

Advanced software packages for beam dynamics simulation *

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Abstract: We are developing highly scalable and systematic software packages for beam dynamics simulations. Both traditional Particle-In-Cell (PIC) methods and advanced direct VLASOV methods have been adopted. For the PIC method, particles are distributed evenly on different processors and space charge effects are included by solving Poisson's equation on a finite mesh. Several Poisson solvers have been developed using Fourier, hp-Finite Element (hp-FEM) and wavelet methods. These solvers can be used in Cartesian and Cylindrical coordinate systems, hp-FEM based solvers can be used on both structured and unstructured meshes. Domain decomposition (DD) has been used to parallelize these solvers and all these solvers have been implemented into the PTRACK code. PTRACK is now widely used for large scale beam dynamics simulations in linear accelerators. For the direct VLASOV method, Semi-LAGRANGE and discontinuous GALERKIN methods scheme have been employed to solve VLASOV equation directly in 1P1V and 2P2V phase spaces. They all use the time splitting scheme proposed by Cheng and Norr. Simulation results will be presented and challenges will be discussed.

1. Introduction

Plasma and charged beams are of great importance in modern science and technology. The research in this field is relying more and more on simulations. Simulating plasma and charged beams has three different methods: microscopic model, kinetic model and fluid model. In the microscopic model, each charged particle is described by 6 variables (x, y, z, v_x, v_y, v_z). Therefore, for N particles, there are $6N$ variables in total. This requires solving the VLASOV equation in $6N$ dimensions, which exceeds the capability of current supercomputers for large N . On the other end is the fluid model which is the simplest model, because it treats the plasma as a conducting fluid with electromagnetic forces exerted on it. This leads to solving the Magneto-hydrodynamics (MHD) equations in 3D (x, y and z). MHD solves for the average quantities, such as density and charge, which makes it difficult to describe the fine structure in the plasma. Between these two models is the kinetic model, which solves for the charge density function by solving the BOLTZMANN or VLASOV equations in 6 dimensions (x, y, z, v_x, v_y, v_z). The VLASOV equation describes the evolution of a system of particles under the effects of self-consistent electromagnetic fields. The model been used in current beam dynamics simulations is the kinetic model. There are two different ways to solve it. The dominant one is the so called Particle-In-Cell (PIC) method, which utilizes the motion of the particles along the characteristics of the VLASOV equation using a Lagrange-Euler approach [1,2]. The PIC method has the advantages of

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speed and easy implementation, but similar to MHD, it is hard to capture the fine structures in the plasma. Furthermore, there is noise associated with the finite number of particles in the simulations. With petascale computing, one-to-one simulation can be realized for 10^9 particles. But for more intense beams, PIC method still uses macro particles. The other way to solve the kinetic model is to solve the VLASOV equation directly. But the challenge is the high dimensions. For example, in order to simulate a beam in 3D, VLASOV equation has to be solved in 6D. This clearly needs peta-scale computing, and peta-scalable algorithms are critical to the success. During the past 5 years, we have developed several software packages to meet these demands. This paper presents our efforts on developing peta-scalable algorithms to simulate charged beams in linear accelerators.

2. Parallel Poisson Solvers

In both PIC and VLASOV approaches, Poisson's equation has to be solved in 2D or 3D to account for the space charge effect. In designing peta-scalable algorithms, it is usually the most challenging part. Therefore, we present our work on this first. Several different methods have been adopted and are given in following:

$$\phi(x, y, z, t) = \sum_{m=-M/2}^{M/2-1} \sum_{p=-P/2}^{P/2-1} \sum_{n=-N/2}^{N/2-1} \phi(m, p, n, t) e^{-icm x} e^{-i\beta p y} e^{-i\gamma n z}$$

2.1. Fourier Method

This is the most standard method for solving the Poisson's equation in box region with Cartesian coordinate system. The potential has been expanded in Fourier series in all three directions. Periodic and Dirichlet zero boundary conditions have been applied in all three directions. Three different domain decomposition methods have been implemented as shown in Figure 1. Using model C, it is easy to use tens of thousands of processors with relatively small grid for space charge calculation. For example, solving the Poisson's equation on 32^3 mesh can use 32 thousands processors with model C, while only one thousand with model B and 32 processors with model A. This makes it possible to use small mesh for the space charge calculation. Since relatively small grid can be used for space charge calculation, good scaling has been obtained and can be found in [3,4].

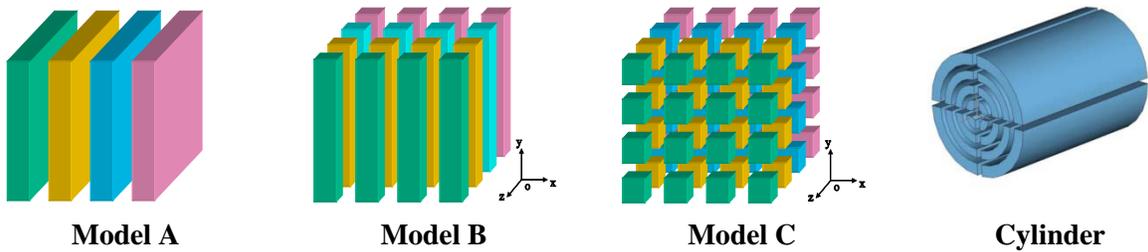


Figure 1. Domain decomposition method for solving Poisson's equation in Cartesian (1, 2 and 3) and Cylinder (4) coordinate systems.

2.2. Fourier Hp-Finite Element Method

This solver is developed for cylindrical coordinate system. The potential is expanded in Fourier series in the axial and circumferential directions, while it uses hp-finite element expansion in the radial direction.

$$\phi(x, y, z, t) = \sum_{m=-M/2}^{M/2-1} \sum_{n=-N/2}^{N/2-1} \sum_{p=0}^P \phi(m, p, n, t) e^{-icm x} e^{-i\beta n z} P_p(y)$$

$$P_p(y) = \begin{cases} \left(\frac{1-y}{2}\right) & p=0 \\ \left(\frac{1-y}{2}\right)\left(\frac{1+y}{2}\right)P_{p-1}^{1,1}(y) & 0 < p < P \\ \left(\frac{1+y}{2}\right) & p=P \end{cases}$$

Domain decomposition in the radial and circumferential directions has been implemented as shown in Figure 1(4). Periodic B.C. has been applied in the axial and circumferential directions and zero Dirichlet B.C. have been applied in the cylinder wall. Detailed method and benchmark results can be found in [2].

2.3. Hp-Finite Element Method on Structured Grid

The hp-Finite Element Method (hp-FEM), originated in the 1940's [6,7,8], has been applied in many different areas. In our VLASOV solvers, a parallel Poisson solver based on hp-FEM on structured grid has been constructed. 2D bases have been shown on the left of the Figure 2(1). The 2D structured mesh is shown in Figure 2(2). Continuous Galerkin (CG) method has been used and zero Dirichlet B.C. has been imposed. The potential distribution is shown in Figure 2(3). Due to the memory limitation, only the iterative solver can be used for solving boundary modes of the 2D Poisson's equation when the mesh is large. Interior modes in each element have been solved directly according to the Shur complement. The discrete system of Poisson's equation can be written as: (b and i correspond to boundary and interior variables)

$$\begin{aligned} (A_{bb} - C_{bi}A_{ii}^{-1}C_{bi}^T)u_b &= f_b - C_{bi}A_{ii}^{-1}f_i \\ u_i &= A_{ii}^{-1}(f_i - C_{bi}^T u_b) \end{aligned} \quad \begin{pmatrix} A_{bb} & C_{bi} \\ C_{bi}^T & A_{ii} \end{pmatrix} \begin{pmatrix} u_b \\ u_i \end{pmatrix} = \begin{pmatrix} f_b \\ f_i \end{pmatrix}$$

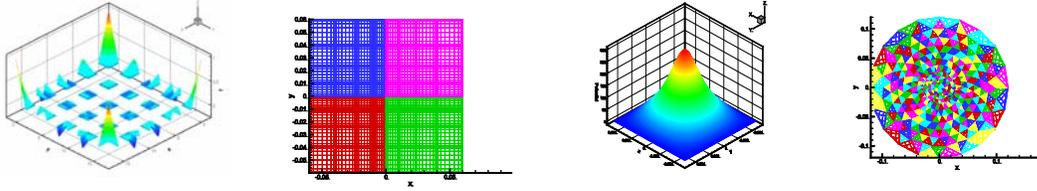


Figure 2. Convergence history with/without preconditioning (left), wavelet coefficients (middle) and 2D structured grid (right).

2.4. Hp-Finite Element Method on Unstructured Grid

In order to solve Poisson's equation in complex geometries, a parallel Poisson solver using hp-FEM on an unstructured grid has been developed recently. Since finite element method (FEM) can handle complex geometry easily, and spectral method can achieve high order accuracy. Combine these two, hp-FEM can handle the complex geometry and also achieve high order accuracy at the same time. The 2D unstructured mesh is shown in Figure 2(4).

The potential can be expressed as

$$f(r, s) = \sum_{i+j \leq p} \psi_{ij}(r, s) \hat{f}_{ij}$$

The continuous Galerkin formula for solving the Poisson's equation is

$$\begin{aligned} \int_V f \cdot \varphi dv &= \int_V \nabla^2 u \cdot \varphi dv \\ &= \int_V [\nabla(\nabla u \varphi) - \nabla u \cdot \nabla \varphi] dv \\ &= \int_{\partial V} \vec{n} \cdot (\nabla u \varphi) dS - \int_V \nabla u \cdot \nabla \varphi dv \\ \int_V \nabla u \cdot \nabla \varphi dv &= \int_{\partial V} \vec{n} \cdot (\nabla u \varphi) dS - \int_V f \cdot \varphi dv \\ \int_{\partial V} \vec{n} \cdot (\nabla u \varphi) dS &= \int_{\partial V} (n_x \varphi \frac{\partial u}{\partial x} + n_y \varphi \frac{\partial u}{\partial y}) dS \end{aligned}$$

3. Beam Dynamics Simulation With PIC Method

In the last several years, we have developed a parallel PIC solver based on the serial version of TRACK, which was developed in the physics division at ANL. Particles have been distributed evenly over all processors, and parallel Poisson solvers described above have been used for the space charge effect. Parallel algorithm and detailed benchmark results can be found in [2,3,4]. As small mesh can be used for calculating space charge effect, PTRACK has achieved good scaling. Recently PTRACK has been used for end-to-end simulation of full LINAC system. It can also be used for one-to-one simulation for some beams such as that in FNAL proton driver. Totally 865M charged particles have been simulated from 50 keV to 2.5 MeV in 325 MHz radio frequency quadrupole of a proton driver at FNAL. Figure 3 shows the comparison of contour in $(\phi, \Delta W/W)$ plane with 1M, 10M, 100M and 865M particles. As can be seen, using large number of particles provides much more accurate information and this is useful to the accelerator design and optimizations. Now PTRACK is being used as workhorse for large scale optimizations.

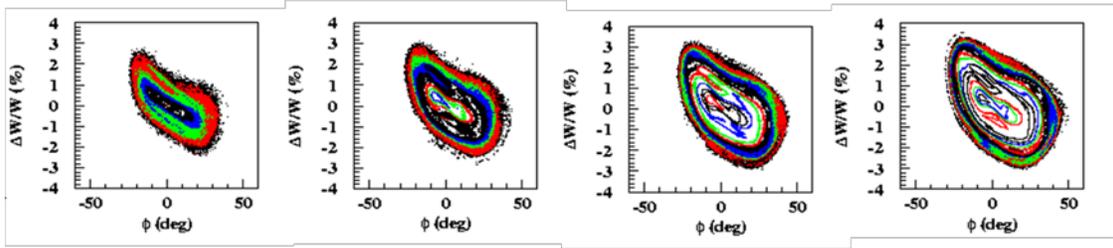


Figure 3. $(\phi, \Delta W/W)$ plane contour with 1M(1), 10M(2), 100M(3) and 865M(4) particles.

4. Beam Dynamics Simulation By Direct Solving Vlasov Equation

In order to overcome the shortcoming of the PIC solvers, we have developed direct VLASOV solvers. The distribution function $f(\vec{x}, \vec{v}, t)$ in phase space is governed by the VLASOV equation.

VLASOV equation in 1P1V phase space

$$\frac{\partial f(x, v, t)}{\partial t} + v(x, t) \frac{\partial f(x, v, t)}{\partial x} + E(x, t) \frac{\partial f(x, v, t)}{\partial v} = 0, \quad E(x, t) = -\frac{\partial \phi(x, t)}{\partial x}, \quad -\Delta \phi(x, t) = \frac{\partial E(x, t)}{\partial x} = \rho(x, t) - 1$$

4.1. VLASOV Equation in 2P2V Phase Space

$$\frac{\partial f}{\partial z} + \frac{\vec{v}}{v_b} \cdot \nabla_{\vec{x}} f + \frac{q}{\gamma_b m v_b} \left(-\frac{1}{\gamma_b^2} \nabla \Phi^s + \vec{E}^e + (\vec{v}, v_b)^T \times \vec{B}^e \right) \cdot \nabla_{\vec{v}} f = 0, \quad -\Delta_x \Phi^s = \frac{q}{\epsilon_0} \int_{R^2} f(z, \vec{x}, \vec{v}) d\vec{v}$$

where Φ^s is the self-consistent electric potential due to charges. \vec{E}^e and \vec{B}^e are external electric and magnetic fields. v_b is the reference beam velocity.

4.2. Numerical Algorithm

The Semi-Lagrangian Method (SLM) [9] has been used for time integration. A plot explains the idea is shown on the left of Figure 4(1). The time splitting scheme has been used for time integration as proposed by Cheng and Knorr [10]. 4D domain decomposition has been adopted as shown in Figure 4(2).

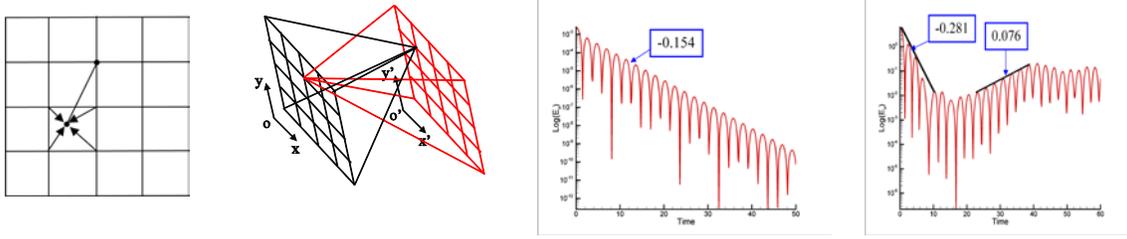


Figure 4. Semi-Lagrange Scheme (1), 4D domain decomposition (2), Linear Landau Damping (3), Strong Landau Damping (4).

4.3. Benchmarks and Simulation Results

The code comprises two major parts: interpolation and space charge (SC) calculation. The SLM performs back tracking and interpolation respectively in the physical and velocity spaces. Each processor has only part of the global mesh for the space charge calculations. The field mesh and space charge mesh are different. This scheme has the advantage of easy implementation and no communication for particle tracking is required. However, this method requires large memory in each processor and intense communication for the parallel Poisson solver.

Figures (3 and 4) in Figure 4 show the time history of $\log(E_x)$ for linear and strong Landau damping. The initial particle distribution function and the related parameters are shown in following:

$$f(0, x, v) = \frac{1}{\sqrt{2\pi}} \exp(-v^2/2)(1 + \alpha \cos(kx)) \quad L = 4\pi, \quad R = [-6, 6], \quad \Delta t = 1/8,$$

$$\forall (x, v) \in [0, L] \times R, \quad \alpha = 0.01, \quad k = 0.5 \quad P = 16, \quad E = 64, \quad 1024 \times 1024 \quad CPU = 256, \quad T \sim 10 \text{ min s}$$

For the linear Landau damping, $\alpha = 0.01$, and for the strong Landau damping, α is 0.5. Clearly they represent different dynamics. The decreasing and increasing rate can be measured and are consistent with theoretical predictions and the work by other researchers.

4.4. 2P2V Simulations

In 2P2V simulations, a proton beam has been simulated through alternating hard edge electric quadrupole channel. The initial emittance is $\varepsilon = 200\pi$ mm mrad, and the energy is $W = 0.2$ MeV. The current of the beam is 0.1 A, and the reference velocity is $v_b = 6.19 \times 10^6$ m/s. The transverse physical space is $[-0.12, 0.12]$ by $[-0.12, 0.12]$, and the velocity space is $[-8 \times 10^5, 8 \times 10^5]$ by $[-8 \times 10^5, 8 \times 10^5]$ m/s. The alternating electric quadrupole field is defined as $\vec{E}^e(x, y, z) = (k_0(z)x, -k_0(z)y)$. Figure 5 compare with PIC simulations, and Figure 6 are contours.

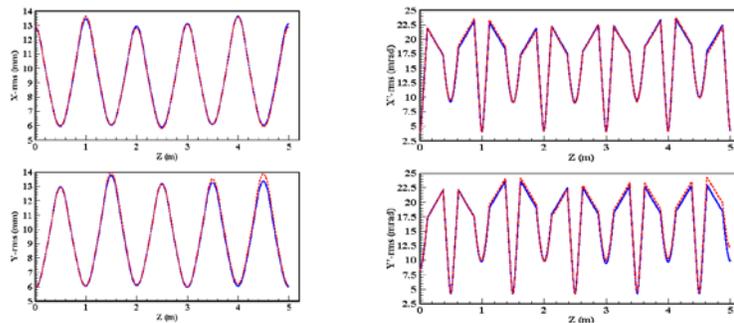


Figure 5. Comparison of TRACK (solid) and VLASOV (dotted) simulations using a Gaussian beam: X_{rms} (left upper), Y_{rms} (lower left), X'_{rms} (upper right), Y'_{rms} (lower right) for a 100 mA proton beam.

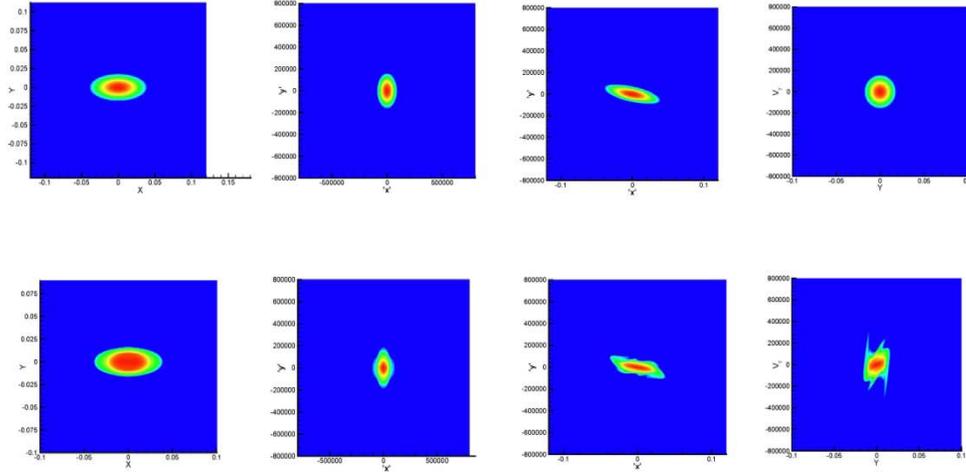


Figure 6. From left to right are contours in the (x, y) , (x, x') , (y, y') and (x', y') planes, from top to bottom correspond to $t=0$ and 3 time period.

5. Summary

This paper presents our researches on developing peta-scalable algorithms for large scale beam dynamics simulations. Both PIC method and direct VLASOV method have been used. Different parallel Poisson solvers have been developed to satisfy the requirement of considering space charge effect in various solvers. Domain decomposition has been adopted for parallelization of the TRACK code. PTRACK has now been used for large scale beam dynamic optimization and real accelerator simulations. These Poisson solvers adopted different numerical techniques in different conditions, such as using Cartesian and Cylindrical coordinate systems, using structure and unstructured grids, etc. Direct VLASOV solvers have been developed for 2D and 4D. A high-order hp-FEM has been used. The advantages and effectiveness of the hp-FEM have been demonstrated. The VLASOV solvers have adopted the Semi-Lagrangian method. Similarly domain decomposition has been used for parallelization of these solvers. Scalable Poisson solvers have been developed with hp-FEM. Linear and strong Landau damping have been studied with direct 2D VLASOV solver, and results clearly captured the physics of these phenomena. Direct 2D VLASOV solver can be applied to study more problems in plasma and charged beams later. Benchmarks of the parallel models have shown good scaling on BlueGene/P at ANL with up to 32k processors. The hp-FEM shows its advantages in these direct VLASOV solvers, such as local interpolation, easy parallelization and long time integration. These developments are encouraging, and more investigation will be done.

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