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The Random Ray Method for neutral particle transport

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ABSTRACT

A new approach to solving partial differential equations (PDEs) based on the method of characteristics (MOC) is presented. The Random Ray Method (TRRM) uses a stochastic rather than deterministic discretization of characteristic tracks to integrate the phase space of a problem. TRRM is potentially applicable in a number of transport simulation fields where long characteristic methods are used, such as neutron transport and gamma ray transport in reactor physics as well as radiative transfer in astrophysics. In this study, TRRM is developed and then tested on a series of exemplar reactor physics benchmark problems. The results show extreme improvements in memory efficiency compared to deterministic MOC methods, while also reducing algorithmic complexity, allowing for a sparser computational grid to be used while maintaining accuracy.

1. Introduction

The method of characteristics (MOC) solves a partial differential equation (PDE) by defining characteristic lines (or curves) along which the PDE is reduced to an ordinary differential equation (ODE). By solving the ODE along a set of discrete characteristic lines (sometimes in conjunction with ray tracing) and iterating on the initial conditions for the lines, a solution to the governing PDE can be numerically estimated. MOC methods are popular in transport applications for problems featuring fine-grained spatial and angular dependencies. Such problems often feature steep gradients, voids, or optically thin regions of low diffusivity where more computationally efficient methods (such as diffusion and short characteristic methods) are subject to significant losses in accuracy or can become subject to ray effects. In these instances, MOC methods featuring long characteristics retain their fidelity as they can accurately capture global effects caused by fine-grained spatial and angular dependencies of the governing PDE.

Typical MOC applications will use a deterministic quadrature composed of many tracks to cover the phase space of the system evenly. The overall fidelity of the simulation is therefore related to the resolution of this quadrature. In this paper, a new stochastic method of track selection is presented wherein no deterministic quadrature is used. Rather, characteristic lines sampled from a uniform random distribution in phase space are followed through the system until termination criteria are met. The new method, known as The Random Ray Method (TRRM), can allow for increases in accuracy due to accumulation of effective resolution over successive iterations, while also reducing computational storage requirements by removing the need to store deterministic quadrature data and starting condition data.

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The new method may be applicable to a range of fields of computational physics that utilize MOC techniques, such as neutron transport [1–4], gamma ray transport [5–7], and astrophysics radiative transfer [8–11]. To provide a preliminary assessment of the general utility of TRRM, the new method will be deployed in the context of a neutron transport application and tested on a set of reactor physics benchmark problems. TRRM will then be compared against a traditional deterministic neutron transport MOC application in order to quantify the benefits of TRRM.

1.1. Example transport problem description

Neutron transport for the purposes of nuclear reactor simulation is an ideal test case for TRRM as there are numerous community benchmark problems available to test the accuracy and performance of new methods. Additionally, there are existing deterministic MOC based applications for neutron transport available to compare the performance of the new method against. Another reason to test the new method in this form is the opportunity for immediate impact on the field of reactor physics, as the potential improvements offered by TRRM may enable high fidelity simulation of a full nuclear reactor core.

Full core simulations can potentially reduce design and construction costs, increase reactor performance and safety, reduce the amount of nuclear waste generated, and allow for much more complex and novel designs. To date, however, the time to solution and memory requirements for a full core high fidelity deterministic 3D calculation have rendered such calculations impractical, even using leadership class supercomputers. However, with High Performance Computing (HPC) architectures evolving rapidly towards exascale, the computational horsepower required to accomplish full 3D reactor simulations may soon be available.

MOC based simulation techniques are currently a field of active research in reactor physics as they have the potential for fast and efficient performance on a variety of next generation HPC systems, including CPU, GPU, and Intel Xeon Phi architectures [12,13]. The task-based and highly vectorizable nature of MOC style simulations allows them to very efficiently utilize the floating point resources of modern hardware architectures – in one test reaching 63% of peak FLOPS available on a CPU node [12]. This is advantageous, as most high performance computing applications are only able to achieve 8 to 20% of peak FLOPS [14], with some neutronics algorithms, such as continuous energy Monte Carlo, often failing to exceed 1% [15]. While 2D MOC has long been used in reactor design and engineering as an efficient simulation method for smaller problems, the transition to 3D has only begun recently, and to our knowledge no 3D MOC based codes are currently used in industry. The delay of the onset of full 3D codes can be attributed to the impossibility of "naively" scaling current 2D codes into 3D due to prohibitively high memory requirements, though there is ongoing work into more optimal 3D MOC methods [1,16–20].

Most current 2D MOC solvers take as input a constructive solid geometry (CSG) format to define the geometry specifications of the reactor. A pre-processing step is then performed which calculates an azimuthal quadrature over the 2D geometry, and converts the CSG definition into a much larger set of tracks and segment specifications known as a "tracking file." Numerical solution to the neutron transport equation can then be solved by sweeping angular fluxes along all tracks in the azimuthal quadrature, attenuating them and tallying their contributions to source regions along the way (as described in subsection 2.2). This method works well for small or medium sized problems in 2D, but the tracking file can be quite large. For example, for a single 2D reactor pin cell with a fine quadrature the tracking file can be over 100 MB. In such 2D methods, the 3rd dimension is assumed infinite and a polar quadrature is used when integrating the characteristic on each 2D segment. This 2D assumption works well for many traditional Pressurized Water Reactor (PWR) designs, but often cannot be applied to many next-generation reactor designs due to a much higher degree of axial heterogeneity or no symmetry basis being present at all (e.g., Pebble Bed reactors). Additionally, the angular flux at the boundaries of each track (i.e., where each track intersects the edge of the computational domain) must be stored in memory between each power iteration. The storage requirements for this can be even more than the requirements for storing the tracking file, especially in high fidelity calculations utilizing many neutron energy groups.

Naive extension of traditional 2D MOC methods into 3D is possible, but will result in unmanageably large tracking files and a large amount of track boundary data. For a full reactor core, this could be in excess of 1 PB of data just to store the tracking and segment information for a fine quadrature. Several advanced methods have been proposed to efficiently extend MOC into 3D. One method, developed by Gunow et al. [13], allows for a more memory-efficient extension into the 3rd dimension by using a 2D tracking file, but ray tracing on the fly in the axial direction using an extruded 2D geometry approach. This method inherently assumes a significant degree of axial homogeneity is present in order to maintain speed, which is often an acceptable assumption for traditional light water reactors. In addition, the performance penalty for extruded geometry is still unclear, and this methodology will not work for geometries lacking high degrees of axial symmetry. Such methods also do not reduce the memory requirements for storing the boundary angular flux data for all tracks. Alternative methods have been proposed, such as 2D MOC + 1D diffusion [21], or grouping similar length segments together to reduce storage overhead [22], though such methods often result in a loss of fidelity or a considerable increase in code complexity. No 3D MOC based methods that offer full 3D geometrical flexibility without considerable overhead have been proposed to date.

In this study, we present a new method of performing characteristic based numerical estimation of PDEs. The new method, known as The Random Ray Method (TRRM), defines ODEs that can be solved along characteristic lines through the phase space of the system (similar to MOC), but uses a stochastic rather than deterministic process for selecting which