Prediction of Neutral Particle Analog Monte Carlo Computational Time with Discrete Ordinates

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General Introduction and Motivation

- Monte Carlo particle transport can be used to find high fidelity results with few approximations
- In order to resolve estimates within acceptable statistical uncertainty, some problems require numerous samples and *long runtimes*
- Figure of Merit (FOM) for a Monte Carlo simulation
  - R is the relative error associated with estimates of quantities of interest
  - T is the total simulation runtime

$$\mathrm{FOM} = \frac{1}{R^2 T}$$

- Variance reduction techniques (VR) attempt to maximize the FOM
  - Most techniques are dependent on non-trivial user supplied parameters

Introduction and Motivation for This Work

- Current state of practice: Hybrid Calculation
  - Find the adjoint function for a response of interest deterministically
  - Use the adjoint to generate weight window bounds (CADIS)
  - This approach may result in bounds that split particles entering a region of high importance so much that the FOM is negatively impacted, known as oversplitting
- Improvements from this work:
  - Completed: Find the expected future time field by solving the future time equations deterministically
  - Next Steps: Use the additional information to mitigate oversplitting in the CADIS approach
- If successful, improved VR parameters are generated leading to *shorter runtimes* with *reduced uncertainties* for Monte Carlo simulations

Mission Relevance

- This work aims to accelerate Monte Carlo particle transport simulation
- The long-term goal is to automate the process to both eliminate the need for expert judgment and reduce the time requirements of the analyst
- By mitigating the issue of long runtimes without requiring expert judgement, high fidelity simulation can be applied to a larger set of problems more readily

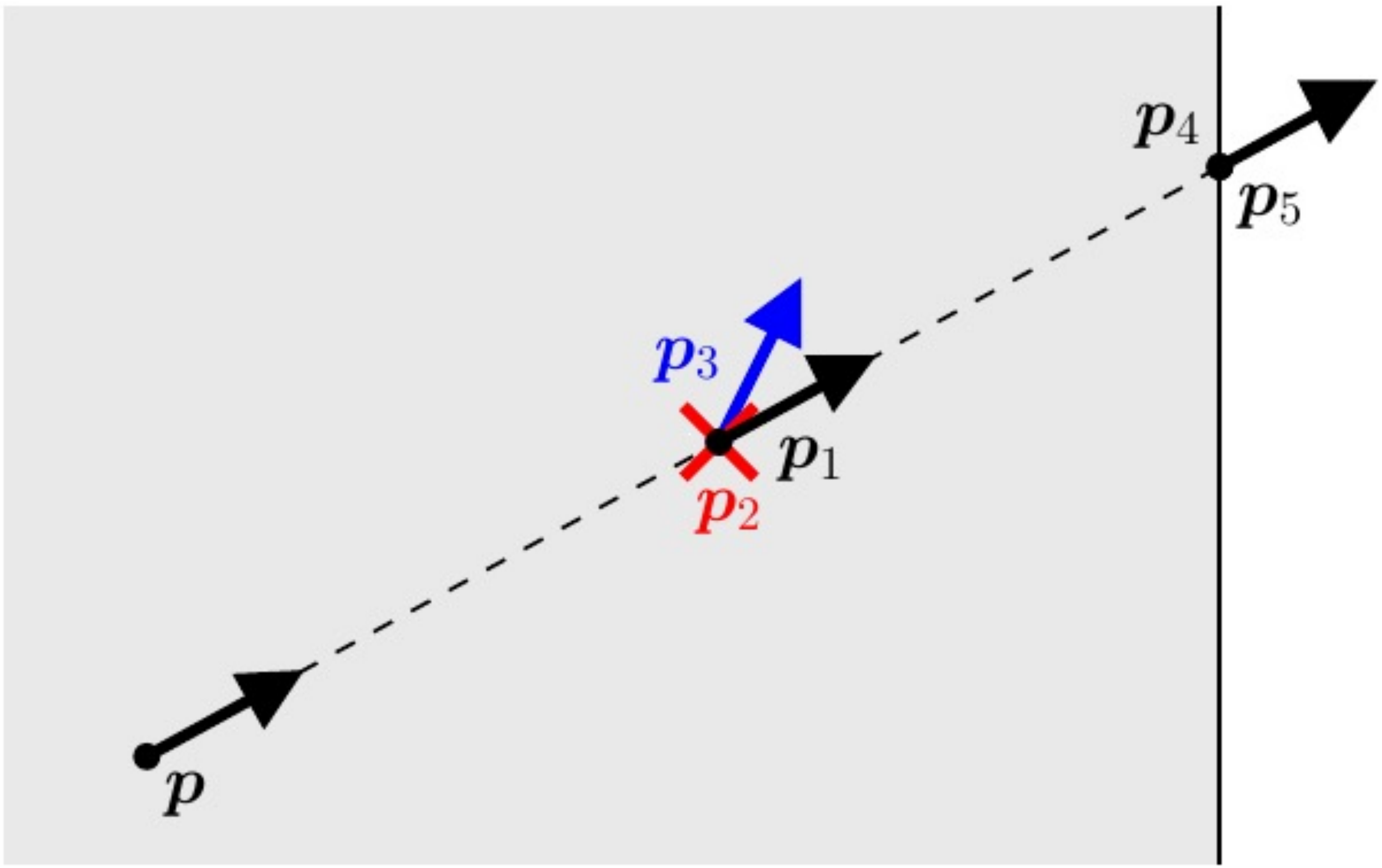
Overview of Technical Approach

- The future time equation (FTE) describing the expected computational time to simulate a Monte Carlo history is derived for non-multiplying analog case
    - Looks like *adjoint* neutron transport equation with special source terms
- Source terms for the FTE are estimated using timers embedded in the Monte Carlo transport routines of the University of Michigan's Hammer code
- The FTE is solved using the Hammer code's 2-D discrete ordinates solver
- Goal: use the solution of the FTE as a heuristic in the generation of weight window bounds for an optimized Monte Carlo simulation

The Role of the Hammer Code

- The Hammer code is a student-driven particle transport framework
- It has both Monte Carlo and deterministic (2-D discrete ordinates) transport capabilities
- It was developed with the goal of being a testbed for advanced hybrid deterministic-Monte Carlo methods
  - Ideal for the implementation of the embedded timer source term estimation, deterministic FTE solution, and, eventually, improved VR parameter generation

Representative Monte Carlo Cell



The Future Time Equation

- Identical to the adjoint neutron transport equation with different source terms (boxed in red)

$$-\boldsymbol{\Omega}\cdot\nabla\Upsilon\left(\boldsymbol{x},\boldsymbol{\Omega},E\right)+\Sigma_t\left(\boldsymbol{x},E\right)\Upsilon\left(\boldsymbol{x},\boldsymbol{\Omega},E\right)=$$

$$\int d\boldsymbol{\Omega}'\int\Sigma_s\left(\boldsymbol{x},\boldsymbol{\Omega}\rightarrow\boldsymbol{\Omega}',E\rightarrow E'\right)\Upsilon\left(\boldsymbol{x},\boldsymbol{\Omega}',E'\right)dE'$$

$$+\boxed{\Sigma_t\left(\boldsymbol{x},E\right)\left(\tau_{\text{trans}}+\tau_{\text{col},W}\right)}$$

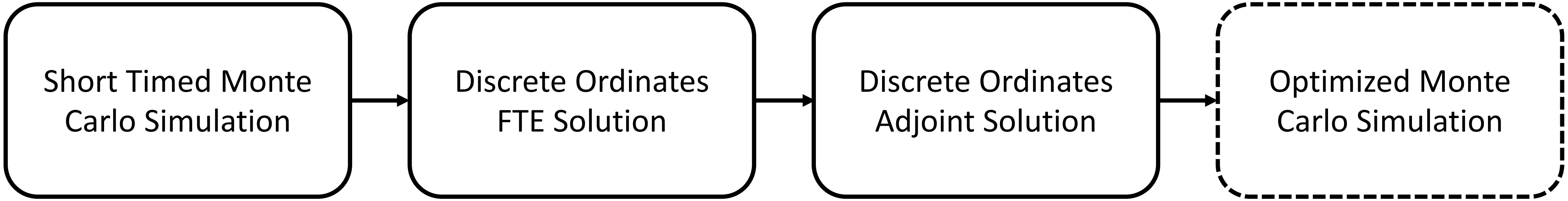
$$\text{where}$$

$$\Upsilon\left(\boldsymbol{x},\boldsymbol{\Omega},E\right)=\boxed{\tau_{\text{trans}}+\tau_{\text{surf}}+\Upsilon_{\text{b}}\left(\boldsymbol{x},\boldsymbol{\Omega},E\right)},\boldsymbol{x}\in\delta\Gamma,\boldsymbol{\Omega}\cdot\boldsymbol{n}>0$$

FTE Time Equation Source Term Estimation

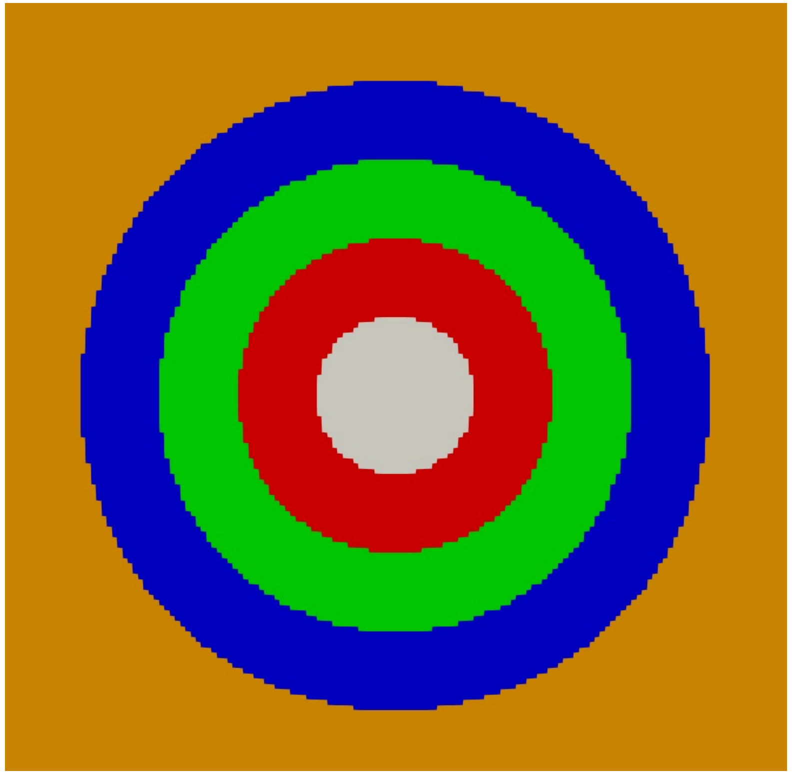
- The source terms to the FTE are the computational time required to process a transport event in the Monte Carlo code, τ_{event}
- Source terms are problem and machine dependent
  - Estimated using timing routines wrapped around transport routines in the Monte Carlo code
  - Timing routines change machine behavior, this adds inherent error

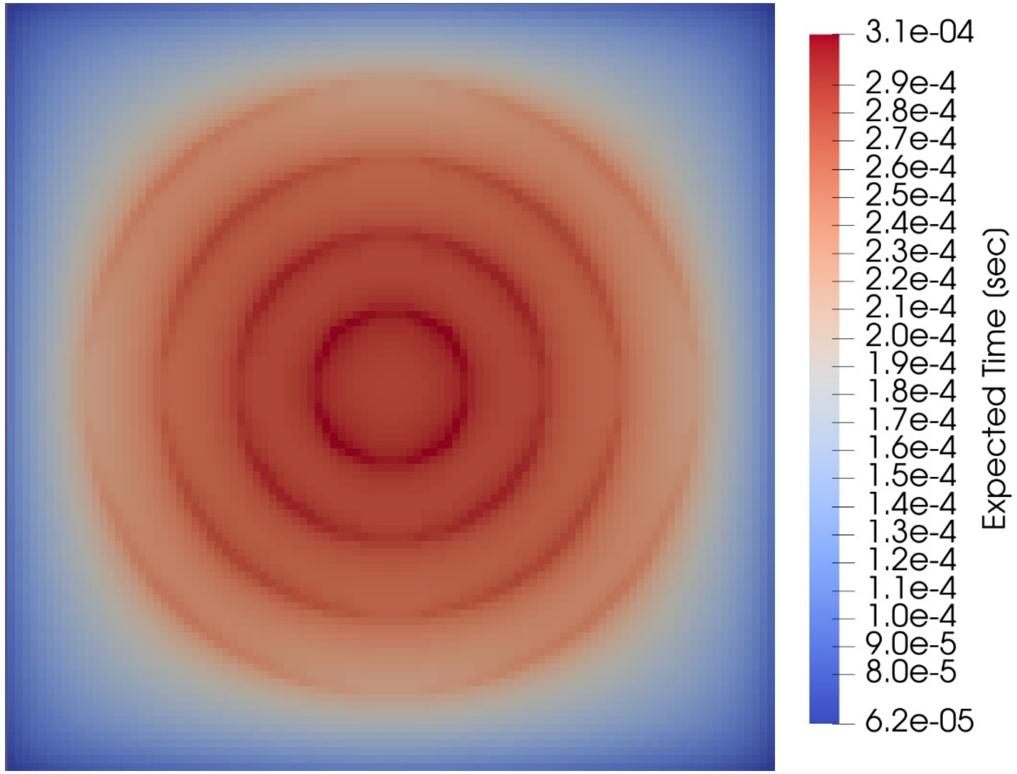
Monte Carlo optimization workflow:



Results: FTE Solution Field

Test Case: 80% scattering and 20% absorbing homogeneous 2-D 10x10 MFP system with four cylindrical surfaces and track length tallying in each cell. Cell ID given on the left and expected future time per history in seconds given on the right.





- Taking the inner product of the future time field and Monte Carlo source intensity gives the expected time per history of the Monte Carlo simulation
- Typical relative errors for test cases are 10-30%, for a point source in the center of the system the above shows 28% error.
- **What is important for VR optimization is the correct shape of the time field**

Expected Impact

- This work demonstrates that:
  - The FTE may be derived for an arbitrary Monte Carlo implementation
  - Embedded timers may be used to estimate FTE source terms
  - The FTE may be solved using a discrete ordinates solver with slight modifications
- This work will be used:
  1. In adjoint terms to keep particles away from high-cost regions of the problem
  2. To quantitatively restrict oversplitting in CADIS weight window generation
- The automated optimization of variance reduction allows Monte Carlo simulation to be applied with a smaller computational burden

MTV Impact

- This work was performed in collaboration with the Los Alamos National Lab Monte Carlo Codes Group (XCP-3) scientist Joel Kulesza
- Following this work, I plan on returning to XCP-3 for a second remote summer internship
- The FTE solver approach currently implemented in the Hammer code, is a general tool that can be incorporated into other hybrid codes to accelerate Monte Carlo simulation

Conclusion

- The goals of this work were to:
    1. Derive the FTE for non-multiplying analog transport in the Hammer code
    2. Implement embedded timers to estimate FTE source terms
    3. Implement a discrete ordinates FTE solver
    4. Use the FTE solution as a heuristic in weight window parameter generation
- Items 1-3 were given in this talk, demonstrating the portability of the FTE approach
- If item 4 is shown to be successful, a new Monte Carlo optimization scheme has been developed
- Automated, general purpose Monte Carlo optimization improves the speed and accuracy of transport simulation results

Next Steps

1. Implement CADIS weight window bound generation in Hammer
2. Implement FTE to improve CADIS approach

   Possible approaches:
   - Use FTE solution to inform maximum splitting across regions
   - Use FTE solution to augment total cross section in adjoint solution
3. Test fully automated optimization workflow for general problems
4. Extend discrete ordinates solver to 3-D

Acknowledgements

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