MODERN DEVELOPMENT IN PARTICLE SIMULATION

J. C. Adam

Centre de Physique Theorique de L'Ecole Polytechnique
Plateau de Palaiseau - 91128 Palaiseau - Cedex - France

ABSTRACT

We review some of the extension that has been made recently to particle codes to allow them to handle low frequency phenomena economically.

1. INTRODUCTION

Over the past few years several attempts have been made to extend the applicability of particle simulation to low frequency phenomena in large systems. Plasma experiments provide many examples of low frequency phenomena in which kinetic effects are important. These examples can be found in inertial confinement experiments ("laser fusion") as well as in magnetic confinement experiments (Tokamac, Mirrors, etc...). The data shown at this school also show that space plasma simulations will also required the use of such models.

The purpose of this paper is to review the diverse approaches that have been used by different authors to allow the use of large time steps in particle simulation. Let us recall that the stability of standard particle models is subject to the constraint $\omega_p\Delta t<1$ due to the use of explicit difference scheme in the equation of motion of particles as well as in the field equation (for the electromagnetic case, which in fact yield also $\omega_o\Delta t<1$, where ω_o is the frequency of the electromagnetic wave). To eliminate this constraint an implicit formulation must be used. This means that the solution is advanced from time $n\Delta t$ to $(n+1)\Delta t$ by backward time differencing from $(n+1)\Delta t$ to $n\Delta t$ instead of forward marching in an explicit scheme.

The organization of this chapter is the following. In the next section we shall review different implicit algorithms because the choice of an efficient one has to be made at the very beginning of the

H. Matsumoto and T. Sato, Computer Simulation of Space Plasmas,

design of an implicit particle code. In section 3 the moment implicit method will be presented and in section 4 we shall present the so called direct approach.

2. IMPLICIT TIME INTEGRATION

This topic has been discussed in details in the literature [Denavit,1981; Cohen et al.,1982; Barnes er al., 1982]. Our presentation will be based on Cohen et al.[1982] which is the most exhaustive.

An implicit time integration scheme may be thought as a low pass filter : one wishes to have an accurate solution for frequencies lower than some value ω_o and suppress as efficiently as possible modes with frequencies higher than ω_o because they cannot be accurately described with the time step chosen. In this optic the ideal implicit scheme should be like an ideal low pass filter i.e. a step function. Much in the same way a low pass filter approaches the step function when the number of coefficient is increased, the more past information is used in an implicit algorithm the sharper is the transition between frequencies correctly described and the ones that are damped.

2.1 First order damping implicit scheme

Such scheme have used in Mason[1981] and in Brackwill and Forslund [1982]. Because the scheme of Brackwill and Forslund[1982] is presented in another chapter of this book and at the end of section 3 we shall restrict our presentation to the scheme of Mason [1081]. For particle motion it writes :

$$x^{n+1} - x^n = v^{n+1/2}\Delta t,$$

$$v^{n+1/2} - v^{n-1/2} = \theta\Delta t a^{n+1} + (1 - \theta) \Delta t \, a^{*n} \qquad (1)$$

$$a^{*n} = \frac{1}{4} (a^{n+1} + 2a^n + a^{n-1})$$

$$0 < \theta < 1$$

Very general technics can be applied to study the stability of this scheme but a "feeling" of its behaviour can be obtained by applying it to the problem of the harmonic oscillator where acceleration and position are related by $\lambda=-\omega_o^2$. Writing all the quantities in (1) as $A=\exp(-i\omega t)$ one can obtain the dispersion relation of this scheme. This dispersion relation can be solved by expansion for $\omega_o\Delta t << 1$. It gives :

$$\mathrm{Re}\,\frac{\omega}{\omega_o} = + [1 - \frac{1}{24} \omega_o\Delta t^2 [2 + 3\theta(\theta + 1)]],$$

$$\mathrm{Im}\ \frac{\omega}{\omega_o} = -\theta\frac{\omega_o\Delta t}{2}$$

For $\theta=0$ this scheme gives phase errors that are twice as large as the standard leapfrog scheme and no damping. The other extreme is $\theta=1$ which correspond to the fully implicit scheme which yields :

$$\mathrm{Re}\ \frac{\omega}{\omega_o} = \pm[1 - \frac{1}{3}(\omega_o\Delta t)^2\ ] \quad \mathrm{Im}\ \frac{\omega}{\omega_o} = -\frac{\omega_o\Delta t}{2} \tag{3}$$

A change in θ allows a control on the damping rate. It should however be emphasized that $\theta\neq1$ implies the storage of field quantities at two times level for a dependence of the damping rate linear in $\omega_o\Delta t$. We shall see in the next subsection that with the same information schemes with a stronger dependence on $\omega_o\Delta t$ can be built. This is desirable since it provides stronger damping at large value of $\omega_o\Delta t$ while keeping it low for small value of $\omega_o\Delta t$.

2.2 Third order damping implicit scheme.

In this section we shall see that by keeping information on enough time levels it is possible to design implicit schemes, with transfer functions that approximate more closely the ideal low pass filter than the preceding scheme.

The first class of algorithms we shall consider is called class C scheme in Cohen et al.[1982]. For the equations of motion of particles it can be written:

$$v^{n+1/2} - v^{n-1/2} = a^n$$

$$x^{n+1} - x^n = v^{n+1/2} + C_o\Delta t(a^{n+1} - a^n) + C_1\Delta t^2(a^n - a^{n-1})... \tag{4}$$

Insight in the behaviour of this scheme can be gained as in the preceding section by appling it to the problem of the harmonic oscillator. The roots of the dispersion relation for small values of $\omega_o\Delta t$ are given by :

$$\begin{aligned}\mathrm{Re}\ \frac{\omega}{\omega_o} &= \pm\ (1 + \frac{1}{2}\ (\omega_o\Delta t)^2(\frac{1}{12} - C_o - C_1\ ...) + O(\Delta t^3)\\ \mathrm{Im}\ \frac{\omega}{\omega_o} &= -\frac{1}{2}(\omega_o\Delta t)^3(C_1 + 2C_2 +...) + O(\Delta t^4)\end{aligned} \tag{5}$$

At this stage the constants C_o, C_1, C_2 ... have to be chosen to give optimal properties to the scheme. It is obvious from (4) that for $C_o=C_1=C_2=...=0$ one recover the standard explicit leapfrog scheme. The algorithm used by Denavit [1981] for advancing particles is

$$V^{n+1} - V^n = \left(\frac{3}{4}a^{n+1} + \frac{1}{4}a^{n-1} \right)\Delta t$$

$$X^{n+1} - X^n = \left(\frac{3}{4} V^{n+1} + \frac{1}{4} V^{n-1} \right)\Delta t \qquad (6)$$

which can be cast in the form of equations (4) with $C_0=9/16$, $C_1=1/8$, $C_2=1/16$. Then from (5) one has :

$$\mathrm{Re}\ \frac{\omega}{\omega_0} = \pm \left(1 - \frac{(\omega_0\Delta t)^2}{3} + \ldots \right) \qquad \mathrm{Im}\ \frac{\omega}{\omega_0} = - \frac{(\omega_0\Delta t)^3}{8} \qquad (7)$$

Another scheme proposed by Denavit writes :

$$V^{n+1} - V^n = \frac{1}{16} \left(9a^{n+1} + 6a^n + a^{n-1} \right)$$

$$X^{n+1} - X^n = \frac{1}{16} \left(9V^{n+1} + 6V^n + V^{n-1} \right)\Delta t \qquad (8)$$

The corresponding coefficient are $C_0=81/256$, $C_1=14/256$, $C_2=1/256$ and (5) gives

$$\mathrm{Re}\ \frac{\omega}{\omega_0} = \pm \left(1 - \frac{7}{48} (\omega_0\Delta t)^2 \right); \quad \mathrm{Im}\ \frac{\omega}{\omega_0} = - \left(\frac{\omega_0\Delta t}{32} \right)^3 \qquad (9)$$

It is instructive to compare the phase properties and damping properties of (6) and (8). In the second scheme the error on the phase (i.e. the real part of ω) has been reduced by almost a factor 2, but simultaneously the damping of unwanted frequencies has been reduced by four.

In Denavit[1981] another scheme is proposed called "C_1 optimized" scheme which is obtained by maximizing the damping of the least damped mode of the dispersion relation of (1) subject to the constraint C_S ($s \geqslant 2$)=0. One then find that for $C_0=0.302$, $C_1=0.04$:

$$\mathrm{Re}\ \frac{\omega}{\omega_0} = \pm \left(1 - 0.13\ (\omega_0\Delta t)^2 \right) \qquad \mathrm{Im}\ \frac{\omega}{\omega_0} = -0.02(\omega\Delta t)^3) \qquad (10)$$

which is not very different of (9) for less storage of information. A last scheme proposed in Denavit[1981] is the "D_1 scheme" which is based on a second order stiffly stable scheme given by Gear[19**] for first order differential equation. It writes :

$$X^{n+1} - X^n = V^{n+1/2}\Delta t$$

$$V^{n+1/2} - V^{n-1/2} = 1/2a^{n+1}\Delta t + 1/2(V^{n-1/2} - V^{n-3/2}), \qquad (11)$$

Solving the dispersion the dispersion relation for a harmonic oscillation as precedingly yields :

$$\mathrm{Re}\left(\frac{\omega}{\omega_o}\right) = \pm\left(1 - \frac{11}{24}(\omega_o\Delta t)^2\right); \quad \mathrm{Im}\left(\frac{\omega}{\omega_o}\right) = 1/2\,(\omega_o\Delta t^3) \qquad (12)$$

Comparison of (12) and (7) shows that the damping rate of high frequencies ($\omega_o\Delta t << 1$) in this scheme is 50 times larger than for the optimized C_1 scheme. However the phase error for ($\omega_o\Delta t << 1$) is also multiply by 4 and becomes much larger than in the case of the standard explicit leapfrog scheme. This means that if one limits the phase error to some maximum value for a given frequency of interest a time step smaller by a factor 2 has to be used. This in turn reduces the damping by 8. Even under this constraint the D_1 scheme remains superior to C_1 scheme but then it becomes twice as expensive.

A recursive formulation of (11) given in Barnes[1982] makes it very attractive in term of storage requirement. It writes:

$$x^{n+1} = x^n + v^{n+1/2}\Delta t$$

$$v^{n+1/2} = v^{n-1/2} + 1/2\bar{a}_n$$

$$\bar{a}^n = 1/2\,(a^{n+1} + a^{n-1}) \qquad (13)$$

The equivalence of (11) and (13) can be readily shown by factoring equation (15a) of Denavit[1981] into two equations (A.B. Langdon private communication);

- the first one corresponds to a low pass filtering, it is the introduction of $\bar{a}$
- a leapfrog step define by the two first of (13).

This scheme is probably one of the most attractive in term of global behaviour (i.e. : phase error, damping, storage requirement)

The schemes that have been described in this section are not directly applicable to a particle simulation. A fully self-consistent implicit particle code would require solving iteratively the system of equations describing the N particles plus the field equations. Such an algorithm is prohibited by storage requirement as well as cost of going iteratively through particle data. Methods have to be devised that uncoupled implicit equations for particle and implicit equations for field.

3. MOMENT METHOD

3.1 Electrostatic case

The essence of the method outlined in Mason[1981] and Cohen et al.[1982] is that the microscopic (particle) and macroscopic (moment equations) representation of plasmas should not differ significantly over a time because field equations depend only on the two first

moment i.e., density and current. The method devised by R. Mason uses the first order damping described in the preceding section : Fluid equations are first integrated using :

$$\tilde{J}_\alpha^{n+1/2} = \tilde{J}_\alpha^{n-1/2} - \frac{1}{m_\alpha} \frac{\partial P_\alpha}{\partial x} - q_\alpha n_\alpha^n E^* \Delta t \qquad (14)$$

$$\tilde{n}_\alpha^{n+1} = n_\alpha^n - \frac{\partial \tilde{J}_\alpha^{n+1/2}}{\partial x} \Delta t \qquad (15)$$

α denotes the particles specifies. E^* is the same linear combination as (1). J_α and P_α are obtained from the particle data by :

$$J_\alpha = \Sigma_p V_{p,\alpha} \qquad P_\alpha = m\Sigma_{\alpha p} V_{p,\alpha}^2$$

Poisson equation is then integrated using the predicted value of $\tilde{n}^{n+1}$. Note however that the integration of (14) necessitates the knowledge of E^* which is a function of $\tilde{E}^{n+1}$ which in turn is a function of $\tilde{n}^{n+1}$

$$\tilde{E}^{n+1} = 4\pi \int_0^x \Sigma_\alpha q_\alpha \tilde{n}_\alpha^{n+1} dx + E^{n+1}(0) \qquad (16)$$

Substitution of (14, 15) into (16) yields an equation for $\tilde{E}^{n+1}$ which can be explicitly in 1D (see Mason[1981]). In a 2D system, (16) must remain in differential form yielding an equation of the following type :

$$\nabla \tilde{E}^{n+1} = f(n^n, J^n, E^n, E^{n-1}) + g(\tilde{E}^{n+1}) \qquad (17)$$

In finite difference representation (17) is a matrix equation as the usual Poisson equation but its coefficients are no longer constant. A method for solving that kind of equation is described in Brackwill and Forslund [1982] for the same algorithm.

It should also be pointed that a difficulty arise due to the pressure gradient term. The only quantity that one can build explicitly at the end of a time step is obtained from particle data with positions define at level n and velocities at level n-1/2. This explicit pressure term introduces a stability condition $\Delta t < \Delta x/V_T$ where V_T is thermal velocity of the plasma. In Mason [1981] this difficulty is alleviated by the use of a predicted value of the pressure term obtained by a local adiabatic approximation in the following way :

- $n_e^{n-1/2}$ is accumulated at half time step
- n^* is built as $n_i(n) - (1/4\pi e)(\partial E^*/\partial x)$ then :
- $P_\alpha = p^{n-1/2}(n^*/n_e^{n-1/2})^3$

this pressure is then used to integrate equation (16) and an iteration over E^* is necessary. In Brackwill and Forslund [1982] a fully implicit pressure term define as $p=n^{n+1}T^n$ is used for stability.

After the E^{n+1} field has been obtained particles are advanced

using Eq. (1) and a new cycle initiated.

Denavit [1981] approach to the same problem is slightly different. One start again with fluid equations

$$\frac{\partial n_\alpha}{\partial t} = - \nabla(n_\alpha U_\alpha) \tag{17a}$$

$$\frac{\partial}{\partial t} (n_\alpha U_\alpha) = \frac{q_\alpha}{m_\alpha} n_\alpha E - \nabla \cdot P_\alpha \tag{17b}$$

$$\nabla \cdot E = 4\pi \Sigma_\alpha n_\alpha e_\alpha \tag{17c}$$

In 1D (17a) and (17c) can be combine to give

$$\frac{\partial E}{\partial t} = 4\pi e \sum_\alpha n_\alpha u_\alpha e_\alpha \tag{18}$$

the algorithm define by equation (6) is then applied to the resolution of the system of equations (17) and (18). It becomes :

$$(n_\alpha u_\alpha)^{n+1} = n_\alpha u_\alpha^n + \frac{3\Delta t}{4} (\delta_\alpha n_\alpha E + F_\alpha)^{n+1} + \frac{\Delta t}{H} (\delta_\alpha n_\alpha E + F_\alpha)^{n-1} \tag{19a}$$

$$E^{n+1} = E^n + \frac{3}{4}\Delta t \Sigma n_\alpha u_\alpha e^{n+1} - \frac{\Delta t}{H} \Sigma n_\alpha u_\alpha e^{n-1}_\alpha \tag{19b}$$

where $F_\alpha = -\nabla \cdot P_\alpha$ and δ_α depends on the charge and mass of each particle specie.

From (19a) and (19b) an explicit expression for the predictor field at E^{n+1} is obtained that depend only on fluid quantities at level n and n-1 except for the pressure term which appear at time level (n+1). This imply that an iterative procedure has to be apply to obtain the field. Fluid quantities are obtained as in Mason method from the particle including the pressure so that the iteration must involve the particle. At each time step the value needed to start the iteration are the ones obtained at the preceding time level. At the end of the iteration Poisson equation is solved to insure error in the resolution of equation (18) do not accumulate over time. According to Denavit the convergence of the scheme is very rapid and a time step can very often be used without iteration. However the only way to ascertain this point is to do at least two iterations. This scheme should be more accurate than the preceding one for the following reasons:

- It uses a third damping order time integration scheme.
- Pressure terms are collected at each level of iteration from particle data (Note that here also the pressure is implicit for stability).

On the side of the drawbacks :

- One has to iterate through particle data which may be expensive.
- Many quantities must be stored at two times levels which is very expensive in term of memory requirement and probably prohibit the use of this scheme in 2D.

3.2 Electromagnetic case.

This topic being developed in another chapter of this book we quote it here only for completeness. The only code that has been built is the one of Brackbill and Forslund use a first order implicit scheme for Maxwell equations which writes

$$B^{n+1} - B^n = - c(\nabla X E^{n+\theta})\Delta t$$

$$E^{n+1} - E^n = c(\nabla X B^{n+\theta})\Delta t - 4\pi J^{n+1/2}\Delta t$$

$$\nabla \cdot E^{n+\theta} = 4\pi N^{n+\theta}$$

$$\nabla \cdot B^n = 0 \qquad (20)$$

$E^{n+\theta}$ is defined by : $E^{n+\theta}=\theta E^{n+1}+(1-\theta)E^n$ and particles an advanced using

$$X^{n+1} = X^n + V^{n+\theta}\Delta t$$

$$V^{n+1} = V^n \pm \frac{q}{m} [\, E^{n+\theta} + \frac{V^{n+1/2} \times B^n}{\Delta t} \,]\Delta t \qquad (21)$$

Plasma density at level $N^{n+\theta}$ and current density at time $J^{n+1/2}$ are obtained from momentum equation according to the scheme

$$N^{n+\theta} = N^n - \nabla \cdot J^{n+\Gamma}(\theta\Delta t)$$

$$J^{n+1/2} = J^n - \nabla \cdot \frac{J^{n+1/2}\ J^n}{N^n} (\Gamma\Delta t)$$

$$+ \frac{q}{m}\ N^{n+1/2}\ E^{n+\theta} + \frac{J^{n+1/2} \times B^n}{c}\ \Gamma\Delta t$$

$$- q_s\ \nabla \cdot \tilde{P}(\Gamma\Delta t) \qquad (22)$$

The density N^n and the current J^n are collected from particle according to the standard definition

$$N^{(n)}(x) = q_p \Sigma_p\ h(X - x_p^n)$$

$$J^{(n+1/2)}(x) = q_p \Sigma_p V^{n+1/2}\ h(X - x_p^{n+1/2})$$

where the summation extends over all the particles p and h is the particle shape function.

The pressure term that appears in equation (22) has to be evaluated implicitly for nonlinear stability. The choice made is $p^{n+1} = N^{n+1}T^n$. The system of equations defined by (20) and (22) is solved iteratively and once convergence as been obtained particles are advanced using (21). Extensive discussion of this algorithm is given in Brackwill and Forslund [1982].

4 DIRECT METHOD

4.1 Electrostatic case

Another kind of approach has been used in Cohen et al. [1982], Friedman et al.[1981] and Langdon et al. [1981]. The method is called direct because moment equations are not used as auxiliary equations. In particular the kinetic stress tensor is not collected. The potential cost of the algorithm is that it can be necessary to iterate through the particles. The algorithm can be described as follows. One start with the D_1 scheme of section 1 for particle motion

$$v^{n+1/2} - v^{n-1/2} = 1/2\, a^{n+1}\Delta t - 1/2\,(v^{n-1/2} - v^{n-3/2}) \qquad (23)$$

The value x^{n+1} of equation (23) can be written as

$$x^{n+1} = 1/2\, a_{n+1}\Delta t^2 + x^{n+1(0)}$$

$$x^{n+1(0)} = x^n + v^{n-1/2}\Delta t - 1/2\,(v^{n-1/2} - v^{n-3/2}) \qquad (24)$$

i.e. as the position obtained from the free streaming motion plus a displacement due to the acceleration. The basis of the direct method is:

1) Compute the charge density $\rho^{(0)}$ obtained from free streaming motion of particle. Since it depends only on quantities defined at t=n or earlier, it is known.

2) Evaluate the change $\delta\rho$ due to the displacement of particle from particle from $x^{n+1(0)}$ to x^{n+1} i.e. $\delta x=(x^{n+1(0)}-x^{n+1})$. As shown in Langdon [1979]. this increment $\delta\rho$ is

$$\delta\rho = - \nabla\cdot[\, \rho^{(0)}_{n+1}(x)\, \delta x(x)] \qquad (25)$$

3) Assume that δx is the same for all the particle having the same $x^{n+1(0)}$. This means the electric field is assumed to be sufficiently uniform spatially to insure that dispersion in velocity is unimportant. Then

$$\delta X \sim 1/2\, \frac{q}{m}\, E^{n+1}(x)\Delta t^2 \qquad (26)$$

4) Replace (26) into (25) to obtain $\delta\rho$

$$\delta\rho = -\nabla\left[\frac{q}{2m} \rho^{(0),n+1}(x)\Delta t^2 E^{n+1}(x) \right]$$

$$= -\nabla\left[\omega_p^2(x)^{(0),n+1} \frac{\Delta t^2}{2} E^{n+1}(x) \right] \qquad (27)$$

5) Solve the Poisson equation at time (n+1)

$$E^{n+1}(x) = \rho^{n+1}(x) = \rho^{(0),n+1} + \delta\rho$$

$$= \rho^{(0),n+1}(x) - \nabla\left(\omega_p^2 (x) \frac{\Delta t^2}{2} E^{n+1}(x) \right.$$

$$\nabla\left[1 + \frac{\omega_p^2 (x)\Delta t^2}{2} \right] E^{n+1}(x) = \rho^{(0),n+1} \qquad (28)$$

the term $1+(\omega_p^2\Delta t^2)/2$ in equation (28) acts as an effective suceptibility which screens the high frequencies. In principle an iterative refinement of the value of the electric field obtained from equation (28) is possible simply by improving the value of the guess $\rho^{(0)}$ (see Langdon et al., 1982].).

At this stage it becomes easy to explain the relationship between the direct and the moment approaches. This relationship has been observed by Mason by eliminating $J^{n+1/2}$ between Eq.15b and 15a and replacing E^* by E^n. Poisson equation then becomes

$$\nabla\cdot E_{n+1} + \frac{q}{m} \Delta t^2 \nabla\cdot(\rho_n E_{n+1}) = \rho_n - \Delta t\nabla\cdot\left(J_{n-1/2} - \frac{q\Delta t}{m}\nabla P_n \right) \qquad (29)$$

the right hand side of this equation is obtained by setting $E^* = 0$ in (14) and therefore correspond to the $\rho^{n+1(o)}$ approximation of the direct method.

While the direct approach is conceptually very simple its practical implementation is very sensitive to the details of the difference schemes, so that it is useful to reformulate the basic algorithm in term of finite size particle.

The density in each cell is defined as

$$\rho_j^{n+1} = \frac{q}{\Delta X} \Sigma_p S(X_p^{n+1} - X_j) \quad , \qquad (30)$$

where p is a summation over particles. The free streaming approximation to X_p^{n+1} is

$$\tilde{X}^{n+1(0)} = X_p^n + V_p^n\Delta t \ .$$

then we may write

$$S(X_p^{n+1} + X_j) = S(X_p^{n+1,(0)} - X_j) + (X_p^{n+1} + X_p^{n+1,(0)}) \frac{\partial S}{\partial \tilde{x}_k} \qquad (31)$$

Note that for a linear spline this expansion is exact as long as the particle does not change of cell during the iteration.

Finally one must evaluate $(X_p^{n+1}-X_p^{n+1,(0)})$ which is done using:

$$X_p^{n+1} - X_p^{n+1,(0)} = \frac{q}{m}\Delta t^2 E^{n+1}(X_p^{n+1}) \qquad (32a)$$

$$\sim \frac{q}{m}\Delta t^2 \Sigma_i S(X_p^{n+1(0)} - X_i) E_i^{(n+1)} \qquad (32b)$$

Note that (32b) is a good approximation of (32a) only if $q E\Delta t^2/mL=\omega_b^2\Delta t^2 \ll 1$, where L is a typical scale length and ω_p is the bounce frequency in the E field for the corresponding scale length. From (30), (31) and (32) one can finally obtain the finite difference form of Poisson equation which writes

$$(\phi_{j+1} - 2\phi_j + \phi_{j-1})^{n+1} = \rho_j^{(0)n+1} - \Sigma_i W_{ij}(\phi_{i+1} - \phi_{i-1})/2\Delta X \qquad (33)$$

where $$\rho_j^{(0),n+1} = \frac{q}{\Delta X}\Sigma_p S(X_p^{(0),n+1} - X_j)$$

and

$$W_{ij} = \frac{q^2\Delta t^2}{m\Delta X} \Sigma_p S(X_p^{(0),n+1} - X_i) \frac{\partial S(X_p^{0,n+1} - X_i)}{\partial X_p} \qquad (34)$$

For a linear shape function W_{ij} is zero if $|i-j|>1$ and since $\partial S/\partial X_p$ is $\pm(1/\Delta X)W_{ij}$ is identical to $\Sigma_p S(X_p^{(0),n+1})$ within a numerical factor. This means that $\rho^{(0),n+1}$ and W_{ij} can be collected simultaneously by no more operations than in a standard particle code. However the resolution of Poisson equation becomes more complicated because (33) is no longer a tridiagonal system with constant coefficient.

4.2 Electromagnetic case.

An extension of the direct method to the electromagnetic case has been suggested by A. B. Langdon [1983] at the 10th numerical simulation meeting. It used D1 scheme for both particles and fields. Equations for particles in the electromagnetic case write

$$X^{n+1} - X^n = V^{n+1/2}\Delta t,$$

$$V^{n+1/2} - V^{n-1/2} = \bar{a}^n\Delta t + (V^{n+1/2} + V^{n-1/2}) \times \frac{qB^2\Delta t}{2mc} \quad , \qquad (35)$$

$$\bar{a}_n = 1/2\bar{a}^{n-1} + \frac{q}{m} E^{n+1}(X^{n+1}) \quad .$$

$$X_{n+1} - X_n = V^{n+1/2}\Delta t$$

$$V^{n+1/2} - V^{n-1/2} = \bar{a}_n^n \Delta t + \left(V^{n+1/2} + V^{n-1/2} \right) \times \frac{qB^2 \Delta t}{2mc} \quad .$$

$$\bar{a}^n = 1/2\bar{a}^{n-1} + \frac{q}{m} E^{n+1}(X^{n+1}) \quad .$$

An approximation $X^{(0),n+1}$ $V^{(0),n+1/2}$ can be obtained for example by

$$X^{(0),n+1} - X^n = V^{(0)n+1/2}\Delta t$$

$$V^{(0),n+1/2} - V^{n-1/2} = 1/2\bar{a}^{n-1}$$

The current at $J^{n+1/2}$ can then be split into two contribution

$$J^{n+1/2} = J^{(0),n+1/2} + \delta J$$

with

$$J^{n+1/2}(X) = \sum_p q_p V_p^{n+1/2} S\left(X - X_p^{n+1/2} \right)$$

$$J^{(0),n+1/2}(X) = \sum q_p V^{(0),n+1/2} S\left(X - X_p^{(0),n+1/2} \right)$$

δJ can then be evaluated as a function of known quantities and of the value of the electric field at level E^{n+1} by expanding the shape function around $X^{(0),n+1/2}$. The simplest differencing scheme (which assumes again that the displacement $\delta X = (X_p^{n+1/2} - X_p^{(0),n+1/2})$ is the same for all the particle in one cell yield

$$\delta J^{n+1/2} = \left(1/4\rho^{(0)} \frac{q}{m} \Delta t \right) \left(I + R \right) \cdot E^{n+1}$$

$$+ \frac{1}{8} \frac{q}{m} (\Delta t)^2 \nabla \times J^{(0)n+1/2} \times \left(I + R \right) \cdot E^{n+1}$$

I and R will be defined later. Note that as in Brackbill and Forslund scheme the magnetic term has been kept centered. This is essential for good energy conservation. Equation for the fields are:

$$c\left(\nabla \times B^{n+1/2} \right) = J^{n+1/2} + \frac{E^{n+1} - E^n}{t}$$

$$c\left(\nabla \times E^n \right) = \frac{B^{n+1/2} - B^{n-1/2}}{\Delta t}$$

$$E^n = \frac{1}{2} \left(E^{n+1} = E^{n-1} \right)$$

B^n necessary to integrate equations (35) is obtained by extrapolation. The spirit is the same as for the electrostatic case

one splits the current necessary in (36) into two parts

$$J^{n+1/2} = J^{(0),n+1/2} + \delta J \tag{37}$$

The contribution $J^{(0),n+1/2}$ is obtained by an extrapolation procedure i.e..

$$J^{(0),n+1/2} = \sum_p q_p V^{(0),n+1/2} S(X - X_p^{(0),n+1/2})$$

where $X^{(0)}$ and $V^{(0)}$ are obtained from

$$X^{(0),n+1} - X^n = V^{(0),n+1/2}\Delta t$$

$$V^{(0),n+1/2} - V^{n-1/2} = 1/2\bar{a}^{n-1}$$

When $J^{n+1/2}$ is defined by

$$J^{n+1/2} = \Sigma_p q_p V_p^{n+1/2} S(X - X_p^{n+1/2}) \quad .$$

δJ is obtained by including in it every thing that is not in $J^{(0),n+1/2}$. This is done by writing

$$V^{n+1/2} \text{ as } V^{(0),n+1/2} + \delta V$$

$$X^{n+1/2} \text{ as } X^{(0),n+1/2} + \delta X$$

and carrying out the necessary expansions. The simplest differencing scheme (which again assumes that the displacement $\delta X=(X_p^{n+1/2}-X_p^{(0),n+1/2})$ is uniform for all te particle within one cell yields

$$\delta J^{n+1/2} = (1/4\rho^{(0)}\frac{q}{m}\Delta t)(I + R)\cdot E^{n+1} \tag{38}$$

$$- \frac{1}{8}\frac{q}{m}(\Delta t)^2\nabla \times J^{(0),n+1/2} \times (I + R)\cdot E^{n+1}$$

I is an identity matrix, while R is a rotation matrix by $-qB^n\Delta t/mc$. When (37) is substitute in (36) with this expression for δJ one obtains a closed system for E^{n+1} and $B^{n+1/2}$. The scheme then proceed in the same way as for the electrostatic case.

5. CONCLUSIONS

We hope to have shown that there are lots of possibilities that have been suggested to overcome the time step limitation imposed by the standard particles method. There is still a great deal of effort needed to make some of the approaches practical, but usually when a code is written it becomes difficult to change it, so that the choice of the algorithm deserve some reflexion....

REFERENCES

DENAVIT, J., J. Comput. Phys., 42, 337, 1981.
Cohen, B..I., LANGDON, A. B., FRIEDMAN, A., J. Comput. Phys., 46, 15, 1982.
BARNES, D. C., KAMIMURA, T., LEBOEUF, J. N., TAJIMA, T., Institute for fusion studies internal report IFSR # 68, 1981.
Gear, C. W., Numerical Initial Value Problems in Ordinary differential equations (Prentice Hall).
MASON, R. J., J. Comput. Phys., 41, 233, 1981.
BRACKBILL, J. V. and FORSLUND, D.,W., J. Comput. Phys., 46, 271, 1982.
FRIEDMAN, A., LANGDON, A. B., COHEN, B. I., Comments on Plasma Physics and control Fusion 6, 225, 1981.
LANGDON, A. B., COHEN, B. I., FRIEDMAN, A., Lawren Livermore Laboratory Univ. of California, Report UCRL 86350, 1982.
LANGDON, A. B., in proceeding of the 10th conference on Numerical of Plasma 1983.
LANGDON, A. B., J. Comput. Phys., 30, 202, 1979.