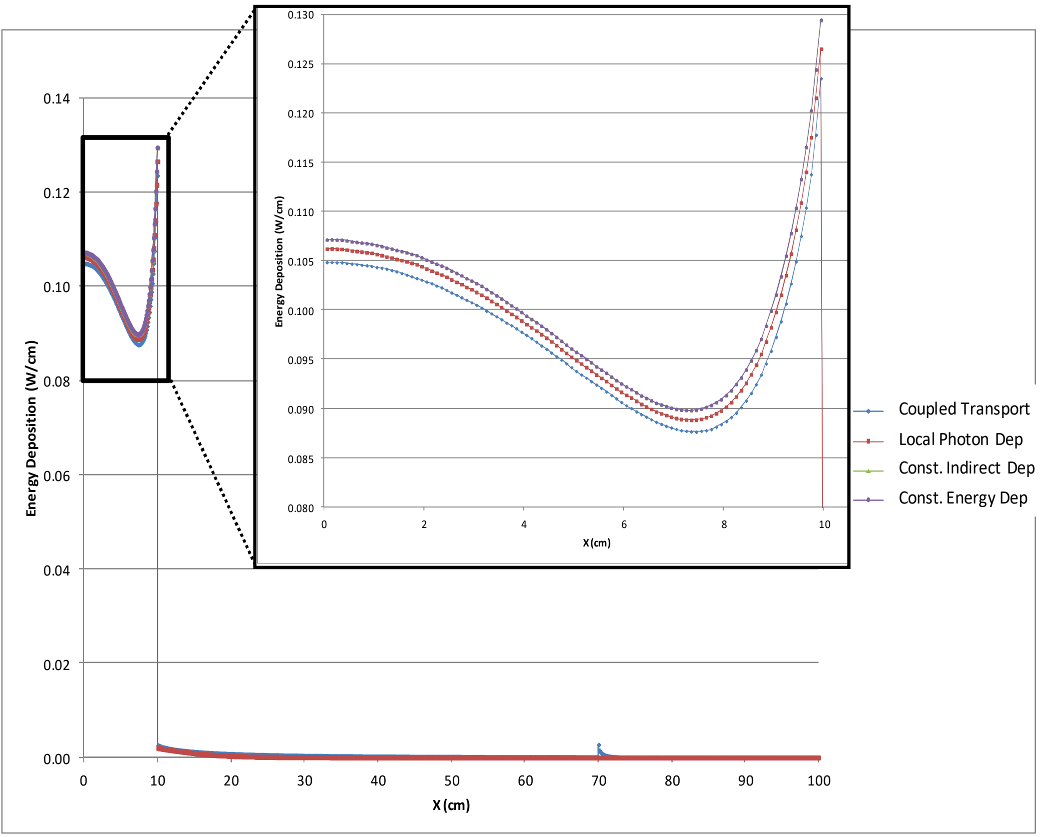


- UO_2/Water Mixture
  - 3% enriched UO_2
  - 11.64 H/U ratio
- Lead
  - ^{204}Pb, ^{206}Pb, ^{207}Pb, ^{208}Pb
  - Nat. abund.
- Polyethylene (CH_2)
  - Natural Carbon
  - H-Polyethylene
- Air
  - ^{16}O
  - Near vacuum

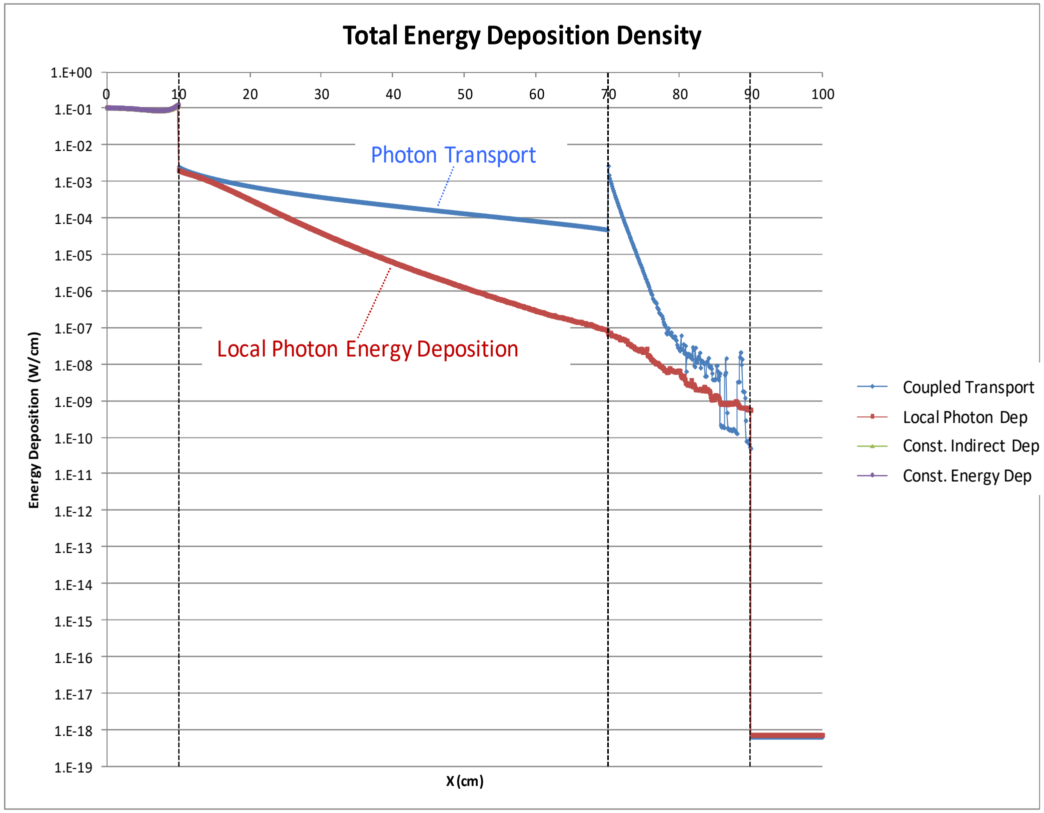
- 50 million neutron histories
  - 5,100 batches (100 discard)
  - 10,000 histories/batch
- $k_{eff} = 1.0390 \pm 0.0002$
- Run on 16 quad-core Xenon Nehalem E5530 procs @ 2.4 GHz
  - Parallel execution on 64 cores
- Results collected over 1000 bin mesh tally
  - Normalized to 1 watt total power

Comparison of In-Line Heating Treatments

Energy Deposition Density in Model



Linear Scale



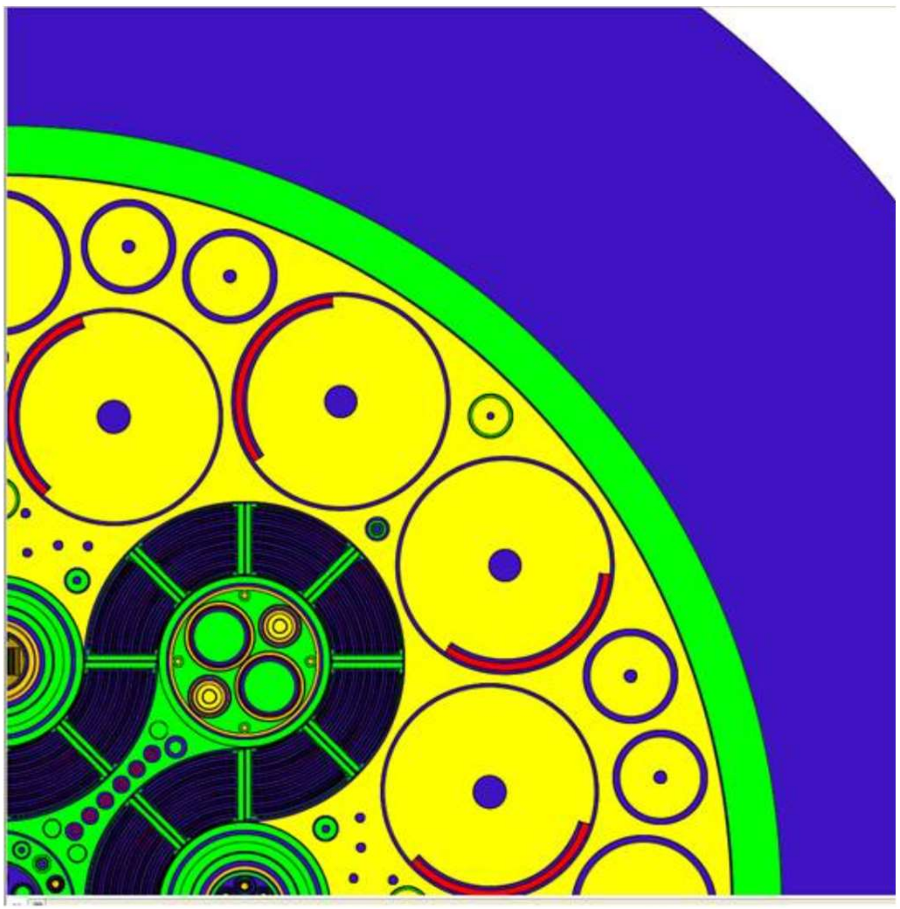
Log Scale

Comparison of In-Line Heating Treatments

	Constant Energy per Fission	Constant Indirect Energy per Fiss.	Local Photon Energy Dep.	Fully Coupled Transport
Total Run Time	**582.08 s**	**580.76 s**	**587.89 s**	**1414.65 s**
Neutron Calc.	582.08 s	580.76 s	587.89 s	958.08 s
Photon Calc.	-	-	-	456.57 s
Energy Deposition Fraction by Region				
Core Total	**100%**	**100%**	**98.85%**	**97.37%**
Neutron	100%	93.55%	90.25%	90.24%
Photon	-	6.45%	8.60%	7.12%
Polyethylene Total	**-**	**-**	**1.15%**	**2.49%**
Neutron	-	-	0.526%	0.527%
Photon	-	-	0.626%	1.96%
Lead Total	**-**	**-**	**2.87×10^{-5}%**	**0.14%**
Neutron	-	-	2.39×10^{-6}%	2.31×10^{-6}%
Photon	-	-	2.63×10^{-5}%	0.135%

Coupled Transport In-Line Heating – Heating by Category

ATR Quarter Core, NE Quadrant
2D Slice (z = 85 – 90 cm)

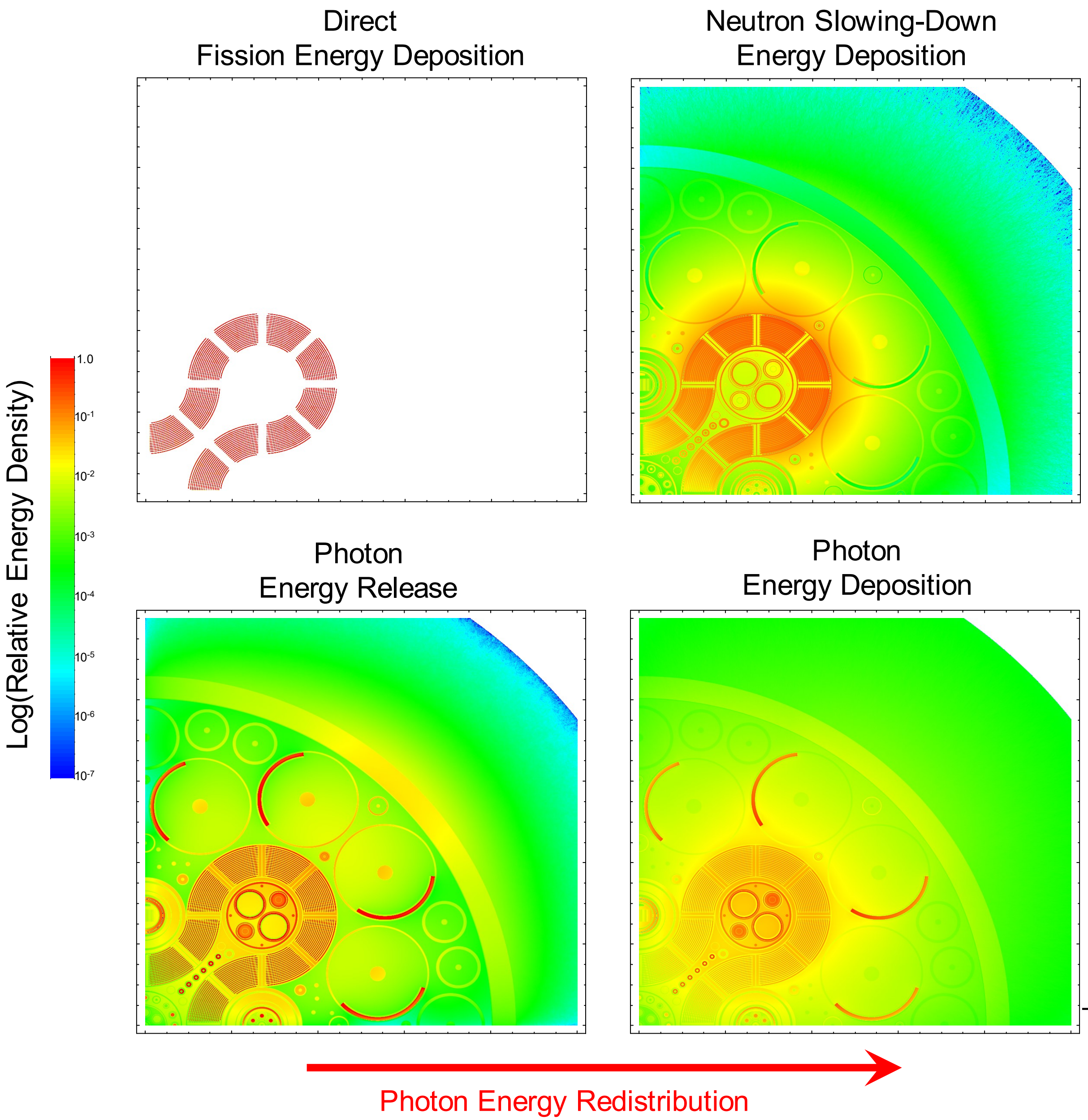


Blue = Water; Red = Hafnium; Green = Aluminum; Yellow = Beryllium

- 3D ATR model created for MC21
  - ~4,000 surfaces
  - ~7,000 components
- 50 million neutron histories
  - 5,100 batches (100 discard)
  - 10,000 histories/batch
- k_{eff} = 0.8367 ± 0.0002
- Results collected over 1 million cell mesh tally (1000 × 1000)

Model and illustration courtesy of C.M. Rodenbush

Coupled Transport In-Line Heating – Heating by Category



Conclusions

- Full paper describes a generalized framework for in-line treatment of energy deposition in Monte Carlo neutron transport calculations.
- Framework gives flexibility to choose, at run-time, from among four self-consistent energy deposition treatments
  - Constant energy release per fission
  - Constant indirect energy release per fission
  - Local photon energy deposition treatment
  - Fully coupled neutron/photon transport energy deposition
- Flexibility allows users to tailor accuracy of energy deposition calculation to be tailored to the needs of a particular application or to meet resource limitations.

Conclusions

- All energy deposition treatments were tested on a simple 1-D core/shield problem.
  - Within the core, all methods agreed to within 3% on integrated energy deposition and 6% on energy deposition density.
  - Treatments without explicit photon transport were 2.5x faster than the reference coupled transport calculation, but significantly under-predicted energy deposition in the shield region.
- Coupled in-line neutron / photon heating calculation for 2D ATR slice was shown
  - Results illustrate energy deposition due to various mechanisms, as well as redistribution effects due to photon transport.