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Physical Effects of Aleph's Semi-implicit Particle-in-cell Algorithm

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Abstract

System-scale kinetic simulation of high-density plasmas in vacuum arc discharges is challenging due to stability constraints placed on the timestep and mesh size in conventional particle-in-cell (PIC) methods. In recent years, an energy-conserving semi-implicit PIC[1,2] (SIPIC) scheme has been implemented in the low-temperature plasma simulation code Aleph [3] that allows the circumvention of the finite-grid instability (FGI) and relaxes the timestep requirement that the electron plasma frequency be resolved. However, how/if the semi-implicit scheme affects the underlying physics of the discharge is not well understood. In this work, the influence of SIPIC on particular quantities of interest in vacuum-arc discharges is investigated and comparisons between analytical theory and explicit electrostatic PIC are made where possible.

Introduction

Energy-conserving Semi-implicit PIC

$$\dot{\boldsymbol{x}} = \frac{\boldsymbol{p}_p}{m_p},$$

$$m_p \dot{\boldsymbol{v}}_p = -\sum_v \nabla S_v(\boldsymbol{x}_p)\phi_v,$$

$$\nabla \cdot \left(1 + C\frac{e^2\Delta t^2}{4\, m_e \epsilon_0}\bar{n}_e\right)\nabla\phi = -\frac{\rho}{\epsilon_0},$$

$$\rho = \frac{1}{V_v}\sum_p S_v(\boldsymbol{x}_p) q_p$$

For $|\boldsymbol{u}_e| < v_{th,e}$, SIPIC is stable against aliasing instabilities

→ $\Delta x > \lambda_{De}$ can be used

If $C \geq 1$, the electron plasma mode is stabilized

→ $\Delta t > \omega_{pe}^{-1}$ can be used

Physical Effects

'Stretches' the Debye length

$$\lambda_{De}^{\mathrm{SI}} = \sqrt{\frac{\epsilon^{\mathrm{SI}} k_B T_e}{n_e e^2}},\ \epsilon^{\mathrm{SI}} = \epsilon_0\left(1 + C\frac{e^2\Delta t^2}{4\, m_e \epsilon_0} n_e\right)$$

'Contracts' plasma frequency

$$\omega_{pe}^{\mathrm{SI}} = \sqrt{\frac{n_e e^2}{\epsilon^{\mathrm{SI}} m_e}},$$

SI cold-plasma dispersion relation (fluid-perspective)

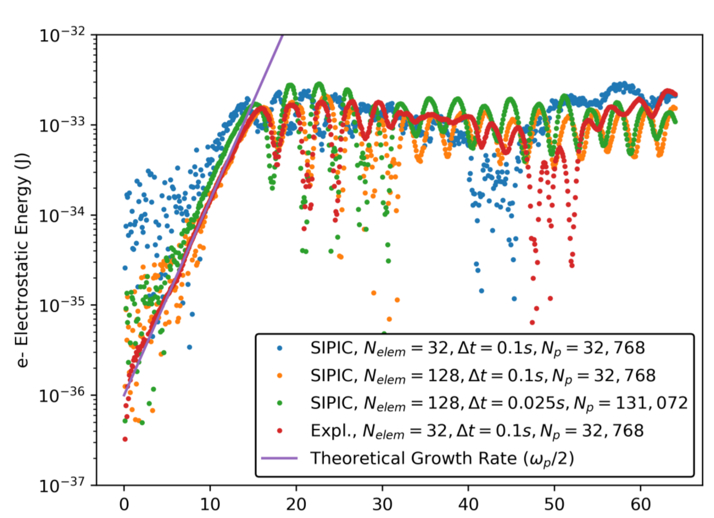
$$1 - \sum_\sigma \frac{{\omega_{pe}^{\mathrm{SI}}}^2}{(\omega - \boldsymbol{u}_0 \cdot \boldsymbol{k})^2} = 0$$

$\omega_{pe} \to \omega_{pe}^{\mathrm{SI}}$ in growth rates derived from fluid equations

Question

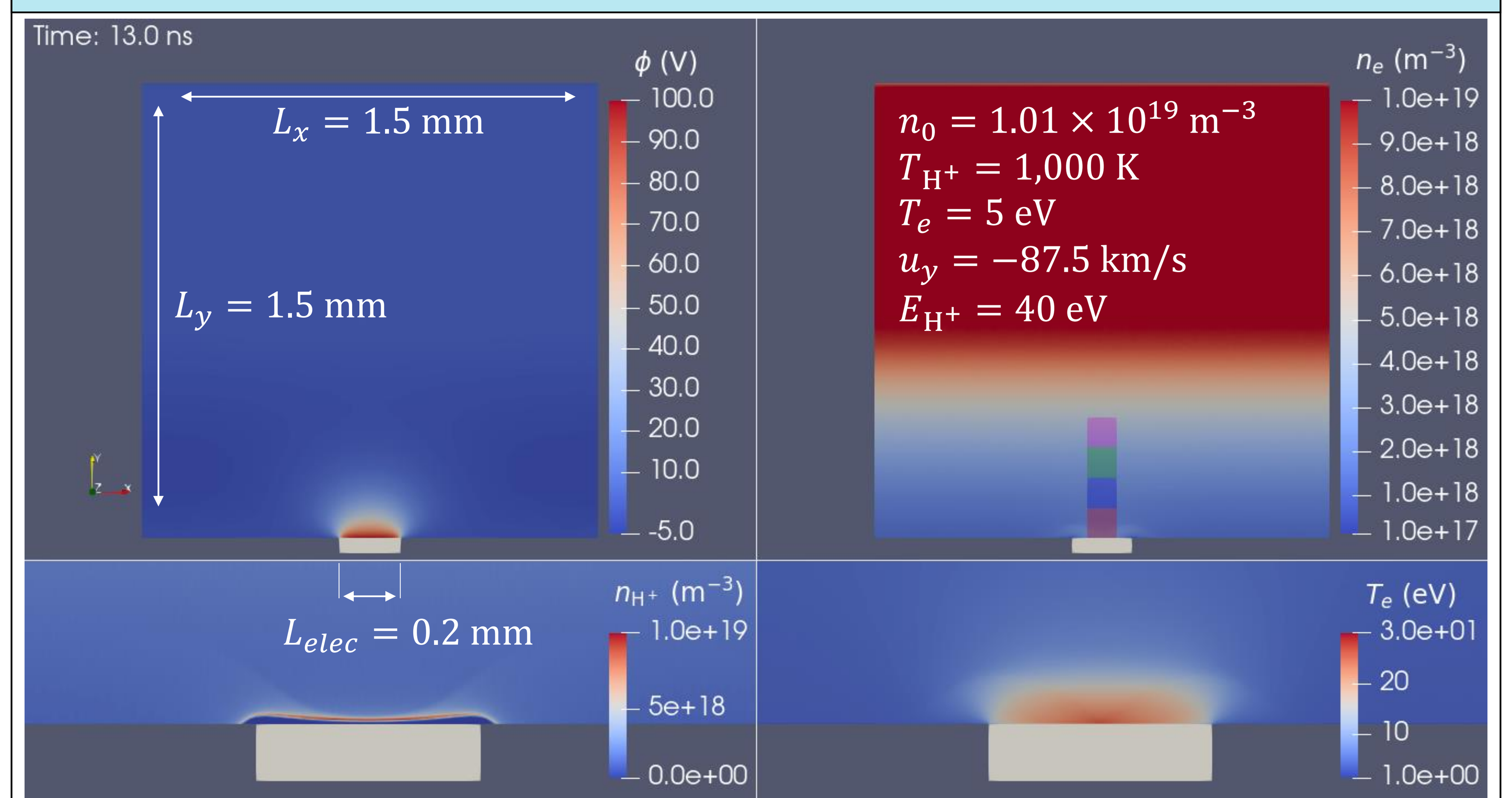
Can we use this algorithm to accurately model surface-plasma interactions in high-density plasma discharges?

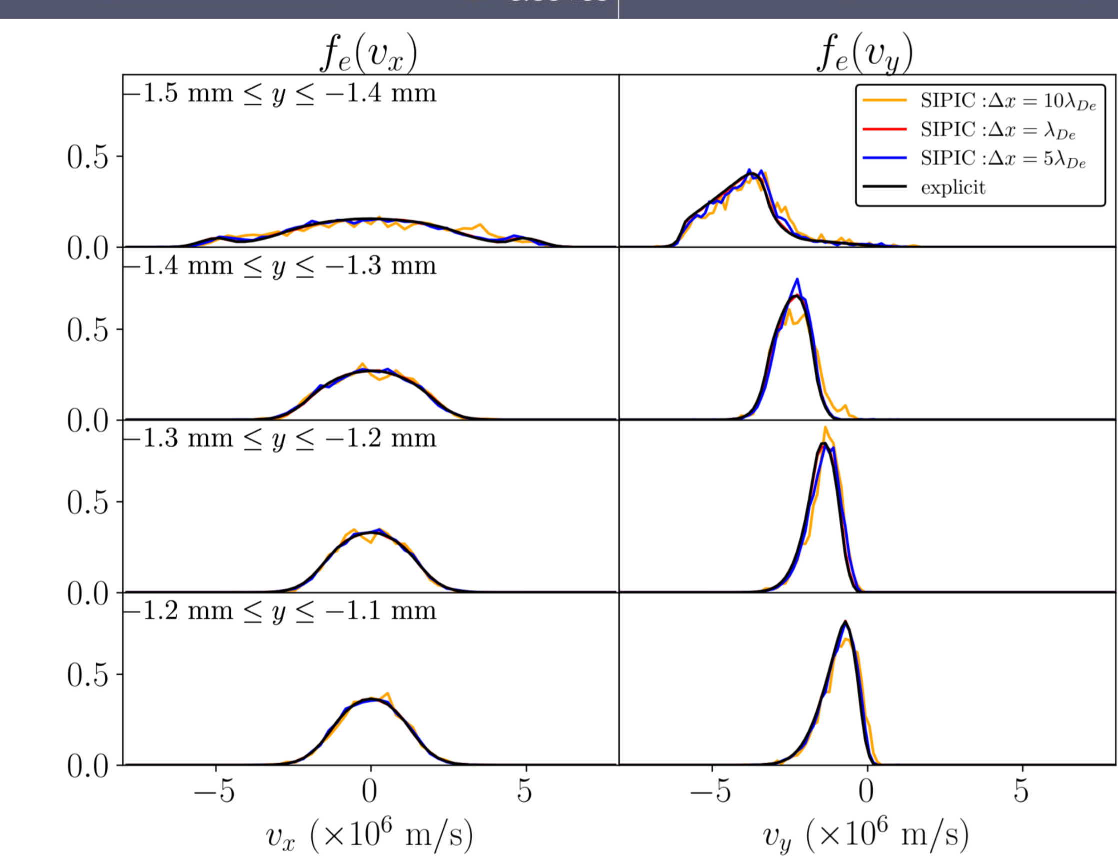
Cold Electron-Electron Two-Stream Instability

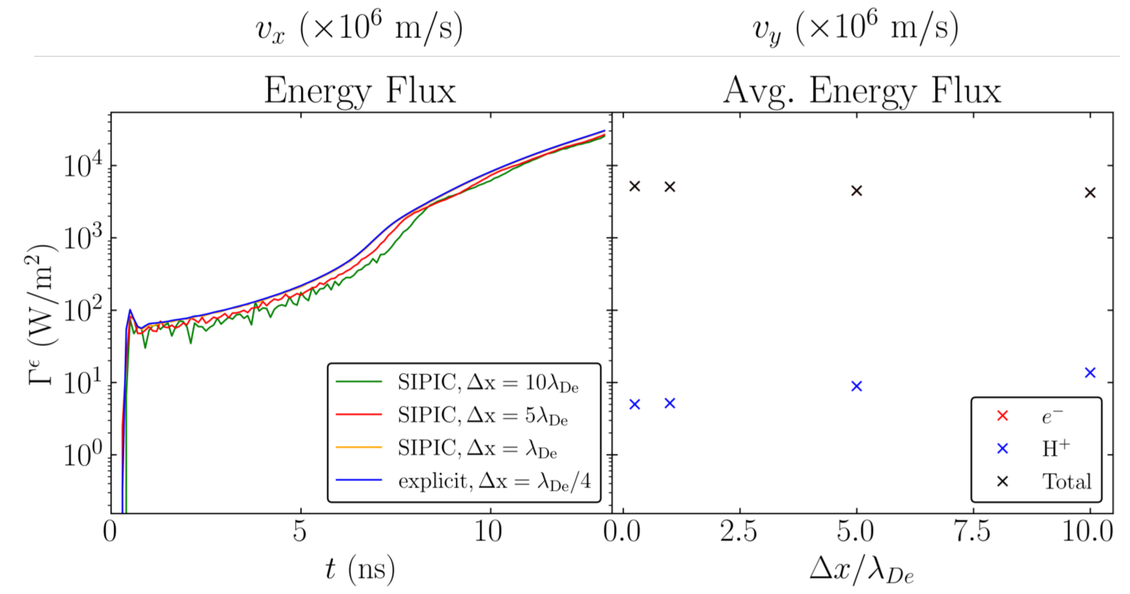


- SIPIC captures growth rate when using the same numerical parameters
  - Much more noisy intrinsically for this problem
  - Can 'refine away' issues
    - element size has biggest effect
- Reason for intrinsic noise is TBD
  - $T_e = 0$ K → $|\boldsymbol{u}_e| > v_{the}$, so FGI may play a role here?

Electron Sheath

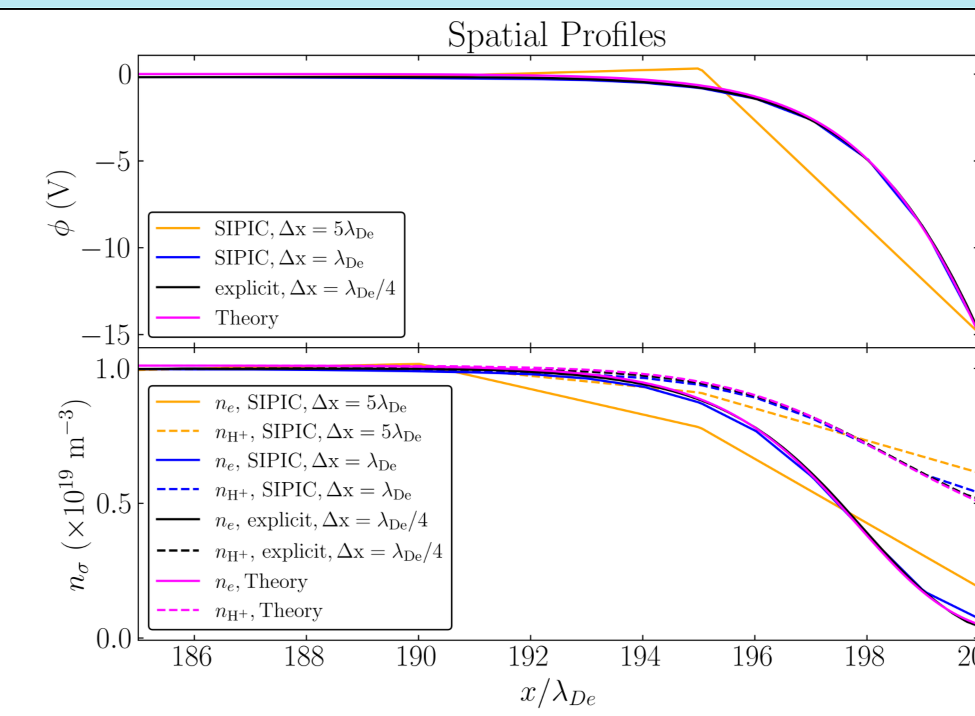


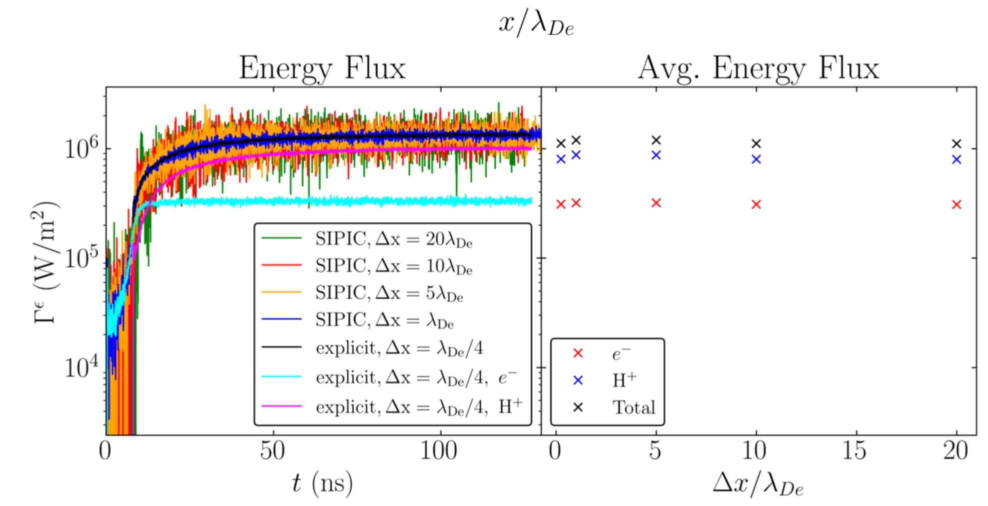




- Explicit PIC is extremely expensive ($\Delta t = 0.2$ ps, $\Delta x = 1.3\ \mu$m)
  - Reached only $\tau_{sim} \sim 13$ ns on 2400 cores in 48 hours
  - SIPIC runs require a fraction of this computational cost
- Energy fluxes and EVDFs are comparable between explicit and SIPIC models regardless of element size ($\Delta x^{\mathrm{SI}} = [\lambda_{De}, 5\,\lambda_{De}, 10\,\lambda_{De}]$)
- Understanding how refinement of N_{ppc} & Δt affect results is WIP

Ion Sheath





- The sheath is poorly resolved spatially as the mesh size increases
  - Mesh refinement near electrodes might be beneficial in real problems
- Energy fluxes are comparable with explicit PIC and SIPIC despite poor resolution of the sheath
- Potential drop from plasma-bulk to wall is the same

Conclusion

Aleph's SIPIC model stretches the Debye length (and/or contracts ω_p)

- Allows for $\Delta t > \omega_{pe}^{-1}$ and $\Delta x > \lambda_{De}$
- Accurately models dense plasmas at a fraction of the computational cost

Regardless of element size, for (electron/ion) sheaths SIPIC shows

- Good agreement of EVDFs near biased electrodes with PIC
- Good agreement of energy fluxes to walls/electrodes

For the cold e-e two-stream instability

- SIPIC captures the growth rate
- Need to refine mesh is troublesome, but may be related to FGI in energy-conserving PIC schemes
- SIPIC may benefit from noise-reducing techniques (C1 elements, time-filtering, etc.)

References

1. Barnes, D. C, "Improved C^1 shape functions for simplex meshes," J. of Comp. Phys., **424** (2021), 109852.
2. Barnes, D. C. and Chacon, L., "Finite spatial-grid effects on energy-conserving particle-in-cell methods," Comp. Phys. Comm. **258** (2021), 107560.
3. Eckert, Z. et al., "Aleph: Highly Scalable Dynamically Load Balanced Unstructured PIC-DSMC Low Temperature Plasma Code," unpublished.

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