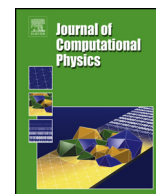




Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Octree particle management for DSMC and PIC simulations. Part I: Basic algorithms

Robert Scott Martin ^{a,*}, Jean-Luc Cambier ^b^a ERC Inc., USA^b In-Space Propulsion Branch, Air Force Research Laboratory, Edwards AFB, CA 93524, USA

ARTICLE INFO

Article history:

Received 8 June 2015

Received in revised form 7 December 2015

Accepted 15 January 2016

Available online xxxx

Keywords:

Plasma simulation

Particle method

Dynamic weight

Phase-space remapping

Octree

PIC

ABSTRACT

The ratio of physical to computationally modeled particles is of critical importance to the fidelity of particle-based simulation methods such as Direct Simulation Monte Carlo (DSMC) and Particle-in-Cell (PIC). Like adaptive mesh refinement for continuum/grid-based simulations, particle remapping enables dynamic control of simulation fidelity in regions of interest so that computational resources can be efficiently distributed within the problem. This is particularly important for simulations involving high dynamic range in the density for one or more species such as problems involving chain-branching reactions like combustion and ionizing breakdown. In this work, a new method of particle remapping is presented which strictly conserves mass, momentum, and energy while simultaneously remaining faithful to the original velocity distribution function through the use of octree binning in velocity space.

© 2016 Published by Elsevier Inc.

1. Introduction

Particle based kinetic simulations such as direct simulation Monte Carlo (DSMC) and particle in cell (PIC) make accessible broad classes of non-equilibrium flow in complex multi-dimensional configurations that are generally inaccessible by other common methods. This is made possible through the efficiency of discrete statistically representative degrees of freedom sampling phase space rather than attempting to uniformly simultaneously track all of phase space as in the case of Vlasov methods. However, particle codes attain this flexibility at the cost of statistical noise. To some extent, this noise can be mitigated through sampling in steady state problems or by increasing the number of particles used, but it remains a fundamental limiting consequence of the method. This issue of statistical noise is exacerbated by problems with large dynamic range as is encountered in flows ranging from the wake behind a bluff body in re-entry [3], electric propulsion plasma plumes [17], and induction delay time for combustion [2].

Aside from simply using more particles, particle remapping methods have long been recognized as an area of critical importance in the simulation of these high dynamic range multiple-length-scale kinetic plasma. The most common approach has been a split that retains velocity and scatters particles in space in a moment preserving way coupled with a pairwise particle merging [8]. Unfortunately in pairwise merging, the resulting particle contains too few degrees of freedom to simultaneously conserve mass, momentum, and energy. To address this issue, the two other common approaches have been to either attempt to select near-neighbors in velocity space for merging to minimize the error in energy conservation or

* Corresponding author.

E-mail address: robert.martin.81.ctr@us.af.mil (R.S. Martin).<http://dx.doi.org/10.1016/j.jcp.2016.01.020>

0021-9991/© 2016 Published by Elsevier Inc.

to use more complex conservation techniques such as merging to grids and redistributing conserved quantities or using complex macro-particles with internal degrees of freedom. A third and considerably less common approach is the ternary merge from 3 or more particles to 2 as noted in References [4,8]. With two particles resulting from the merge, enough degrees of freedom are then available to preserve mass, momentum and energy simultaneously. The primary weakness of this method is perceived to be the difficulty in finding three near neighbors in velocity space such that thermalization of the velocity distribution is avoided.

In Reference [10], the authors describe combining the ternary merge techniques with velocity space octree binning to inhibit numerical thermalization. The approach was then applied to several sample problems including beams crossing in a potential well and electrostatic DC-discharge to demonstrate the advantage of octree binning over a naive random pair-selection. In this work, the methods have been ported from the original MATLAB prototype implementations into a newly developed thermophysics universal research framework (TURF) [11] which enables much higher fidelity and multidimensional applications in a unified C++/CUDA toolset. The methods have been further refined with focus on verifying multidimensional validity and ensuring that particle real-to-computational weights are clustered close to the target weight required for a goal number of particles per cell without scattering some particles to high and low weights even after repeated application of the methods. Two different high fidelity versions of the DC-discharge are then used to demonstrate the necessity of particle weight adaptation and the minimal impact on simulation results. Unlike the MATLAB version, the implementation in TURF also enables collection of relevant timing data to demonstrate the relative cost of aggressive application of the particle weight managements algorithms. Relative to the baseline simulation cost per iteration, the cost of particle management is a significant additional fraction. However, this fraction can be quickly overwhelmed by unconstrained growth in computational cost due to increasing particle counts. The cost is also negligible compared to the cost required for even a modest reduction in statistical noise from adjusting traditional global particle weight.

The work presented here in Part I represents the groundwork for a broader set of research centered around this approach for adaptive particle remapping in kinetic models. The next step, Part II, focuses on minimizing recursive dependency in construction of the octree data structures so that the techniques may be applied efficiently in a massively parallel nature on general purpose graphics processing units. In future work (Part III), conservation of higher-order moments as well as mixed spatial-velocity moments such as angular momentum will be considered.

2. Adaptive octree particle weight management algorithms

2.1. Introduction

As described in Section 1, very large dynamic range of plasma densities makes for a particular challenge in retaining accuracy in particle-based methods. A means of reconstructing the phase space from a stochastic description in order to minimize noise and increase accuracy (including for rare events) must be developed.

The standard approach of merging of particles [8] uses pair-wise coalescence (2:1 ratio), i.e. constructs a new particle with average properties from two initial ones. This approach is very simple and very fast and also conserves mass by simply summing the computational weight of the individual constituents. However, it cannot simultaneously conserve momentum and kinetic energy. This can be easily visualized by considering two particles of equal mass, statistical weight and opposite velocity vectors; the resulting single particle would have the combined mass but a zero momentum (which is correct, the momentum of the center of mass remaining the same) and zero kinetic energy (which is clearly incorrect, since the original particles have velocities).

This error can be reduced by selecting particles that are near each other in velocity space [8], but this adds an additional cost of the procedure and the error remains a fundamental consequence of the reduction of degrees of freedom; it is never fully removed. An acceptable error tolerance tunable parameter is chosen and potential merges are rejected if they introduce error beyond the tolerance. Because more potential merges are rejected as the tolerance is lowered, this represents a natural tradeoff between the ability of the algorithm to control computational cost and conservation accuracy. Reference [18] explores using a k-dimensional tree spanning not only velocity space, but also physical space for near neighbor selection. This allows the merge to be independent of physical computational mesh size. The impact of several choices of conserved quantity were also investigated in this work with an apparent preference towards full energy conservation at the expense of momentum conservation in observed in two-stream instability cases.

As a result of this inherent limitation on simultaneous momentum and energy conservation, various sophisticated models have also been designed to mitigate the error in momentum or energy, e.g.: Hewett used computational particles with internal energy in which the error could be accumulated [6]; Assous and then Welch designed methods of merging values to grid nodes and redistributing the moments to particles [1,20]. Although exact energy and momentum conservation is possible with these methods, they are considerably more complicated than the original naive 2:1 merge.

Having identified the lack of sufficient degrees of freedom in the merged resultant particle as the source of the error, a simple method which relies on the generation of a pair of particles was devised [4]. The particle pair provides the required freedom to conserve all moments up to 2nd order exactly. The pair of resultant particles have the same mean momentum as the originals, but they also have additional equal and opposite components of velocity in addition to the mean momentum such that energy is conserved. This method would obviously provide no benefits if starting from 2 particles, but an effective 2:1 reduction could be achieved by merging 4 particles into 2. An arbitrary number of initial particles can be considered,

Download English Version:

<https://daneshyari.com/en/article/4967988>

Download Persian Version:

<https://daneshyari.com/article/4967988>

[Daneshyari.com](https://daneshyari.com)