Commun. Comput. Phys. Vol. **16**, No. 3, pp. 599-611
doi: 10.4208/cicp.070813.280214a September 2014

Parallelization of an Implicit Algorithm for Multi-Dimensional Particle-in-Cell Simulations

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Received 7 August 2013; Accepted (in revised version) 28 February 2014

Abstract. The implicit 2D3V particle-in-cell (PIC) code developed to study the interaction of ultrashort pulse lasers with matter [G. M. Petrov and J. Davis, Computer Phys. Comm. 179, 868 (2008); Phys. Plasmas 18, 073102 (2011)] has been parallelized using MPI (Message Passing Interface). The parallelization strategy is optimized for a small number of computer cores, up to about 64. Details on the algorithm implementation are given with emphasis on code optimization by overlapping computations with communications. Performance evaluation for 1D domain decomposition has been made on a small Linux cluster with 64 computer cores for two typical regimes of PIC operation: ”particle dominated”, for which the bulk of the computation time is spent on pushing particles, and ”field dominated”, for which computing the fields is prevalent. For a small number of computer cores, less than 32, the MPI implementation offers a significant numerical speed-up. In the ”particle dominated” regime it is close to the maximum theoretical one, while in the ”field dominated” regime it is about 75-80 % of the maximum speed-up. For a number of cores exceeding 32, performance degradation takes place as a result of the adopted 1D domain decomposition. The code parallelization will allow future implementation of atomic physics and extension to three dimensions.

PACS: 52.38.-r, 52.38.Ph, 52.50.Jm

Key words: Particle-in-cell, Maxwell equations, MPI, lasertarget interaction.

1 Introduction

The particle-in-cell (PIC) codes are ubiquitous and have many applications covering diverse scientific areas such as astrophysics, plasma physics, microelectronics and chemistry [1–3]. PIC codes are also at the forefront of simulation tools for modeling laser-matter interactions since they can adequately model both the laser radiation and the response of the material allowing a self-consistent description of particles and fields. One

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example is the interaction of short-pulse lasers with thin foils, which are routinely used in laboratories around the world for particle acceleration, x-ray generation, and other scientific endeavors such as laser nuclear physics.

The modeling of short-pulse lasers interacting with thin foils faces a host of challenges. Typically, the electromagnetic fields of the laser exceed the atomic field strength and the material becomes instantaneously ionized by Optical Field Ionization. The resulting dense plasma may be opaque for the laser radiation and the material starts to act as a "mirror". The electromagnetic fields can not penetrate the plasma they created and decay inside the material on a scale length of only 10-50 nm, which can be up to three orders of magnitude smaller than the thickness of the foil [4]. In addition, the spatial distribution of the material is highly non-uniform: the target is very dense and concentrated in a narrow region of the computational domain (see Fig. 1), contrary to other problems in which the plasma is distributed uniformly. As a result, the numerical solution of the problem requires high spatial resolution and the number of particles is often prohibitively large. The problem is pushed to the extreme in virtually every numerical aspect, which makes the simulations computationally intensive and numerical algorithms challenging. PIC codes can run for days, sometimes weeks, which is a great impetus for development of efficient and robust PIC codes.

In terms of numerical approach, PIC codes fall into two general categories: explicit and implicit. In explicit PIC information (particle positions and fields) is used only from previous time levels for physical quantities that are already calculated, which makes it straightforward and computationally efficient (per time step). All quantities, electromagnetic field components, current density and particle push are arranged in space and time in the most optimal way and are advanced sequentially in a single sweep. It is, however, subject to severe numerical stability constraints [1–3, 5]. In contrast, implicit PIC codes include information from the next time level, which is more involved and requires some extra logistic and programming efforts, but the payoff can be substantial: the numerical stability improves dramatically, and the number of particles, temporal and spatial resolution requirements are greatly relaxed. In implicit PIC the computational cost per time step for the particles and field update is higher compared to explicit PIC, but implicit PIC can advance with larger time step, use a computational grid with larger cell size and use smaller number of particles. Implicit PIC codes with application to laser-target interactions first appeared in the early 80's [6, 7]. Since then, numerous codes have been developed over the years: ANTHEM [8], AVANTI [9, 10], MACROS [11], DADIPIC [12], OSIRIS [13], LSP [14, 15], CELESTE3D [16], and more recently, iPIC3D [5]. Many of those codes are widely used and are constantly evolving both in terms of applications and numerical implementation. Markidis et al. proposed muti-scale simulations with large dynamic range for studying phenomena spanning over large time scale [5]. Advanced implicit PIC codes have emerged incorporating novel adaptive techniques [17] and adding critical features such as energy conserving schemes [18].

The implicit PIC code, developed at the Naval Research Laboratory (NRL) [19, 20] for studying laser-matter interactions, is powerful enough to handle real-world problems