Journal of Computational Physics 363 (2018) 178–199

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

A parallel electrostatic Particle-in-Cell method on unstructured tetrahedral grids for large-scale bounded collisionless plasma simulations

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ARTICLE INFO

Article history:
Received 16 May 2017
Received in revised form 4 February 2018
Accepted 7 February 2018
Available online 21 February 2018

Keywords:
Bounded collisionless plasma simulation
Parallel Particle-In-Cell (PIC)
Unstructured PIC
Finite volume Multi-Point Flux
Approximation Poisson solver
Parallel GMRES

ABSTRACT

An unstructured electrostatic Particle-In-Cell (EUPIC) method is developed on arbitrary tetrahedral grids for simulation of plasmas bounded by arbitrary geometries. The electric potential in EUPIC is obtained on cell vertices from a finite volume Multi-Point Flux Approximation of Gauss' law using the indirect dual cell with Dirichlet, Neumann and external circuit boundary conditions. The resulting matrix equation for the nodal potential is solved with a restarted generalized minimal residual method (GMRES) and an ILU(0) preconditioner algorithm, parallelized using a combination of node coloring and level scheduling approaches. The electric field on vertices is obtained using the gradient theorem applied to the indirect dual cell. The algorithms for injection, particle loading, particle motion, and particle tracking are parallelized for unstructured tetrahedral grids. The algorithms for the potential solver, electric field evaluation, loading, scatter-gather algorithms are verified using analytic solutions for test cases subject to Laplace and Poisson equations. Grid sensitivity analysis examines the L^2 and L^∞ norms of the relative error in potential, field, and charge density as a function of edge-averaged and volume-averaged cell size. Analysis shows second order of convergence for the potential and first order of convergence for the electric field and charge density. Temporal sensitivity analysis is performed and the momentum and energy conservation properties of the particle integrators in EUPIC are examined. The effects of cell size and timestep on heating, slowing-down and the deflection times are quantified. The heating, slowing-down and the deflection times are found to be almost linearly dependent on number of particles per cell. EUPIC simulations of current collection by cylindrical Langmuir probes in collisionless plasmas show good comparison with previous experimentally validated numerical results. These simulations were also used in a parallelization efficiency investigation. Results show that the EUPIC has efficiency of more than 80% when the simulation is performed on a single CPU from a non-uniform memory access node and the efficiency is decreasing as the number of threads further increases. The EUPIC is applied to the simulation of the multi-species plasma flow over a geometrically complex CubeSat in Low Earth Orbit. The EUPIC potential and flowfield distribution around the CubeSat exhibit features that are consistent with previous simulations over simpler geometrical bodies.

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https://doi.org/10.1016/j.jcp.2018.02.011

1. Introduction

Particle-in-Cell (PIC) methods using unstructured grids and parallelization offer flexibility to perform large-scale computations of collisionless plasmas in domains with complex geometries. The algorithmic and mathematical issues for parallelized unstructured PIC implementations involve all aspects of a PIC cycle: gather/scatter, particle search and motion, potential and electric field evaluation, boundary conditions in bounded and unbounded plasmas, and quality of simulation due to artificial collisions and heating. There have been few implementations of electrostatic and electromagnetic PIC on unstructured grids and an even smaller number of parallelized ones. A three-dimensional parallel, electromagnetic PIC method on non-uniform hexahedral grids was developed by Wang et al. [1,2]. The method is based on a finite volume formulation with hexahedral cells that are connected with cubic cells, distorted to fit the complex geometries. Each hexahedral is mapped one to one to a unit cube in the logical Cartesian space. The gather/scatter procedures are performed in the Cartesian space using a charge conserving weighting scheme by Villasenor and Buneman [3]. The code has been applied to ion beam neutralization [4]. Wu et al. [5] developed a 3d finite element, parallelized, electrostatic code using unstructured tetrahedral grids with dynamic domain decomposition. Petillo et al. [6] developed a finite element electromagnetic PIC code on structured and unstructured grids and applied to electron guns. A three-dimensional PIC code on unstructured tetrahedral grids coupled with a finite element electrostatic solver and a frequency-domain electromagnetic solver was developed by Pavarin et al. [7] and applied to the simulation of a cylindrical cusped-plasma accelerator [8]. Alternative approaches addressing complex geometries without using unstructured meshes include conformal mapping [9] and adaptive mesh refinement [10]. Unstructured PIC simulations present a potential for increased artificial collisions and numerical heating due to the exerted self-force on particles [11]. Bettencourt [12] suggested an algorithm that allows controlling the amount of the self-force. Gatsonis and Spirkin [13] presented the mathematical formulation and implementation of an electrostatic PIC method on unstructured 3d Delaunay–Voronoi tetrahedral grids (UPIC3dE). The duality of the Delaunay–Voronoi grid was used in [13] effectively in the gather/scatter, potential solver, particle mover, and sampling step of the UPIC3dE cycle but imposed restrictions due to the required quality of the Delaunay discretization in 3D.

To take advantage of available general-purpose tetrahedral grid generators and multi-platform shared-memory multiprocessing computers including GPUs, this work presents a new mathematical formulation of a parallelized electrostatic PIC method on unstructured tetrahedral grids (EUPIC). All algorithms of the EUPIC are parallelized and implemented using OpenMP methodology allowing large-scale plasma computations with complex geometrical domains on multiprocessors. The grid structure used in EUPIC involves the tetrahedral cells, which scale with the local Debye length and the indirect dual cells formed by connecting the centroids of each adjoining face to the midpoints of the edges shared and then connecting the centroids of the faces to the centroids of the tetrahedra to which these faces belong. Charge assignment to the vertices of the tetrahedra (or nodes) and electric-field weighting to the particle follows [13]. The evaluation of the electric potential follows the finite volume formulation of the integral Gauss law in [13] but is performed using the indirect dual cell as the Gaussian surface. The potential is assumed to vary linearly within a cell, which makes our formulation consistent with the Multi-Point Flux Approximation (MPFA) family of methods [14]. The potential on conductors driven by external circuits is evaluated by a finite volume MPFA of the integral Gauss law, the charge conservation law and Kirchhoff's lumped circuit law. Unlike previous approaches [13,15,16] during an EUPIC iteration a single extended system of algebraic equations is solved providing the potential on all nodes of the domain, including externally driven, Dirichlet and Neumann nodes. The solution is obtained by the restarted generalized minimal residual method (GMRES) solver with an incomplete LU preconditioner with zero fill-ins (ILU(0)) following [17]. GMRES is parallelized in EUPIC with OpenMP using a combination of node-coloring and level-scheduling approaches. The nodal electric field is evaluated by a finite volume MPFA of the integral definition for the electric field [13]. For a Dirichlet or driven-circuit boundary node the electric field is corrected by use of the nodal surface charge, which is evaluated by a finite volume MPFA of Gauss' Law. The particle integrator in EUPIC follows Buneman's time-centered leapfrog formulation [18]. The particle search-locate algorithm is performed using an optimized version of an algorithm developed for Direct Simulation Monte Carlo method on tetrahedra [19]. Particle injection from surfaces in EUPIC follows [13]. Periodic boundary conditions are also implemented in EUPIC for a number of pairs of periodic surfaces by mirroring the grids and translating particles between two periodic surfaces. Nodal macroscopic properties are evaluated using a super-cell that consist of all tetrahedral cells surrounding a node taking into account particles with different weights. The methods and algorithms in EUPIC are validated and verified with an extensive set of test cases. Grid sensitivity analysis is performed to identify the order of accuracy for the potential and electric field evaluation. The effects of particles/cell, grid scaling, and timestep on the numerical heating, the slowing-down time, and the deflection time are investigated by performing simulations of fully ionized electron–positive ion plasmas in a grounded box with periodic boundary conditions. Laframboise's results [20] on current collection by cylindrical Langmuir probes in collisionless plasmas are used for verification of EUPIC simulations in the orbital motion limited and thin sheath regimes. Finally, EUPIC is used for a simulation of the plasma flow around a CubeSat in Low Earth Orbit.

2. Electrostatic unstructured particle in cell in 3D (EUPIC) methodology

The EUPIC method solves the electrostatic Vlasov–Poisson system for a multi-species fully ionized plasma [21,22]. The single-particle distribution function for species s particles, gives the average number of particles in a volume $d^3rd^3v \equiv$