Diffusion coefficients and critical spectrum methods in Serpent

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Overview

- Some diffusion coefficient calculation and critical spectrum methods
- Traditional group constant generation methods in Serpent
- Other studies on diffusion coefficients and critical spectrum methods
- Work in progress on diffusion coefficients and critical spectrum methods in Serpent
- Preliminary results
- Summary

Some diffusion coefficient calculation and critical spectrum methods

- Diffusion coefficient methods
  - Outflow: easy to calculate, approximate
  - Inflow: generally requires P_1 flux spectrum not present in Monte Carlo or P_0 transport calculations
- Critical spectrum and diffusion coefficient methods
  - B_1: buckling search to calculate diffusion coefficients and critical spectrum
  - P_1: similar to B_1 but without one buckling dependent coefficient
- Critical spectrum methods
  - CASMO-4 method: buckling search using already calculated diffusion coefficients to calculate critical spectrum

The traditional Serpent way

- Group constants other than diffusion coefficient
  - Spatially homogenized group constants tallied into fine energy groups
  - Energy group condensation into macro energy groups by flux-weighting
    - In lattice calculation spectrum (`INF_`)
    - In leakage corrected spectrum calculated from B_1 fundamental mode equations using the fine energy group constants (`B1_`)
    - The B_1 spectrum is used in many deterministic lattice transport codes
- Diffusion coefficients
  - Out-scattering diffusion coefficients tallied into fine energy groups and condensed into macro energy groups by flux-weighting (`INF_DIFFCOEF`)
  - B_1 diffusion coefficients solved from B_1 equations and condensed into macro energy groups by B_1 flux-weighting (`B1_DIFFCOEF`)
- Fine energy group division affects `INF_DIFFCOEF` and all `B1_` group constants

Other studies on diffusion coefficients and critical spectrum methods

- Comparisons of one-step P_0 transport calculations and two-step transport–nodal diffusion calculations against Monte Carlo reference with LWR cases [4][3][1][5][2]
- Comparisons of different transport approximations and leakage correction methods (some names vary from publication to publication)
  - No transport correction (use total cross section), out-scattering and in-scattering transport corrections
  - No leakage correction, P_1, B_1 and CASMO-4 critical spectrum methods

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[4] S. Choi & D. Lee. "*Impact of Inflow Transport Approximation on Reactor Analysis.*". In proc. Mathematics and Computation (M&C), Supercomputing in Nuclear Applications (SNA) and Monte Carlo (MC) international conference (M&C+SNA+MC 2015). 2015.

[3] S. Choi et al. "*Impact of inflow transport approximation on light water reactor analysis.*". Journal of Computational Physics **299** (2015), 352–373.

[1] D. Lee, S. Choi, & K. S. Smith. "*On the Diffusion Coefficient of Two-step Method for LWR analysis.*". In proc. Transactions of the Korean Nuclear Society Autumn Meeting. 2015.

[5] S. Choi & D. Lee. "*Investigation of Diffusion Coefficient Calculation Methods for Two-Step LWR Analysis.*". In proc. PHYSOR2016. 2016.

[2] S. Choi et al. "*On the diffusion coefficient calculation in two-step light water reactor core analysis.*". Journal of Nuclear Science and Technology **54**.6 (2017), 705–715.

Other studies on diffusion coefficients and critical spectrum methods

- It was found that the inflow transport approximation for one-step calculations and combination of inflow transport approximation (and inflow diffusion coefficients) and CASMO-4 leakage correction method for two-step calculations produced consistently best results
- In P_0 transport solutions, the transport approximation also affects the transport solution
- In two-step Monte Carlo–nodal diffusion solutions the transport approximation only affects the calculated diffusion coefficients not used in the Monte Carlo calculation
- Also Ref. [6] states that instead of B_1 critical spectrum method and diffusion coefficients, in-scattering diffusion coefficients should be used to get accurate results for LWR calculations

[6] K. S. Smith. "*Nodal diffusion methods and lattice physics data in LWR analyses: Understanding numerous subtle details.*". Progress in Nuclear Energy **101** (2017), 360–369.

Other studies on diffusion coefficients

- A way to calculate more accurate diffusion coefficients using Monte Carlo calculated transport correction coefficients was published in Ref. [7]
- A general way to calculate in-scattering diffusion coefficients in an infinite geometry using cumulative migration method (CMM) was published in Refs. [8] and [9]
- The methodology was recently improved in Ref.[10].
- The original CMM method was included in Serpent 2.1.27 (`CMM_DIFFCOEF`)
- Serpent has also an option to calculate diffusion coefficients from user given transport to total cross section curve (`TRC_DIFFCOEF`)

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[7] B. R. Herman et al. "*Improved diffusion coefficients generated from Monte Carlo codes.*". In proc. International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering (M&C 2013). 2013.

[8] Z. Liu et al. "*A cumulative migration method for computing rigorous transport cross sections and diffusion coefficients for LWR lattices with Monte Carlo.*". In proc. PHYSOR2016. 2016.

[9] Z. Liu et al. "*Cumulative migration method for computing rigorous diffusion coefficients and transport cross sections from Monte Carlo.*". Annals of Nuclear Energy **112** (2018), 507–516.

[10] Z. Liu, K. Smith, & B. Forget. "*Group-wise tally scheme of incremental migration area for cumulative migration method.*". In proc. PHYSOR2018. 2018.

Work in progress on diffusion coefficients and critical spectrum methods in Serpent

- On-going work to replicate selected results of Ref. [2] using Serpent– Ants [11] calculation chain
- Only two-step Monte Carlo–nodal diffusion against Monte Carlo reference
- No leakage correction with out-scattering and in-scattering (CMM) diffusion coefficients
- Leakage correction and diffusion coefficients using P_1 and B_1 methods
- CASMO-4 leakage correction with out-scattering and in-scattering (CMM) diffusion coefficients
- First results with external scripts
- Selected methods will be implemented in Serpent
- The improved CMM methodology already implemented, testing for implicit capture mode ongoing

[2] S. Choi et al. "*On the diffusion coefficient calculation in two-step light water reactor core analysis.*". Journal of Nuclear Science and Technology **54**.6 (2017), 705–715.

[11] V. Sahlberg & A. Rintala. "*Development and first results of a new rectangular nodal diffusion solver of Ants.*". In proc. PHYSOR2018. 2018.

Preliminary results

Modified VERA-5A problem center assembly two-group constants with CMM diffusion coefficients and CASMO-4 leakage correction

Method	D_1 (cm)	D_2 (cm)	$\Sigma_{a,1}$ $(\frac{1}{cm})$	$\Sigma_{a,2}$ $(\frac{1}{cm})$	$\nu\Sigma_{f,1}$ $(\frac{1}{cm})$	$\nu\Sigma_{f,2}$ $(\frac{1}{cm})$	$\Sigma_{s,1\to 2}$ $(\frac{1}{cm})$
C4 & CMM	1.40295	0.41195	0.00891	0.07455	0.00540	0.09525	0.01816

Differences of other methods compared with CMM diffusion coefficients and CASMO-4 leakage correction

Method	D_1 (%)	D_2 (%)	$\Sigma_{a,1}$ (%)	$\Sigma_{a,2}$ (%)	$\nu\Sigma_{f,1}$ (%)	$\nu\Sigma_{f,2}$ (%)	$\Sigma_{s,1\to 2}$ (%)
No & out	5.69	–9.07	0.64	0.03	0.32	0.03	1.24
C4 & out	5.82	–9.05	0.10	0.00	–0.04	0.00	0.20
No & CMM	–0.20	–0.03	0.64	0.03	0.32	0.03	1.24
B1	–2.17	–3.24	–0.01	0.00	0.03	0.00	–0.01
P1	–1.59	–3.21	0.00	0.00	0.03	0.00	0.00

Summary

- Serpent currently supports calculation of diffusion coefficients with outscattering, B_1 and CMM/TRC methods
- Serpent currently supports critical spectrum calculation with B_1 method
- Study for other methods/method combinations underway with Serpent–Ants calculation chain
- Selected methods will be implemented in Serpent

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