Development of Molecular Dynamics (MD) code for Study of miso-scale plasma physics

Yu-Chao Huang(黃禹超)
Mao-Syun Wong (翁茂勛), Shih-Hung Chen (陳仕宏)
Department of Physics, National Central University, Zhongli, Taiwan

Abstract

An accurate description of light-matter interaction in strongly coupled region is indispensable for meso-scale physics that concerning many predominant topics such as HHG, nuclear processes and near-field microscopy. Many plasma study were done with Particle-in-Cells (PIC) simulation, therefore, plasma collision and plasma micro-field were neglected or added in an artificial way. The goal of the study is to develop a Molecular Dynamics (MD) code for studying the laser proton acceleration. The MD code will be integrated with the PIC code, which can be used to study a wider range of meso-scale plasma behaviors.

Introduction

There are three main regions in laser-matter interaction depending on the temperature and density of the target. In particular, the interaction between **low intensity laser ($< 10^{10}\ W/cm^2$)** and matter belongs to **strongly coupled** region of which **short-range** interactions dominate **long-range** interactions. **Particle-in-Cells** method has been widely used for modeling weakly coupled systems, but the lack of short-range force prohibit its application for strongly coupled systems. Therefore, a hybrid method, which combine **Molecular Dynamics** simulation and **Particle-in-Cells simulation** is implemented for modeling the strongly coupled systems, it's called **Microscopic Particle-in-Cells method (MicPIC).** In this poster we study the process of plasma formation in droplet using PIC simulation with field ionization. The prospect is to incorporate Molecular Dynamics into our simulation to study light-matter interaction in strongly coupled region

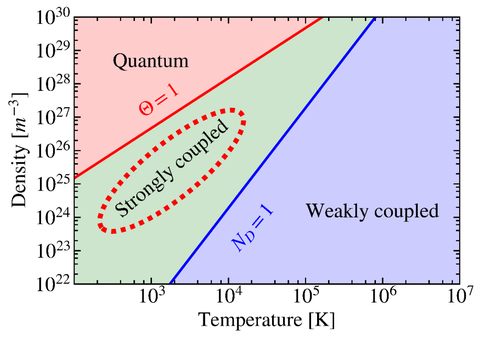


Figure 1. Three regions of Laser-Plasma interaction which is characterized by Debye number(N_D) and degeneracy(Θ). Strongly coupled region lies between $N_D \lesssim 1$ and $\Theta > 1$.

E_F: Fermi energy
λ_D: Debye length
n: Density

Debye Number

$$N_D = \frac{4\pi}{3} n\lambda_D^3 = \frac{4\pi}{3}\frac{(\varepsilon_0 k_B T)^{3/2}}{\sqrt{n}e^3} \quad (1)$$

Degeneracy Parameter

$$\Theta = {k_B T}/{E_F} = \frac{2m_e k_B T}{\hbar^2 (3\pi^2 n)^{2/3}} \quad (2)$$

	MD	PIC
Pros	• nanometer target • Collision • plasma micro-field	• $O(N_p) = \alpha N_p + \beta(N)$ • Wave propagation • $N_p \sim 10^{11}$
Cons	• $O(N_p) = 10N_p^2 - N_p$ • EM wave propagation • $N_p \sim 10^6$	• Short-range interaction • Many body collision • Plasma micro-field

Table 1. MicPIC inherit the advantages of MD and PIC simulations for simulating light-matter interactions with $\sim 10^{11}$ particles. The simulation time is **linearly scaled** with $O(N_p, N_n) = \alpha N_p + \beta(N) + \gamma N_p N_n$.

N_p: Number of particles
N_n: Number of neighbors
α, γ: constants
β: A function of N (*e.g.* $5N^3\ log_2\ N^3$)
N: # of gird (*e.g.* $N \times N \times N$)

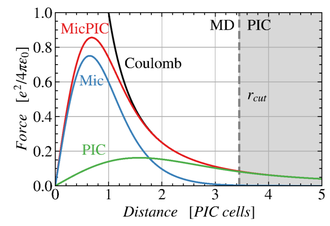
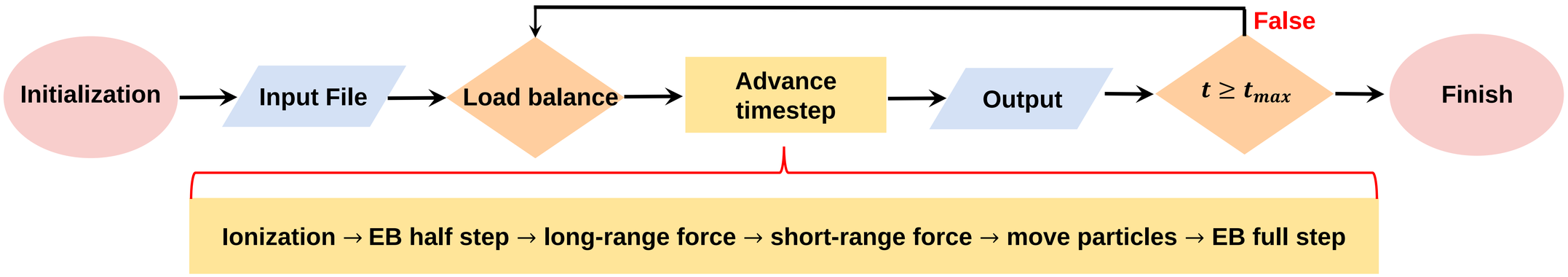
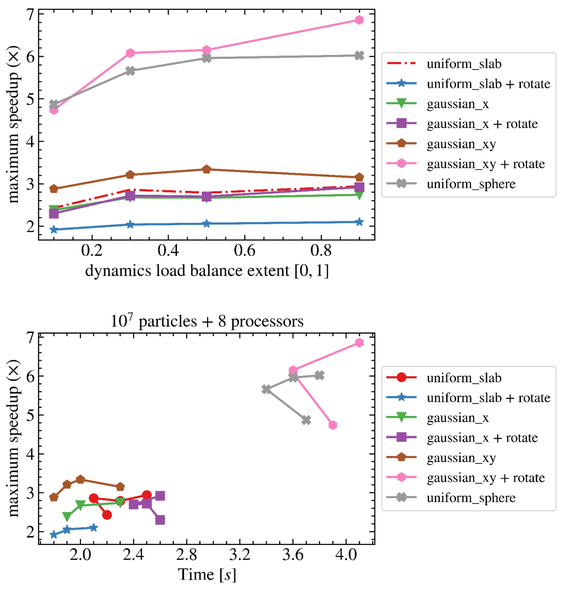


Figure 2. Coulomb force decompose into Mic force and PIC force.

MD Simulation



Development and validation



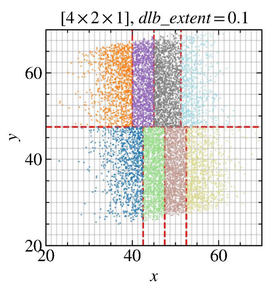


Figure 5. Parallelization efficient and maximum speedup comparison with different distribution

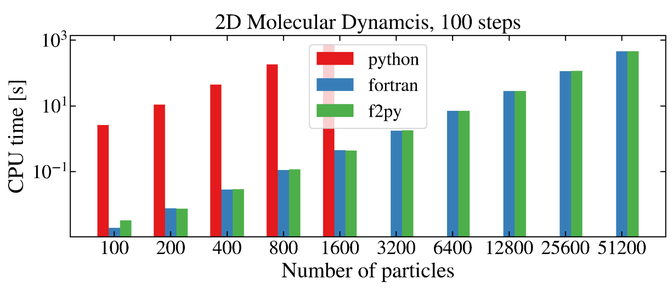


Figure 6. Compare execution speed of different language. Finally, we chose f2py since it is simple but also fast both in serial and parallel code.

From the benchmark of execution speed from different language, we decided to use f2py as primary language from our MD code, since it's fast and also easy to implement (see Figure 6). We then use different initial distribution to benchmark our dynamics load balance scheme, as you can see in Figure 5, it perform well under many different distributions. Finally, we also tested our code and compare with theoretical solution of RDF for Lenard-Jones fluid [4].

$$g(r^*, T^*, \rho^*) = 1 + (r^*)^{-2}\exp[-(a + r^* + b)]\sin(c * r^* + d) + (r^*)^{-2}\exp[-(gr^* + h)]\cos(k * r^* + l) \quad when\ r^* < 1 \quad (3)$$

$$g(r^*, T^*, \rho^*) = sexp[-(m * r^* + n)^4] \quad when\ r^* \leq 1 \quad (4)$$

where $a, b, c, d, g, h, k, l, m, n$ *are the adjustable parameters as a function of temperature and density.*

Figure 7. Results of RDF(Radial Distribution Function) in Lenard-Jones fluid compare to theory fit.

Conclusion

1. Using highly parallelized Molecular Dynamics enable us to study wide range of plasma dynamics in highly coupled region.
2. Further incorporation of Molecular Dynamics into our PIC simulation is an imminent task to study light-matter interaction in strongly coupled region.

Reference

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