

An updated approach for calculation of diffusion coefficient

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Outline

- Derivation of diffusion coefficient – a quick reminder
- Updated collapsing scheme
- Numerical example
- Conclusions

Getting diffusion coefficient from P1 equations

- Multi-group P1 equation in 1D:

$$\frac{d}{dx} \phi_{1,g} + \Sigma_{t,g} \phi_{0,g} = \sum_{g'} \Sigma_{s0,g' \rightarrow g} \phi_{0,g'} + S_{0,g}$$
$$\frac{1}{3} \frac{d}{dx} \phi_{0,g} + \Sigma_{t,g} \phi_{1,g} = \sum_{g'} \Sigma_{s1,g' \rightarrow g} \phi_{1,g'} + S_{1,g}$$

- ϕ_0 and ϕ_1 – 0th and 1st flux moments
- Σ_0 and Σ_1 – 0th and 1st 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 $\rightarrow S_{1,g} = 0$
 - Using Fick's law:

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$$J_g = - D \frac{d}{dx} \phi_{0,g}$$

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

Getting diffusion coefficient from P1 equations

- Multi-group P1 equation in 1D:

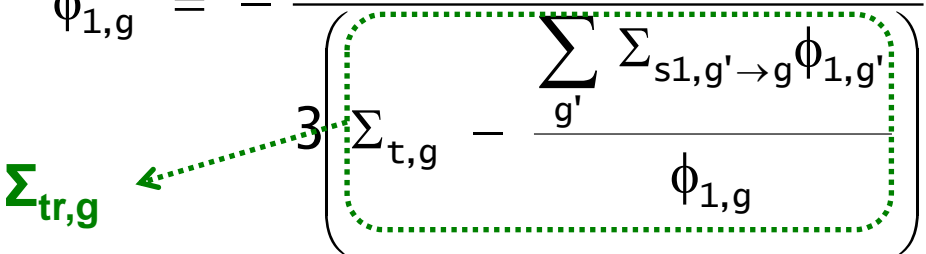
$$\frac{d}{dx} \phi_{1,g} + \Sigma_{t,g} \phi_{0,g} = \sum_{g'} \Sigma_{s0,g' \rightarrow g} \phi_{0,g'} + S_{0,g}$$

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Out-scatter approximation

- Complexities in calculations of Σ_{tr}
 - ϕ_1 is needed
 - ϕ_1 is not always available
- Additional assumption:

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

- Then:

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

- Typical out-scatter form of $\Sigma_{tr,g}$

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

Advantages of out-scatter approximation

- Simplicity

In Serpent:

- $\Sigma_{t,g}$ and $\Sigma_{s0,g}$
 - Sampled using standard tallies
- μ_g
 - Sampling of the incident and emergent directions for scattered neutrons

Generation of few-group diffusion coefficients

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

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

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

**Option 2:
Collapsing of D_g**

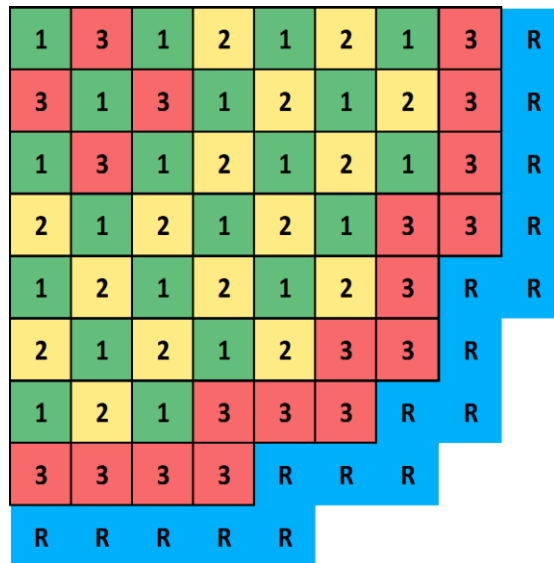
$$D_g = \frac{1}{3 \Sigma_{tr,g}} \Rightarrow D_G = \frac{\sum_{g \in G} D_g \phi_g}{\sum_{g \in G} \phi_g}$$

- Previously in Serpent:

$$\Sigma_{tr,G} = \Sigma_{t,G} - \hat{\mu}_G \Sigma_{s,G} \Rightarrow D_G = \frac{1}{3 \Sigma_{tr,G}} \quad \leftarrow \text{Equivalent to Option 1}$$

Numerical example

- Consider 2D model of a PWR core
- Generate and compare few-group XS and diffusion coefficients
 - With Serpent and HELIOS2
- Perform nodal diffusion calculations with DYN3D code
 - Using few-group XS generated by Serpent and HELIOS
- Verify DYN3D results vs. full core Serpent solution



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

Diffusion coefficients calculated by Serpent: Difference between Option 1 and 2

	type 1	type 2	type 3	reflector
D_1	-25%	-26%	-26%	-37%
D_2	-11%	-11%	-11%	-11%

- The effect on full core results will be demonstrated later

Comparison of few-group XS: Serpent vs. HELIOS, % difference

XS type	D_1	D_2
Fuel 1	0.00	-0.16
Fuel 2	0.30	-0.16
Fuel 3	0.28	-0.15
Reflector	3.32	0.10

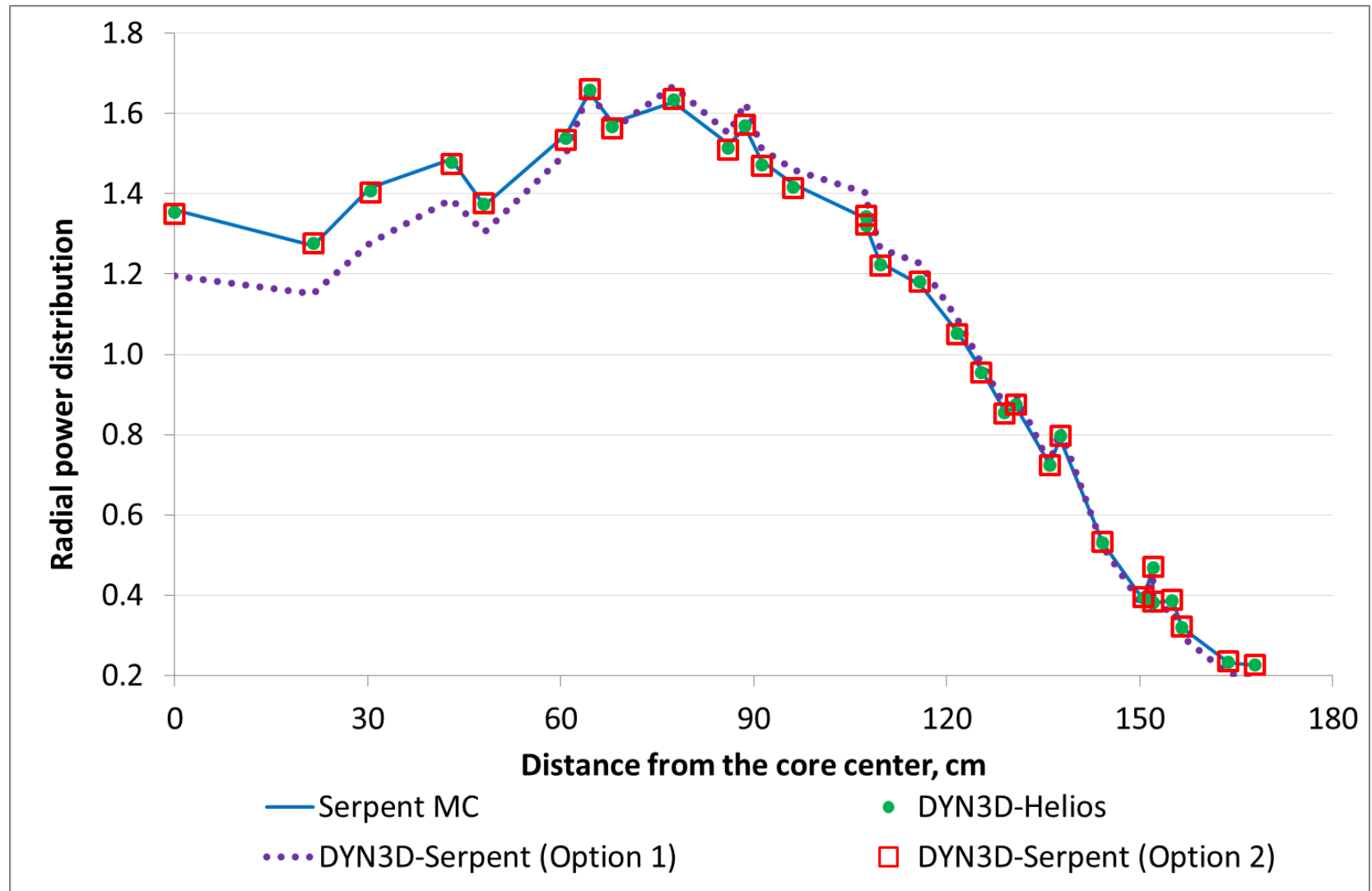
- ENDF/B-VII based data libraries
- D_G was generated via collapsing fine-group D_g
 - 177-group in HELIOS
 - 70-group in Serpent

Full core results: k-eff

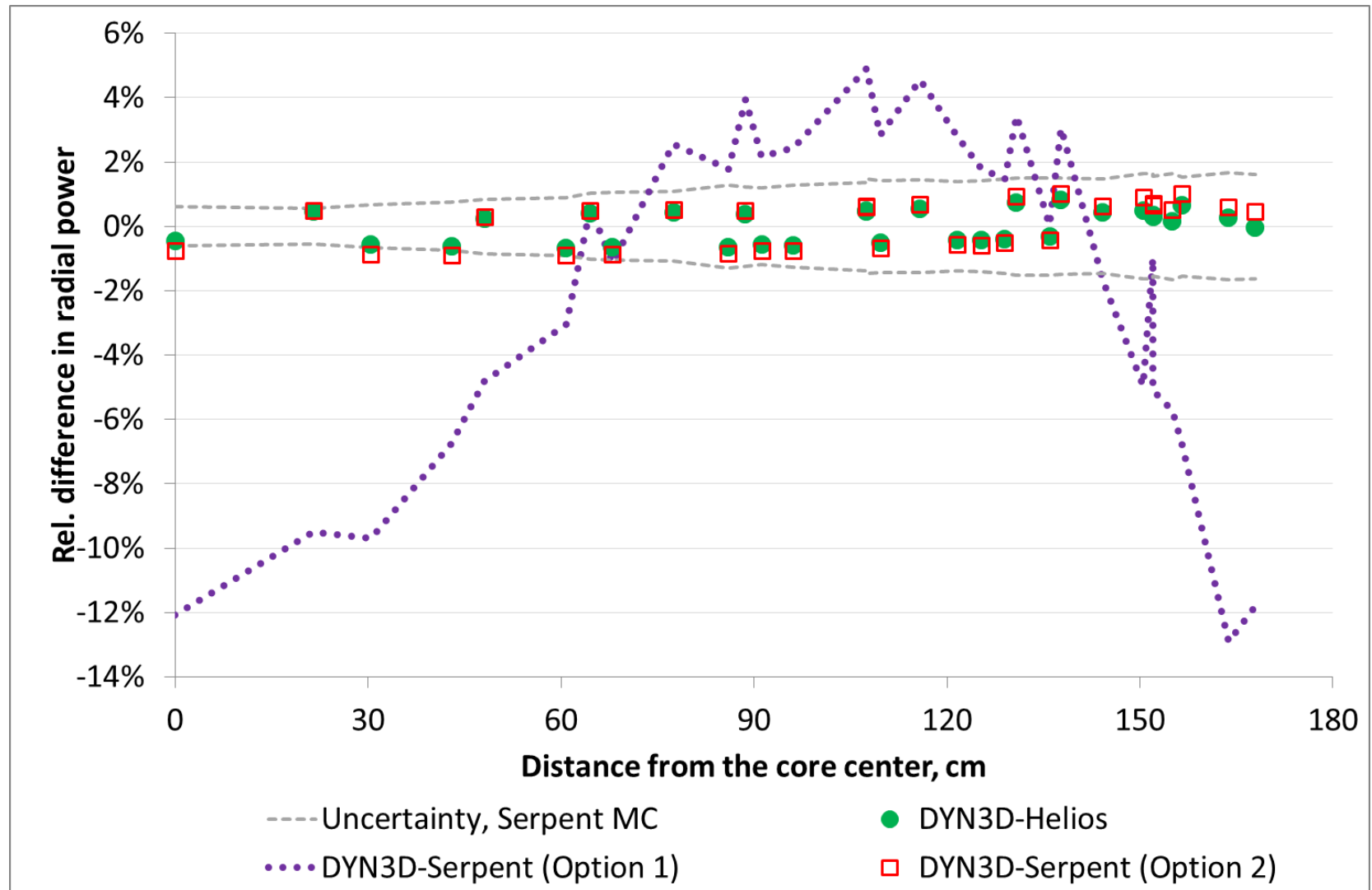
	k-eff	% difference
Serpent full core MC	1.00187±0.00004	Reference
DYN3D-Serpent	1.00016	-0.17
DYN3D-Helios	0.99998	-0.19

- 15 independent full core Serpent simulations
 - for estimation of radial power distribution + uncertainties

Full core results: radial power distribution



Full core results: radial power distribution



Conclusions

- Correct collapsing of diffusion coefficient is important
- Leads to consistent 3D nodal diffusion results
- Updated approach was recently implemented in Serpent 2
- HELIOS users: FYI

Thank you for your attention!