Oak Ridge National Laboratory

Adapting CLUTCH Methodology to Multigroup TSUNAMI-3D for Eigenvalue Sensitivity Calculations

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Outline

1. Introduction
2. Methodology
3. Results
4. Conclusions

Introduction

- TSUNAMI-3D sequences within SCALE code system provide different capabilities to determine the sensitivity to k_{eff}
  1. Adjoint-based perturbation theory with Multigroup (MG) KENO transport
  2. The iterated fission probability method (IFP) with continuous energy(CE) transport, available with both KENO and Shift transport
  3. The Contributon-Linked eigenvalue sensitivity/Uncertainty estimation via Tracklength importance CHaracterization method (CLUTCH) with CE transport, available with KENO codes
- Each method has benefits and limitations depending on the problem

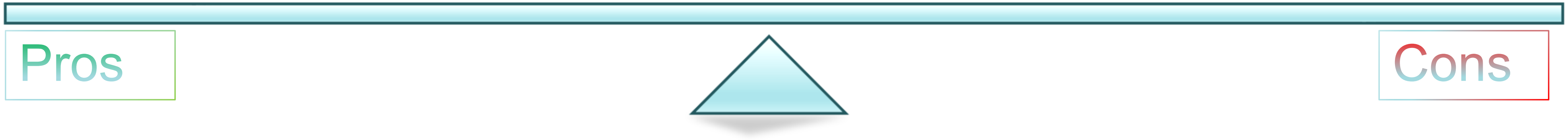
Introduction

- Conventional MG TSUNAMI-3D
  - Forward and adjoint KENO transport to estimate flux moments on a mesh
  - Post-process flux/flux moments with SAMS to calculate sensitivities
  - Mesh selection is important for accurate sensitivity results

Relatively shorter runtime compared to CE KENO transport

Suffer memory issues when the calculation requires high resolution mesh

Convergence issues with KENO adjoint depending on the problem

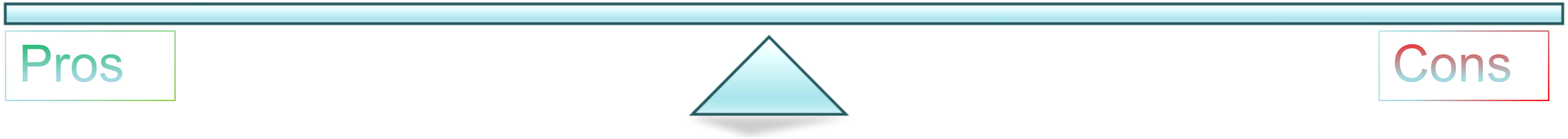


Introduction

- MG TSUNAMI-3D with Contributon Method
  - No adjoint KENO transport
  - Mesh-free adjoint-weighting of tallies during the forward KENO transport
  - Importance of an event determined by
    - simulating the secondary particles at the site of the event
    - then tracking the number of fission neutrons created by each secondary particle

Smaller memory footprint

Runtime penalty due to the simulation of secondary particles



Its initial implementation in KENO in previous SCALE versions evaluated as an impractical approach for the production calculations, retained for research purposes.

Introduction

- The IFP method
  - Mesh-free adjoint-weighting of tallies during the forward CE KENO transport
  - Need to store reaction rates and data from collisions for every neutron for several generations

Pros

Accurate sensitivity results with enough neutrons in each generation

Cons

Intolerable level of memory requirement for complex problems

Relatively longer runtime compared to CLUTCH

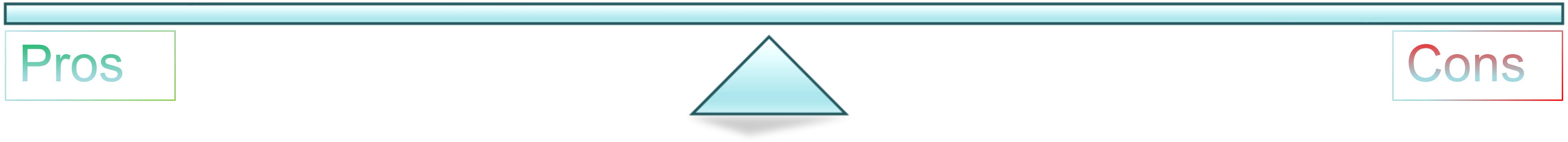
Introduction

- CLUTCH method
  - Mesh-free adjoint-weighting of tallies during the forward CE KENO transport
  - Use approach from the Contributon theory to estimate importance
  - Does not simulate the secondary particles as Contributon method does
  - Track how many fission neutrons are created by the primary neutron after the reaction of interest

Small and manageable memory

Reasonable runtime compared to Contributon and IFP

difficulties in generating accurate sensitivities for systems with large reflectors and hydrogenous materials



Introduction

- Objective: Adapt CE CLUTCH method to MG TSUNAMI-3D to enhance MG sensitivity capabilities for k_{eff}
  - Eliminate explicit KENO adjoint calculation
  - Eliminate memory-demanding mesh flux moment tallies
  - Manageable runtime and memory for sensitivity tallies provided by the CLUTCH methodology
  - Enable faster sensitivity calculations for k_{eff}
- This adaptation allows MG sensitivity calculations with Shift, ORNL’s next-generation high-performance Monte Carlo transport code, which currently does not offer any sensitivity capabilities with MG transport.

Methodology

- Eigenvalue sensitivity due to a small perturbation in a macroscopic cross section given by

$$S_{k,\Sigma_x} = \frac{\Sigma_x}{k}\frac{\delta k}{\delta \Sigma_x} = \frac{< \Phi^* \left(\lambda \frac{\delta F}{\delta \Sigma_x} - \frac{\delta B}{\delta \Sigma_x}\right) \Phi >}{< \Phi^* F \Phi >}$$

- Each term in above equation calculated by CLUTCH as well as other methods in TSUNAMI to determine the sensitivity coefficients;
  - Denominator term (adjoint-weighted fission source term)
  - Three functions that describe different forms of the inner product for $\boldsymbol{\Phi\Phi^*}$ in the numerator;
    - Collisional term
    - Fission source term
    - Scattering source term

- Neutron importance of events and reaction rates for every collision calculated by CLUTCH during the neutron's lifetime

- After particle's death, this information is combined to calculate tally scores for each term

Methodology

- Contributon theory used by CLUTCH to estimate the neutron importance

$$\phi^*(\tau_s) = \frac{\lambda}{Q_s}\int_V G(\tau_s \rightarrow r)F^*(r)\, dr$$

  - No secondary particle generation in the calculation of transfer function, $\boldsymbol{G(\tau_s \rightarrow r)}$
  - Track how many fission neutrons are created by the primary neutron after the reaction of interest
  - IFP-like approach used to estimate $\boldsymbol{F^*(r)}$ weighting function
  - Both collision ($\sum_{i=m}^{M}\left[\boldsymbol{w_i}\left(\frac{\upsilon\Sigma_f}{\Sigma_t}\right)_{i+1}\boldsymbol{F^*(r_{i+1})}\right]$)and track-length ($\frac{\lambda}{w_m}\sum_{i=m}^{M}\left[\boldsymbol{w_i\bar{\upsilon}\Sigma_{f_i}\mathcal{F}(l_i)}\right]$)estimators used for importance calculation

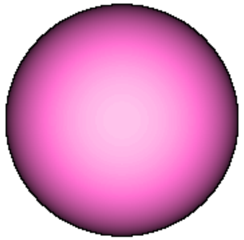
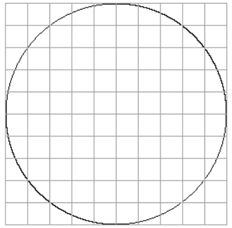
- Collisional term $(\boldsymbol{\Sigma_x(r_m, E_m)\phi(\tau_m)\phi^*(\tau_m)})$, use collision estimated neutron importance
- Fission term $(\boldsymbol{\bar{\upsilon}\Sigma_f(r_m, E_m)\phi(\tau_m)\phi^*(r_m, E', \hat{\Omega}')})$, use track-length estimated neutron importance
- Scattering source term $(\boldsymbol{\Sigma_s(r_{m-1}, E_{m-1})\phi(\tau_{m-1})\phi^*(\tau_m)})$, use track-length estimated neutron importance
- Denominator term (adjoint-weighted fission source term, calculated by fission term from all particles in each generation)

Methodology

- Use existing CLUTCH framework designed for CE transport, but with some updates in MG transport

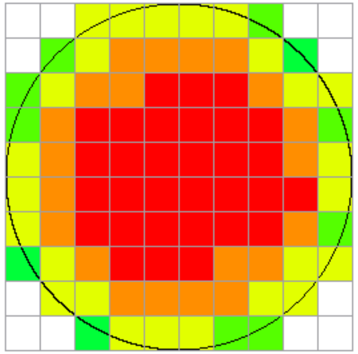
Missing features in MG KENO required by CLUTCH		Updates in MG KENO
Operate with mixture cross sections to simulate the physical events (no nuclide-specific information)	→	Provide nuclide-specific information where CLUTCH implementation stores and requires nuclide information to process sensitivity tallies
Fission nuclide not known	→	Use fission probabilities of all fissile nuclides in the mixture to select the fission nuclide, and use this information in fission source term tally scores
Collided nuclide not known	→	Use corresponding reaction cross section for all nuclides in the mixture where collision occurs, and update scattering source term tally scores for all these nuclides with their non-absorption probability
	→	Use mixture's neutron production cross section in importance calculations
No F*(r) calculation capability	→	Load previously calculated F*(r) from an external file

Results

- HMF-001-001 used as a test case for the new MG CLUTCH methodology
- MacBook Pro with 2.9 GHz 6-Core Intel Core i9, 32 GB memory used as the test platform
- TSUNAMI-3D calculations repeated with the following methods to evaluate the code performance in terms of accuracy, runtime and memory requirement:
  - TSUNAMI-3D, MG conventional, uniform coarse mesh (10 x 10 x 10)
  - TSUNAMI-3D, MG conventional, uniform fine mesh (50 x 50 x 50)
  - TSUNAMI-3D, CE CLUTCH, F*(r) calculation on uniform 10 x 10 x 10 mesh
  - TSUNAMI-3D, CE IFP

Results



- CE CLUTCH computed F*(r) importance used in MG CLUTCH (no F*(r) calculation currently available in MG CLUTCH)
- CE CLUTCH and IFP calculations used 5 latent generations
- In all calculations
  - ENDF/B-VII.1 MG and CE libraries
  - 500 total generations
  - 50 generations skipped
  - 20,000 neutrons per generation
  - Sensitivities tallied in 252-group SCALE multigroup energy structure
- No parallel transport calculation

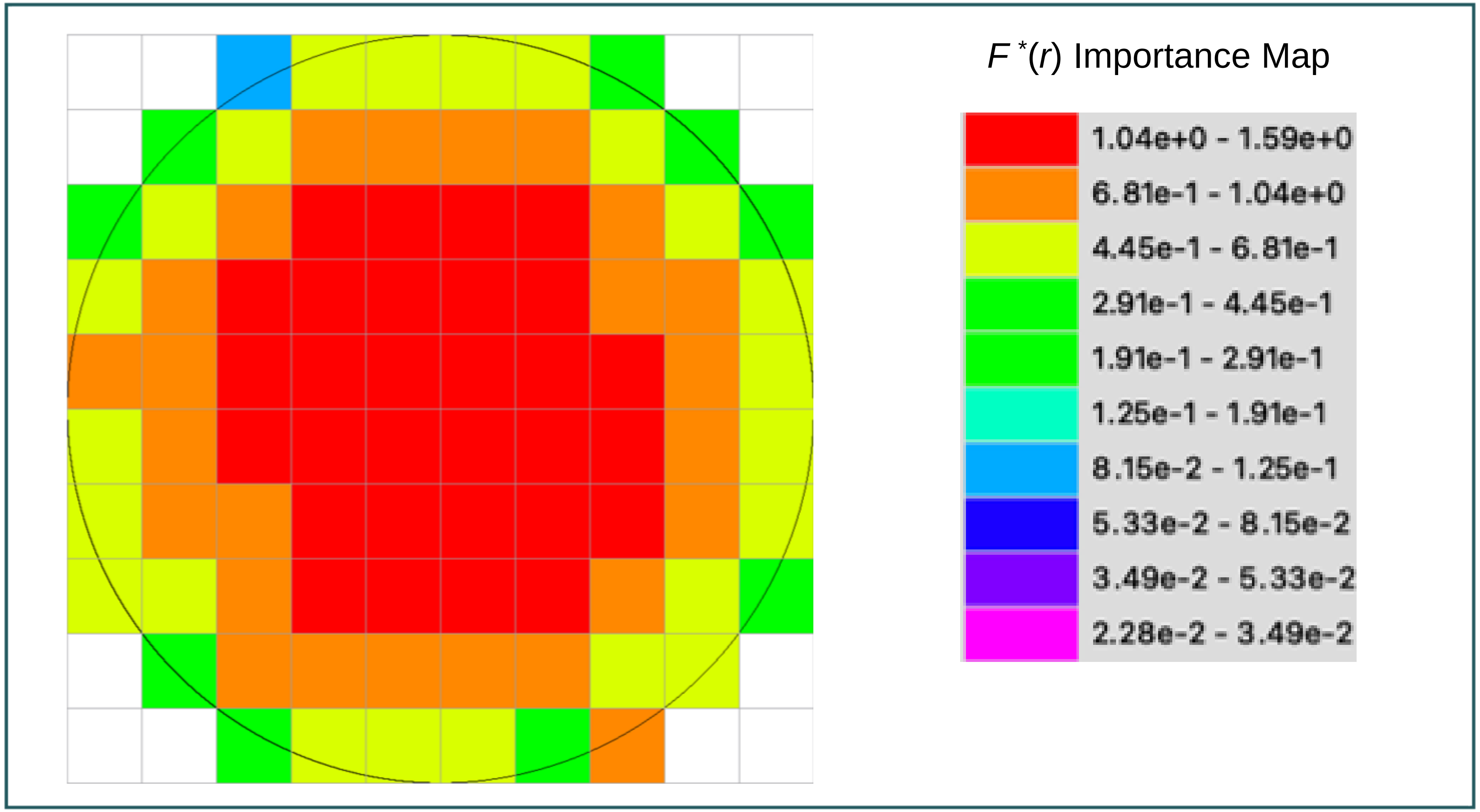
Results

- Sensitivity coefficients

Nuclide	MG CLUTCH		CE CLUTCH			IFP		
	S	σ_S	S	σ_S	% diff.	S	σ_S	% diff.
^{235}U	0.80153	0.00064	0.80173	0.00065	−0.02	0. 80446	0.00161	−0.36
^{238}U	0.01759	0.00005	0.01764	0.00013	−0.29	0.01713	0.00035	2.68
^{234}U	0.00751	0.00004	0.00727	0.00006	3.23	0.00748	0.00016	0.46

Results

- CE CLUTCH computed F*(r) used in both CE and MG CLUTCH calculations



Results

- Code performance comparison

Method	Runtime (min)	Peak Memory (GB)
IFP	10.65	1.253
CE CLUTCH	5.75	0.970
MG CLUTCH	5.72	0.870
MG conventional (coarse mesh, 10 × 10 × 10)	2.86 (forward) 4.62(adjoint) 7.58 (total)	0.848
MG conventional (fine mesh, 50 × 50 × 50)	10.29 (forward) 12.21 (adjoint) 22.50 (total)	4.038

Conclusions

- CLUTCH method adapted to MG KENO transport as an alternative sensitivity tally calculation approach within TSUNAMI sequence
- The new method provides encouraging results for being able to generate accurate sensitivity coefficients as those of other TSUNAMI-3D sequences for the critical experimental system HMF-001-001
- More testing is needed for other types of systems and materials (i.e., thermal and intermediate energy ranges and different moderators and reflectors) after enabling implicit sensitivity calculation capability in MG CLUTCH
- Better runtime results could be obtained after optimizing the CLUTCH framework for MG CLUTCH
- Expected that MG runtime performance will be more attractive compared to CE runtimes for more complicated models
- Methodology will be added to estimate F*(r) weighting function internally in MG CLUTCH calculations

Acknowledgment

This work was supported by the Nuclear Criticality Safety Program, funded and managed by the National Nuclear Security Administration for the Department of Energy.

Questions

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