DEVELOPING PETA-SCALABLE ALGORITHMS FOR BEAM DYNAMIC SIMULATIONS*

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Abstract

Peta-scalable software packages for beam dynamic simulations are being developed and used at Argonne national laboratory. The standard Particle-In-Cell (PIC) method and direct Vlasov solvers in up to 4 dimensions have been developed and benchmarked with respect to each other. Both of them have successfully run on 32 thousands processors on BG/P at Argonne Leadership Computing Facility. Peta-scale computing facility at ANL provides suitable environment for simulating beams in large scale. We have simulated charged beams through traditional PIC method as well as direct solving of the Vlasov equation in higher dimensions. Several scalable Poisson solvers have been developed and incorporated with these methods. High-order numerical methods have been adopted for solving the Poisson and Vlasov equations. Preliminary results on direct Vlasov solvers have been obtained in up to 4 dimensions. Domain decomposition method has been used for the parallelization in these software packages, and good scaling has been achieved. These packages have been successfully applied in end-to-end simulation of linear accelerators and large scale accelerator design optimizations. There are still lots of places can be improved for the PIC method and lots of challenges exist in the direct Vlasov solvers, therefore, more efforts are needed in both algorithms and applications.

INTRODUCTION

Plasma and charged beams are of great importance in modern science and technology. Their researches become more and more rely on the 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 fast 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 beam in 3D, Vlasov equation has to be solved in 6D. This clearly needs peta-scale computing, and the 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.

PARALLEL POISSON SOLVERS

In both 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:

Fourier Method

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

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.

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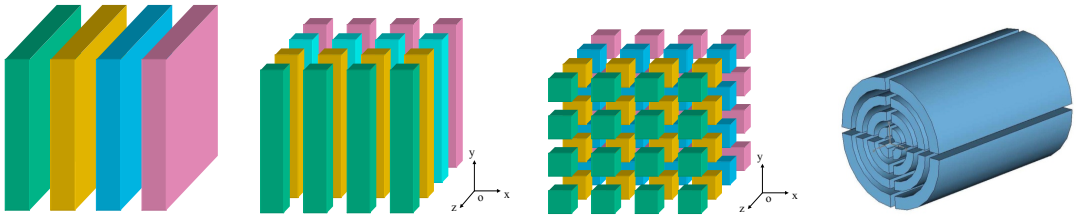

Model A Model B Model C Cylinder

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

Three different domain decomposition methods have been implemented as shown in Fig.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].

Fourier hp-Finite Element Method

This solver is developed for cylinder 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.

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

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

Domain decomposition in the radial and circumferential directions has been implemented as shown in the Fig. 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].

Hp-Finite Element Method on Structured Grid

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 Fig. 2(1). The 2D structured mesh is shown in Fig. 2(2). Continuous Galerkin (CG) method has been used and zero Dirichlet B.C. has been imposed. The potential distribution is shown in Fig. 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)

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

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

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

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 Fig. 2(4).

The potential is expressed as

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

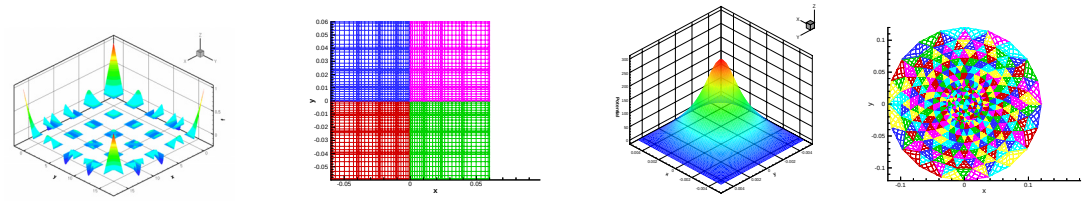

Figure 2: 2D expansion functions (1), 2D structured mesh (2), potential in 2D (3) and 2D structured mesh (4).

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

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

BEAM DYNAMIC SIMULATION WITH PIC METHOD

In the last several years, we have developed a parallel PIC solver based on the serial version, TRACK, which was developed in 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 and 4]. As small mesh can be used for calculating space charge effect, PTRACK has achieved good scaling as shown in Table 1. 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 has been used as workhorse for large scale optimizations.

BEAM DYNAMIC SIMULATION BY DIRECT SOLVING VLASOV EQUATION

In order to overcome the shortcoming of the PIC solvers, we have developed direct Vlasov solvers. The

Table 1: Weak scaling of PTRACK

CPU	Time/cell	Particle #	Parallel Efficiency
256	384	55M	100%
512	384	220M	100%
1024	388.7	220M	98.8%
2048	400.6	440M	95.8%
4096	385	880M	99%

distribution function $f(\vec{x},\vec{v},t)$ in phase space is governed by the Vlasov equation.

Vlasov equation in 1P1V phase space

In 1P1V phase space, the non-dimensional Vlasov equation can be written as following:

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

Vlasov equation in 2P2V phase space

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 $p_x,p_y\ll p_b$

where $p_b=\gamma mv_b$ 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:

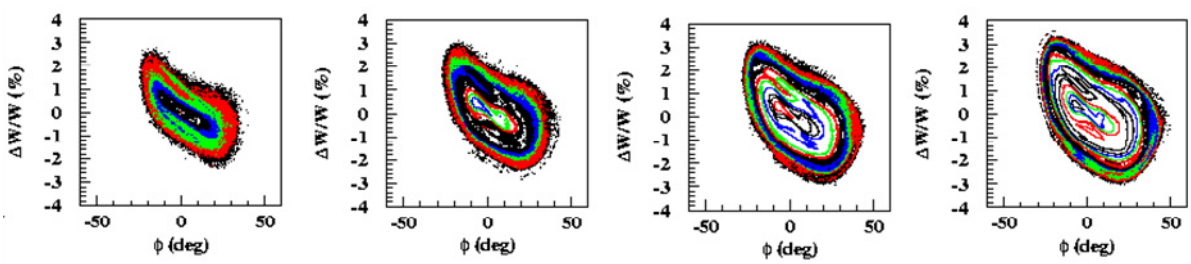

Figure3: $(\varphi,\Delta W/W)$ plane contour with 1M(1), 10M(2), 100M(3) and 865M(4) particles

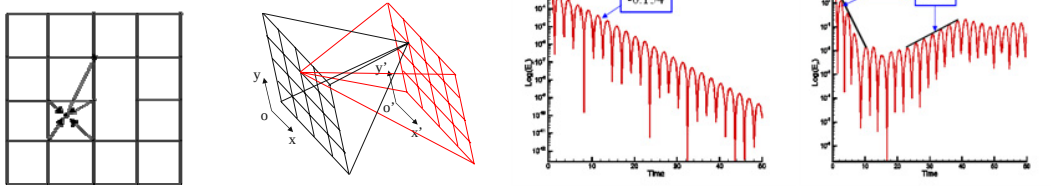

Figure 4: Semi-Lagrange Scheme (1), 4D domain decomposition (2), Linear Landau Damping (3), Strong Landau Damping (4)

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

Coupled with Poisson's equation

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

,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.

Numerical Algorithm

The Semi-Lagrangian Method (SLM) [9] has been used for time integration. A plot explains the idea has been shown on the left of Fig. 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 Fig. 4(2).

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

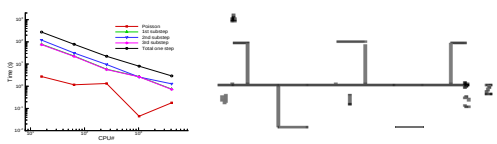

Figure 5: Scaling of 2P2V Vlasov solver (left) and alternating electric focusing force (right)

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.

Good scaling has been achieved. The right plot in Fig. 5(left) 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.

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

$$f(0,x,v)=\frac{1}{\sqrt{2\pi}}\exp(-v^2/2)(1+\alpha\cos(kx))$$
$$\forall(x,v)\in[0,L]\times R,\quad \alpha=0.01,\quad k=0.5$$
$$L=4\pi,\quad R=[-6,6],\quad \Delta t=1/8,$$
$$P=16,\quad E=64,\quad 1024\times1024$$
$$CPU=256,\quad T\sim10\ \min s$$

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

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 $v_b=6.19\times10^6$ 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 $\vec{E}^e(x,y,z)=(k_0(z)x,-k_0(z)y)$ and shown in Fig. 5(right).

Figure 6 shows the comparison of TRACK (solid) and Vlasov (dotted) simulations using a Gaussian beam: *Xrms*(*left upper*), *Yrms*(*lower–le ft*), *X'rms*(*upper right*), *Yr'ms*(*lower right*) for a 100 mA proton beam. As can be seen, they match each other quite well. Figure 7 shows the beam contours in (x, y), (x, x'), (y, y') and (x', y') phase planes at t=0 and 1 time period. More detailed information on 1P1V and 2P2V Vlasov simulations can be found in [2].

SUMMARY

This paper presents our researches on developing peta-scalable algorithms for large scale beam dynamic simulations. Both PIC method and direct Vlasov method have been used. Different parallel Poisson solvers have been developed to satisfy the requirement of counting space charge effect in various solvers. Domain decomposition has been adopted for parallelization of TRACK code. PTRACK has now

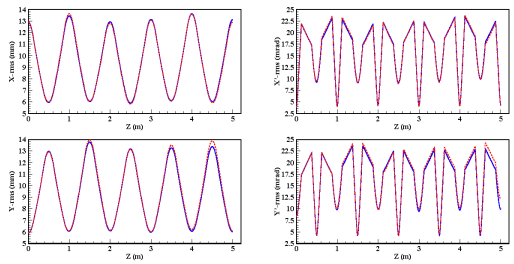

Figure 6: Comparison of TRACK (solid) and Vlasov (dotted) simulations using a Gaussian beam: Xrms(left-upper), Yrms(lower-left), X'rms(upper-right), Y'rms(lower-right) for a 100 mA proton beam.

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 explorations are encouraging, and more investigation will be done.

REFERENCES

[1] P.N. Ostroumov, V. N. Aseev, and B. Mustapha. Phys. Rev. ST. Accel. Beams 7, 090101 (2004).

[2] J. Xu and P.N. Ostroumov, Computer Physics Communications, 178 p.290-300 (2008).

[3] J. Xu, B. Mustapha, V.N. Aseev and P.N. Ostroumov, Phys. Rev. ST. Accel. Beams 10, 014201 (2007).

[4] J. Xu, B. Mustapha, V. N. Aseev and P.N. Ostroumov, HB 2008, Nashville, Tennessee, USA, Aug. 25- 29, (2008).

[5] M. Gutnic, M. Haefele, I. Paun and E. Sonnendrücker, Comput. Phys. Comm., 164, 214-219 (2004).

[6] E. Sonnendrücker, J. Roche, P. Bertrand and A. Ghizzo, J. Comput. Phys., 149, 201 (1998).

[7] F. Filbet, E. Sonnendrücker, Vol.16, No.5, 763-791 (2006).

[8] M.O. Deville, P.F. Fischer and E.H. Mund, High-Order Methods for Incompressible Fluid Flow, Cambridge University Press, Cambridge (2002).

[9] J.S. Hesthaven and T.Warburton, Nodal Discontinuous Galerkin Methods: Algorithms, Analysis and Applications, Springer, New York (2008).

[10] G.E. Karniadakis and S.J. Sherwin, Spectral/hp element methods for CFD, Oxford University Press, London (1999).

[11] Robert, Atmos. Ocean. 19, 35 (1981).

[12] C.Z. Cheng and G. Knorr, J. Sci. Comp., 22, 330 (1976).

[13] Xu, P.N. Ostroumov, "Solving 2D2V Vlasov Equation with High Order Spectral Element Method", Communication in Computational Physics, (2010).

Acknowledgments

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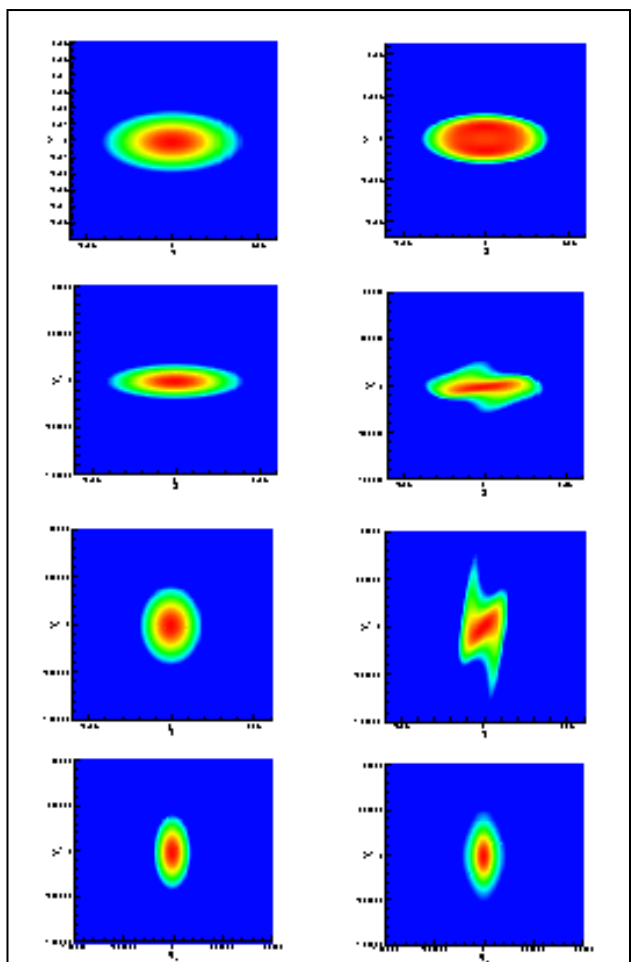

Figure 7: From top to bottom are contours in the (x, y), (x, x'), (y, y') and (x', y') planes, from left to right correspond to t=0 and 1 time period.