

Scalable Arbitrary-Order Pseudo-Spectral Electromagnetic Solver

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Abstract— Numerical simulations have been critical in the recent rapid developments of advanced accelerator concepts. Among the various available numerical techniques, the Particle-In-Cell (PIC) approach is the method of choice for self-consistent simulations from first principles, and although the fundamentals of the PIC method were established decades ago, improvements or variations still continue to arise nearly continuously. While spectral methods have been popular in the early PIC codes, the finite-difference time-domain method has become dominant. Recently, a novel parallelization strategy was proposed that takes advantage of the local nature of Maxwell equations that has the potential to combine spectral accuracy with finite-difference favorable parallel scaling. Due to its compute-intensive nature combined with adjustable accuracy and locality, the new solver promises to be especially well suited for emerging exascale systems. The new solver was recently extended to enable user-programmability of the spatial and temporal order of accuracy at runtime, enabling a level of scalability and flexibility that is unprecedented for such codes.

Keywords— *High-Performance Computing, Particle-in-Cell Codes, Pseudo-Spectral Solver, Maxwell Equations Solver, Computational Scalability, Exascale Computing.*

I. INTRODUCTION

The accepted methods for self-consistent modeling of beams and plasma are based on Particle-in-Cell (PIC) formulations that provide the natural mapping of plasma interactions to a computational resource and are used with great success in various regimes. The standard formulation uses finite differences in both space and time (FDTD) of Maxwell's or other relevant equations and for certain traditional problems these methods scale very well to 100K processors or more. Fields on a staggered grid are used, giving second order accuracy. However discretization errors in current techniques perturb the representation of a very high quality particle beam required for advanced design.

A novel method for the parallelization of electromagnetic Pseudo-Spectral Analytical Time Domain (PSATD) solvers [3] has been proposed and prototyped [4], opening the way for our family of solvers that combine the favorable parallel scaling of

standard FDTD methods with the accuracy and stability advantages of pseudo-spectral methods. The new solver and parallelization schemes take advantage of the properties of FFTs and Maxwell's equations (i.e. the finite speed of light), to allow the use of local FFTs while limiting communications of data within guard regions between neighboring computational subdomains. The PSATD solver also relaxes constraints on time step, particle shape factor, and digital filtering, reducing compute time by producing stable simulations for parameters where FDTD fails. The new solver is named PSAOTD for "Pseudo-Spectral Arbitrary-Order Time-Domain". At the limit of spatial derivative of infinite order, the PSAOTD is equivalent to the PSATD solver.

To demonstrate the effectiveness of this solver, we have implemented a 2D PSAOTD solver in the PIC framework Warp [5], which also has a conventional FDTD solver. Figures 1 and 2 illustrates the respective properties of the FDTD and PSAOTD solvers, and parallelization potential using an expanding electromagnetic unit pulse that physically produces a sharp circular wave front. Numerical dispersion in the FDTD solver produces unphysical ripples propagating anisotropically at subluminal velocity even at the Courant timestep where dispersion is best. The PSATD solver does not exhibit numerical dispersion, producing the correct behavior regardless of time step.

In this poster, we highlight a scalable algorithm that mitigates significant unphysical effects from discretization errors. Traditionally, such a move would compromise the scalability of the PIC method and render the calculation intractable with required accuracy and spatial resolution. The key to our approach is the use of our new solver to take advantage of multilevel parallelism in emerging systems by naturally subdividing the computational domain and workload in a way that is optimally assigned to the heterogeneous computational resources.

Our PSAOTD implementation presented here tackles the bottlenecks normally associated with traditional FFT (fully spectral) solvers. In fact, our research involves an error analysis and better understanding of the performance tradeoff between domain decomposability, the solver’s robustness and accuracy, and code scalability.

The PSATD solver is currently running in a variety of computational platforms. In this poster, we will present our latest scalable performance results obtained on a CRAY XC30, Hopper, at the National Energy Research Scientific Computing Center (NERSC). The PSATD will be used at the production level in 2D and 3D, and applied to significant DOE mission relevant applications including free electron lasers, coherent synchrotron radiation and laser plasma acceleration. Comparisons to FDTD solvers already in Warp will quantify both the improved scalability and the improved accuracy.

II. GREATER IMPACT

Our scalable arbitrary-order pseudo-spectral electromagnetic solver has the potential to improve substantially the accuracy and efficiency (in FLOPS and Joules) of most electromagnetic plasma simulations and hence to enable simulations, not otherwise possible, which are required in areas like experimental and space plasmas (e.g. space weather), as well as fusion devices. Our future research agenda will include an on-line autotuner for the PSATD solver to provide performance portability and adaptability in future exascale systems.

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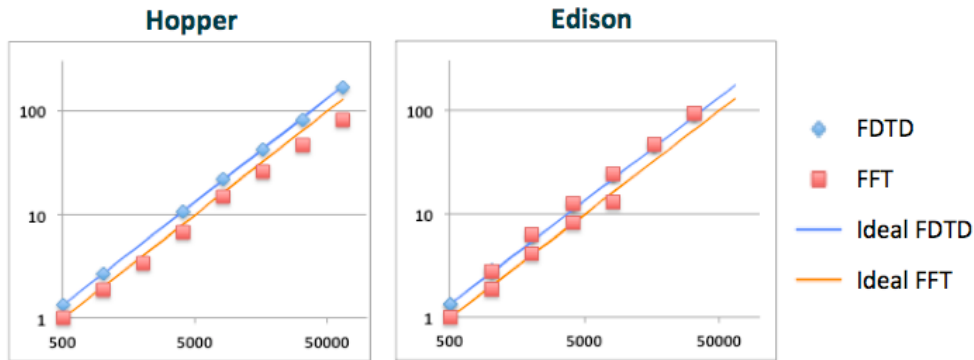


Figure 1: Strong scaling of Warp’s spectral PIC solver on a test problem of a 4,096x4,096 2-D plasma with periodic boundary conditions and 64 macroparticles/cell on NERSC’s Hopper and Edison supercomputers , number of cores is shown on the x-axis.

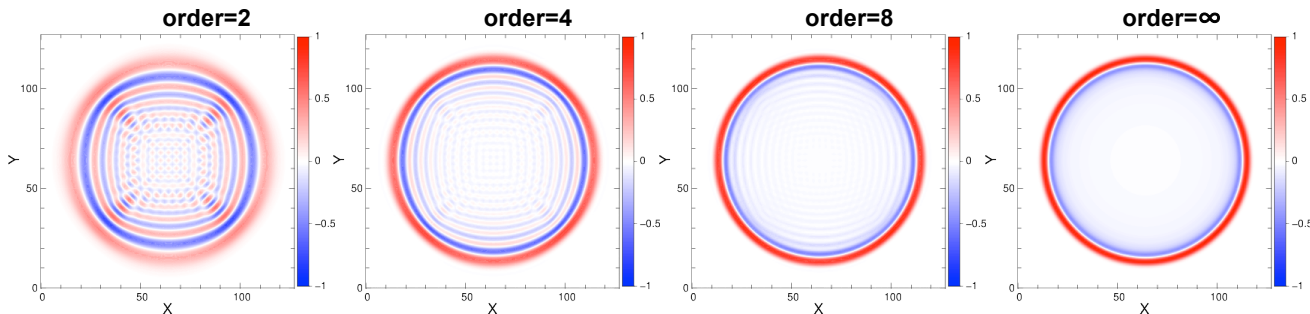


Figure 2: Snapshots from an expanding electromagnetic unit pulse on a 128x128 grid, using the PSAOTD solver with the order of accuracy set to respectively 2, 4, 8 and infinity. The latter setting is equivalent to using the PSATD solver. For all, the time step was set to $\Delta t = 50\Delta x = 1000\delta t$. Spurious effects due to inaccuracy are reduced as the order is increased.