# SOLVING THE VLASOV EQUATION FOR BEAM DYNAMICS SIMULATION*

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*Abstract*

This paper presents the development of parallel direct Vlasov solvers using the Spectral Element Method (SEM). There are several benefits to the direct method over the standard PIC approach for solving the Vlasov equation, such as avoiding the noise associated with a finite number of particles and the capability to capture the fine structure in the plasma. The most challenging aspect of the direct Vlasov solver is the size of the problem where the computational cost increases as $N^{2d}$, where d is the dimension of the physical space and N the number of mesh nodes per dimension. We show that the SEM method has several advantages, such as easy interpolation due to local element structure and long time integration due to its high order accuracy. Domain decomposition in high dimensions is used for parallelization, includes scalable parallel 2D Poisson solvers. Benchmarks and simulation results are reported in two dimensions in both the physical and velocity spaces (2P2V).

## INTRODUCTION

Plasma and charged particle simulations have great importance in science. There are three different approaches to simulate plasmas: the microscopic model, the kinetic model and the 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 very large N. On the other end is the fluid model which is the simplest 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. Due to computer speed limitations, MHD is currently the most popular approach in plasma simulations. 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. This paper deals with the kinetic model.

There are two different ways to solve the kinetic model. The most popular one is to represent the beam bunch by macro particles and push the macro particles along the characteristics of the Vlasov equation. This 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]. In principle, it simplifies the Partial Differential Equation (PDE) to an Ordinary Differential Equation (ODE). The interaction between charged particles, which is called the space charge force, is handled by solving Poisson's equation. Then the electric field from the potential solution can be computed. The PIC method has the advantages of speed and easy implementation, but similar to MHD, it is hard to calculate fine structures in the plasma. Furthermore, there is noise associated with the finite number of particles in the simulation. This noise decreases very slowly, as $1/\sqrt{N}$, when the number of particles N is increased.

The other way to solve the kinetic model is to solve the Vlasov equation directly. This can overcome the shortcomings of the PIC method, but due to the high dimensional nature of the Vlasov equation, numerical simulations have generally been conducted in low dimensions such as 1P1V or the axisymmetric case [3, 4]. Recently, 2P2V simulations have been reported [5]. We have applied SEM which can achieve high order accuracy than [5] and developed scalable Poisson and Vlasov solvers to make use of the BG/P supercomputer at ANL.

## VLASOV EQUATION

The distribution function $f(\vec{x},\vec{v},t)$ in phase space is governed by the Vlasov equation. In beam dynamics, a simplified model can be deduced in 2P2V form as a paraxial model based on the following assumptions:

- The beam is in a steady-state: All partial derivatives with respect to time vanish;
- The beam is sufficiently long so that the longitudinal self-consistent forces can be neglected;
- The beam is propagating at a constant velocity $v_b$ along the propagation axis z;
- Electromagnetic self-forces are included;
- $\vec{p}=(p_x,p_y,p_z)$, $p_z \sim p_b$ and $p_x, p_y << p_b$

where $p_b=\gamma m v_b$ is the beam momentum. It follows in particular that

$$\beta \approx \beta_b = (v_b/c)^2,\ \gamma \approx \gamma_b = (1-\beta_b^2)^{-1/2}$$

- The beam is narrow: the transverse dimensions of the beam are small compared to the characteristic longitudinal dimension. The paraxial model can be written as:

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

Coupled with Poisson's equation

$$-\Delta_{\vec{x}}\Phi^s=\frac{q}{\varepsilon_0}\int_{R^2} f(z,\vec{x},\vec{v})d\vec{v}$$

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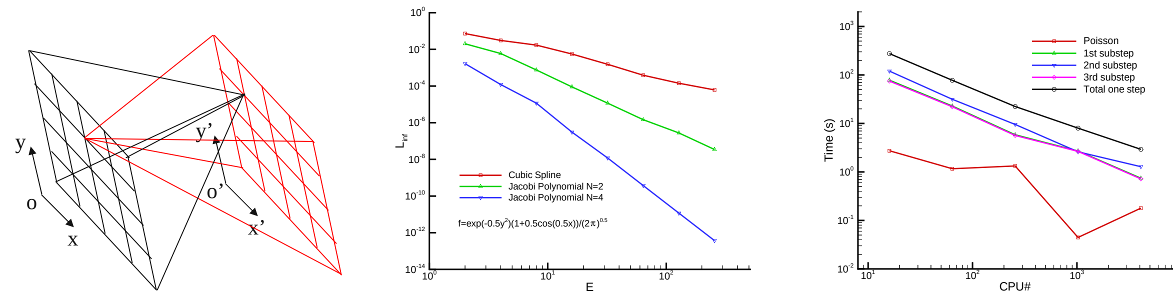


Figure 1: 4D domain decomposition (left), Interpolation errors vs. element number (middle) and strong scaling in 2P2V simulation (right).

Where $\Phi^s$ 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.

## NUMERICAL METHOD

The Spectral Element Method (SEM) originated in the 1980's [6, 7, 8], and has been applied in many different areas. It has been used for interpolation and solving Poisson's equation. The Semi-Lagrangian Method (SLM) [9] has been used for time integration. The time splitting scheme has been used for time integration as proposed by Cheng and Knorr [10]. It combines the flexibility of the finite element method and the high-order accuracy of the spectral method. The SEM is characterized by its close relation with orthogonal polynomials and Gaussian quadrature. The SEM shows great advantages compared to other methods in many application areas.

## PARALLEL SOLVERS

### *Parallel Poisson Solvers*

Domain decomposition has been used for 2D Poisson solvers with Dirichlet boundary conditions. Due to memory limitation only the iterative solver has been developed for solving boundary modes of the 2D Poisson's equation. Interior modes in each element have been solved 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)

$$\begin{pmatrix} A_{bb} & C_{bi} \\ C_{bi}^T & A_{ii} \end{pmatrix} \begin{pmatrix} u_b \\ u_i \end{pmatrix} = \begin{pmatrix} f_b \\ f_i \end{pmatrix}$$

$$(A_{bb} - C_{bi} A_{ii}^{-1} C_{bi}^T) u_b = f_b - C_{bi} A_{ii}^{-1} f_i$$

$$u_i = A_{ii}^{-1} (f_i - C_{bi}^T u_b)$$

Table 1: Scaling 2D Poisson Solver (E=64, P=4)

| CPU | 16 | 64 | 256 | 1024 | 4096 |
|---|---|---|---|---|---|
| Time (s) | 286 | 68 | 17.2 | 4.08 | 1.66 |
| PE | 1.0 | 1.0 | 1.0 | 1.0 | 0.673 |

### *Parallel Algorithms*

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. Figure 1 (left) shows the domain decomposition in 4D for 2P2V simulations.

## BENCHMARKS AND SIMULATION RESULTS

### *Benchmarks*

Table 1 shows the benchmark results for the 2D Poisson solver. Good scaling has been achieved. Figure 1 (middle) compares the interpolation errors with cubic spline, Jacobi polynomial with P=2 and 4. Clearly using a Jacobi polynomial gives much better results, which is good to use in the Semi-Lagrangian scheme. The right plot in Fig. 1 shows the strong scaling results for both the Poisson and Vlasov solvers in 2P2V simulations. It shows that the Vlasov solver can have good scaling because the most time consuming part is the interpolation. And since the interpolations are local on each processor, there is no communication between different processors. So even when the scaling of the Poisson solver becomes worse with 4k processors, the overall scaling is still good.

### *2P2V Simulations*

In 2P2V simulations, a proton beam has been simulated through alternating hard edge electric quadruple 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 $[-8\times10^5, 8\times10^5]$ by $[-8\times10^5, 8\times10^5]$ m/s. The alternating electric quadruple field is defined as $\vec{E}^e(x,y,z) = (k_0(z)x, -k_0(z)y)$.

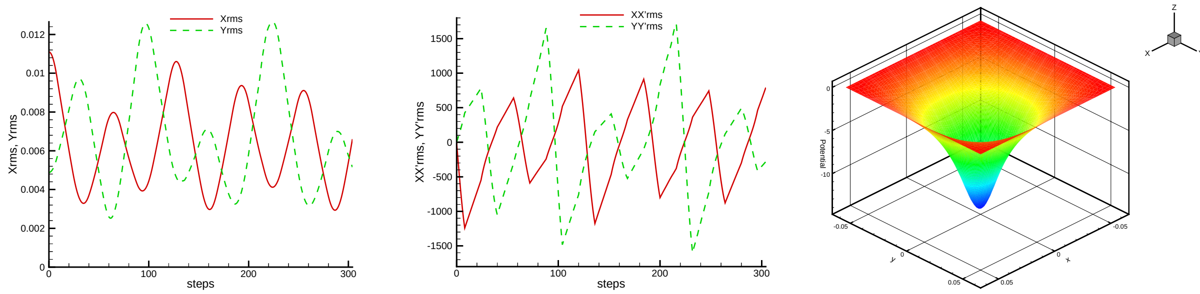


Figure 2: RMS for X and Y (left), RMS for XX' and YY' (middle), potential (right).

The left plot in Fig. 2 shows the $X_{rms}$ and $Y_{rms}$ values, the middle plot is for $XX'_{rms}$ and $YY'_{rms}$, the right one is the potential distribution. Since the initial beam distribution is Gaussian (not a KV distribution), the RMS envelope is not periodic with the amplitude fluctuating from one period to the next. Figure 3 shows the beam contours in (x, y), (x, x'), (y, y') and (x', y') phase planes at z=0 and 192 steps.

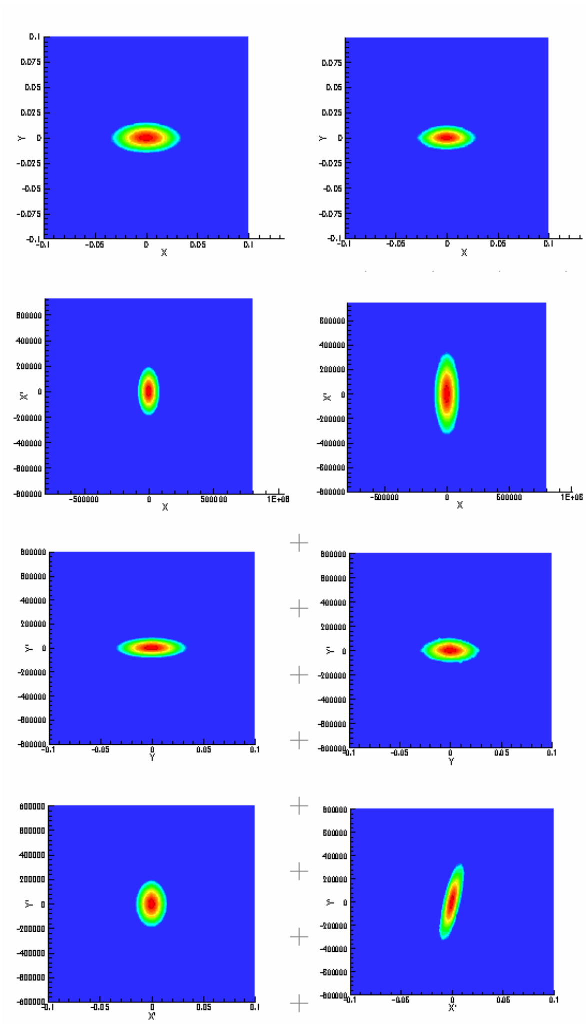

Figure 3: From top to bottom are contours in the (x, y), (x, x'), (y, y') and (x', y') planes, from left to right correspond to z=0 and 192 time steps.

## SUMMARY

This paper presents our first efforts to develop parallel direct Vlasov solvers with a high-order SEM. The advantages and effectiveness of the SEM have been demonstrated. A 2P2V Vlasov solver has been successfully developed using the Semi-Lagrangian method. Domain decomposition has been used for parallelization of these solvers. Scalable Poisson solvers have been developed within. Benchmarks of the parallel models have shown good scaling on BlueGene/P at ANL with up to 4k processors. The SEM shows its advantages in these direct Vlasov solvers, such as local interpolation, easy parallelization and long time integration. These first explorations are encouraging, and higher dimensional problems are under investigation and will be reported in the near future. We will also compare transport of 4D transverse emittance DC beam using the Vlasov approach with the ray tracing (PIC) method.

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