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# Computer-Assisted Particle-in-Cell Code Development

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**Abstract**

This report presents a new approach for an electromagnetic Particle-in-Cell (PIC) code development by a computer: in general PIC codes have a common structure, and consist of a particle pusher, a field solver, charge and current density collections, and a field interpolation. Because of the common feature, the main part of the PIC code can be mechanically developed on a computer. In this report we use the packages FIDE and GENTRAN of the REDUCE computer algebra system for discretizations of field equations and a particle equation, and for an automatic generation of Fortran codes. The approach proposed is successfully applied to the development of 1.5-dimensional PIC code. By using the generated PIC code the Weibel instability in a plasma is simulated. The obtained growth rate agrees well with the theoretical value.

Keywords: PIC code, Particle code, Program generation, Particle simulation, Computer-assisted simulation, Plasma simulation, Weibel instability

# 1 Introduction

Particle-in-cell (PIC) codes are widely used for simulations in plasma physics[1]–[7]. The PIC code is a powerful research tool. A physicists' requirement is to obtain a reliable PIC code but not to construct it by themselves. So far many researchers have constructed PIC codes for their own purposes by themselves.

However the PIC code has a common structure: a PIC code consists of a particle pusher, a field solver, charge and current density collections, and a field interpolation. Because of the common feature, the main part of the PIC code can be mechanically developed on a computer. We proposes a new approach for an electromagnetic PIC code development by a computer. In this report we use the packages FIDE[8] and GENTRAN[9] of the Reduce computer algebra system[10] for discretizations of field equations and a particle equation and for Fortran code generation. In order to complete a PIC code development, the parts of code generated automatically are combined with hand-written remaining parts doing such things like the input/output or initial setup.

The proposed approach has been successfully applied to the development of a 1.5-dimensional(D) PIC code. By using the generated PIC code the Weibel instability in a plasma is simulated. The growth rate obtained by the simulation agrees well with the theoretical value.

By using this approach, a PIC code development is more efficient and the code development time can be reduced. In addition, a source PIC code is available to a user. Therefore a user can check a reliability of the code by himself, and can change the code. In plasma simulations minor changes of the code are performed frequently: for example, the initial conditions, or the boundary conditions, or the total number of super particles employed, or the plasma parameters may be changed. Such flexibility can be realized in our approach, however not in a black-box package system.

# 2 PIC code development

## 2.1 PIC code structure

The structure of a PIC code is well established, and the PIC code consists of the initial setup, an interpolation of fields on every particle, a particle pusher, a collection of a particle charge and/or a current density on every space grid cell, and the integration of field equations. These subprocesses are repeated until the final result is obtained as follows:

(1) Initial preparation.

(2) Interpolation of electromagnetic fields ($\boldsymbol{E}$ and $\boldsymbol{B}$) on every particle.

(3) Particle pusher: solve a relativistic equation of motion for every particle.

(4) Obtain a particle charge density ($\rho_e$) and/or a current density ($\boldsymbol{J}$) on every space

grid cell.

(5) Field solver: integrate field equations.

(6) Repeat (2) to (5) until the end condition specified is satisfied.

The detail structure of a PIC code will be discussed again in the end of this section.

## 2.2 A 1.5-D PIC code development

In this report we focus on an electromagnetic 1.5-D PIC code in which field equations are solved by a finite difference method, and a space grid is a uniform. After a suitable normalization, we obtain the following system of partial differential equations for the electromagnetic field:

$$\frac{\partial E_x}{\partial t} = -J_x \tag{1}$$

$$\frac{\partial E_y}{\partial t} = -\frac{B_z}{\partial x} - J_y \tag{2}$$

$$\frac{\partial B_z}{\partial t} = -\frac{E_y}{\partial x} \tag{3}$$

The fields of $E_x(x,t), E_y(x,t)$ and $B_z(x,t)$ are obtained from current densities $J_x(x,t)$ and $J_y(x.t)$ which are computed in every grid point.

For every superparticle $p$ with the position $\mathbf{x}_p(t)$ and the velocity $\mathbf{v}_p(t)$ the equations of motion, after a suitable normalization, are

$$\frac{d\,\gamma \mathbf{v}_p}{dt} = -(\mathbf{E}_p + \mathbf{v}_p \times \mathbf{B}_p), \qquad \frac{d\mathbf{x}_p}{dt} = \mathbf{v}_p, \tag{4}$$

where $\gamma$ is the relativistic factor.

For solving the particle equations of motion we use the Buneman scheme[11], which is widely used in many PIC codes. First we introduce the notation

$$\mathbf{u} = \gamma \mathbf{v}.$$

Here we assume that $\mathbf{u}$ on the time step $n - 1/2$ and the electromagnetic fields on the time step $n$ are known. Then the Buneman procedure proceeds as follows:

$$\mathbf{u}^- = \mathbf{u}^{n-1/2} - \mathbf{E}^n \Delta t/2 \tag{5}$$

$$u_x^{'} = u_x^- + u_y^- \tau \tag{6}$$

$$u_y^+ = u_y^- - u_x^{'} s \tag{7}$$

$$u_x^+ = u_x^- + u_y^- \tau \tag{8}$$

$$\mathbf{u}^{n+1/2} = \mathbf{u}^- - \mathbf{E}^n \Delta t/2 \tag{9}$$

where

$$\tau = -\frac{B_z^n \Delta t}{2\gamma^-} \tag{10}$$

$$s = \frac{2\tau}{1+\tau^2} \tag{11}$$

$$(\gamma^-)^2 = 1 + (\mathbf{u}^-)^2. \tag{12}$$

The velocity is calculated from

$$\mathbf{v}^{n+1/2} = \frac{\mathbf{u}^{n+1/2}}{\gamma^{n+1/2}}, \tag{13}$$

where

$$(\gamma^{n+1/2})^2 = 1 + (\mathbf{u}^{n+1/2})^2.$$

The particle position is advanced by

$$\mathbf{x}^{n+1} = \mathbf{x}^n + \mathbf{v}^{n+1/2}\Delta t. \tag{14}$$

According to the Buneman scheme, the equation of motion is easily discretized by FIDE[8], which is a package for discretization of partial differential equations and for manipulations (rearrangement and simplification) of discretized equations. Then GENTRAN[9] package is used to generate a Fortran code solving the difference equations.

We use a uniform grid (see Fig.1) $x_i = i\Delta x, i = 0, \cdots, N+1$ with the boundaries at $x_1 = 0$ and $x_N$. The quantities $E_x, E_y, J_x$ and $J_y$ are defined in the grid points $x_i$ . The magnetic field $B_z$ is defined in the grid points $x_{i+1/2} = x_i + \Delta x/2$.

In Eq. (4) we need to know the values of electromagnetic field components at the position of every particle. For electromagnetic field interpolation we employ the area weighting method[2]-[4],[6]. Let a particular particle $p$ is at the position $x_p$. First we need to know in which cell this particle appears. If we denote

$$i_p = \lfloor x_p/\Delta x \rfloor + 1,$$

then the particle is in the cell $(x_{i_p}, x_{i_p+1})$. Now the particle is assumed to have the size $\Delta x$, same as the grid step. The electrical field on the particle is given by the combination of the field values in the grid points $x_{i_p}$ and $x_{i_p+1}$ weighted by the lengths of the intersections of the artificial particle cell with cells $(x_{i_p-1/2}, x_{i_p+1/2})$ and $(x_{i_p+1/2}, x_{i_p+3/2})$ (see Fig.1). The electric field $\mathbf{E}_p$ on the particle $p$ is then

$$\mathbf{E}_p = \frac{\mathbf{E}_{i_p} S_1 + \mathbf{E}_{i_p+1} S_2}{\Delta x}, \tag{15}$$

where

$$S_2 = x_p - (i_p - 1)\Delta x, \qquad S_1 = \Delta x - S_2.$$

For the magnetic field $B_z$ which is defined in the grid points $x_{i+1/2}$ we need to use a slightly different procedure. If we denote

$$i'_p = \left\lfloor \frac{x_p - \Delta x/2}{\Delta x} \right\rfloor + 1,$$

then the particle is in the cell $(x_{i'_p+1/2}, x_{i'_p+3/2})$. The value of magnetic field on the particle is given by combination of its values in the grid points $x_{i'_p+1/2}$ and $x_{i'_p-3/2}$ weighted by the lengths of the intersections of the artificial particle cell with cells $(x_{i'_p}, x_{i'_p+1})$ and $(x_{i'_p-1}, x_{i'_p+2})$. If $B_{zp}$ is the magnetic field on the particle $p$, then

$$B_{zp} = \frac{B_{z,i'_p-1/2}S'_1 + B_{z,i'_p+3/2}S'_2}{\Delta x}, \tag{16}$$

where

$$S'_2 = x_p + \Delta x/2 - i'_p \Delta x, \qquad S'_1 = \Delta x - S'_2.$$

The current density is defined in the grid points $x_i$ and is calculated from particles appearing in the cell $(x_{i_p}, x_{i_p+1})$. If we have again a particle $p$ at the position $x_p$ with the charge $Q_p$ and the velocity $\mathbf{v}_p$, then it contributes to the values of current density at the points of $x_{i_p} and x_{i_p+1}$ as follows:

$$\mathbf{J}_{i_p} = \frac{Q_p \mathbf{v}_p S_1}{\Delta x^2}, \tag{17}$$

$$\mathbf{J}_{i_p-1} = \frac{Q_p \mathbf{v}_p S_2}{\Delta x^2}. \tag{18}$$

The field equations are discretized by the time centered difference scheme by FIDE. Then GENTRAN is used to generate a Fortran code for the difference equations:

$$\frac{B^{n-1/2}_{z,i+1/2} - B^{n-1/2}_{z,i-1/2}}{\Delta t} = -\frac{E^n_{y,i+1} - E^n_{y,i}}{\Delta x} \tag{19}$$

$$\frac{E^{n+1}_{x,i} - E^n_{x,i}}{\Delta t} = -J^{n+1/2}_{x,i} \tag{20}$$

$$\frac{E^{n+1}_{y,i} - E^n_{y,i}}{\Delta t} = -\frac{B^{n+1/2}_{z,i+1/2} - B^{n+1/2}_{z,i-1/2}}{\Delta x} - J^{n+1/2}_{y,i} \tag{21}$$

The magnetic field $B_z$ on the time layer $n$, which is required during the particle integration, is obtained by an average

$$B^n_{z,i+1/2} = \frac{1}{2}\left(B^{n+1/2}_{z,i+1/2} + B^{n-1/2}_{z,i+1/2}\right). \tag{22}$$

Equations (19)–(21) are converted to the following Fortran program by FIDE and GENTRAN:

```
      do 25005 i=0,n+1
          abzo(i)=abz(i)
25005 continue
      do 25006 i=1,n
          abz(i)=(abzo(i)*dx-(ae(2,i+1)*dt)+ae(2,i)*dt)/dx
25006 continue
      do 25007 i=1,n
          ae(1,i)=ae(1,i)-(aj(1,i)*dt)
25007 continue
      do 25008 i=1,n
          ae(2,i)=
     &     (abz(i-1)*dt-(abz(i)*dt)+ae(2,i)*dx-(aj(2,i)*dt*dx))/
     &     dx
25008 continue
```

Particle integration and field integration are two main components of the PIC algorithm. For one time step these two integrations can be simply outlined as:

1. *Particles integration*: for every particle $p$.
   (a) *preparation step*: calculate electric and magnetic fileds $\mathbf{E}_p$ and $B_{z,p}$ on the particle $p$ according to (15) and (16).
   (b) *integration step*: calculate the new velocity $\mathbf{u}^{n+1/2}$ and the new position $\mathbf{x}^{n+1}$ of the particle according to the Buneman procedure (5)-(14).
2. *Field integration*:
   (a) *preparation step*: calculate the current density in all grid points $x_i$: over all particles $p$ sum their contributions $\mathbf{J}_{i_p}$ and $\mathbf{J}_{i_p+1}$ given by (17) and (18).
   (b) *integration step*: from the difference schemes (19)-(21) calculate the new values of electromagnetic fields components $\mathbf{E}_i^{n+1}$ and $B_{z,i+1/2}^{n+1/2}$.
   (c) *magnetic field averaging step*: calculate $B_{z,i-1/2}^{n}$ according to Eq. (22).
   (d) *electric field correction*: solve the Poisson equation to compensate the difference between the charge density obtained from the electric field and that from the particle charge assignment [1]. The Poisson equation is also discretized by FIDE and rearranged to set the matrix elements. The generated source code by GENTRAN is combined with a matrix solver which is prepared separately in this report.

In this report we use the periodic boundary condition in the $x$ space.

## 2.3 Example simulation result – the Weibel instability

In the Weibel instability[12]–[14] an anisotropic thermal energy is converted to a magnetic field energy. A magnetic field perturbation, whose wave number is $k$, causes the filamentation of the electron stream in a direction perpendicular to both $k$ and $B_z$. The filamentation amplifies the perturbation of $B_z$. During the growth of $B_z$ an inductive electric field decelerates the electrons. In the Weibel instability the plasma has an anisotropic temperature, and the temperature in the direction perpendicular to both $k$ and $B_z$ is larger than those in other directions.

Consequently the electron energy is converted to the magnetic field energy in the Weibel instability. The linear growth rate $\Gamma$ is obtained in a long wavelength limit [12]:

$$\Gamma = \sqrt{\frac{1}{2}\left[\omega_p^2 + k^2c^2 - \sqrt{(\omega_p^2 + k^2c^2)^2 + 4u_t^2\omega_p^2k^2}\right]} \tag{23}$$

Here $\omega_p$ is an electron plasma frequency, and $u_t$ the electron thermal speed in the direction perpendicular to both $k$ and $B_z$. For example, we use the following parameter values: the

electron number density $10^{18}/\text{cm}^3$, the electron thermal speed in $y$ direction $u_t = 0.25c$, the electron thermal speed in $x$ direction $u_{tx} = 0.0125c$, and $c$ is the speed of light. The excited perturbation wave number is about 0.002cm, and $\Gamma$ obtained by Eq. (23) is $1.20 \times 10^{13}$ /sec. The $\Gamma$ obtained by the simulation is $1.16 \times 10^{13}$ /sec that agrees well with the above theoretical value. Figure 2 presents $B_z$ profiles for several time shots, and Fig. 3 shows an electron particle map in the phase space $v_x$-$v_y$ plane. Figure 3 demonstrates that the initial anisotropic Maxwell distribution function tends to relax to an isotropic distribution function.

## 2.4 Evaluation of computer assisted PIC code development

In order to evaluate the effectiveness of the computer assisted PIC code development, first we present the detail process of the PIC algorithm in this subsection:

(1) Initial preparation: the variables declaration, the particle distribution, initialization of the field variables. Depending on a problem considered, a random number generator may be required.

(2)Time step $\Delta t$ computation: $\Delta t$ is determined from a stability condition, for example, the Courant condition[15].

(3) Interpolation of electromagnetic fields ($\mathbf{E}$ and $\mathbf{B}$) on every particle: find the grid cell to which the particle belongs.

(4) Particle pusher: solve $\mathbf{v}_p$ and $\mathbf{x}$ for every particle.

(5) Impose the boundary condition for the particle position: for example, in the example case presented in the previous section, the periodic boundary conditions are used, therefore particles moving beyond one boundary return from the other boundary.

(6) Obtain a particle density ($\rho_\mathbf{e}$) and/or a current density ($\mathbf{J}$) in every space grid.

(7) Impose the boundary condition for ($\rho_\mathbf{e}$) and ($\mathbf{J}$).

(8) Field solver: integrate field equations.

(9) Impose the boundary condition for $\mathbf{E}$ and $\mathbf{B}$.

(10) Output the computed data.

(11) Repeat (2) to (10) until the specified end condition is satisfied.

In the above steps, the steps (4) and (8) as well as the steps of (3) and (6) are the main part of the PIC code, and are developed by FIDE and GENTRAN except for the array declaration and the declarations like `subroutine`, `return`, and `end` statements, as partially shown in the former subsection. The steps (3) and (6) depend on the interpolation method specified by users. We employed the area weighting method for the steps (3) and (6) based on Eqs. (15)

and (16). One can also prepare several library routines for 1-D, 2-D and 3-D versions of a specified interpolation method. In the step (2) one can specify the $\Delta t$ controller by himself, however the Courant condition $\Delta t \leq \Delta x/max(\mathbf{v}_p, c)$ is rather general in PIC simulations. The $\Delta t$ control routine can be prepared by hand as a library routine and can be combined to the generated part. The steps (5), (7) and (9) are closely related to the used boundary conditions. The periodic and reflecting boundary conditions are popular in many PIC simulations. The routines for the boundary conditions can be prepared by hand. If the boundary conditions are special, users can modify the routine after the computer assisted generation. The data output routine in the step (10) is not general, and users should perform additional preparations for data processing. The step (1) for the initial preparation can have different forms. A routine for the step (1) and a main routine are not large nor general. It is practical to leave these routines to be developed by users. It should be mentioned that the core part of the 1.5-D PIC code was developed by a computer in our approach.

# 3 Discussions and summary

In this report we presented a new approach to develop a PIC code on a computer, and successfully developed an example 1.5-D PIC code, which was used to simulate the Weibel instability. This approach helps in the development of a PIC code in an essential point: the core part of the PIC code can be developed by a computer. Therefore the time-consuming work of a program coding and dubugging can be reduced and optimized[16], and the one can focus on the particular physical problem in hands. We believe that our approach presents the effective method of PIC code development.

In particle simulation, there are several other methods[3]–[6]: a particle-particle particle-mesh one ($P^3M$), a particle-particle one without a space grid, etc. Similar approach can be applied to the development of codes implamenting these methods.

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**Figure Captions**

Fig. 1 A mesh sturucture used in a 1.5D PIC simulation. A sign × shows a particle position in the mesh.

Fig. 2 Magnetic field ($B_z$) profiles for the Weibel instability by using the developed 1.5D PIC code. $B_z$ grows in time. Here $\omega_{pe}$ is an electron plasma frequency.

Fig. 3 Particle maps in the phase space ($V_x, V_y$) for the Weibel instability. In the Weibel instability an anisotropic particle distribution causes the instability and the particle energy is converted to the purely growing magnetic field. According to this conversion, the particle distribution anisotropy is moderated.

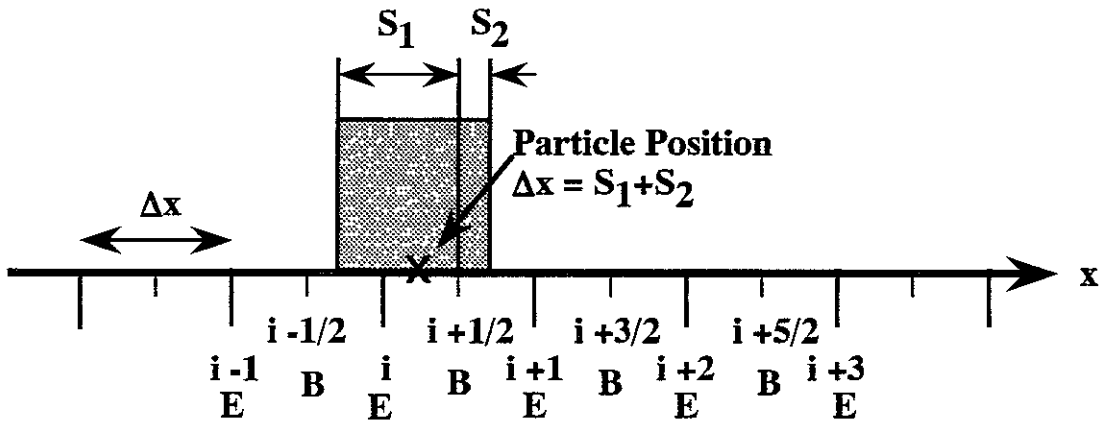
S1
S2
Particle Position
Δx = S1+S2
Δx
x
i -1/2
i +1/2
i +3/2
i +5/2
i -1
E
B
i
E
B
i +1
E
B
i +2
E
B
i +3
E

Fig.1

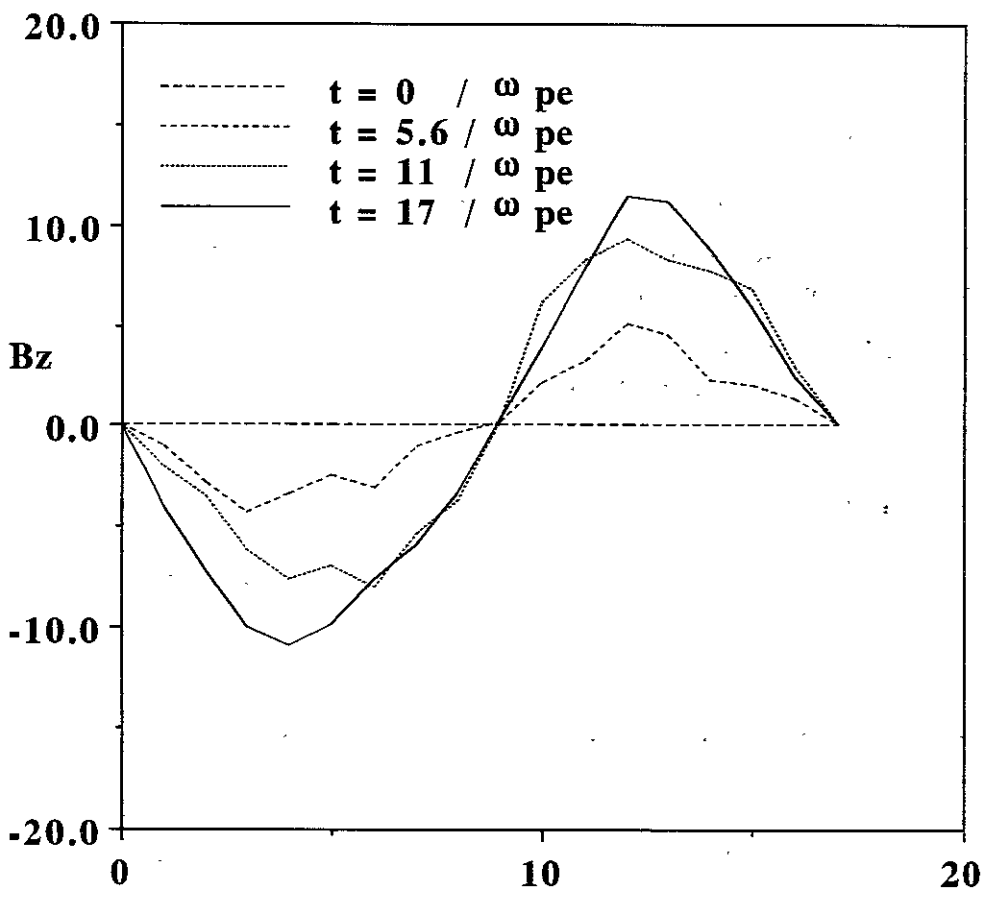
20.0
10.0
0.0
-10.0
-20.0
Bz
0
10
20
X
t = 0 / ω pe
t = 5.6 / ω pe
t = 11 / ω pe
t = 17 / ω pe

Fig.2

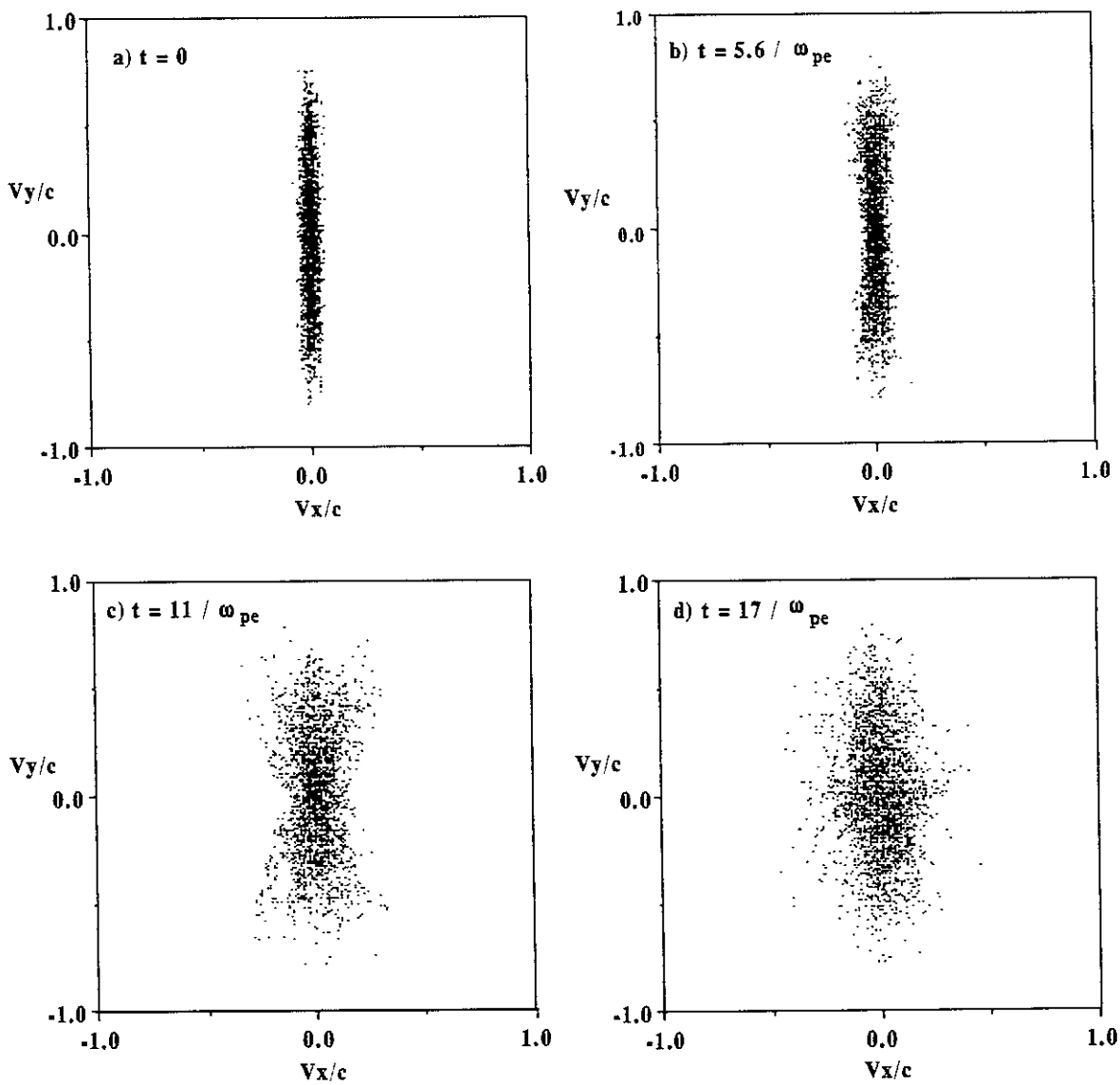


Fig.3

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