Hybrid-Delta Tracking on a Structured Mesh in MCATK

Joanna Piper Morgan^{1,2}, Travis J. Trahan¹, Colin J. Josey¹, Timothy P. Burke¹, & Kyle E. Niemeyer² ¹Los Alamos National Laboratory, XCP-3; ²The Center for Exascale Monte Carlo Neutron Transport (CEMeNT) at Oregon State University

Background

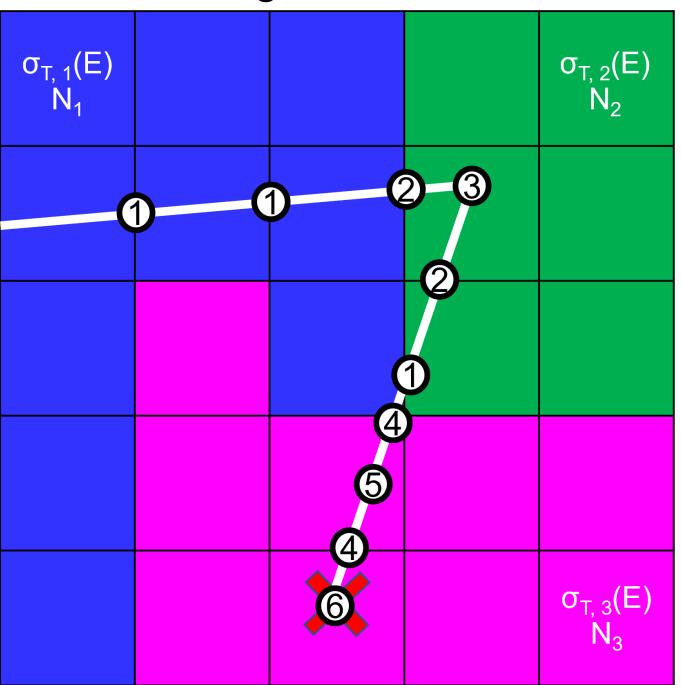
The Monte Carlo Application ToolKit [1] (MCATK) is a Monte Carlo particle transport code that commonly uses surface tracking on a structured mesh to compute scalar fluxes. The structured mesh makes distance-to-boundary calculations cheap compared to simulations using a constructive solid geometry. MCATK's standard algorithm computes the total cross-section of all isotopes in a cell every time a particle moves between cells. Computationally expensive lookup and interpolation functions are called at every boundary crossing. When cell sizes are small compared to a neutron mean free path, often this cross-section lookup finds that a particle does not collide in the cell. This process repeats until a collision occurs.

Hybrid-Delta Tracking

We introduce a hybrid-delta tracking algorithm (based off Woodcock-delta tracking [2]) to eliminate the macroscopic cross section lookup at surface crossings while still performing standard surface tracking. Thus, we can keep the computationally performant components of MCATK—surface tracking on a structured mesh—while decreasing the number of cross section lookups.

This also allows us to use a track-length tally to compute scalar fluxes on the mesh instead of a collision estimator as is required in standard Woodcock delta tracking. This boons variance reduction as track length estimators are more accurate than collision estimators. This hybrid-delta tracking approach requires limited alteration to MCATK's tracking algorithm which enables rapid implementation across its transport modes.

Consider the region defined in Figure 1 with three materials shown in blue, green, and pink presented in Figure. A particle enters the region from the left and undergoes transport with operations required at every σ_{τ, 2}(Ε) σ_{τ, 1}(Ε) distance to a boundary or



collision. For this hypothetical problem using Hybrid-Delta tracking we have reduced the number of total cross section lookups to find from ten to three.

Figure 1. A material region in a structured mesh where each color represents a different material with a different number density total cross section

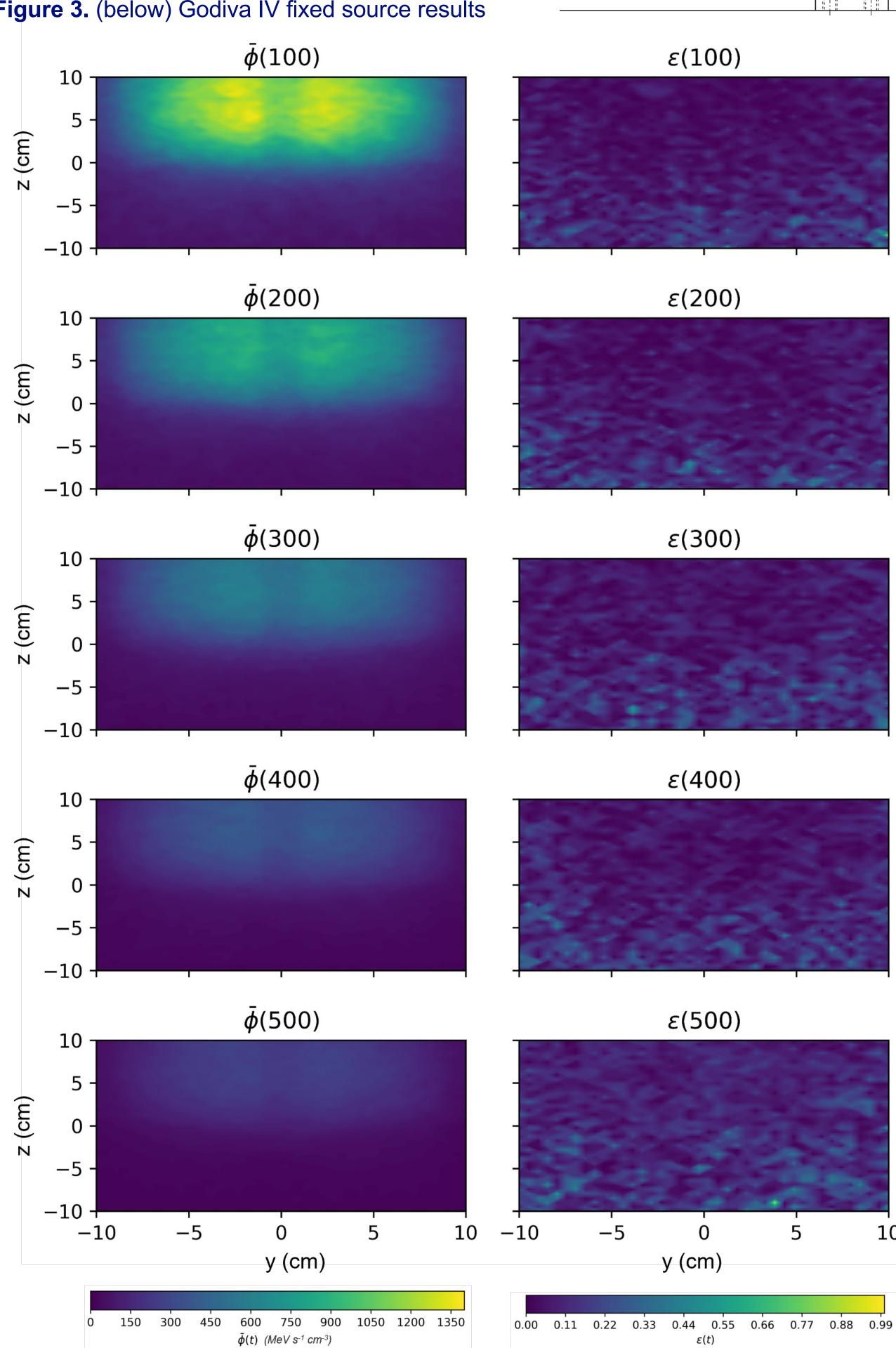




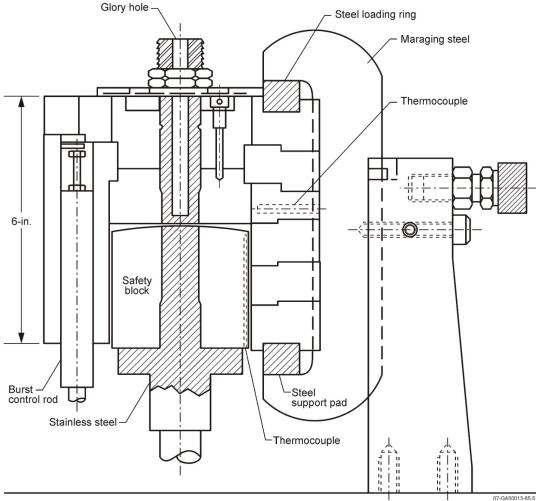
Benchmarks

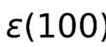
We investigated the performance of hybrid-delta tracking on a series of benchmark problems: one from the Godiva IV (shown in Figure 2) experiment and two from the MUSiC experiment [3]. All three are materially complex, having between 48 and 125 isotopes over the whole model, and implement a structured tracking mesh imposed on the geometry. The minimum mesh cell dimension is 1 mm in the fissile region of each problem.

Figure 2. (left) Godiva IV Figure 3. (below) Godiva IV fixed source results









k-eigen Simulations

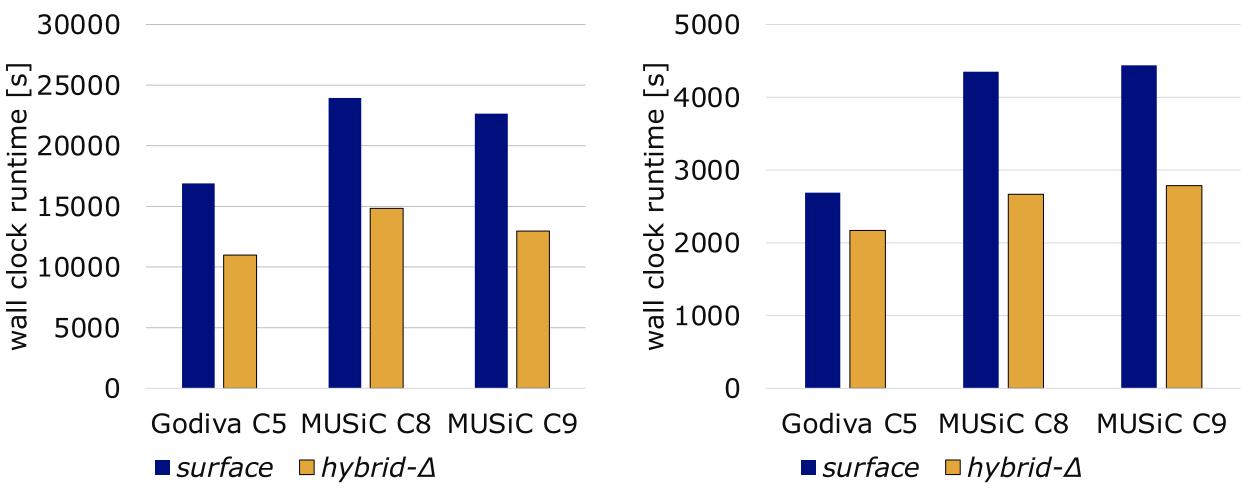


Figure 4. wall clock runtime of benchmark problems in a (left) k-eigen value problem and (right) fixed source problem

Conclusions & Future Work

Hybrid-delta tracking on a structured mesh improves run time in large and materially complex simulations like the ones we benchmarked: 1.5 to 1.75X speed-up for k-eigenvalue and 1.2 to 1.6X speed-up for fixed source problems. The solutions found with hybrid-delta tracking match to within three standard deviations of solutions found with MCATK's standard algorithm. We expect further optimizations will improve speed-up for these algorithms.

In MCATK we have already extended the hybrid delta tracking algorithm to work with multi-temperature data and Photons and hope to include this algorithm in the next version release. We expect that this work will increase the overall performance of MCATK when delta tracking is appropriately used in problems that warrant it.

Citations

[1] T. Adams, S. Nolen, J. Sweezy, A. Zukaitis, J. Campbell, T. Goorley, S. Greene, and R. Aulwes. "Monte Carlo Application ToolKit (MCATK)." Annals of nuclear energy, 82, pp. 41–47 (2015)

[2] E. R. Woodcock, T. Murphy, P. Hemmings, and T. C. Longworth. *Techniques used* in the GEM code for Monte Carlo neutronics calculations in reactors and other systems of complex geometry. Argonne National Laboratory, Lemont USA (1965).

[3] J. B. Briggs, editor. International Handbook of Evaluated Critical Safety Benchmark *Experiments*. Nuclear Energy Agency, NEA/NSC/DOC(95)03/I, Paris, France (2020)

Acknowledgments

Research presented in this poster was supported by the Laboratory Directed Research and Development program of Los Alamos National Laboratory under project number 20220084DR.

This work was supported by the Center for Exascale Monte-Carlo Neutron Transport (CEMeNT) a PSAAP-III project funded by the Department of Energy, grant number: DE-NA003967.

The authors would like to R. Arthur Forster for the discussions that inspired this work as well as Theresa Cutler, Travis Smith, and Robert Weldon Jr. for providing benchmark problem input files.