TRIANGLE-BASED QUASI-DIFFUSION NODAL SOLVER EMPLOYING SERPENT'S HOMOGENIZED GROUP CONSTANTS

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Serpent User Group Meeting

October 28th 2020

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Outline

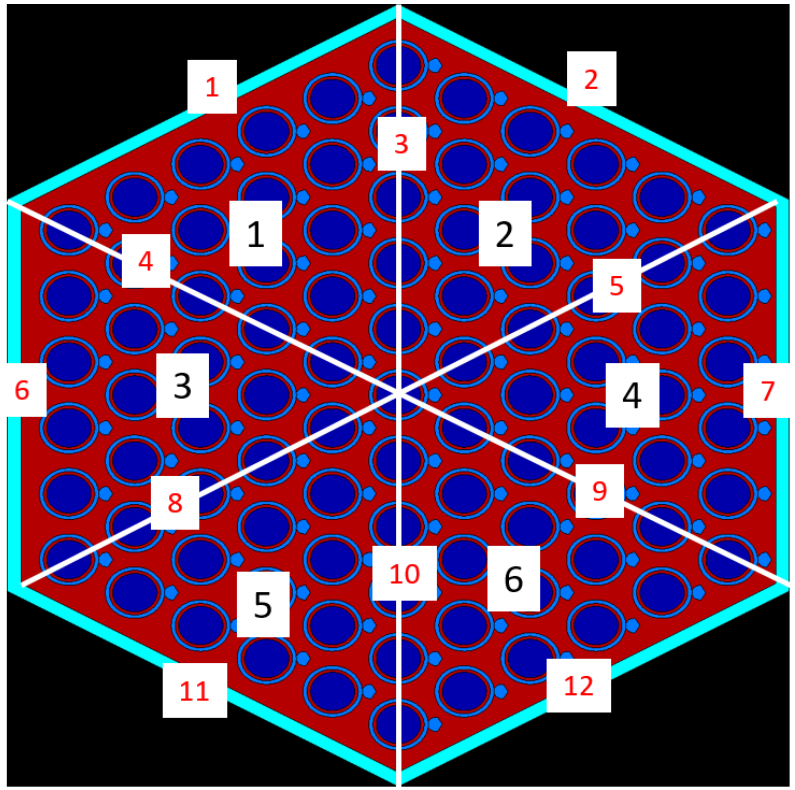
What Covered in this Presentation

- Background
- Derivation of Quasi-diffusion Equation
- Formulation of Triangle-based Quadratic Expansion Method (TQEM)
- Iteration Scheme for TQEM-CMFD
- Serpent Model
- Results
- Conclusion

Background

What Motivates this Work

- Hundreds of different material composition in SFR subassemblies ➔ cause a large heterogeneity effect at assembly interface
- Quasi-diffusion methods proved to improve accuracy in nodal solver (Y. Xu, V. Seker, T. Downar, 2020)
- Triangular nodes provide better resolution than hexagonal nodes (1 hex = 6 triangles)
- This method is proposed for SFR analysis in PARCS utilizing group constants from Serpent



Derivation of Quasi-diffusion Equation

Start with the Boltzman Transport Equation

Multigroup transport equation:

$$\hat{\Omega} \cdot \nabla \psi_g(\vec{r}, \Omega) + \Sigma_{t,g}(\vec{r}) \psi_g(\vec{r}, \hat{\Omega}) = S_g(\vec{r}, \hat{\Omega}) \qquad (1)$$

Integrate Equation (1) along $d\Omega \in 4\pi$ to obtain 0th angular moment of transport equation:

$$\nabla \cdot \vec{J}_g(\vec{r}) + \Sigma_{t,g}(\vec{r}) \phi_g(\vec{r}) = S_{0,g}(\vec{r}) \qquad (2)$$

Multiply Equation (1) by Ω, and again integrate along $d\Omega \in 4\pi$ to obtain 1st angular moment of transport equation:

$$\int_{4\pi} \hat{\Omega}\hat{\Omega} \cdot \nabla \psi_g(\vec{r}, \hat{\Omega})\, d\Omega + \Sigma_{t,g}(\vec{r}) \vec{J}_g(\vec{r}) = \vec{S}_{1,g}(\vec{r}) \qquad (3)$$

Derivation of Quasi-diffusion Equation

Eddington Factors

Introduce Eddington factors/tensors:

$$E_{uv,g} = \frac{\int_{4\pi} \Omega_u \Omega_v \, \psi_g(\vec{r}, \hat{\Omega}) d\Omega}{\int_{4\pi} \psi_g(\vec{r}, \hat{\Omega}) d\Omega}$$

$$\vec{\vec{E}}_g = \begin{bmatrix} E_{xx,g} & E_{xy,g} & E_{xz,g} \\ E_{yx,g} & E_{yy,g} & E_{yz,g} \\ E_{zx,g} & E_{zy,g} & E_{zz,g} \end{bmatrix}$$

Important features of Eddington Factors:

- Diagonal elements $\in [0,1]$, generally close to 1/3, and sum up to 1
- Off-diagonal elements $\ll$ diagonal elements, so practically can be neglected in calculation

Derivation of Quasi-diffusion Equation

Final Form of Quasi-diffusion Equation

- Inserting Eddington factors into the first moment equation (Eq. 3):

$$\vec{J}_g(\vec{r}) = -\frac{\vec{\vec{E}}}{\Sigma_{tr,g}} \cdot \nabla\phi_g(\vec{r}) \qquad (4)$$

- Neglecting the off-diagonal terms, we can obtain directional diffusion coefficient:

$$\vec{D}_g = \left(D_{xg}, D_{yg}, D_{zg}\right) = \hat{x}\frac{E_{xx,g}}{\Sigma_{tr,g}} + \hat{y}\frac{E_{yy,g}}{\Sigma_{tr,g}} + \hat{z}\frac{E_{zz,g}}{\Sigma_{tr,g}}$$

Where Transport cross-section, $\Sigma_{tr,g} = \Sigma_{t,g} - \Sigma_{s1,g}$

- Substituting the net current defined before (Eq.4) into zeroth moment equation (Eq. 2) results in:

$$-\left(D_{x,g}\frac{\partial^2}{\partial x^2} + D_{y,g}\frac{\partial^2}{\partial y^2} + D_{z,g}\frac{\partial^2}{\partial z^2}\right)\phi_g(\vec{r}) + \Sigma_{t,g}(\vec{r})\phi_g(\vec{r}) = S_{0,g}(\vec{r})$$

Where: $D_{u,g} = \frac{E_{uu,g}}{\Sigma_{tr,g}}$

Formulation of Triangle-based Quadratic Expansion Method (TQEM)

Polynomial Expansion in Triangle nodes

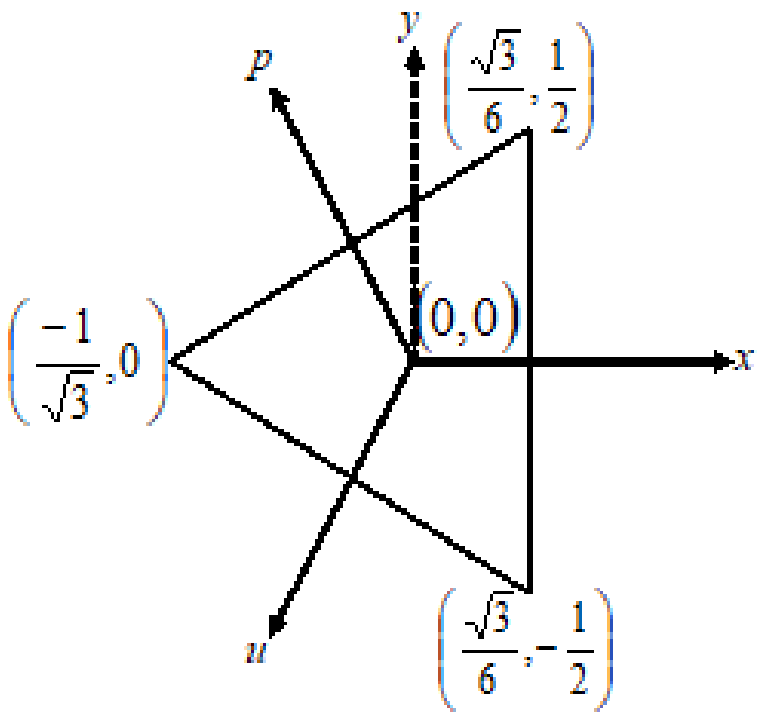
- Coordinate transformation for triangle

$$u(x,y) = -\frac{1}{2}\left(x + \sqrt{3}\,y\right)$$

$$p(x,y) = -\frac{1}{2}\left(x - \sqrt{3}\,y\right)$$

- Polynomial Expansion function for scalar flux

$$\phi_g(x,y) = a_1 + a_2 x + a_3 y + a_4 (x^2 + y^2)$$



Formulation of Triangle-based Quadratic Expansion Method (TQEM)

Constraints to Solve

The 4 terms of polynomial expansion need 4 constraint for each triangular node, each axial plane and each energy group:

1. Node-average flux
2. Surface-p continuity
3. Surface-x continuity
4. Surface-u continuity

- To solve for the nodal equations, instead of using the one-node and two-node approach like conventional nodal methods, TQEM utilizes the whole plane approach

Formulation of Triangle-based Quadratic Expansion Method (TQEM)

Why Quadratic Polynomial is Used

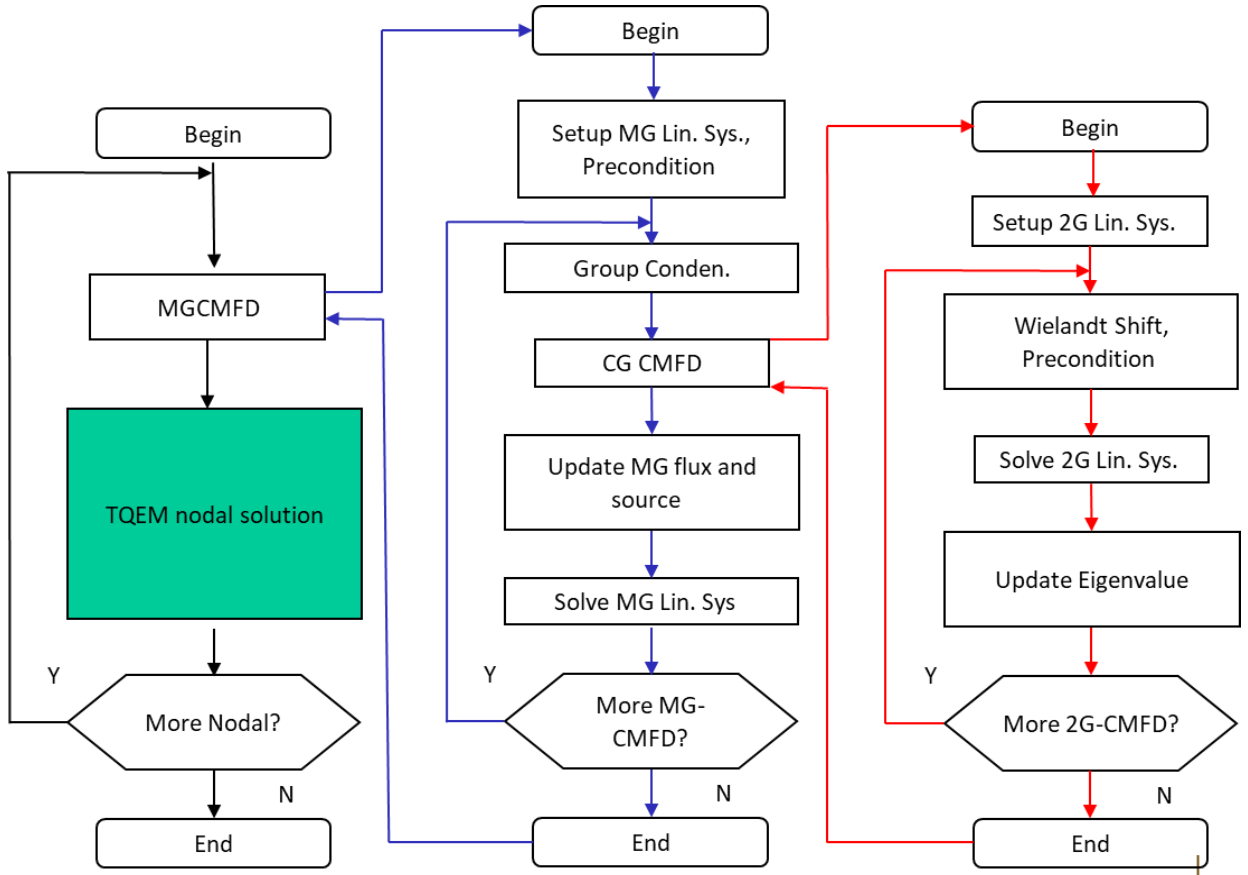
1. The flux distribution in fast reactors is smoother than that in the thermal reactors (mean free path of fast neutrons is significantly longer than thermal neutrons)
2. Constraint equations can be minimized, and the requirement of corner point fluxes can be avoided

Formulation of Triangle-based Quadratic Expansion Method (TQEM)

Primary variable	Equation
Node Average Flux	$\bar{\bar{\phi}}_g = \frac{4}{\sqrt{3}} \int_{-1/\sqrt{3}}^{\sqrt{3}/6} \int_{y_u(x)}^{y_p(x)} \phi_g(x,y)\ dy$
Surface-x Average Flux	$\bar{\phi}_{xg} = \int_{-1/2}^{1/2} \phi_g\left(\frac{\sqrt{3}}{6}, y\right)\ dy$
Surface-u Average Flux	$\bar{\phi}_{ug} = \frac{2}{\sqrt{3}} \int_{-1/\sqrt{3}}^{\sqrt{3}/6} \phi_g\left(x, y_u(x)\right)\ dy$
Surface-p Average Flux	$\bar{\phi}_{pg} = \frac{2}{\sqrt{3}} \int_{-1/\sqrt{3}}^{\sqrt{3}/6} \phi_g\left(x, y_p(x)\right)\ dy$
Surface-x Average Current	$\bar{J}_{xg} = -\frac{D_{xg}}{h} \int_{-1/2}^{1/2} \frac{d}{dx}\phi_g\left(\frac{\sqrt{3}}{6}, y\right)\ dy$
Surface-u Average Current	$\bar{J}_{ug} = \frac{1}{h} \int_{-1/\sqrt{3}}^{\sqrt{3}/6} \frac{1}{\sqrt{3}}\frac{d}{dx}\phi_g\left(x, y_u(x)\right) + \frac{d}{dy}\phi_g\left(x, y_u(x)\right)\ dy$
Surface-p Average Current	$\bar{J}_{pg} = \frac{1}{h} \int_{-1/\sqrt{3}}^{\sqrt{3}/6} \frac{1}{\sqrt{3}}\frac{d}{dx}\phi_g\left(x, y_p(x)\right) - \frac{d}{dy}\phi_g\left(x, y_p(x)\right)\ dy$

Iteration Scheme

Utilizing Multi-level CMFD Acceleration



Serpent Model

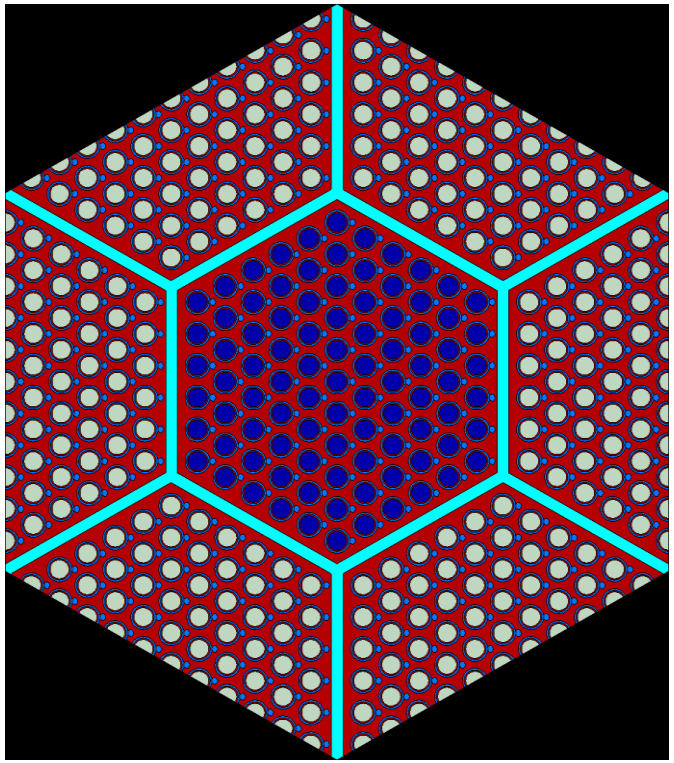
Serpent features and capabilities for this work

- Triangle geometry was developed by Serpent team as of late 2019 – early 2020 (**surf tric**)
- The standard group constants in triangle geometry can be obtained similar to other implemented geometries
- Heterogeneous solutions (node average fluxes, surface fluxes and currents) for ADF generation in a triangle geometry can be obtained through **set adf** option in triangle surface
- Eddington Factors can be obtained using **set eddi** option in the latest version of Serpent

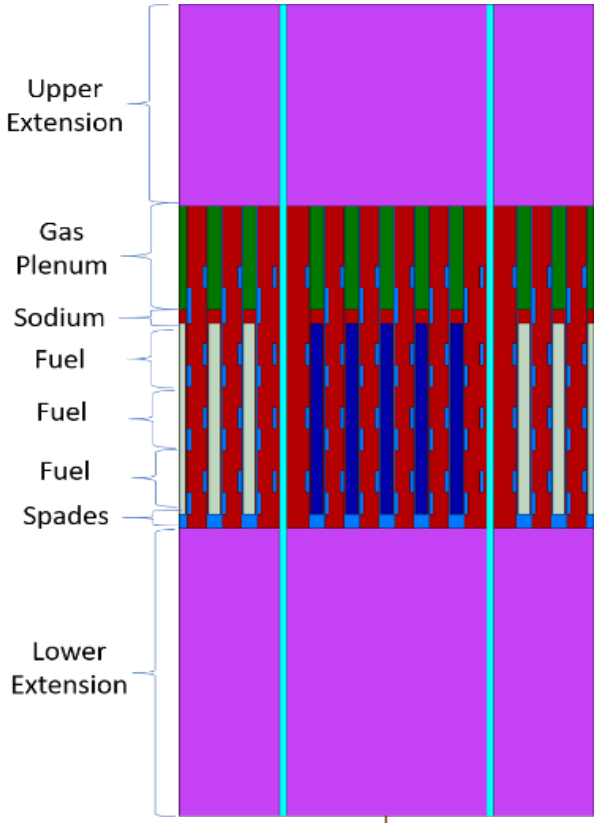
Serpent Model

3D 4-Hex Assemblies Model of EBR-II Reactor

Radial View

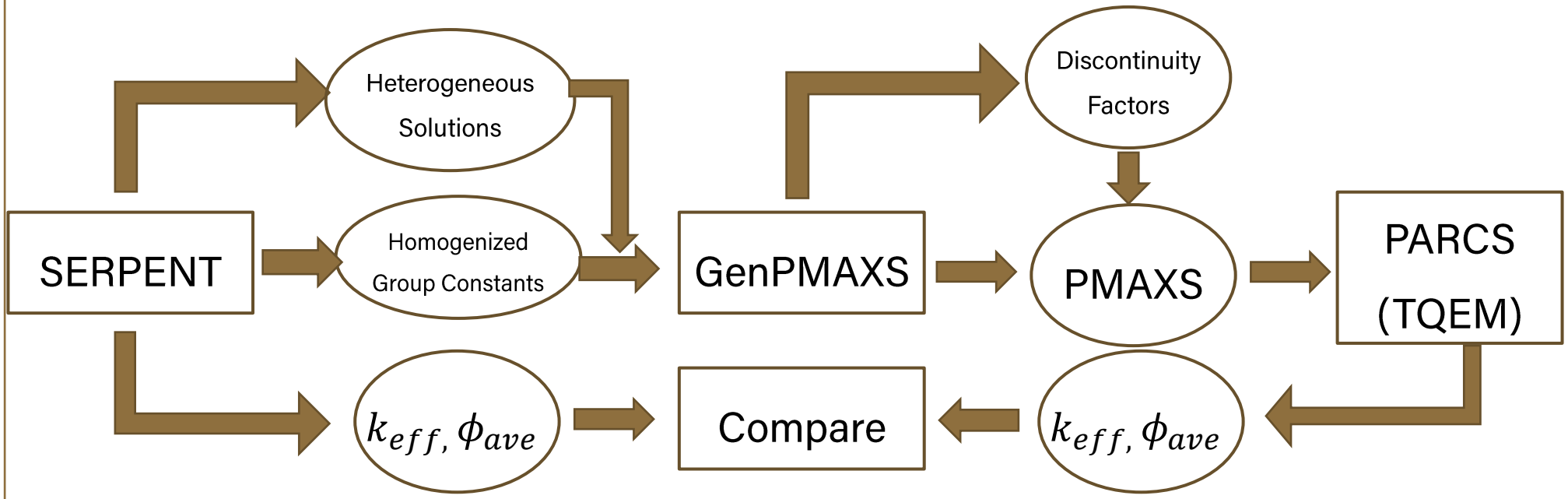


Axial View



Serpent Model

Test Procedures



Results

k_{eff} Comparison

Serpent keff	ADF	Diffusion	TQEM keff	TQEM Error (pcm)
1.01356 ± 0.00003	Off	Standard	1.0248817	1132.17
	Off	QD	1.0201777	661.77
	On	Standard	1.0135600	0.00
	On	QD	1.0135600	0.00

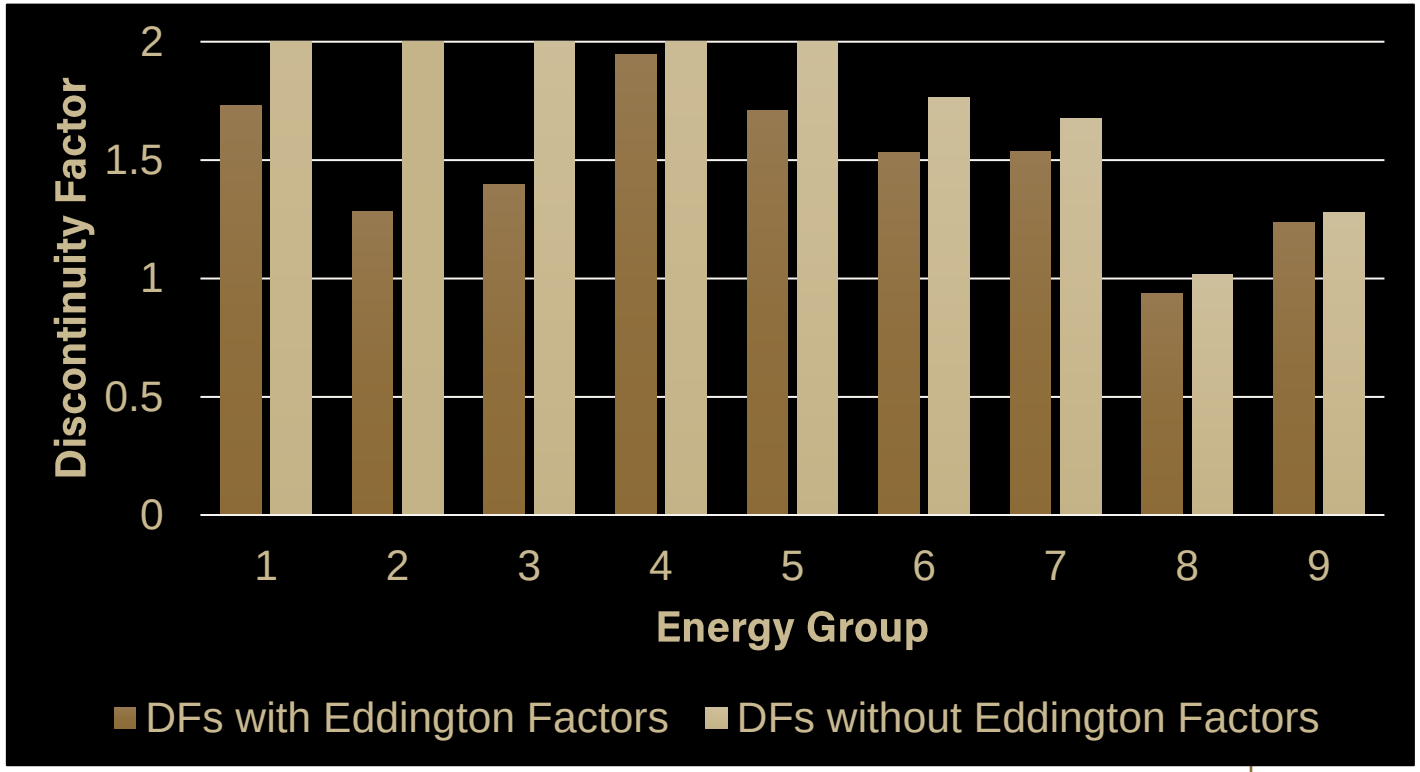
Results

Node-averaged Flux Relative Error

ADF	Diffusion	Average Error	Maximum Error	RMS Error
Off	Standard	6.9111E-02	9.9623E-01	1.5522E-01
Off	QD	4.5373E-02	4.2777E-01	1.5259E-01
On	Standard	7.7345E-09	3.1532E-07	6.9842E-08
On	QD	7.2300E-09	2.9542E-07	6.4999E-08

Results

Comparison of group-wise discontinuity factors on the bottom reflector facing vacuum boundary, with and without Eddington factors included



Conclusion

- Utilizing Serpent group constants and heterogeneous solutions, the TQEM method can reproduce the exact Serpent k-eff and fluxes
- Quasi-diffusion provide significant improvement of the results in nodal solver when ADFs are not available
- With ADFs included, the quasi-diffusion method can make the ADFs to be closer to unity, therefore increasing the calculation stability

THANK YOU

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