

GPU-ACCELERATED 3D TIME-DOMAIN SIMULATION OF RF FIELDS AND PARTICLE INTERACTIONS*

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Abstract

The numerical simulation of electromagnetic fields and particle interactions in accelerator components can consume considerable computational resources. By performing the same computation on fast, highly parallel GPU hardware instead of conventional CPUs it is possible to achieve a 20x reduction in simulation time for the traditional 3D FDTD algorithm. For structures that are small compared to the RF wavelength, or that require fine grids to resolve, the FDTD technique is constrained by the Courant condition to use very small time steps compared to the RF period. To avoid this constraint we have implemented an implicit, complex-envelope 3D ADI-FDTD algorithm for the GPU and demonstrate a further 5x reduction in simulation time, now two orders of magnitude faster than conventional FDTD codes. Recently, a GPU-based particle interaction model has been introduced, for which results are reported. These algorithms form the basis of a new code, NEPTUNE, being developed to perform self-consistent 3D nonlinear simulations of vacuum electron devices.

INTRODUCTION

Existing approaches to 3D simulation of vacuum electronic rf drivers for accelerators typically rely on particle-in-cell (PIC) methods based on the finite-difference time-domain (FDTD) algorithm. Present implementations target parallel execution on multi-core CPUs or CPU clusters to achieve acceptable performance, yet simulations commonly take many hours to complete. In this paper we describe results from a new code, NEPTUNE, under development at the Naval Research Laboratory. The new code achieves two orders of magnitude improvement in electromagnetic simulation performance by combining an improved algorithm with an implementation using high performance GPU hardware. Particle beam simulation algorithms for the GPU are presently under development.

A limitation of the FDTD technique when applied to slow-wave vacuum electron devices is due to the Courant condition. For the simple case of a 3D grid of cells of uniform size, this condition may be expressed as $c\Delta t < h/\sqrt{3}$ where h is the cell size in each direction, and Δt is the integration time step. Structure dimensions are typically small compared to the rf wavelength, which requires that the FDTD grid use small cells to resolve the geometry, therefore $h \ll \lambda$. Consequently, due to the Courant limit,

the time step that must be employed is correspondingly small, often needing a minimum of 100 time steps to solve for each rf period. To alleviate this problem, we use an implicit ADI-FDTD algorithm [1, 2] to solve for the fields represented in complex envelope form. While this takes additional computation per time step, this is more than compensated by the increase in time step size that may be used.

3D FDTD ALGORITHM

The basic time-stepping FDTD algorithm on the conventional Yee grid can be written in a very simple form

$$E_x^{n+1/2} = E_x^{n-1/2} + \frac{\Delta t}{\epsilon_x} [\delta_y H_z^n - \delta_z H_y^n - J_x^n] \quad (1)$$

$$H_x^{n+1} = H_x^n + \frac{\Delta t}{\mu_x} [\delta_z E_y^{n+1/2} - \delta_y E_z^{n+1/2}] \quad (2)$$

where superscripts denote the time step and centered difference operators with respect to the coordinates are defined for a discrete field f^n as

$$(\delta_y f)_{(i,j,k)}^n = \frac{f_{(i,j+1/2,k)}^n - f_{(i,j-1/2,k)}^n}{y_{j+1/2} - y_{j-1/2}} \quad \text{etc.} \quad (3)$$

Field quantities have subscripts to denote the spatial location in grid cells. Electric fields are stored on cell edges and offset by a half time step,

$$E_{x(i+1/2,j,k)}^{n+1/2} \quad E_{y(i,j+1/2,k)}^{n+1/2} \quad E_{z(i,j,k+1/2)}^{n+1/2},$$

while magnetic fields are associated with cell faces,

$$H_{x(i,j+1/2,k+1/2)}^n \quad H_{y(i+1/2,j,k+1/2)}^n \quad H_{z(i+1/2,j+1/2,k)}^n.$$

In our implementation, we use Finite Integration Theory to support both dielectric and permeable materials, and non-uniform grids. The time-advance formulas are simple and provide a good test for the performance of GPUs.

The present implementation uses C++ with Nvidia's CUDA toolkit (www.nvidia.com/cuda) to perform the core computations on compatible graphics hardware. High-level operations, including geometry definition and control of the time-loop are implemented in Lua (www.lua.org) providing full scripting capability. The following example simulation demonstrates the effectiveness of the approach.

We modeled a 3D photonic bandgap cavity, based on the MIT design [3]. A periodic array of cylindrical metal rods creates a stopband, preventing propagation of TM radiation. Removal of a single rod at the center creates a defect that can confine a resonant mode, while removing additional rods allows coupling to the external waveguide.

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The model is represented using an approximately uniform grid, $268 \times 34 \times 334$, with over 3 million cells. For this model, the Courant condition limits the time step for FDTD simulation to $c\Delta t \approx 0.006\lambda$. For the simulation we excite the structure via the waveguide, ramping the input signal smoothly over the first 100 rf periods to limit the signal bandwidth. The simulation is continued for an additional 100 rf periods to ensure a steady state is reached. Figure 1 shows the field excited after 200 rf periods computed by FDTD.

Running on a Nvidia GTX 480 graphics card this simulation took 94.6s, completing 33417 time steps. This represents a raw performance metric of $1076 \text{ Mcells} \times \text{steps/s}$, or effectively less than 1ns per time step per cell. A more meaningful performance metric is $6.4 \text{ Mcells} \times \text{periods/s}$. i.e. one second of computation can advance fields on a grid of 3×10^6 cells by just over 2 rf periods. This represents more than an order of magnitude improvement compared to an equivalent single-CPU simulation.

3D CE-ADI-FDTD ALGORITHM

In order to circumvent the restriction in time step due to the Courant condition, we chose to use the ADI-FDTD algorithm [4]. This algorithm solves tridiagonal equations to advance the electric fields implicitly by a half time step, followed by an explicit magnetic field half-step. The second half time-step proceeds similarly. From this scheme we derived two new schemes. First, a leapfrog variant [1] that solves tridiagonal equations for both electric and magnetic fields, but advancing by a full time step each time; second, a hybrid scheme [2] that requires tridiagonal solution only for the electric field updates as in the original scheme, but by full time-steps in a leapfrog scheme, using a simplified form of the equations. This second scheme is used here.

The hybrid scheme starts from a set of initial complex envelope fields $E_{x,y,z}^{n-1/2}$, $\hat{E}_{x,y,z}^n$, $H_{x,y,z}^n$, and advances them according to the following set of equations, where $\theta \equiv \omega\Delta t/4$ characterizes the center frequency of the envelope representation,

$$\begin{aligned} & \left[(1 - i\theta)^2 - \left(\frac{\Delta t}{2} \right)^2 \epsilon^{-1} \delta_y \mu^{-1} \delta_y \right] \Delta E_x^n \\ & = \frac{\Delta t}{\epsilon} [\delta_y H_z^n - \delta_z H_y^n] + 4i\theta E_x^{n-1/2} \end{aligned}$$

$$H_z^{n+1/2} = \frac{1 + i\theta}{1 - i\theta} H_z^n + \frac{\Delta t}{2\mu(1 - i\theta)} [\delta_y E_x^{n+1/2} - \delta_x \hat{E}_y^n]$$

$$\begin{aligned} & \left[(1 - i\theta)^2 - \left(\frac{\Delta t}{2} \right)^2 \epsilon^{-1} \delta_z \mu^{-1} \delta_z \right] \Delta \hat{E}_x^{n+1/2} \\ & = \frac{\Delta t}{\epsilon} [\delta_y H_z^{n+1/2} - \delta_z H_y^{n+1/2}] + 4i\theta \hat{E}_x^n \end{aligned}$$

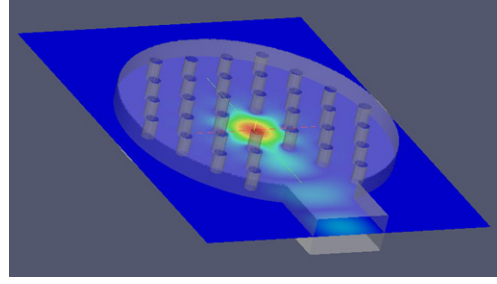


Figure 1: Converged FDTD field solution for a 3D photonic bandgap cavity excited via a waveguide.

$$\begin{aligned} H_y^{n+1} & = \frac{1 + i\theta}{1 - i\theta} H_y^{n+1/2} \\ & + \frac{\Delta t}{2\mu(1 - i\theta)} [\delta_x E_z^{n+1/2} - \delta_z \hat{E}_x^{n+1}] \end{aligned}$$

where we solve systems of equations for the change in the complex amplitudes of the electric fields, defined by

$$\begin{aligned} \Delta E_x^n & \equiv E_x^{n+1/2} - E_x^{n-1/2} \\ \Delta \hat{E}_x^{n+1/2} & \equiv \hat{E}_x^{n+1} - \hat{E}_x^n. \end{aligned}$$

The operators that must be inverted are tridiagonal due to the discrete second derivative terms, and are solved in practice using the dual-sweep Thomas algorithm.

Implementing the tridiagonal matrix algorithm for the GPU proved challenging. Each tridiagonal solution progresses in a direction through the grid aligned with one of the three coordinate axes, so that a two-dimensional array of these solutions can be implemented independently in parallel. In a naive implementation, a single GPU thread is assigned to perform each tridiagonal solve in isolation, and the implementation follows the serial case. This proved sufficient for two of the coordinate directions, however in the third direction each solve must operate on a contiguous region of GPU memory, known to give poor performance due to constraints in the GPU memory model. Solution time was almost a factor of ten greater in this direction. We therefore modified the tridiagonal algorithm to operate cooperatively with parallel threads to ensure that memory accesses were properly coalesced, and achieved performance within a factor of two of the other two directions.

We applied the CE-ADI-FDTD algorithm to the same cavity example as before, only now our time step is not constrained by the Courant condition. Also, since we are solving only the envelope field, it is also not necessary to finely resolve the rf period, and we found that the time step could be increased to on the order of the rf period while capturing the time-evolution of the transient.

Figure 2 shows a sequence of solutions as the distance between the two metal rods that form the coupling aperture is varied. Fields are normalized in each case to the central cavity peak field, so that the relative magnitude of the cavity field and the waveguide fields is apparent. In the high-Q case, where the rods are closer together, the standing wave

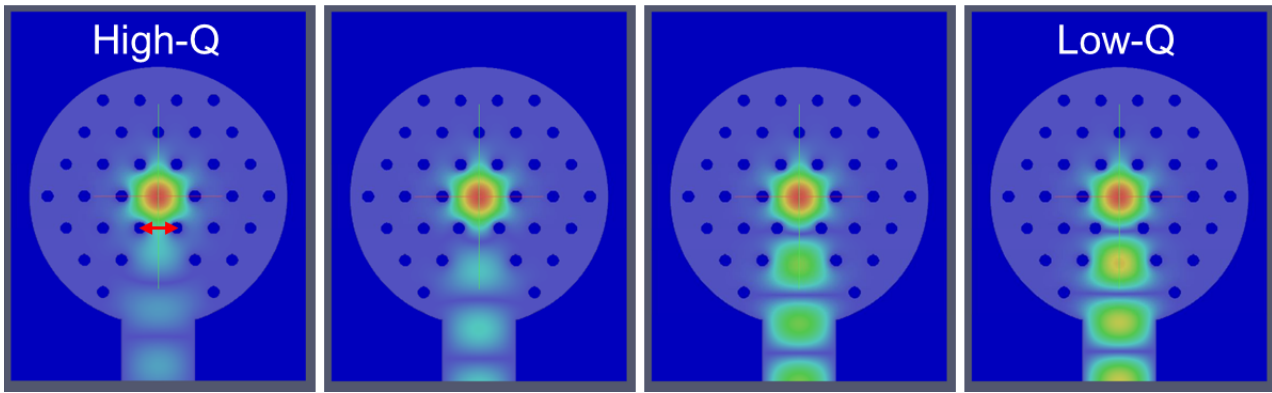


Figure 2: Simulations of "MIT" cavity using the 3D CE-ADI-FDTD algorithm, as size of the coupling aperture is varied.

field in the waveguide is much smaller than in the low-Q case, for the same peak cavity field.

For a time step $c\Delta t = 0.25\lambda$, simulation using the CE-ADI-FDTD method took 32.3s to complete 800 time steps, while for $c\Delta t = \lambda$, the same simulation took just 8.3s (200 steps). While this gives a raw performance of only 73.6 Mcells \times steps/s, due to the extra computation for each implicit time step, it corresponds to a simulation rate of 73.6 Mcells \times periods/s. i.e. one second of computation can advance fields on a grid of 3×10^6 cells by over 24 rf periods, an order of magnitude faster than the equivalent FDTD simulation.

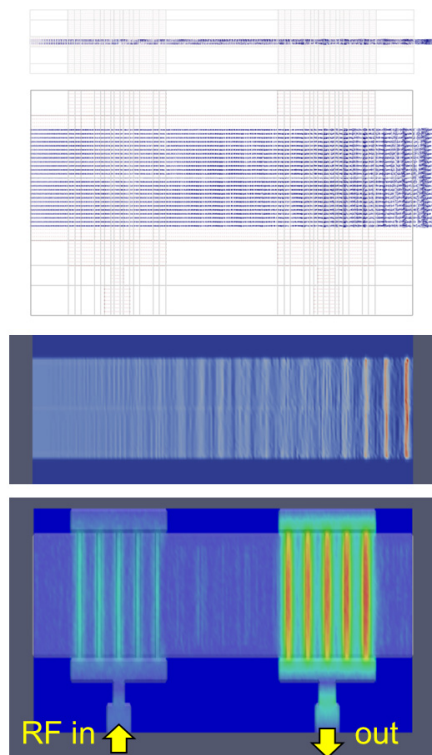


Figure 3: Example of particle simulation

PARTICLE SIMULATION

We have recently implemented a full particle-in-cell algorithm, coupled self-consistently with the FDTD algorithm. Figure 3 displays results of a simulation of a two-cavity sheet-beam extended interaction klystron (EIK), showing side and plan views of the particles, and plan views of the longitudinal current and rf field respectively. The model is discretized using 525,000 cells, and the simulation was run with around 190,000 particles for 2000 rf periods, with $c\Delta t = 0.0075\lambda$ (267,000 time steps). The full simulation took 15 minutes, with approximately 6 minutes for the fields and 9 minutes for the particles, effectively 10ns per particle push.

CONCLUSION

The high performance achievable using low-cost GPU hardware for the simulation of accelerator structures and vacuum electronic devices has been demonstrated. Self-consistent interaction of fields with a particle beam, implemented on the GPU, holds promise for further research.

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