PARALLEL THREE-DIMENSTIONAL PIC CODE FOR BEAM-BEAM SIMULATION IN LINEAR COLLIDERS *

M.A. Boronina, V. D. Korneev, V.A. Vshivkov, ICM&MG SB RAS, Novosibirsk, Russia

Abstract

We present our parallel 3D3V particle-in-cell code for the numerical simulations of ultrarelativistic charged beams in supercolliders. In the algorithm we employ the three-dimensional set of Maxwell equations and the Vlasov-Liouville equation for the distribution function of beam particles in 6-dimensional phase space. The code allows performing numerical experiments with an arbitrary density distribution, beam crossing angle and relative offset. We present the results of numerical simulations of colliding beams using dummy parameters and parameters close to the ones of the newest ILC project.

INTRODUCTION

Today numerical simulation of charged particle beam dynamics in supercolliders is based on the slice model. The colliding beams are divided into slices of macroparticles. The particles of each beam receive a kick of the 2D fields of counter beam and change their motion. Usually the transversal field of each slice is calculated with Basetti-Erskine equations or as the derivative of 2D potential. The Poisson equation with boundary conditions or the Green function can be used to obtain the potential [1]. Standard ways of parallelizing are based on the slice decomposition, when one or few slices are assigned to one processor. Another way is two-dimensional domain-decomposition approach, when each processor contains one rectangular block domain. But this method is not effective when particles move far from their positions during time step. This problem can be avoided by using particle-field decomposition [2].

Reduction to the 2D problem can not completely cover the three-dimensional and longitudinal effects in particular, which can play significant role in cases of superhigh densities. Besides, the model complicates simulations of the beams crossing at angle.

In our 3D algorithm we employ the Vlasov-Liouville equation for the distribution function of beam particles, the three-dimensional set of Maxwell equations and new methods for initial and boundary conditions calculations [3, 4], which automatically account for such difficulties. We solve these equations by using the particle-in-cell (PIC) method and the leapfrog scheme.

From the mathematical point of view the main problem of the three-dimensional modeling is the presence of the high relativistic factor values (the field gradients are high), the convergence conditions for the leapfrog scheme

and the necessarily big number of particles in 3D cell. Thus the parallel algorithm is based on the mixed Euler-Lagrangian decomposition in order to achieve good load balancing and to reduce computation time. With the advances of the code it will be possible to apply it for one-passage beam-beam simulations in linear colliders with supercritical parameters.

COMPUTATIONAL METHODS

We consider the motion of counter charged electron/positron beams in rectangular domain. The motion takes place in vacuum in self consistent electromagnetic fields taking into account the external focusing field of collider. Each beam is defined by its shape, sizes, coordinates in space and time, number of particles, non-linear density distribution. The problem can be described by Vlasov's kinetic equation for the distribution function of electrons and positrons and the set of Maxwell's equations:

$$\frac{\partial f_{+,-}}{\partial t} + \vec{v}\,\frac{\partial f_{+,-}}{\partial \vec{r}} + \vec{F}_{+,-}\,\frac{\partial f_{+,-}}{\partial \vec{p}} = 0$$

$$\mathrm{rot}\vec{E} = -\frac{1}{c}\frac{\partial \vec{H}}{\partial t}$$

$$\mathrm{rot}\vec{H} = \frac{4\pi}{c}\,\vec{j} - \frac{1}{c}\frac{\partial \vec{E}}{\partial t}$$

$$\mathrm{div}\vec{E} = 4\pi\rho$$

$$\mathrm{div}\vec{H} = 0$$

Three-dimensional Maxwell's equations allow calculating the beams movement regardless of the collective motion direction.

We use dimensionless variables (the characteristic length L_0 of the beam is 1 cm and the characteristic speed v of the particles is the speed of light). We apply particle-in-cell method with PIC form factor and the leap-frog scheme. All the components are calculated at the half-step time and space grids. In this case all the derivatives involved in the equations are written with central differences, and this scheme provides second order accuracy by time and space. We apply the Villancenor-Buneman scheme in order to calculate the currents, this method satisfies precisely the Gauss's law in final differences and thus significantly reduces the approximation error and makes the algorithm more robust.

PARALLEL ALGORITHM

The quality of results, obtained with PIC method, increases with increasing of particle number in cell, usually 10^2-10^3 particles are taken. The high values of relativistic factor lead to the high gradients and thus many small spatial steps, this fact leads by-turn to the high total number of particles. The convergence condition makes the problems worse: the smaller time-step is – the smaller spatial step has to be. The huge total number of particles requires much RAM resources, which one processor cannot provide. All these facts necessitate creating of the well-balanced 3D parallel code of high scalability.

The spatial domain is divided uniformly into stripes along the y axis. The collective particle motion takes place in longitudinal direction, thus the quantity of interprocessor communications will be smaller in comparison with case of decomposition along the z-axis. Each subdomain is assigned to a group of $1..N_0$ processors, each processor in the group has the same spatial grid data, and the particles corresponding to the physical subdomain are divided evenly between all the processors of the group. Such a way of parallelizing yields even particle distribution within the group due to using many processors in the high-density regions of the domain (see Fig.1).
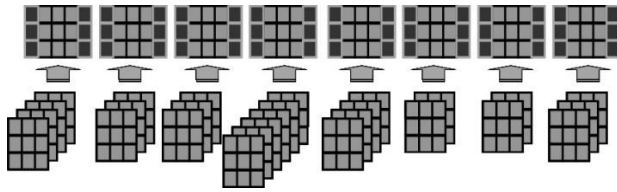

Figure 1: Decomposition structure.

In order to calculate initial and boundary electric fields each processor computes its own density 3D array and sends to the corresponding main processor of the group. Each main group processor calculates its own field 3D arrays and sends it to all the main processors, after the procedure it broadcasts the obtained field data within its own group.

The main group processors use Maxwell equations to compute new fields and broadcast them within their own groups. When the particle leaves the corresponding subdomain, the algorithm sends its parameters to one of the neighbor processors.

It is necessary to calculate the initial particle distribution twice. First the master processor computes the particle number in each of N_0 groups, determines the most optimal processor distribution of given N processors among these groups and the maximum particle number in every processor. Then the master creates the initial particle parameters and sends the packs of parameters to each of N processors until all the particles are distributed.

SIMULATION RESULTS

The algorithm described has been tested using analytical solution for the particle motion through a cylindrical beam with Gaussian density distribution in the transversal directions:

$$\rho\left(\mathrm{r}, \mathrm{z}\right) = \frac{\mathrm{Ne}}{2\pi\sigma^2 \mathrm{l}} \mathrm{e}^{-\frac{\mathrm{r}^2}{2\sigma^2}}.$$

In this case the deflection angle of the particles after the interactions conforms to the following expression [5]:

$$\alpha = \mathrm{p_r} / \mathrm{p_z} = -\frac{2\mathrm{Ne}^2}{\mathrm{rcp_z}}\left(1 - \mathrm{e}^{-\frac{\mathrm{r}^2}{2\sigma^2}}\right).$$

We used $\sigma = 6.25 \cdot 10^{-2}$ cm, cylinder radius $R = 3\sigma$, cylinder length $l = 0.05$ cm. $Q_{beam} = -Ne$, $N = 10^{10}$, $Q_{part} = e = 4.8 \cdot 10^{-10}$ esu, relativistic factor of all the particles $\gamma = 6.85 \cdot 10^3$. Spatial grid: 40x40x40, spatial step $h_x = h_y = 0.025$, $h_z = 0.0025$, time step $5 \cdot 10^{-4}$, number of model particles in the beam $J = 4 \cdot 10^6$. Fig.2. demonstrates the absolute values of the analytical solution (line), the numerical solution (crosses) for the deflection angle after 90 time steps.
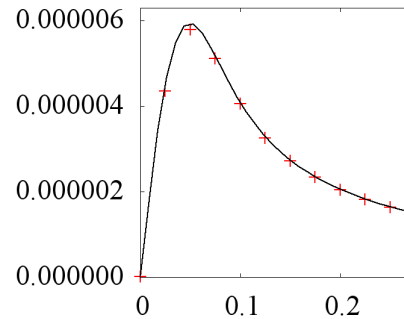

Figure 2: Absolute value of the angle deflection, analytical and numerical solutions.

This data can be obtained with PC in an hour. However, in case of focused beams the highly non-linear beam density distribution and the hour-glass effect force to use spatial grid with higher resolution and, as a consequence, smaller time step and more computing steps.

We present an example of numerical simulations for two counter monoenergetic beams, focused in the center of interaction region of length $L_z = 0.2$ cm. The vertical size of the domain is $L_x = L_y = 2 \cdot 10^{-4}$ cm.

The density distributions of the beams in the crossover plane are described by Gaussian law with $\sigma_x^* = \sqrt{\varepsilon_x \beta_x^*} = \sigma_y^* = 3.9 \cdot 10^{-6}$ cm, the emittances $\varepsilon_x = \varepsilon_y = 10^{-9}$ cm, and the beta-function values $\beta_x^* = \beta_y^* = 1.5 \cdot 10^{-2}$ cm, $\sigma_z = 1.5 \cdot 10^{-2}$ cm. We consider a case of vertical beam displacement $\Delta y = 10^{-5}$ cm ~ $3\sigma_x$.

05 Beam Dynamics and Electromagnetic Fields

D06 Code Developments and Simulation Techniques

The transverse momenta x′ and y′ conform to Gaussian law with $\sigma^*_{x'} = \sqrt{\varepsilon_x/\beta^*_x} = \sigma^*_{y'} = 2.6 \cdot 10^{-4}$. The charges of the beams are opposite, $Q_1 = -Q_2 = 2 \cdot 10^{10}e$, relativistic factors of all the particles are $\gamma = 4 \cdot 10^5$ [6].

We used $J = 10^7$ particles for 100 x 100 x 100 grid. Such parameters cannot be taken using standard domain decomposition in three-dimensional case. 64 processors were distributed in 20 groups, so the minimum number of processors in a group was 1 and the maximum was 14. The computation time equaled to 18 hours at Siberian Super Computer Center (SSCC), 576 4-core processors Intel Xeon E5450/E5540/X5670.
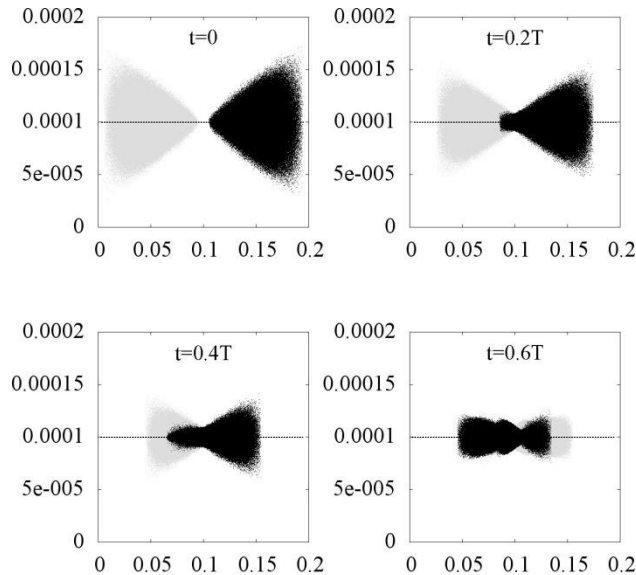

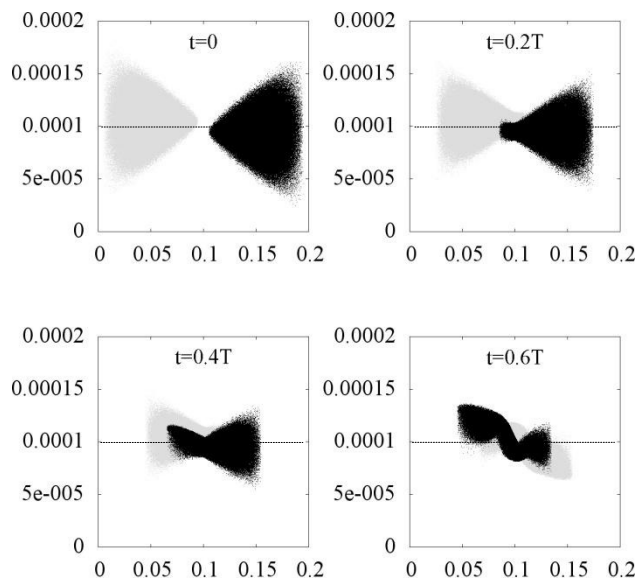Figure 3: Beam evolution, coordinates (z, x).

Figure 4: Beam evolution, coordinates (z, y).

The beam shapes in different instants of time: t=1/5T, t=2/5T, t=3/5T, t=4/5T, where T=0.1 is the complete single passage time, are shown at Fig. 3, 4 with black color. Fig. 3. shows beam coordinates (z,x) and illustrates symmetric motion of the beam with a focusing effect of the opposite beam field. Fig. 4. shows beam coordinates (z,y) and points the kink-instability evolution. The grey color shadows coordinates of the counter beam.

CONCLUSION

New three-dimensional model and the corresponding parallel code for beam-beam simulation with high gamma-factors $(10^3 - 10^5)$ has been developed. The algorithm is based on the domain and particle decomposition and allows performing numerical experiments for spatial grids 200x200x200 and particle number 10^8. The simulation results are in correspondence with existing theory.

REFERENCES

[1] Anderson E. B., Banks T. I., Rogers J. T., "ODYSSEUS: A Dynamic Strong-Strong Beam-Beam Simulation for Storage Rings", International Computational Accelerator Physics Conference (1998).

[2] Ji Qiang, Stefan Paret, "Poisson Solvers for Self-Consistent Multi-Particle Simulations", ICFA Mini-Workshop on Beam-Beam Effects in Hadron Colliders, March 18-22 (2013).

[3] M. Boronina, V. Vshivkov, E. Levichev, S. Nikitin, V. Snytnikov, "3D PIC Method Development For Simulation Of Beam-Beam Effects In Supercolliders", Proceedings of Particle Accelerator Physics (2007), pp. 3366-3368.

[4] V.A. Vshivkov, M.A. Boronina. Three-dimensional simulation of ultrarelativistic charged beams dynamics: study of initial and boundary conditions. Matem. Mod, V. 24, 2, (2012), pp. 67-83.

[5] Mauro Pivi, "Beam-Beam Effects in Future Linear Colliders", US Particle Accelerator School, January 22-26, 2007, Houston, Texas.

[6] Karsten Buesser, "The International Linear Collider", arXiv:1306.3126v1 (2013).