A Comparison between the Simulation Efficiency of a Poisson and Coulomb based Particle Solver

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Introduction & Methods

Under rarefied conditions, where CFD assumptions are no longer fulfilled, particle movement is commonly simulated by integrating individual trajectories of theoretical ”superparticles”. The implementation of external fields accelerating charged particles is also rather straightforward. But with rising charge densities, particle-particle interactions become more important - a phenomenon often referred to as ”space charge”. There are two main distinct approaches to including these interactions: Particle in Cell (PIC) wherein the Poisson equation is being solved and Coulomb algorithms which approximate the sum of individual forces between charged particles.

In this study, an NO REMPI laser plasma expansion (single pulse) was simulated using the PIC based open source code PICLas[1] and the Ion Dynamics Simulation Framework IDSimF[2]. For IDSimF, both the Barnes-Hut tree approach with $\theta = 0.6$ and the FMM (Fast Multipole Method) were utilized.
In all simulations $\sim 10^5$ particles were started in a sphere with radius 1cm at quasineutrality. Ions are at room temperature and photoelectrons possess 1.5eV residual kinetic energy. Results are being compared at $t = 4 \cdot 10^{-8}$ s and $4 \cdot 10^{-7}$ s, with a full sum calculation as a reference.

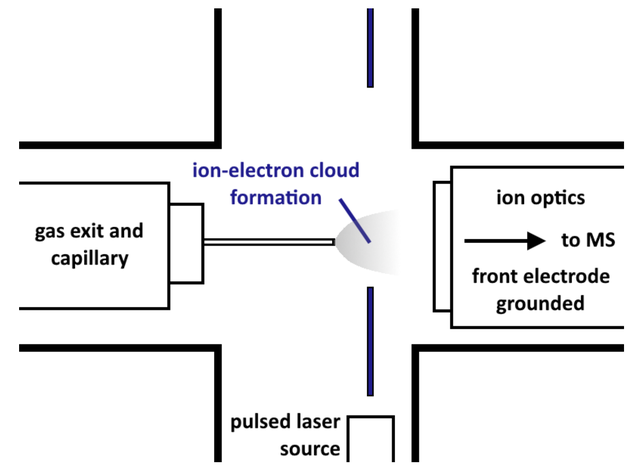


Figure 1: NO REMPI laser experiment

Results

The main difficulty with this kind of expansion simulation is the highly dynamic electron density distribution. Due to escaping fast photoelectrons a potential is generated that decelerates the electrons and ”recaptures” some portion of them. Whether the respective simulations could accurately describe this process was used as a proxy to gauge the validity of simulation results. The percentage of photoelectrons ”retained” within a spherical area of radius 1.5mm around the origin was therefore used as a quality indicator (QI).
Measures of accuracy and runtime are given in **Table 1**:

Table 1: Runtime vs accuracy in four different scenarios

	$\theta = 0.6$ tree	FMM	PICLas	full sum
wall time*	30.7min	15.2h	1.77d	19.3d**
CPU time	84.4min	50.8h	$\sim$ 71d	65.0d**
QI $t = 4 \cdot 10^{-8}$ s	0.02%	1.26%	24.3%	0.84%
QI $t = 4 \cdot 10^{-7}$ s	0	15.5%	28.9%	N/A

*Due to a higher degree of parallelization, PICLas was run on 40 cores while all IDSimF simulations were carried out using 4 (5 for full sum) cores.
**Extrapolated values, only 500 timesteps were calculated with the full sum of interactions.

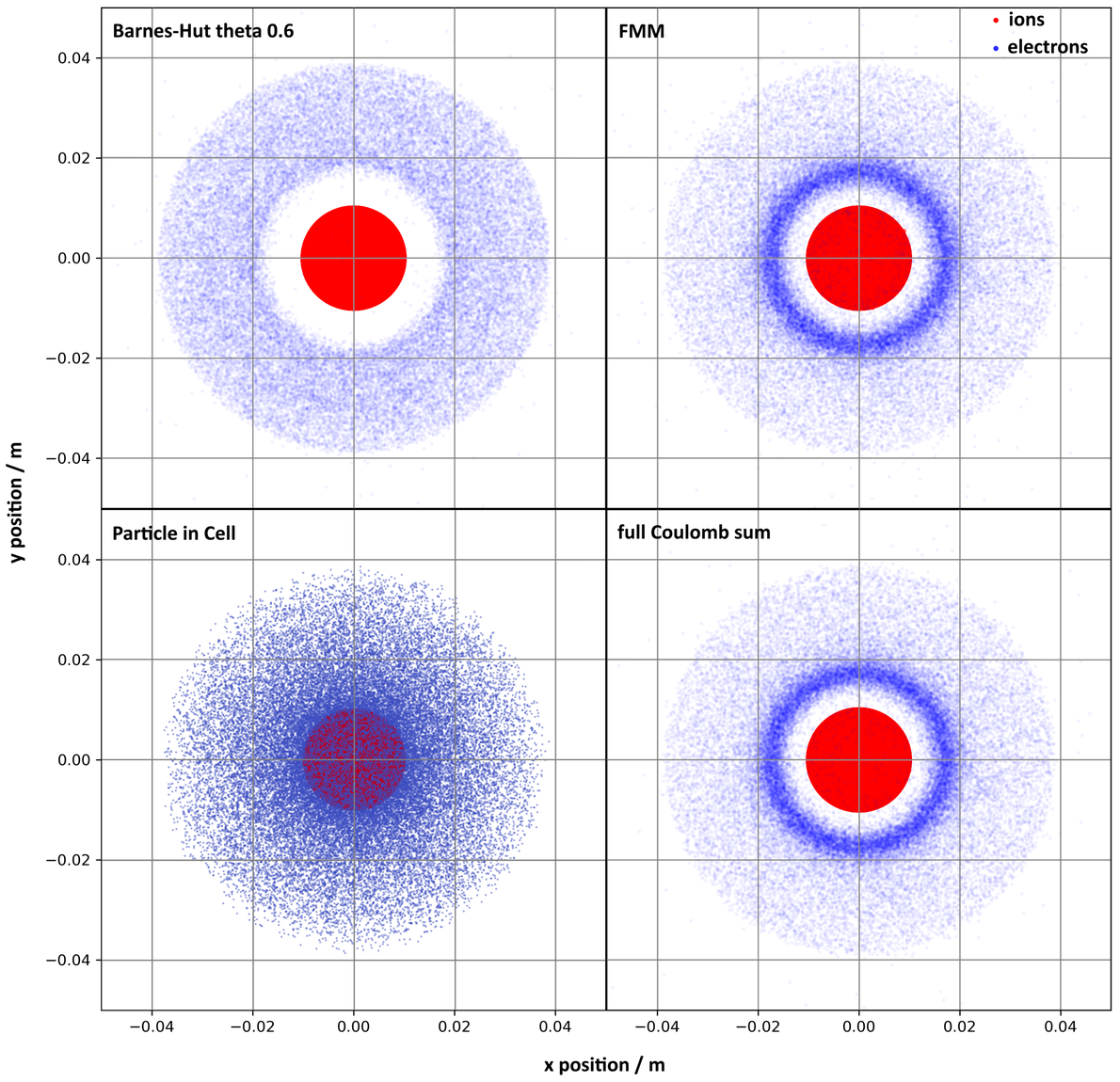
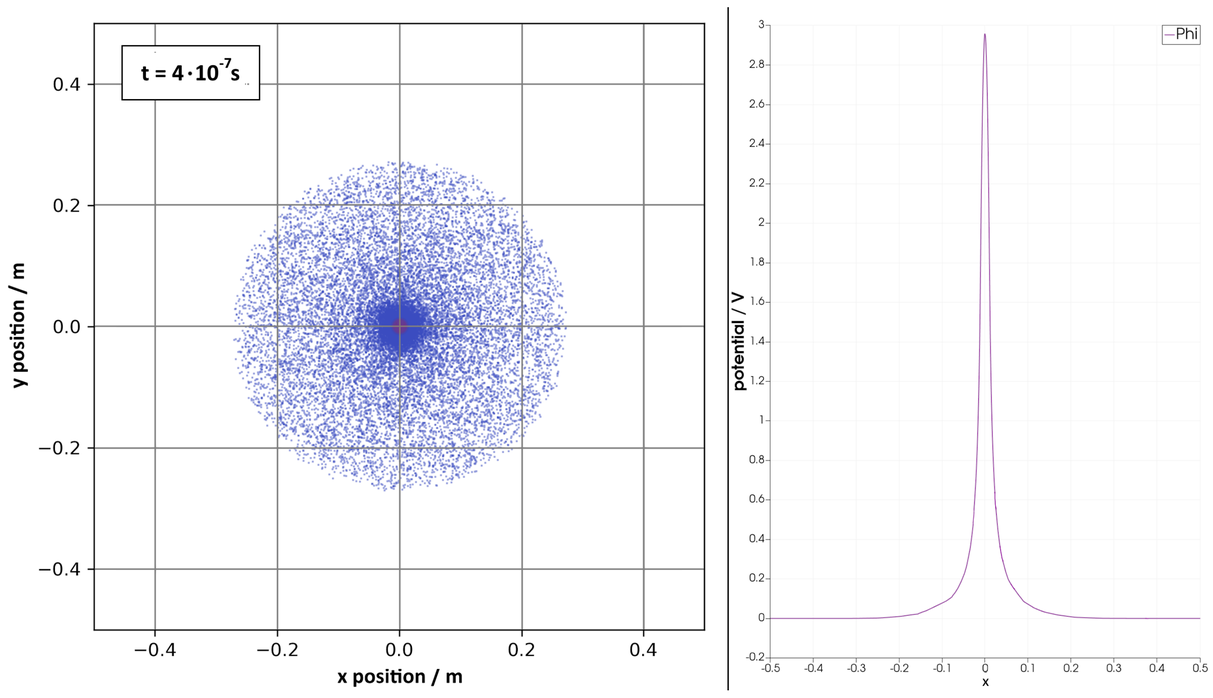


Figure 2: Slice through the particle distribution after $4 \cdot 10^{-8}$ s



It becomes fairly obvious from just the visualization alone that the FMM simulation shows the greatest overlap with the full sum reference (which approaches the exact force on each particle). While the treecode doesn’t seem able to even reproduce the oscillating photoelectron effect, PICLas seems to overestimate the ion-electron interaction. The insane computational cost of the PIC code is also currently being looked into.

Figure 3: The positive ion cloud potential recaptures a portion of photoelectrons

Conclusion and Outlook

Further investigation of the simulation problem at hand revealed a general weakness of simple treecodes. Due to the dipole nature of electrostatic interactions between ions and electrons, charge to center-of-charge calculations are no longer adequate. Thus, the implementation of dipole and quadrupole moments at the ends of the tree structure is planned. As for the direct results: The photoelectrons that are not able to escape the generating electrostatic field oscillate around the ion cloud with a frequency that agrees with the theoretical value of the short-lived plasma. The aim is to take these results and decouple individual electron and ion movement in order to assess the kinetic energy distribution of ions following the ensuing ”Coulomb explosion”.

Literature and COI Declaration

[1] PICLas; Fasoulas, S., Munz, C.D., Pfeiffer, M., Beyer, J., Binder, T., Copplestone, S., Mirza, A., Nizenkov, P., Ortwein, P. & Reschke, W. (2019). *Physics of Fluids*, *31*(7), 072006.
[2] IDSimF; ion dynamics simulation framework; https://idsimf.readthedocs.io/en/latest/

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