Algorithms And Software Engineering Schemes for Radiation Transport on Heterogeneous Compute Architectures

By Joanna Piper Morgan

Candidate for Doctor of Philosophy in Mechanical Engineering
Advisor: Dr. Kyle Niemeyer

Abstract

Predicting the movement of neutrons through space and time is important when modeling inertial confinement fusion, pulsed neutron sources, and nuclear criticality safety experiments, among other systems. Practical solutions to the transport equation are typically found via Monte Carlo or deterministic methods, or clever combinations of the two. Both these families of methods prove computationally challenging, particularly for highly time-dependent systems, as the quantities of interest are functions of seven independent variables: space, velocity, and time. Modern high-performance computers (HPC) with heterogeneous architectures (CPUs and GPUs) are enabling high-fidelity modeling of these systems. To exploit new architectures efficiently, software portability schemes are required. In this talk I will discuss both novel numerical methods and software engineering design for deterministic (S_N) and Monte Carlo transport on modern HPCs. First, I will introduce and analyze an alternative space-parallel (non-sweeping) iteration algorithm for 1D time-dependent transport on GPUs, making comparisons to a more traditional iteration algorithm. I will also present a method for converging these iterations in fewer cycles for highly scattering problems. I found that the space-parallel algorithm operates better on modern GPUs and allows use of vendor supplied libraries instead of manually writing GPU functions. I show that as time step size is decreased the space-parallel algorithm will converge in fewer iterations, and that a second moment method can be used to converge the space-parallel algorithm in the scattering limit. Second, I show how a Python and Numba enabled software engineering scheme allows for rapid numerical methods development and deployment at scale in a new open-source Monte Carlo transport application called, MC/DC. I will present performance data from GPUs and CPUs for a full transient reactor accident simulation. I will also discuss the rapid development of several hybrid Woodcock-delta tracking methods to demonstrate the benefits of the software engineering scheme and novel methods.

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Also on Zoom: https://tinyurl.com/joannadefense

School of Mechanical, Industrial and Manufacturing Engineering

Oregon State University