Comparative Study of Explicit vs. Implicit Particle-in-Cell schemes for Plasma Sheath Simulations

Davide Curreli and Jon Drobny

Nuclear, Plasma, and Radiological Engineering University of Illinois at Urbana-Champaign, 104 S Wright Street, Urbana, IL 61801

60th Annual Meeting of the APS-DPP, November 2018, Portland, OR

Goals and Motivation

Particle-in-Cell Codes

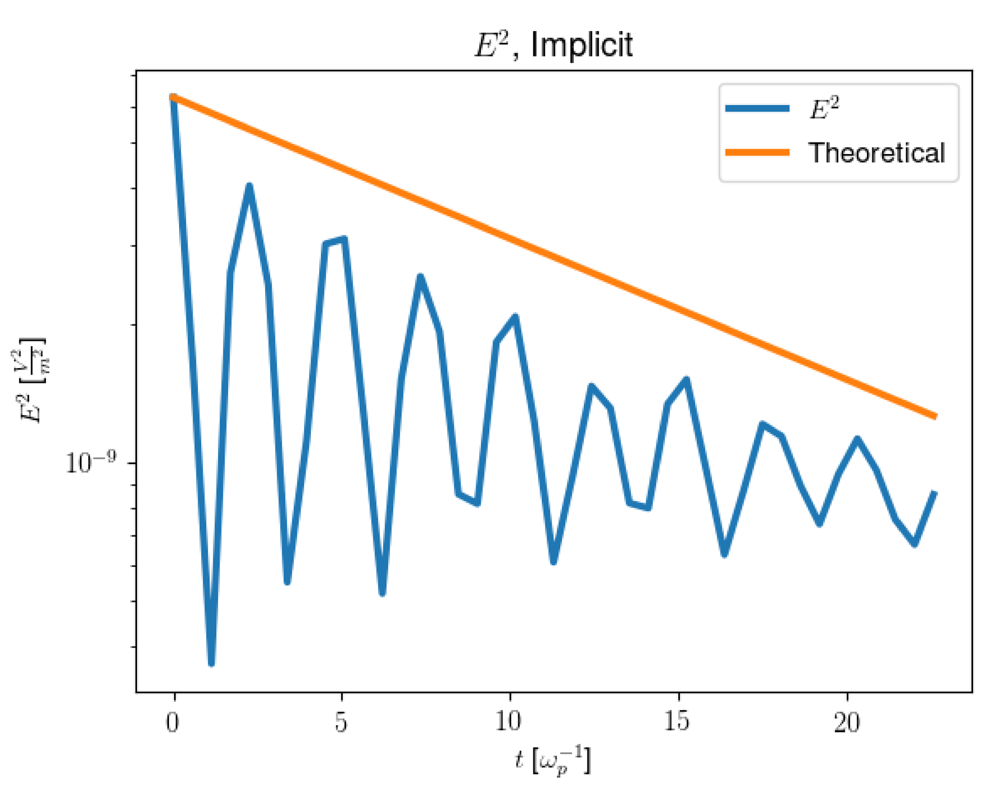
Particle-in-Cell is a particle-based method for solving the transport equations of a fluid such as a plasma. Flowing quantities, such as charge, are tracked with particles, while grid quantities, such as electric field, are applied to the grid from the particle positions. Particle-in-Cell codes are useful for resolving physics at length scales smaller than possible with fluid equations and are particularly well-suited to coupling with other, particle-based codes such as binary collision-approximation codes.

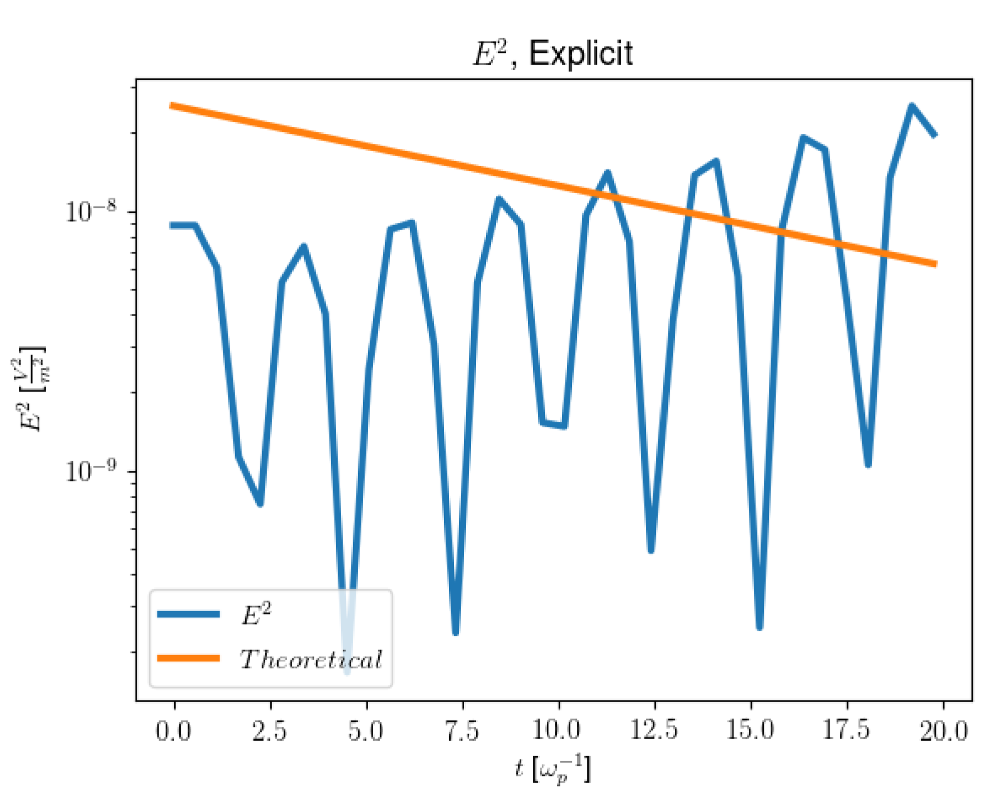
Implicit and Explicit Codes

Traditional particle-in-cell codes use explicit solvers, which have stability criteria. Implicit methods, on the other hand, are universally stable. This makes them useful for multi-scale simulations where one must resolve physics at vastly different timescales, such as the electron and ion timescales in a plasma sheath. Presented is an implicit particle-in-cell code based on the discretization of Chacon et al.[1] tested against theoretical instability calculations and used for modeling a 1D plasma sheath.

Implicit and Explicit Codes for Large Time Steps

Explicit solvers have stability criteria that are easy to exceed with large time steps. Although they may be more costly, implcit methods can remain stable for any timestep.





Above, a landau damping test case is solved using an implicit (top) and explicit (bottom) method. The implicit method correctly reproduces the correct damping rate, while the explicit method exhibits a numerical instability. Plasma physics problems are often multiscale, and the ability to produce correct physics at larget time scales would allow for faster simulation of mixed ion-electron plasmas, since the electron timescale need not be completely resolved in the implicit case.

Governing Equations of Implicit and Explicit PIC Codes

Implicit PIC

$$\frac{\partial f}{\partial t} + v \cdot \nabla f + q(E + v \times B) \cdot \frac{\partial f}{\partial p} = 0$$

Presented is an implicit PIC based on the Vlasov-Ampere system(above). Such a formulation of the particle-in-cell is intrinsically electromagnetic, unlike the classical Vlasov-Poisson PIC.

$$\varepsilon_0 \frac{\partial E}{\partial t} + j - \langle j \rangle = 0$$

In 1D, the charge continuity expression can be integrated directly to find the implicit PIC field update equation. The constant of integration, $\langle j \rangle$, is the *current densty bias*, or the average current. In periodic boundary conditions this term is constant in time.

$$\frac{E^{n+1} - E^n}{\Delta t} = \frac{1}{\varepsilon_0}\left(\langle j \rangle - j^{n+1/2}\right)$$

$$\frac{x_i^{n+1} - x_i^n}{\Delta t} = v_i^{n+1/2}$$

$$\frac{v_i^{n+1} - v_i^n}{\Delta t} = \frac{q_i}{m_i} E^{n+1/2}(x_i^{n+1/2})$$

Crank-Nicholson discretization uses half-time steps for the particle update step.

$$E^{n+1/2}(x_i^{n+1/2}) = \sum_j S(x_j - x_i^{n+1/2}) \frac{E^n + E^{n+1}}{2}$$

$$j^{n+1/2} = \sum_i \frac{q_i v_i^{n+1/2} W(x_i^{n+1/2})}{\Delta x}$$

Field interpolation for the particles and particle weighting to currents is shown above.

Explicit PIC

$$\nabla^2 \varphi = -\frac{\rho}{\varepsilon_0}$$

Traditional particle-in-cell codes are based on the Vlasov-Poisson system.

$$\rho = \sum_i \frac{q_i}{\Delta x} W(x_i)$$

$$E_j = \frac{\varphi_{j+1} - \varphi_{j-1}}{2\Delta x}$$

$$E^{n+1/2}(x_i^{n+1/2}) = \sum_j S(x_j - x_i^{n+1/2}) E_j^{n+1/2}$$

Electric fields are found via direct differentiation of the electric potnetial from Poisson's equation based on weighted charge densities.

$$\frac{x^{n+1/2} - x^{n-1/2}}{\Delta t} = v^n$$

$$\frac{v^{n+1} - v^n}{\Delta t} = \frac{q}{m} E^{n+1/2}(x^{n+1/2})$$

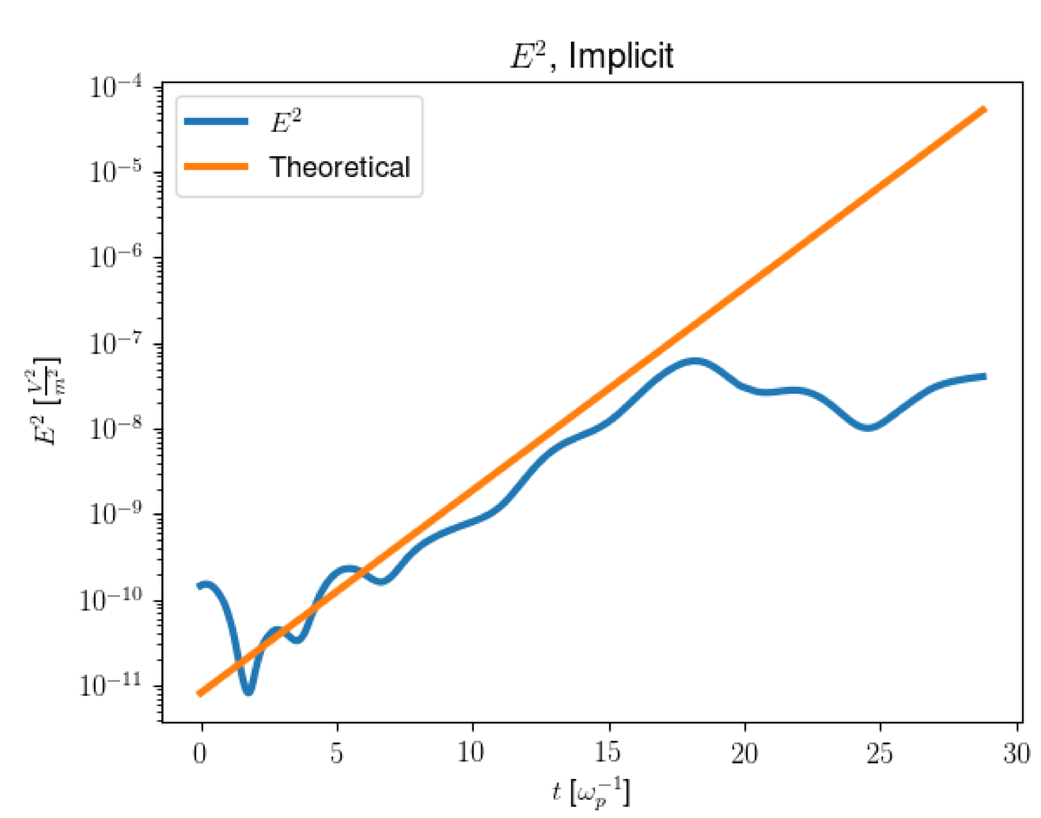
A Boris-Buneman (leapfrog) scheme is used to update the particles. This scheme is more stable than other simple numerical schemes (e.g. Euler Forward).

The classical particle in cell suffers from grid heating, stability problems, and is not intrinisically an electromagnetic method. In order to support electromagnetic effects, an additional current weighting (on top of the charge density weighting) and magnetic field solver must be added to the framework to support proper handling of electromagnetic effects. For these reasons, explicit particle-in-cell codes suffer when used to study long timescale physics.

Theoretical Validation of Implicit PIC

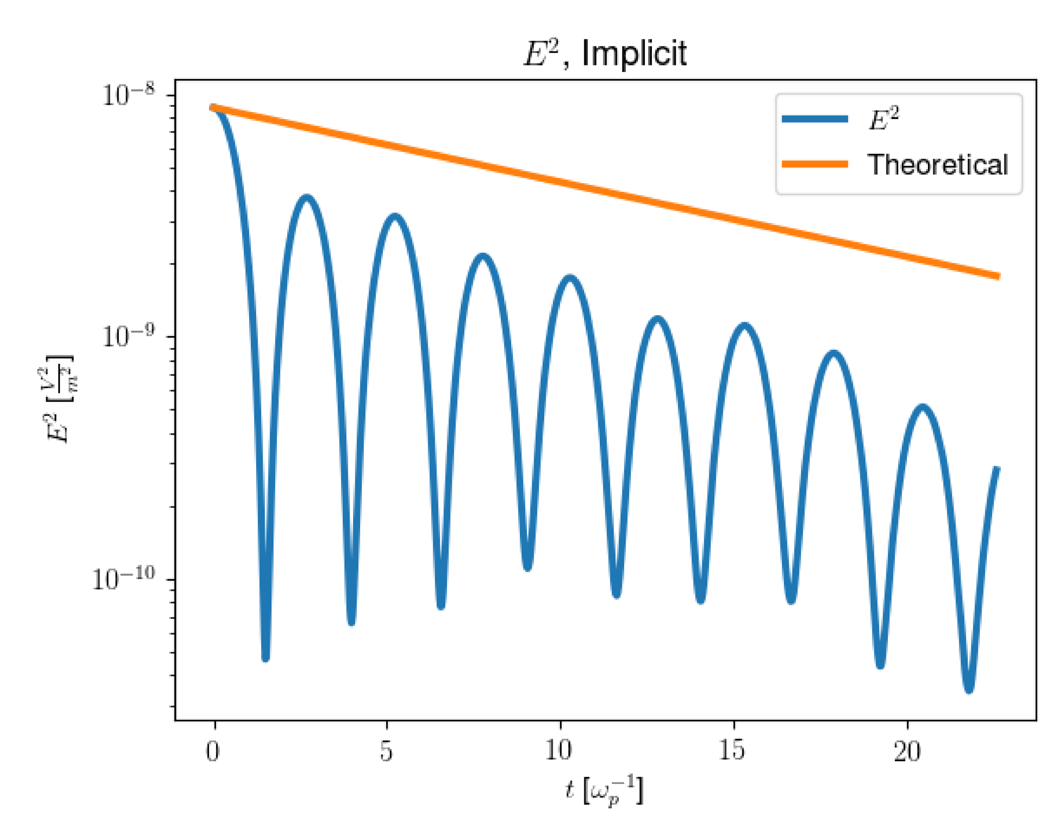
Bump-on-Tail Instability

The bump-on-tail instability occurs when a small population of a larger, mostly thermalized population has a drift speed substantially different from the majority population. The two interacting streams produce an instability.



Landau Damping

Landau damping is a classical hot plasma effect used to validate plasma codes. An initial density perturbation (of a sinusoidal nature) is damped via particle-wave interaction with a characteristic growth rate.

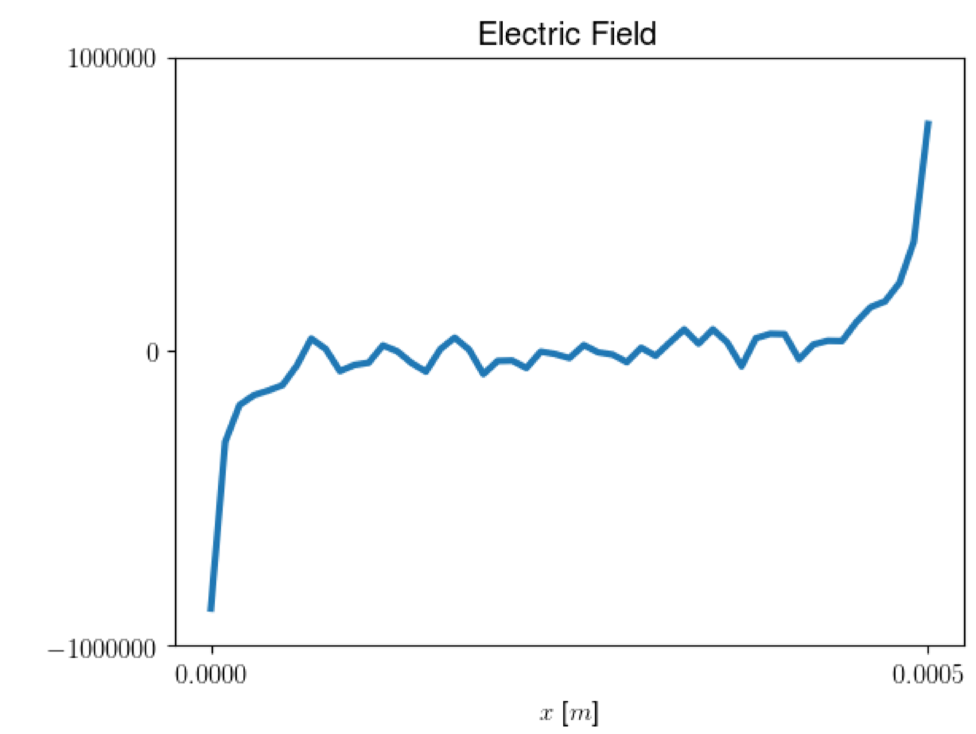


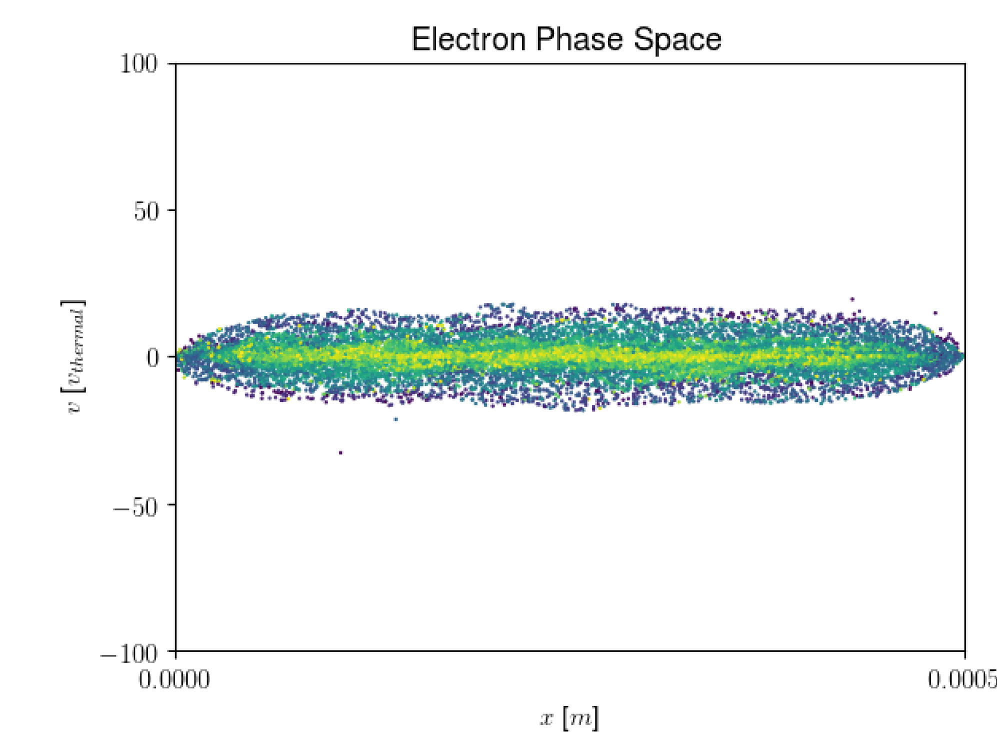
Plasma Sheath

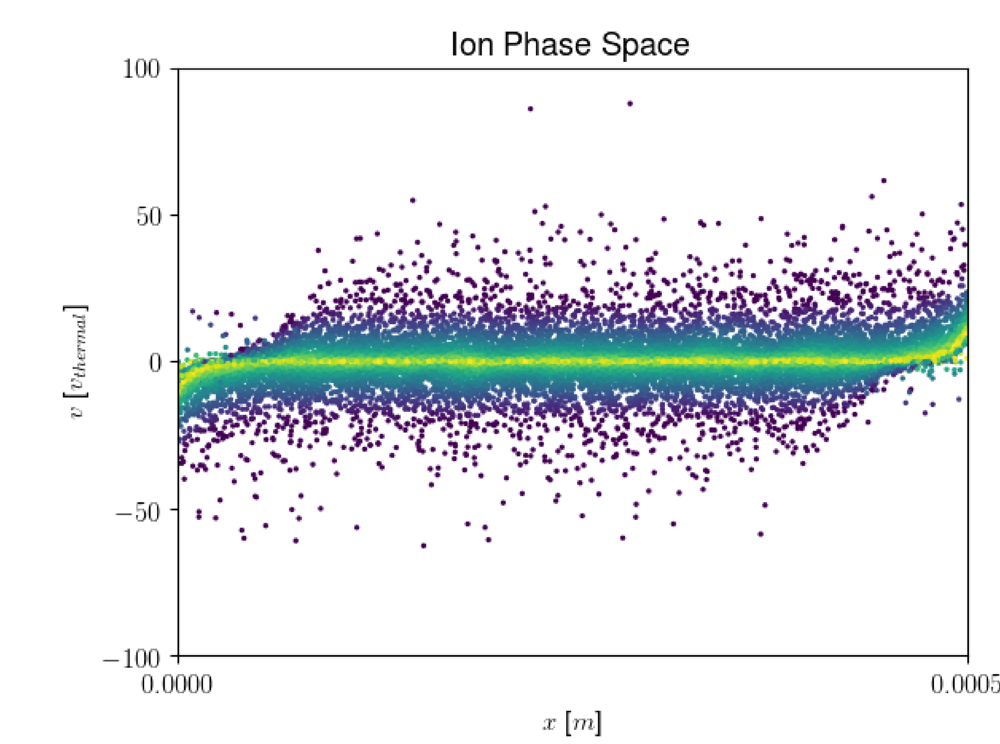
Using Dirichlet-Dirichlet Boundary Condtions, and the appropriate flux boundary conditions on the current, the implicit PIC can model, in kinetic-kinetic mode, the 1D plasma sheath. Extending the model to include magnetic effects is trivial given the model's basis on the Vlasov-Maxwell system instead of the Vlasov-Poisson system.

Implicit methods are advantageous because they remain stable at large time steps. For a kinetic-kinetic simulation, both the electron and ion timescales must be fully resolved. In an explicit PIC, stability criteria must also be satisfied for both populations. Since the Implicit PIC is universally stable, the electron timescale need only be resolved as finely as necessary for the sheath to evolve properly.

Particles are reinitialized using an ideal source that spans the box.







References and Acknowledgements

[1] L. Chacón et al., J. Comput. Phys., 230 (2011) 7018-7036.

The authors would like to thank Dr. Chacón for valuable discussions on the implicit particle-in-cell discretization.