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Massively parallel microscopic particle-in-cell

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ABSTRACT

The microscopic particle-in-cell (MicPIC) method was developed to model classical light–matter interaction in strongly-coupled plasma systems. It effectively overcomes the limitations of the particle-in-cell and molecular dynamics techniques by combining them into a single, unified framework to solve for both electromagnetic wave propagation and atomic-scale collision processes in a self-consistent treatment. Its effective time complexity is $\mathcal{O}(N)$, where N is the number of model particles, which is ideal for studying the dynamics of large ensembles. In this paper, we show that through massively parallel, distributed computations, current implementations of the MicPIC approach can handle up to 10^{11} particles on an IBM Blue Gene/Q computer with 65 536 physical cores. This allows modelling volumes of matter of approximately 1 μm^3 at solid gold density, opening a wealth of potential applications of MicPIC in nanophotonics, diffractive X-ray imaging, and strong-field science.

1. Introduction

When intense laser light interacts with solid-density materials, ionization occurs [1,2]. In the first (inner) ionization mechanism, bound electrons are promoted to a conduction state where they can freely move throughout the solid. In the (outer) ionization stage, they gain enough energy to overcome the work function and leave the material. While they are accelerated by the laser field, electrons in the conduction state can also free further electrons through laser-assisted impact ionization or share their energy with the lattice ions via electron–ion collisions [3,4]. This results in a modification and/or destruction of the material, which is of great interest for industrial and clinical applications, such as laser surgery [5–7], thin-film deposition [8], laser cutting and welding [9,10], and laser-writing of channels and waveguides in solids [11,12]. Laser heating of electrons and ions lifts the quantum degeneracy of solids and, to a good approximation, the particle interactions and dynamics can be treated classically.

Modelling the laser-driven plasma dynamics created during laser-induced material modification and machining processes [13–16] presents researchers with the difficulty of resolving light–matter interaction on both the microscopic and macroscopic length scales. Microscopic phenomena require precise knowledge of the properties and trajectories of individual particles, whereas the macroscopic scale necessitates lengths large enough to account for electromagnetic wave propagation effects. Given that the interatomic distance in a solid-density material is on the order of an ångström and that typical laser wavelengths are in the extreme ultraviolet (XUV, $\sim$ 100 nm) to the mid-infrared (MIR, a few μm) range, bridging the microscopic and macroscopic realms requires resolving roughly four orders of magnitude in length [17]. Furthermore, a 1 μm^3 volume of material at solid density contains approximately $10^{10} - 10^{11}$ particles, depending on the material composition. This presents a true challenge for computer modelling. A massively parallel approach to the microscopic particle-in-cell (MicPIC) method is currently the only avenue to meet all of these requirements.

The simulation of particle systems has a history which dates back to work on diffusion [18]. Classical treatment of systems of interacting particles in more modern cases is typically done using one of two most popular methods. The first such method, *molecular dynamics* (MD), is well-suited to studying the dynamics in systems with dimensions on the order of a few nanometres, where the electrostatic approximation is justified. This involves $\mathcal{O}\left(N^2\right)$ operations (N being the number of simulation particles), whereby each particle is subjected to the binary Coulomb force from all the others. While this method has been shown to work well for cluster nanoplasmas [19,20], chemical physics [21,22], and materials science [23,24], it does not account for electromagnetic radiation. The computational cost is also prohibitive on systems consisting of more than $\sim 10^6$ particles. The hierarchical tree [25] and particle–particle/particle-mesh (P^{3}M) [26] methods were developed to overcome this limitation but they also rely on the electrostatic approximation. MD, tree, and P^{3}M methods are thus limited to simulate light–matter interaction in spatial domains whose size is only a small fraction of the laser wavelength, where

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radiation propagation effects like source depletion, retardation, and non-dipolar excitation can be neglected.

The second method, *Particle-in-cell* (PIC), is a veteran in the field of computational plasma physics. It is formally treated in the works of Eastwood and Hockney [26] and Birdsall and Langdon [27] (see also [28]). It improves upon MD by being $\mathcal{O}(N)$ and by including electromagnetic wave propagation explicitly. Charged particles or ensembles thereof (superparticles) are imposed upon a grid through the construction of weighted charge and current densities, used as sources in Maxwell equations. The electromagnetic field is then time-evolved using the *finite-difference time-domain* (FDTD) method [29]. Finally, the motion of the particles is computed with the Lorentz force by interpolating the electromagnetic field at the location of each particle. In PIC, particles do not interact directly, but through the meshed electromagnetic field that contains all the field contributions from the particles. The advantage of this is the resulting $\mathcal{O}(N)$ scaling. However, a single PIC particle averages over tens of thousands of physical particles and its size is much larger than the atomic length scale. As a result, short range interactions, such as two- and many-body collisions, and plasma micro fields cannot be resolved adequately. Advanced PIC schemes include statistical, Monte Carlo particle collision models based on binary-collisions theories to account for the underestimated short-range particle interactions [30–35]. Still, the applicability of these methods is limited to simulating the dynamics of low-density, near-collisionless plasmas.

The newer tool *MicPIC* [36,37,17] effectively combines the MD and PIC approaches in a two-stage scheme in order to circumvent the electrostatic approximation in the former and the lack of fine-grained details in the latter. Large scale effects are treated with the traditional PIC approach, where each particle corresponds to an atom, ion, or electron. For computational efficiency the size of the PIC particles is chosen much larger than the atomic length scale. When particles come close to each other, the local electric field of each PIC particle is corrected with a short-range electrostatic contribution in the fashion of MD to account for the underestimated part in PIC. The result is a fully electromagnetic simulation method capable of accounting for collisions at the microscopic scale for individual charged particles. Initially, this approach could handle a maximum of $\sim 10^6$ particles in serial runs [17,36,37]. In this paper, we report the use of MicPIC for massively parallel simulations with up to $\sim 10^{11}$ particles, opening new avenues for large-scale modelling in nanophotonics, diffractive X-ray imaging, and strong-field science.

The paper is organized as follows. First in Section 2, we build on the approaches developed for PIC. The need to correct for short range interactions is novel; in addition to PIC there is the need to develop parallelization schemes for short range corrections. We discuss how MicPIC incorporates distributed memory parallelism with short range force corrections for simulations with large numbers of processes. Next in Section 3, we present a theoretical analysis of the expected scaling of MicPIC with respect to the different simulation parameters. We follow up in Section 4 by testing parallel MicPIC in different scenarios on mid and large scale supercomputer systems to assess MicPIC's strong and weak parallel scaling characteristics, respectively. Final conclusions are given in Section 5.

2. Method

Below, we present the important theoretical and numerical aspects of the parallel MicPIC approach in four subsections. First, we briefly discuss the theoretical approach to the MicPIC method and how it expands upon PIC. The serial version of MicPIC was discussed extensively in [17]. Next, we describe the MicPIC algorithm with focus on those components that are parallelized. The following section discusses these main components in more detail, including the numerical algorithms used in MicPIC to compute forces, fields, and particle motion. The final section is dedicated to how MicPIC is parallelized.

2.1. Theoretical approach

MicPIC is inspired by the *particle–particle/particle-mesh* (P^3M) approach. P^3M interpolates long-range forces on a coarse-grained mesh and later corrects the individual inter-particle forces for separations less than some cutoff value to shape the effective short-range interactions [26]. The P^3M technique was developed to solve the Poisson equation, which applies to situations where the electrostatic approximation is justified. It is thus equivalent to MD, but with an $\mathcal{O}(N)$ scaling. MicPIC effectively extends the P^3M scheme by being fully electrodynamic. Electromagnetic radiation and long-range particle interactions are taken care of by the PIC method while short-range corrections to the local field of each particle is performed through the use of a local, electrostatic MD approach, applied only within a small cutoff radius as in P^3M. Generalization to fully relativistic short-range corrections is possible and subject to future research.

To ensure smooth particle interactions with minimal numerical noise, MicPIC's particles are represented by Gaussian charge density distributions with identical, physical width w_0. Therefore, the charge distribution associated with the ith particle is

$$\rho_i\left(\vec{r}, w_0\right) = q_i g\left(\left\|\vec{r} - \vec{r}_i\right\|, w_0\right), \tag{1}$$

where $g\left(\vec{r}, w\right) = (1/\pi^{3/2} w^3)\exp(-\vec{r}\cdot\vec{r}/w^2)$ is a normalized Gaussian function, and q_i and $\vec{r}_i$ are the particle charge and position vector, respectively. As emphasized in previous publications (see, e.g., [36,37,17,38]), for charges in close encounters the physical width parameter w_0 emulates the screening of Coulomb interactions associated with the effective shielding of Coulomb singularities by quantum uncertainty and the finite width of the particle wavefunctions.

The first level of the MicPIC method is identical with the PIC method. For efficient long-range force calculations, numerical particles are represented on a coarse mesh by a wide charge density distribution $\rho_i^{PIC} = \rho_i\left(\vec{r}, w_{PIC}\right)$, with $w_{PIC} > w_0$. The total current density distribution associated with the particle ensemble is then defined as

$$\vec{j}^{PIC} = \sum_i \rho_i^{PIC}\vec{v}_i, \tag{2}$$

where $\vec{v}_i$ is the velocity vector of the ith particle. This current density then acts as a source term in the microscopic Maxwell equations. In MicPIC, the meshed electromagnetic fields obey the microscopic Faraday and Maxwell–Ampère relations:

$$\nabla\times\vec{e}^{PIC} = -\partial_t\vec{b}^{PIC} \tag{3}$$

$$\nabla\times\vec{b}^{PIC} = \mu_0\vec{j}^{PIC} + \frac{1}{c^2}\partial_t\vec{e}^{PIC}. \tag{4}$$

Ultimately, the PIC electromagnetic field acts back on the individual particles through the Lorentz force:

$$\vec{f}_i^{PIC} = \int \rho_i^{PIC}\left(\vec{e}^{PIC} + \vec{v}_i\times\vec{b}^{PIC}\right)d^3r, \tag{5}$$

which leads to new particle positions $\vec{r}_i$ and velocities $\vec{v}_i$ and, in turn, to a new current via Eq (2). In $\vec{f}_i^{PIC}$, the ith particle feels the effect of all the other particles through the electromagnetic field induced by the total particle current $\vec{j}^{PIC}$.

The numerical integration of Eqs (2)–(5) is self-consistent and includes important collective wave propagation effects like scattering, interference, retardation, and absorption. However, we