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GPU-Accelerated, Energy-Conserving Full and Hybrid PIC Simulations for Space and Astrophysical Plasmas

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Full and hybrid particle-in-cell (PIC) simulations are powerful tools for exploring the kinetic-scale dynamics of space and astrophysical plasmas, including phenomena such as wave–particle interactions, kinetic instabilities, and magnetic reconnection. Full PIC simulations provide a first-principles description of both ions and electrons as particles, offering detailed insight into microscopic plasma processes. Hybrid PIC models, in contrast, treat ions kinetically while modeling electrons as a fluid, significantly reducing computational cost while retaining key ion-scale physics. Together, these approaches enable the study of a wide range of plasma regimes, from fully kinetic to fluid-kinetic hybrid systems.

Despite their strengths, conventional PIC and hybrid codes often suffer from the accumulation of numerical errors in the conservation of local charge and total energy during long-term or large-scale simulations. These errors can distort physical results and limit the predictive power of the simulations. To address this challenge, we introduce Full EPIC-GOD and Hybrid EPIC-GOD, two novel GPU-accelerated PIC codes that enforce strict conservation of local charge and total energy—properties often neglected in existing implementations.

Both codes employ a fully implicit algorithm involving nonlinear iteration between particle motion and field updates. Instead of the commonly used Jacobian-Free Newton–Krylov (JFNK) method in implicit PIC simulations, we adopt a more straightforward iterative predictor–corrector scheme based on simple Picard iteration. While JFNK offers better stability for stiff systems, it is computationally complex and difficult to implement. Our Picard-based method achieves rapid convergence while maintaining low algorithmic complexity, and potential convergence issues are mitigated using adaptive time stepping, which dynamically adjusts the time step to maintain a nearly constant iteration count. This adaptive approach enhances robustness while keeping the implementation clean and efficient.

Additionally, we introduce a novel energy-conserving interpolation scheme for evaluating the Lorentz force on particles. Unlike many conventional approaches that require sub-cycling or orbit-averaging to maintain energy conservation when particles cross cell boundaries, our method uses a synchronized global time step and a single iterative loop. This eliminates the need to store intermediate particle states and achieves accurate energy conservation with computational cost comparable to explicit schemes.

We validate both codes through a comprehensive set of test problems—including plasma waves, kinetic instabilities, collisionless shocks, and magnetic reconnection—demonstrating excellent agreement with analytic and benchmark results. Optimized with OpenACC for multi-GPU platforms, both codes show substantial performance gains over CPU-only implementations, enabling large-scale, long-duration simulations with high physical fidelity.

By combining exact conservation properties with high computational efficiency and scalability, Full EPIC-GOD and Hybrid EPIC-GOD provide a reliable and versatile simulation framework for advancing our understanding of collisionless plasma phenomena in heliospheric, planetary, and astrophysical environments.

References

[1] Kim, S. et al., Computer Physics Communications, 315, 109726 (2025)