An updated approach to calculation of diffusion coefficients

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Outline

- Diffusion coefficient from P1 equations
- Different forms of transport correction
- Numerical example
- Conclusions

Getting diffusion coefficient from P1 equations

- Multi-group P1 equation in 1D:

$$\frac{d}{dx}\phi_{1,g} + \Sigma_{t,g}\phi_{0,g} = \sum_{g'}\Sigma_{s0,g'\to g}\phi_{0,g'} + S_{0,g}$$

$$\frac{1}{3}\frac{d}{dx}\phi_{0,g} + \Sigma_{t,g}\phi_{1,g} = \sum_{g'}\Sigma_{s1,g'\to g}\phi_{1,g'} + S_{1,g}$$

- ϕ_0 and ϕ_1 – 0^{th} and 1^{st} flux moments
- Σ_0 and Σ_1 – 0^{th} and 1^{st} moments of scattering XS
- Σ_t – total XS
- S - sources

Getting diffusion coefficient from P1 equations

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- Diffusion coeff. can be derived from the 2nd equation:
  - Assuming isotropy of the sources → $S_{1,g} = 0$
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$$J_g = -D\frac{d}{dx}\phi_{0,g}$$

$$\phi_{1,g} = -\boxed{\frac{1}{3\left(\Sigma_{t,g} - \frac{\sum_{g'}\Sigma_{s1,g'\to g}\phi_{1,g'}}{\phi_{1,g}}\right)}}\frac{d}{dx}\phi_{0,g}$$

Getting diffusion coefficient from P1 equations

- Multi-group P1 equation in 1D:

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In-scatter $\Sigma_{tr,g}$

Complexities in calculations of diffusion coefficient

$$\Sigma_{t,g} - \frac{\sum_{g'} \Sigma_{s1,g' \to g} \phi_{1,g'}}{\phi_{1,g}}$$

- Current spectra is needed - not easy to calculate
- What can be done? Examples:
  - Out-scatter approximation
  - Replacing ϕ_1 by ϕ_0
  - Hydrogen transport correction
  - P1 spectral calculations

Some relevant references:

- Yamamoto et al. “Simplified Treatments of Anisotropic Scattering in LWR Core Calculations”, Journal of Nuclear Science and Technology 45, 2008.

- Herman et al. “Improved Diffusion Coefficients Generated From Monte Carlo Codes”, Proc. MC2013, Sun Valley, 2013.

- Choi et al., “Impact of inflow transport approximation on light water reactor analysis,” Journal of Computational Physics 299, 2015.

Out-scatter approximation

Out-scatter approximation

- Additional assumption:
  - P1 in-scatter and out-scatter sources are equal

$$\sum_{g'} \Sigma_{s1,g'\rightarrow g}\phi_{1,g'} \approx \sum_{g'} \Sigma_{s1,g\rightarrow g'}\phi_{1,g}$$

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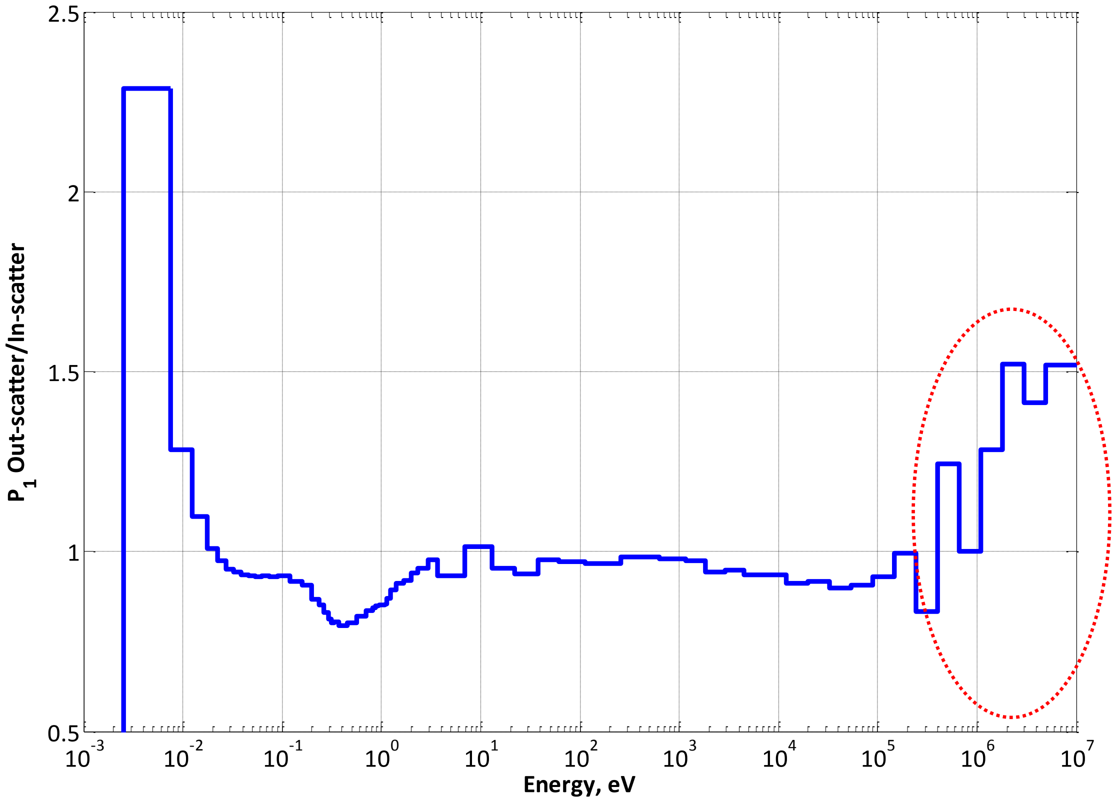
- Then:

$$\frac{\sum_{g'} \Sigma_{s1,g'\to g}\phi_{1,g'}}{\phi_{1,g}} \approx \frac{\sum_{g'} \Sigma_{s1,g\to g'}\phi_{1,g}}{\phi_{1,g}} = \frac{\sum_{g'} \Sigma_{s1,g\to g'}\cancel{\phi_{1,g}}}{\cancel{\phi_{1,g}}} = \sum_{g'} \Sigma_{s1,g\to g'} = \Sigma_{s1,g}$$

- Typical out-scatter form of $\Sigma_{tr,g}$
  - Knowledge of current spectra is not required
  - Current Serpent approach

$$\Sigma_{tr,g} = \Sigma_{t,g} - \Sigma_{s1,g} = \Sigma_{t,g} - \hat{\mu}_g \Sigma_{s0,g}$$

Out-scatter approximation



- Out-scatter and in-scatter sources are not everywhere close (ratio is shown)
- Difference in fast region can result in “too strong” transport correction
  - Serpent results: UO_2 PWR assembly, current spectra from 0-D P1 equation (modified B1)

Hydrogen transport correction

Hydrogen transport correction

- Idea:
  - Obtain H-transport correction curve: Σ_{tr}/Σ_{T}
  - From H-only slab with a fixed fission source
  - Use the H-correction curve to modify Σ_{tr} from lattice calculations

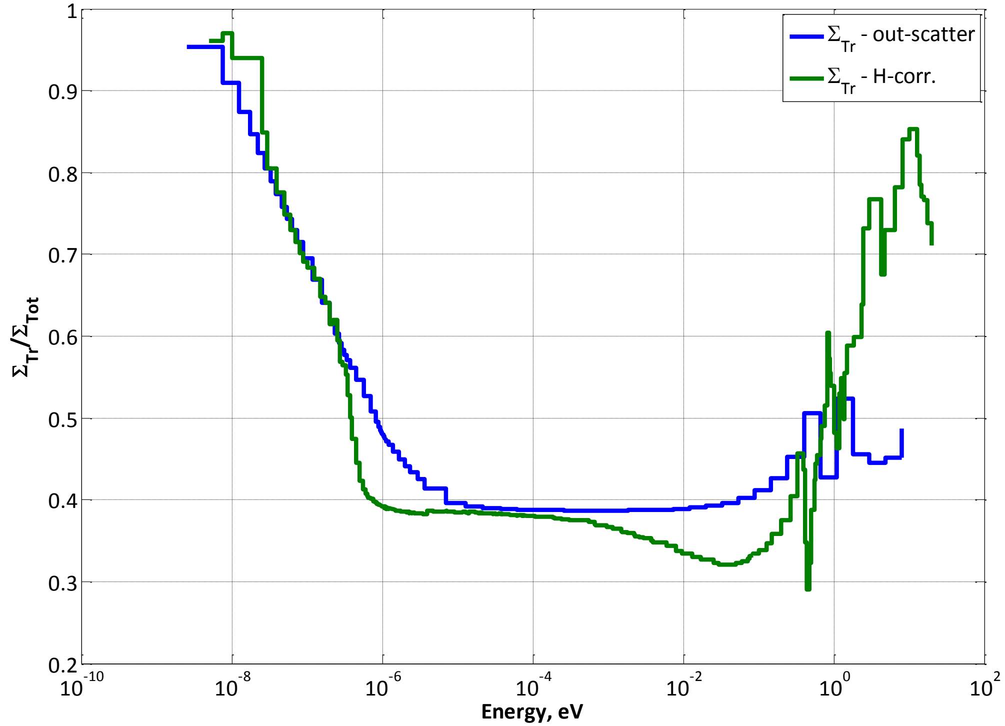
- Assumption:
  - H is a major source for scattering anisotropy ($\mu \approx 2/3A$)

- Procedure:

  1. Calculate $\sum_{tr,all}, \sum_{tr,H}, \sum_{T,H}$
  2. Calculate $\sum_{tr.H}^{corr} = \sum_{T,H} \times \text{Correction curve}$
  3. Calculate $\sum_{tr.all}^{corr} = \sum_{tr,all} - \sum_{tr,H} + \sum_{tr.H}^{corr}$

- Described in details in MC2013 paper by Bryan Herman
  - “Improved Diffusion Coefficients Generated From Monte Carlo Codes”

Hydrogen transport correction curve



- Available in version 2.1.27
- H_2O curve is shown

Diffusion coefficient: Serpent vs. Casmo

	Casmo	Serpent		
		Out-scatter	H-correction	B1
g1	1.47534	1.55880	1.48000	1.44966
g2	0.42139	0.41320	0.43040	0.44533
g1	-	**5.7%**	**0.3%**	-1.7%
g2	-	-1.9%	2.1%	5.7%

Some test problems

2D PWR core

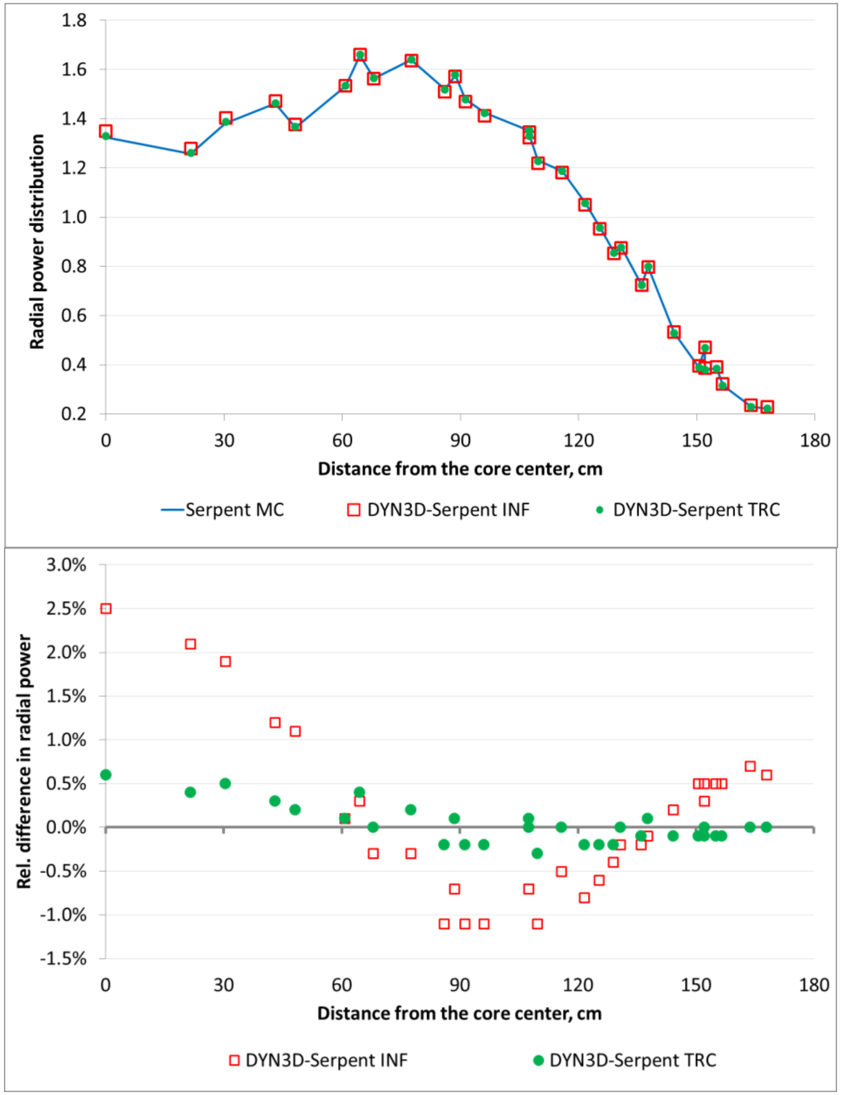
1	3	1	2	1	2	1	3	R
3	1	3	1	2	1	2	3	R
1	3	1	2	1	2	1	3	R
2	1	2	1	2	1	3	3	R
1	2	1	2	1	2	3	R	R
2	1	2	1	2	3	3	R	
1	2	1	3	3	3	R	R	
3	3	3	3	R	R	R		
R	R	R	R	R				

Reference PWR Core

1 – 3.1w/o U-235 + 16 WABAs
2 – 2.3w/o U-235
3 – 2.3w/o U-235
R – Reflector

- Serpent - few-group XS + reference solution
- DYN3D - nodal diffusion calculations
- Verify DYN3D results vs. full core Serpent solution

2D PWR core: Radial power distribution



3D PWR core – OECD MOX benchmark

	1	2	3	4	5	6	7	8
A	U 4.2% (CR-D) 35.0	U 4.2% 0.15	U 4.2% (CR-A) 22.5	U 4.5% 0.15	U 4.5% (CR-SD) 37.5	M 4.3% 17.5	U 4.5% (CR-C) 0.15	U 4.2% 32.5
B	U 4.2% 0.15	U 4.2% 17.5	U 4.5% 32.5	M 4.0% 22.5	U 4.2% 0.15	U 4.2% (CR-SB) 32.5	M 4.0% 0.15	U 4.5% 17.5
C	U 4.2% (CR-A) 22.5	U 4.5% 32.5	U 4.2% (CR-C) 22.5	U 4.2% 0.15	U 4.2% 22.5	M 4.3% 17.5	U 4.5% (CR-B) 0.15	M 4.3% 35.0
D	U 4.5% 0.15	M 4.0% 22.5	U 4.2% 0.15	M 4.0% 37.5	U 4.2% 0.15	U 4.5% (CR-SC) 20.0	M 4.3% 0.15	U 4.5% 20.0
E	U 4.5% (CR-SD) 37.5	U 4.2% 0.15	U 4.2% 22.5	U 4.2% 0.15	U 4.2% (CR-D) 37.5	U 4.5% 0.15	U 4.2% (CR-SA) 17.5	
F	M 4.3% 17.5	U 4.2% (CR-SB) 32.5	M 4.3% 17.5	U 4.5% (CR-SC) 20.0	U 4.5% 0.15	M 4.3% 0.15	U 4.5% 32.5	
G	U 4.5% (CR-C) 0.15	M 4.0% 0.15	U 4.5% (CR-B) 0.15	M 4.3% 0.15	U 4.2% (CR-SA) 17.5	U 4.5% 32.5	Assembly Type CR Position Burnup [GWd/t]	
H	U 4.2% 32.5	U 4.5% 17.5	M 4.3% 35.0	U 4.5% 20.0			Fresh Once Burn Twice Burn	

CR-A	Control Rod Bank A
CR-B	Control Rod Bank B
CR-C	Control Rod Bank C
CR-D	Control Rod Bank D
CR-SA	Shutdown Rod Bank A
CR-SB	Shutdown Rod Bank B
CR-SC	Shutdown Rod Bank C
CR-SD	Shutdown Rod Bank D
O	Ejected Rod

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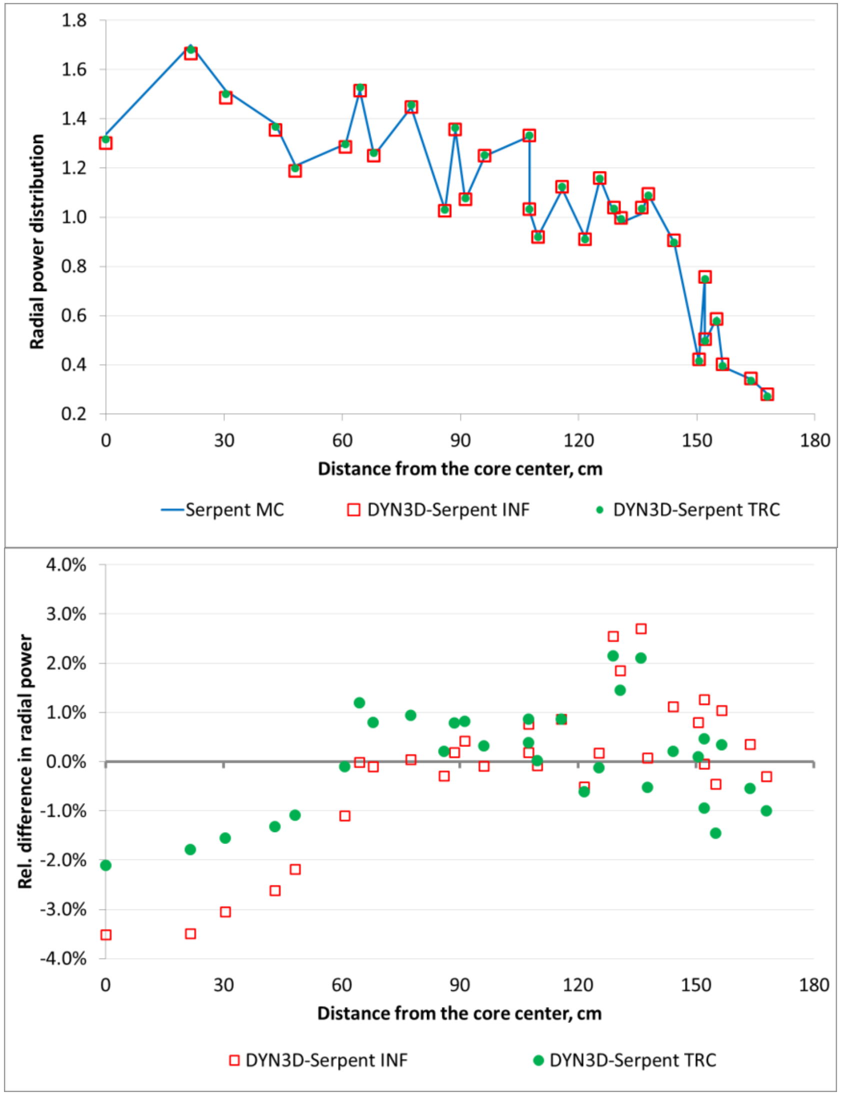

Summary and future work

- H-transport correction was implemented in Serpent 2.1.27
- LWR diffusion coefficients are consistent with Casmo
- Somewhat improved nodal diffusion results…
- But some other factors should be accounted for
  - Discontinuity factors
  - Reflector models
  - Leakage correction
- H-like correction can be used for other scatters
  - deuterium, graphite, …
  - importance (anisotropy) decreases with A ($\mu \approx 2/3A$)
  - further investigation is required

Thank you!

Generation of few-group diffusion coefficients

- $\Sigma_{tr,g}$ can be used for the generation of $\mathbf{D_G}$ in two ways:

Option 1:
Collapsing of $\boldsymbol{\Sigma_{tr,g}}$

$$\Sigma_{tr,G} = \frac{\sum_{g \in G} \Sigma_{tr,g} \phi_g}{\sum_{g \in G} \phi_g} \Rightarrow D_G = \frac{1}{3\Sigma_{tr,G}}$$

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Option 2:
Collapsing of D_g

$$D_g = \frac{1}{3\Sigma_{tr,g}} \Rightarrow D_G = \frac{\sum_{g \in G} D_g \phi_g}{\sum_{g \in G} \phi_g}$$

HZDR