Modelling of 1D DC Discharges Using Various Particle-in-Cell Schemes

N. Savard[1], G. Fubiani[2], M. Dehnel[1,3]
D-Pace[1], LAPLACE/CNRS[2], SIRC[3]

Introduction

Charge- and energy-conserving implicit particle-in-cell (PIC) codes offer the potential to use larger time steps and smaller cell sizes compared to explicit methods[1]. Although non-linear iterations increase computational cost, reducing spatial and temporal resolution while maintaining similar particles-per-cell (PPC) can, in principle, lower overall runtime. However, studies of self-consistent discharges indicate that accuracy is often degraded[2], and there is limited evidence that implicit methods can outperform explicit PIC in higher dimensions at comparable accuracy. Some promise has been demonstrated for static sheaths in 1D with binomial smoothing[3], but concerns remain about efficiency when iterative solvers are required for the particle mover.

In this work, we present a 1D discharge sustained by a constant arc voltage and thermionic cathode current. We compare momentum-conserving (MC-PIC), energy-conserving (EC-PIC), and implicit nearest-grid-point (INGP) charge-and-energy conserving methods for accuracy and computational performance.

Results

A non-uniform grid is used for EC-PIC and INGP of 256 cells derived by:

$$x(\xi) = L\left[\left(\frac{\xi-1}{N_x-1}-1\right)-\left(\frac{1}{N_x-1}-\frac{\Delta x_{min}}{L}\right)\frac{\sin\left(\frac{2\pi(\xi-1)}{N_x-1}\right)}{\sin\left(\frac{2\pi}{N_x-1}\right)}\right]$$

Explicit methods use a time step of 6 ps, whereas the INGP method uses 120 ps which still results in a collision ratio of < 1% per time step. A background of He is assumed with allowed elastic, excitation, and ionization collisions for e + He -> e + He, along with elastic and charge-exchange collisions for He^+ + He -> He^+ + He. Binomial smoothing can be implemented with INGP.

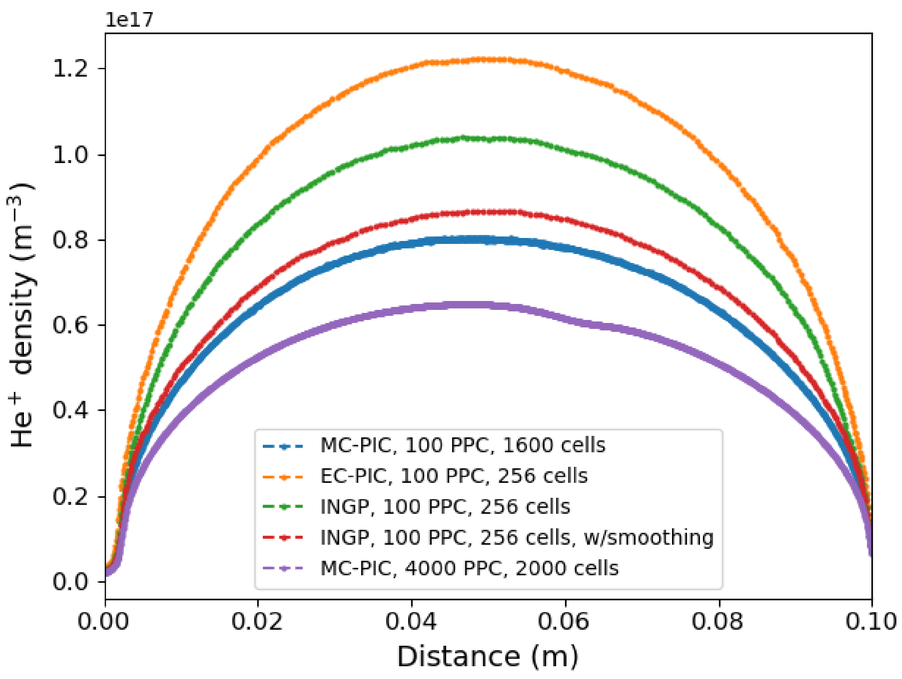

Fig 1: Time-averaged He^+ density for various converged simulations.

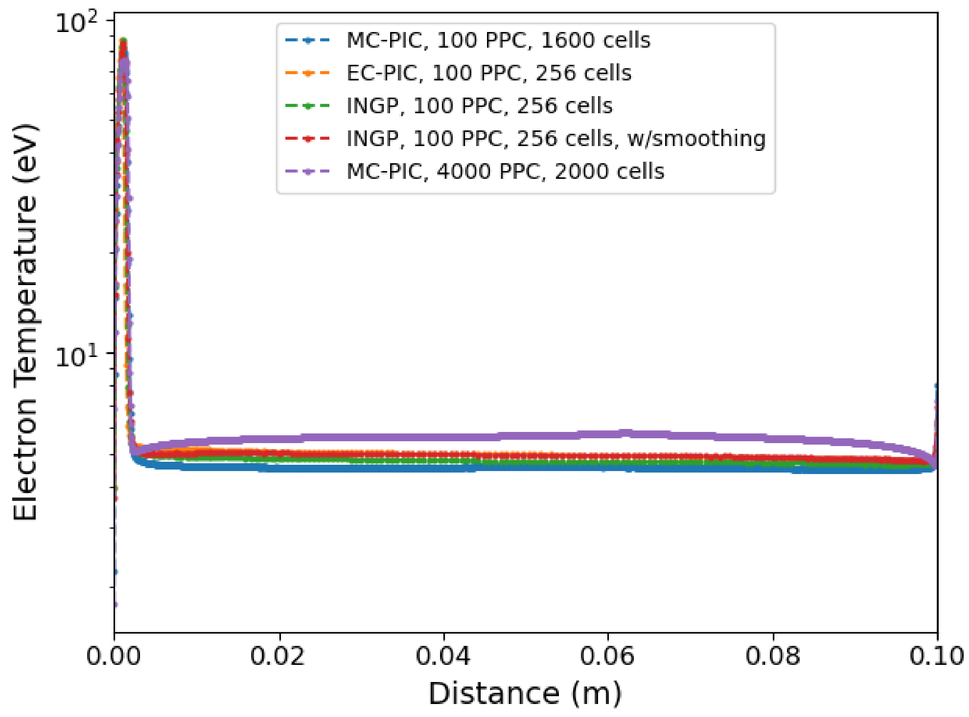

Fig 2: Time-averaged electron temperature for various converged simulations.

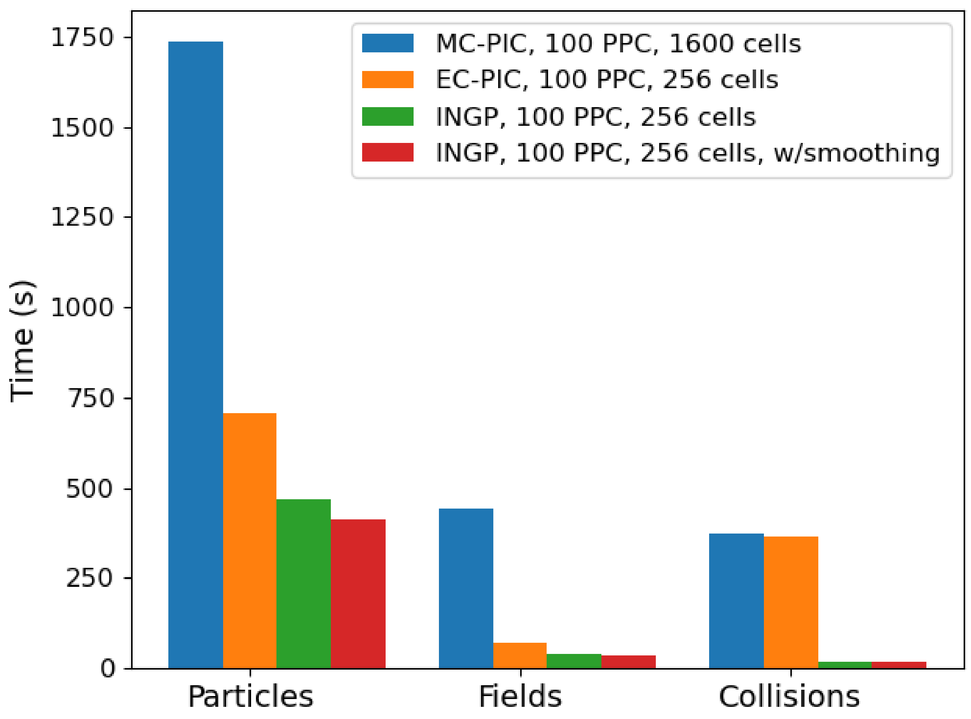

Fig 3: Real simulation time for particle operations (mover, charge deposition), fields (Gauss' law), and collisions (null collision Monte-Carlo) for various simulations. Each simulation done with 2 MPI ranks with 16 OpenMP threads per rank. Each OpenMP thread corresponds to a single CPU.

Conclusion

Reducing particle number and cell resolution decreases accuracy compared to well-resolved simulations. The INGP method offers faster runtimes, especially with binomial smoothing, but the need for Picard iterations in higher dimensions could make the particle mover up to three times slower[2,3]. This raises doubts that implicit methods can achieve both the speed and accuracy of MC-PIC, though they may be suitable when very low-resolution runs are acceptable.

References

1. D Eremin, "An energy-and charge-conserving electrostatic implicit particle-in-cell algorithm for simulations of collisional bounded plasmas", *J. Comp. Phys.* (2022)
2. N Savard *et al*, "Impact of particle number and cell size in fully implicit charge- and energy-conserving particle-in-cell schemes", *Phys. Plasmas* (2025)
3. N Savard *et al*, "Impact of particle number and cell size on energy-conserving PIC applied to RF-driven bounded plasmas", *Submitted to J. Appl. Phys.*