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:

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

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

• \( \phi_0 \) and \( \phi_1 \) – 0th and 1st flux moments
• \( \Sigma_0 \) and \( \Sigma_1 \) – 0th and 1st moments of scattering XS
• \( \Sigma_t \) – total XS
• \( S \) - sources
Getting diffusion coefficient from P1 equations

• Multi-group P1 equation in 1D:

\[
\frac{d}{dx} \phi_{1,g} + \Sigma_{t,g} \phi_{0,g} = \sum_{g'} \Sigma_{s_0, g' \rightarrow g} \phi_{0,g'} + S_{0,g}
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\]

• Diffusion coeff. can be derived from the 2\textsuperscript{nd} equation:
  – Assuming isotropy of the sources $\rightarrow S_{1,g} = 0$
  – Using Fick’s law:
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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- Diffusion coeff. can be derived from the 2\textsuperscript{nd} equation:
  - Assuming isotropy of the sources \( \rightarrow S_{1,g} = 0 \)
  - Using Fick's law:
    \[
    J_g = -D \frac{d}{dx} \phi_{0,g}
    \]
    \[
    \phi_{1,g} = -\left( \frac{1}{3} \Sigma_{t,g} - \frac{1}{\phi_{1,g}} \sum_{g'} \Sigma_{s1,g'\rightarrow g} \phi_{1,g'} \right) \frac{d}{dx} \phi_{0,g}
    \]
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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    \[
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    \]
    \[
    \phi_{1,g} = -\frac{1}{\Sigma_{t,g} - \sum_{g'} \Sigma_{s1,g'\rightarrow g} \phi_{1,g'}} \frac{d}{dx} \phi_{0,g}
    \]
Complexities in calculations of diffusion coefficient

\[ \sum_{i,g} - \frac{\sum_{s1,g' \rightarrow g} \phi_{1,g'}}{\phi_{1,g}} \]

- Current spectra is needed - not easy to calculate

- What can be done? Examples:
  - Out-scatter approximation
  - Replacing \( \phi_1 \) by \( \phi_0 \)
  - Hydrogen transport correction
  - P1 spectral calculations
Some relevant references:


Out-scatter approximation
Out-scatter approximation

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

\[
\sum_{g'} \sum_{s_1, g' \rightarrow g} \phi_{1, g'} \approx \sum_{g'} \sum_{s_1, g \rightarrow g'} \phi_{1, g}
\]
Out-scatter approximation

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

\[ \sum_{g'} \Sigma_{s1,g' \to g} \phi_{1,g'} \approx \sum_{g'} \Sigma_{s1, g \to g'} \phi_{1,g} \]

- Then:

\[ \frac{\sum_{g'} \Sigma_{s1,g' \to g} \phi_{1,g'}}{\phi_{1,g}} \approx \frac{\sum_{g'} \Sigma_{s1, g \to g'} \phi_{1,g}}{\phi_{1,g}} = \sum_{g'} \Sigma_{s1,g \to g'} = \Sigma_{s1,g} \]

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

\[ \Sigma_{tr,g} = \Sigma_{t,g} - \Sigma_{s1,g} = \Sigma_{t,g} - \mu_g \Sigma_{s0,g} \]
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: \( \frac{\Sigma_{tr}}{\Sigma_T} \)
  – From H-only slab with a fixed fission source
  – Use the H-correction curve to modify \( \Sigma_{tr} \) from lattice calculations

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

• Procedure:
  1. Calculate \( \Sigma_{tr,all}, \Sigma_{tr,H}, \Sigma_{T,H} \)
  2. Calculate \( \Sigma_{tr,H} = \Sigma_{T,H} \times \text{Correction curve} \)
  3. Calculate \( \Sigma_{tr,all} = \Sigma_{tr,all} - \Sigma_{tr,H} + \Sigma_{tr,H}^{corr} \)

• 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$_2$O curve is shown
**Diffusion coefficient: Serpent vs. Casmo**

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<th>Casmo</th>
<th>Serpent</th>
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<td>1.55880</td>
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<td></td>
<td></td>
<td>g1 - 5.7%</td>
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<td>g2 - 1.9%</td>
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Some test problems
2D PWR core

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

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
2D PWR core: Radial power distribution
### 3D PWR core – OECD MOX benchmark

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<td>U 4.5% (CR-S)</td>
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<td>U 4.5%</td>
<td>M 4.0%</td>
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<td>U 4.2%</td>
<td>U 4.2%</td>
<td>M 4.3%</td>
<td>U 4.5% (CR-B)</td>
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<td>U 4.5%</td>
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<td>U 4.2%</td>
<td>M 4.0%</td>
<td>U 4.2%</td>
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<td>17.5</td>
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</table>
| F | M 4.3% | U 4.2% (CR-S) | M 4.3% | U 4.5% (CR-S) | U 4.5% | M 4.3% | U 4.5% | CR-A | Control Rod Bank A
|   | 32.5  | 17.5 | 17.5 | 20.0 | 0.15 | 0.15 | 32.5 | CR-B | Control Rod Bank B
|   | 17.5  | 0.15 | 0.15 | 0.15 | 17.5 | 32.5 | 17.5 | CR-C | Control Rod Bank C
|   | 0.15  | 0.15 | 0.15 | 0.15 | 0.15 | 0.15 | 0.15 | CR-D | Control Rod Bank D
|   | U 4.5% (CR-C) | M 4.0% | U 4.5% | M 4.3% | U 4.2% (CR-S) | U 4.5% | CR-SA | Assembly Type
|   | 0.15  | 32.5 | 17.5 | 17.5 | 32.5 | 17.5 | 17.5 | CR-SA | Shutdown Rod Bank A
|   | U 4.2% | U 4.5% | M 4.3% | M 4.3% | U 4.2% | CR-SD | CR-SC | B | CR-SC | Shutdown Rod Bank C
|   | 32.5  | 17.5 | 35.0 | 20.0 | 17.5 | 32.5 | 17.5 | B | O | Ejected Rod

- Serpent - few-group XS + reference solution
- DYN3D - nodal diffusion calculations
- Verify DYN3D results vs. full core Serpent solution
3D PWR core: Radial power distribution
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 $D_G$ in two ways:

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

$$
\Sigma_{tr,G} = \sum_{g \in G} \Sigma_{tr,g} \phi_g 
\Rightarrow
D_G = \frac{1}{3 \Sigma_{tr,G}}
$$
Generation of few-group diffusion coefficients

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**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 $D_g$

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