On the Effect of the Diffusion Coefficient Treatment in Finite Difference Schemes of the Diffusion Equation

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Presented at ANS Student Conference, Richmond, VA, April 6th, 2019

The Continuous Energy Diffusion Equation

$$-\underline{\nabla}\cdot D(\underline{r},E)\underline{\nabla}\phi(\underline{r},E)+\Sigma_t(\underline{r},E)\phi(\underline{r},E)=\sum_{g'=1}^{G}\int_{g'}^{g'-1}dE'\Sigma_s(\underline{r},E'\rightarrow E)\phi(\underline{r},E')$$

$$+\chi(E)\sum_{g'=1}^{G}\int_{g'}^{g'-1}dE'\nu_f(E')\Sigma_f(\underline{r},E')\phi(\underline{r},E')+S_{ext}(\underline{r},E)$$

- A simplification of the Neutron Transport Equation
- Derivation of this equation is based on Fick's law, which requires assumptions about the conditions of the problem
- Nonetheless provides a workable approximation of the Neutron Transport Equation that does not overly tax computational resources
- For these reasons, facilitates scholarly inquiry

Multi-Group Diffusion Equation

$$-\underline{\nabla}\cdot D_g(\underline{r})\underline{\nabla}\phi_g(\underline{r})+\Sigma_{tg}(\underline{r})\phi_g(\underline{r})$$
$$=\sum_{g'=1}^{G}\Sigma_{sg'\to g}(\underline{r})\phi_{g'}(\underline{r})+\chi_g\sum_{g'=1}^{G}\nu_{fg'}\Sigma_{fg'}(\underline{r})\phi_{g'}(\underline{r})+S_{ext,g}(\underline{r})$$

- A simplification of the Neutron Transport Equation
- Accounts for multiple energy types
- Can account for one-, two-, and three-dimensional problems
- Assumes static, unchanging, time-independent nature

Simplifying the area of numerical interest

- Reduce to one energy group to simplify the equation
- Compress three dimension space, r, down to one dimension, x

$$-\frac{d}{dx}\left(D(x)\frac{d\phi}{dx}\right)+\Sigma_a(x)\phi(x)=S(x)$$

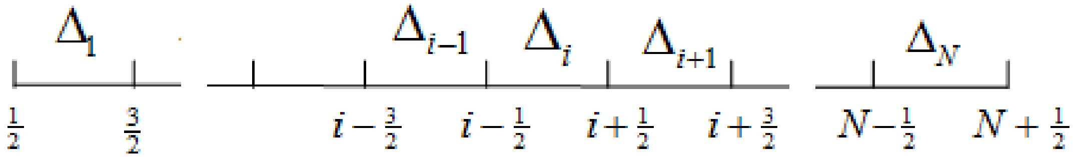
macro-absorption

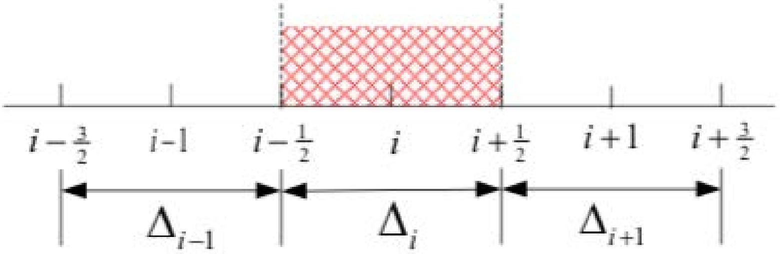
The diffusion coefficient

source

Numerical Discretization

- Divide the domain of interest into N meshes
- Integrate, such that any given mesh will contain only constants.





- Integration proceeds rather smoothly Except for the diffusion term
- Following integration, solve for any given mesh, i, by arranging it into a tridiagonal matrix between its neighboring meshes

Numerical Discretization

- Integrating the diffusion equation over the mesh $(x_{i-1/2}, x_{i+1/2})$

$$-\left[D\left(x_{i+\frac{1}{2}}\right)\frac{d\phi}{dx}\bigg|_{x_{i+\frac{1}{2}}} - D\left(x_{i-\frac{1}{2}}\right)\frac{d\phi}{dx}\bigg|_{x_{i-\frac{1}{2}}} \right] + \int_{\Delta x_i} dx\Sigma_a(x)\phi(x) = \int_{\Delta x_i} dxS(x)$$

- Most terms fall cleanly within the original mesh scheme

$$-\left(D_{i+\frac{1}{2}} \frac{\phi_{i+1} - \phi_i}{\Delta x_{i+\frac{1}{2}}} - D_{i-\frac{1}{2}} \frac{\phi_i - \phi_{i-1}}{\Delta x_{i-\frac{1}{2}}} \right) + \Sigma_{a,i}\phi_i \Delta x_i = S_i \Delta x_i$$

- Approximate thusly:

$$\Delta x_{i+\frac{1}{2}} = \frac{1}{2}\left(\Delta x_i + \Delta x_{i+1}\right), \quad \Delta x_{i-\frac{1}{2}} = \frac{1}{2}\left(\Delta x_{i-1} + \Delta x_i\right)$$

- Approximation of the diffusion coefficient calls for a more nuanced study

Approximating the Diffusion Coefficient

1. Arithmetic Mean of Neighboring Meshes:

$$D_{i+\frac{1}{2}} = \frac{D_{i+1} + D_i}{2}$$

2. Arithmetic Mean of Neighboring Meshes Weighted for Mesh Size:

$$D_{i+\frac{1}{2}} = \frac{D_{i+1}\Delta x_{i+1} + D_i \Delta x_i}{\Delta x_{i+1} + \Delta x_i}$$

3. Harmonic Mean of Neighboring Meshes:

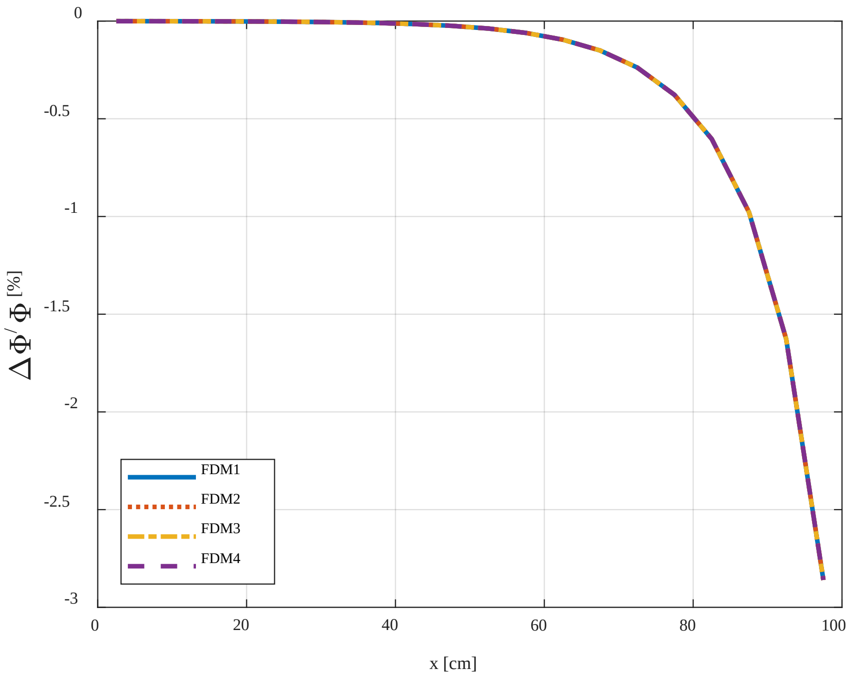
$$D_{i+\frac{1}{2}} = \left(\frac{\frac{1}{D_i} + \frac{1}{D_{i+1}}}{2} \right)^{-1}$$

4. Harmonic Mean of Neighboring Meshes with Weighted Mesh Size:

$$D_{i+\frac{1}{2}} = \left(\frac{\frac{\Delta x_i}{D_i} + \frac{\Delta x_{i+1}}{D_{i+1}}}{\Delta x_{i+1} + \Delta x_i} \right)^{-1}$$

Test and Result – One Material Problem

- One-region one-dimensional problem
- Compared analytic solution to each of the four treatments of the diffusion coefficient
- Error increased as it approached the vacuum boundary on the right side
- Did not yield conclusive judgment about which treatment of the diffusion coefficient minimizes error



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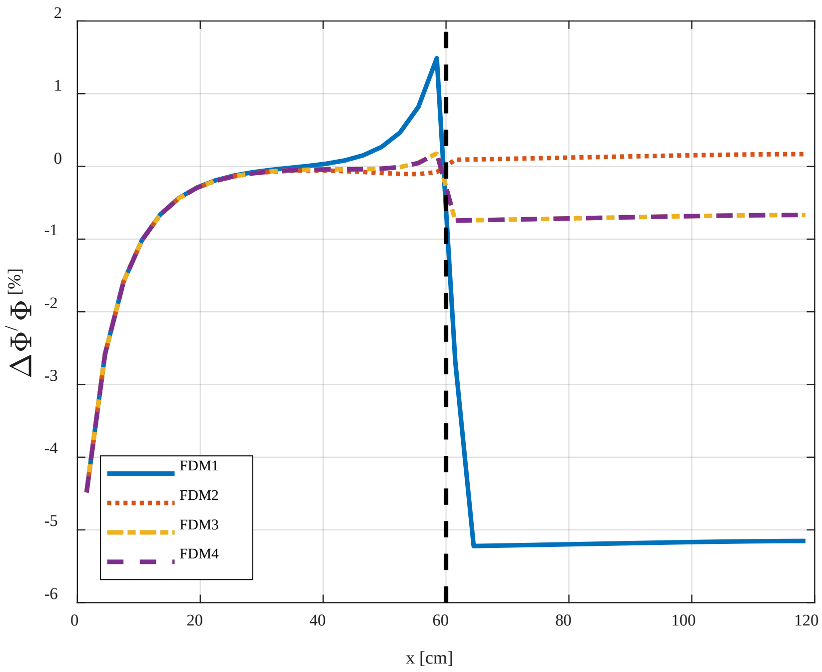
Test and Result – Two Materials Problem

- Two-region one-dimensional problem
- Yielded clear results about which treatment of the diffusion coefficient showed least deviation from the analytic solution

$$D_{i+\frac{1}{2}} = \frac{D_{i+1}\Delta x_{i+1} + D_i \Delta x_i}{\Delta x_{i+1} + \Delta x_i}$$



Conclusions

- Considering a simplified, one-dimensional problem arithmetic mean weighted for mesh size produced the most accurate approximation
- More study is necessary to confirm these findings

References

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