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A Deterministic Particle Method for Transport Diffusion Equations: Application to the Fokker–Planck Equation

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This paper deals with a general deterministic particle method for the approximation of transport-diffusion equations. The method is applied to a Fokker–Planck equation which models fast ion transport. © 1989 Academic Press, Inc.

1. INTRODUCTION

It is well known that particle methods are a powerful tool for the simulation of numerous phenomena involved in such diversified areas as astrophysics, plasma physics, semi-conductor physics, and hydrodynamics (for example, see [1–3]).

From a mathematical point of view these methods can be interpreted as numerical approximation methods for transport equations.

This paper is not intended to explain in detail the principles of these methods. For more details on this, we refer to published works [1–4], which also give convergence analysis. Particle methods are particularly suitable for the treatment of transport terms; this is not the case for diffusion terms. Several authors propose to treat these terms by Monte Carlo methods [5, 6]. Another possibility is to assign a time-varying "weight" to each particle to simulate the diffusion term effect [7]. A third possibility, which is dealt with in this paper, is to consider diffusion terms as nonlinear transport terms, thus following an idea developed in [8–10]. The problem is then reduced to a transport equation which can be resolved by general techniques of particle approximations.

First we study the following diffusion equation:

$$\frac{\partial f}{\partial t} - \sigma \frac{\partial^2 f}{\partial x^2} = 0$$

$$f(x, 0) = f_0(x)$$

$$(x, t) \in R \times [0, T].$$

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We supply a stability criterion and compare the exact solution with the approximated one. We then study the equation:

$$\frac{\partial f}{\partial t} - \sigma \frac{\partial}{\partial x}\left((1-x^2)\frac{\partial f}{\partial x}\right) = 0$$

$$f(x, 0) = f_0(x)$$

$$(x, t) \in [-1, 1] \times [0, T].$$

We explain how the approximation of this equation by a particle method extends f by symmetry conditions in the neighbourhood of 1 and -1. This procedure, which is specific to particle approximation, is not related to the usual boundary condition problem.

Naturally, this particle method was not developed to compete with finite difference or finite element methods which remain, at present, most suitable to solve diffusion equations. As a matter of fact, the treatment of boundary conditions with particle methods is not yet fully clarified.

However, we can generalize the use of particle methods to the case of transport-diffusion equations for which the diffusion term is not dominant. We are especially concerned with the transport of fast ions. This phenomenon is modelled with a Fokker–Planck equation of the type

$$\frac{\partial f}{\partial t} + \mu v \frac{\partial f}{\partial x} + \frac{\partial}{\partial v}(a(v) f) + \frac{\partial}{\partial \mu}\left((1-\mu^2)\, c(v) \frac{\partial f}{\partial \mu}\right) = 0$$

$$f(x, v, \mu, 0) = f_0(x, v, \mu),$$

$a(v)$ and $c(v)$ being given functions.

We see that if the diffusion term

$$\frac{\partial}{\partial \mu}\left((1-\mu^2)\, c(v) \frac{\partial f}{\partial \mu}\right)$$

is taken into account, it appears as a correction to the fast ion equations of motion considered in phase space:

$$\dot{x} = \mu v$$

$$\dot{v} = a(v)$$

$$\dot{\mu} = 0.$$

In other words, we can say that the diffusion term acts as a self-consistent force field. We deal with the example of protons and alpha particles slowing down in boron–deuterium–tritium and deuterium–tritium plasmas [11].

2. Treatment of Diffusion Equation

2.1. *Formulation*

The 1-dimensional diffusion equation can be written

$$\frac{\partial f}{\partial t} - \sigma \frac{\partial^2 f}{\partial x^2} = 0,$$
$$f(x, 0) = f_0(x),$$
$$(x, t) \in R \times [0, T],$$

σ being a given constant.

We can further assume: $f > 0$, in which case this diffusion equation can be written in the form of a nonlinear transport equation:

$$\begin{aligned} &\frac{\partial f}{\partial t} + \frac{\partial}{\partial x}(F(f)f) = 0, \\ &f(x, 0) = f_0(x), \\ &(x, t) \in R \times [0, T], \end{aligned} \tag{1}$$

with

$$F(f) = -\sigma \frac{1}{f} \frac{\partial f}{\partial x} = \sigma \frac{\partial}{\partial x}\left(\mathrm{Log}\left(\frac{1}{f}\right)\right).$$

Let $F_t(\xi) = x(\xi, t)$ be the transformation that associates to each ξ the unique solution of the characteristic differential equation associated with (1),

$$\begin{aligned} &\dot{x}(t) = F(f(x(t), t)), \\ &x(0) = \xi, \end{aligned} \tag{2}$$

and let

$$J(\xi, t) = \frac{\partial x}{\partial \xi}(\xi, t)$$

be the Jacobian of this transformation.

Equation (1) can then be written, in a Lagrangian point of view,

$$\frac{1}{J(\xi, t)} \frac{d}{dt}(J(\xi, t)\, f(x(\xi, t), t)) = 0,$$
$$f(x(\xi, 0), 0) = f_0(\xi),$$

from which we deduce

$$J(\xi, t)\, f(x, t) = f_0(\xi). \tag{3}$$

A "weak" formulation equivalent to this relation consists in finding a function $f = f(x)$ such as to yield, for any function sufficiently regular and with compact support,

$$\int_R f(x,t)\,\varphi(x)\,dx = \int_R f_0(\xi)\,\varphi(x(\xi,t))\,dx. \tag{4}$$

2.2. *Particle Approximation*

The basic principle of particle methods is to approximate the function f_0 by a linear combination of Dirac functions [4, 12]. By means of a numerical integration formula, we can assign for any function ψ which is sufficiently regular and with compact support,

$$\int_R f_0(\xi)\,\psi(\xi)\,d\xi = \sum_{j=1}^{N} \omega_j f_0(\xi_j)\,\varphi(\xi_j), \tag{5}$$

from which we deduce a "weak" approximation of f_0,

$$\tilde{f}_0(\xi) = \sum_{j=1}^{N} \omega_j f_0(\xi_j)\,\delta(\xi - \xi_j).$$

Replacing f_0 by $\tilde{f}_0$ in Eq. (4) we obtain

$$\int_R f(x,t)\,\varphi(x)\,dx = \sum_{j=1}^{N} \omega_j f_0(\xi_j)\,\varphi(x(\xi_j,t)),$$

which yields a "weak" approximation $\tilde{f}$ of f,

$$\tilde{f}(x,t) = \sum_{j=1}^{N} \omega_j f_0(\xi_j)\,\delta(x - x_j(t)),$$

where $x_j(t) = x(\xi_j, t)$ is the solution of the differential equation

$$(1 \leqslant j \leqslant N)\begin{cases} \dot{x}_j(t) = F(f(x_j(t),t)) = \sigma \dfrac{\partial}{\partial x}\left(\operatorname{Log}\left(\dfrac{1}{f(x_j(t),t)}\right)\right) \\ x_j(0) = \xi_j. \end{cases} \tag{6}$$

We obtain an approximation in the usual sense of f by replacing $\tilde{f}$ by its convolution product $\hat{f} = \tilde{f} * \zeta_\varepsilon$ with a "shape" function ζ_ε, i.e., an even function with a support $[-\varepsilon, \varepsilon]$ and such that $\int \zeta_\varepsilon(x)\,dx = 1$. Then we have

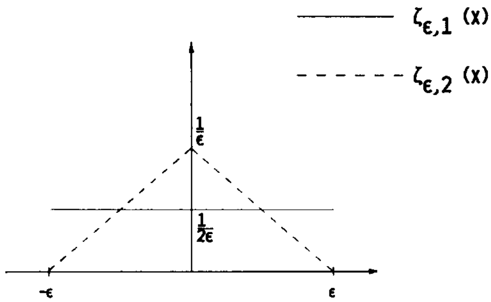
$$\hat{f}(x,t) = \sum_{j=1}^{N} \omega_j f_0(\xi_j)\,\zeta_\varepsilon(x - x_j(t)).$$

Examples of "shape" functions are given in [1, 4]. We mainly use the "gate" function,

$$
\begin{aligned}
&\zeta_{\varepsilon,1}(x)=\frac{1}{2\varepsilon}, && |x|\leqslant\varepsilon,\\
&\zeta_{\varepsilon,1}(x)=0, && \text{otherwise,}
\end{aligned}
\tag{7}
$$

and the "hat" function,

$$
\begin{aligned}
&\zeta_{\varepsilon,2}(x)=\frac{\varepsilon-|x|}{\varepsilon^2}, && |x|\leqslant\varepsilon,\\
&\zeta_{\varepsilon,2}(x)=0, && \text{otherwise.}
\end{aligned}
\tag{8}
$$



Let us assume ζ_ε is differentiable; if we substitute $\hat{f}$ for f in the expression of the nonlinear term $F(f)=\sigma(\partial/\partial x)(\mathrm{Log}(1/f))$ we obtain a "natural" evaluation of $F(f)$ which is:

$$
F(\hat{f}(x_j(t),t)=-\sigma\,\frac{\sum_{k=1}^{N}\omega_k f_0(\xi_k)\,\zeta'_\varepsilon(x_j(t)-x_k(t))}{\sum_{k=1}^{N}\omega_k f_0(\xi_k)\,\zeta_\varepsilon(x_j(t)-x_k(t))}.
$$

Equations (6) then appear as a coupled differential system, for $1\leqslant j\leqslant N$,

$$
\begin{aligned}
&\dot{x}_j(t)=-\sigma\,\frac{\sum_{k=1}^{N}\omega_k f_0(\xi_k)\,\zeta'_\varepsilon(x_j(t)-x_k(t))}{\sum_{k=1}^{N}\omega_k f_0(\xi_k)\,\zeta_\varepsilon(x_j(t)-x_k(t))}\\
&x_j(0)=\xi_j.
\end{aligned}
\tag{9}
$$

We observe that this type of approximation preserves the integral of f throughout time:

$$
\int_R \hat{f}(x,t)\,dx=\int_R f_0(\xi)\,d\xi=\sum_j \omega_j f_0(\xi_j).
$$

Regarding the convergence properties of this type of approximation the reader is referred to [4].

2.3. Discretization in Time and Stability

The differential equation system (9) is approximated by an explicit Euler scheme:

$$\frac{x_j^{n+1}-x_j^n}{\Delta t}=-\sigma\frac{\sum_{k=1}^N \omega_k f_0(\xi_k)\,\zeta_\varepsilon'(x_j^n-x_k^n)}{\sum_{k=1}^N \omega_k f_0(\xi_k)\,\zeta_\varepsilon(x_j^n-x_k^n)}.$$

Let us suppose that Eq. (1) is discretized by a finite difference scheme with steps of Δx, Δt for $(x, t)\in[-L, L]\times[0, T]$ ($2L=N\,\Delta x$ and $T=M\,\Delta T$). The Courant–Friedrichs–Levy (CFL) stability condition would then be written

$$\underset{1\leqslant j\leqslant N}{\mathrm{Max}}\,(\underset{1\leqslant n\leqslant M}{\mathrm{Max}}\,|F(f(j\,\Delta x, n\,\Delta t))|)\leqslant\frac{\Delta x}{\Delta t}.$$

By analogy with this criterion, it seems suitable to assume

$$\underset{1\leqslant j\leqslant N}{\mathrm{Max}}\,(\underset{1\leqslant n\leqslant M}{\mathrm{Max}}\,|F(f(x_j^n, n\,\Delta t))|)\leqslant\frac{\varepsilon}{\Delta t}.$$

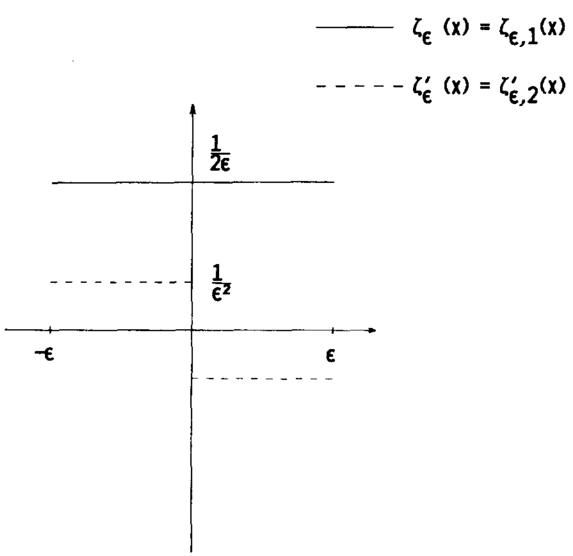
In practice this criterion means that a particle may not cover a length greater than ε during one time step. We then obtain

$$\sigma\underset{1\leqslant j\leqslant N}{\mathrm{Max}}\left(\underset{1\leqslant n\leqslant M}{\mathrm{Max}}\left(\left|\frac{\sum_{k=1}^N \omega_j^0 f_0(\xi_j)\,\zeta_\varepsilon'(x_j^n-x_k^n)}{\sum_{k=1}^N \omega_j^0 f_0(\xi_j)\,\zeta_\varepsilon(x_j^n-x_k^n)}\right|\right)\right)\leqslant\frac{\varepsilon}{\Delta t}. \tag{10}$$

For the sake of simplicity, let us assume that (see definitions (7) and (8)):

$$\zeta_\varepsilon=\zeta_{\varepsilon,1}\qquad\text{and}\qquad\zeta_\varepsilon'=\zeta_{\varepsilon,2}'.$$

This leads to



Let $\mathcal{N}_j^n = \{x_k^n, x_j^n - \varepsilon \leqslant x_k^n \leqslant x_j^n + \varepsilon\}$ and $N_j^n = \text{card}(\mathcal{N}_j^n)$. We have

$$\left| \sum_{k=1}^{N} \omega_k f_0(\xi_k)\, \zeta_\varepsilon(x_j^n - x_k^n) \right| = \frac{1}{2\varepsilon} \sum_{k \in \mathcal{N}_j^n} \omega_k f_0(\xi_k)$$

and

$$\left| \sum_{k=1}^{N} \omega_k f_0(\xi_k)\, \zeta'_\varepsilon(x_j^n - x_k^n) \right| < \frac{N_j^n}{\varepsilon^2} \operatorname*{Max}_{k \in \mathcal{N}_j^n} (\omega_k f_0(\xi_k)).$$

Hence,

$$\sigma \operatorname*{Max}_{1 \leqslant j \leqslant N} \left(\operatorname*{Max}_{1 \leqslant n \leqslant M} \left| \frac{\sum_{k=1}^{N} \omega_k f_0(\xi_k)\, \zeta'_\varepsilon(x_j^n - x_k^n)}{\sum_{k=1}^{N} \omega_k f_0(\xi_k)\, \zeta_\varepsilon(x_j^n - x_k^n)} \right| \right)$$
$$< \frac{2}{\varepsilon} \sigma \operatorname*{Max}_{1 \leqslant j \leqslant N} \left(\operatorname*{Max}_{1 \leqslant n \leqslant M} \left(N_j^n \frac{\operatorname{Max}_{k \in \mathcal{N}_j^n} (\omega_k f_0(\xi_k))}{\sum_{k \in \mathcal{N}_j^n} \omega_k f_0(\xi_k)} \right) \right).$$

A sufficient condition for the stability criterion (10) to be confirmed is then

$$\frac{2}{\varepsilon} \sigma \operatorname*{Max}_{1 \leqslant j \leqslant N} \left(\operatorname*{Max}_{1 \leqslant n \leqslant M} \left(N_j^n \frac{\operatorname{Max}_{k \in \mathcal{N}_j^n} (\omega_k f_0(\xi_k))}{\sum_{k \in \mathcal{N}_j^n} \omega_k f_0(\xi_k)} \right) \right) < \frac{\varepsilon}{\Delta t}. \tag{11}$$

We observe that this criterion is the less restrictive as $\omega_k f_0(\xi_k)$ is a constant for any k. Multiplying f by a constant if necessary, we can assume that

$$\int_R f_0(\xi)\, d\xi = 1.$$

Changing the variable,

$$r = C(\xi) = \int_{-\infty}^{\xi} f_0(u)\, du,$$

in expression (5) yields

$$\int_R f_0(\xi)\, \psi(\xi)\, d\xi = \int_0^1 \psi(C^{-1}(r))\, dr,$$

Thus, using a numerical equiweighted integration formula on $[0, 1]$, provides

$$\int_R f_0(\xi)\, \psi(\xi)\, d\xi \simeq \frac{1}{N} \sum_{j=1}^{N} \psi(C^{-1}(r_j)).$$

Assume we solve the N equations:

$$r_j = C(\xi_j) = \int_{-\infty}^{\xi_j} f_0(u)\, du;$$

we then obtain

$$f_0(\xi)=\frac{1}{N}\sum_{j=1}^{N}\delta(\xi-\xi_j).$$

In this case we have, for any k, $\omega_k f_0(\xi_k)=1/N$ and criterion (11) becomes

$$\sigma\frac{\Delta t}{\varepsilon^2}<\frac{1}{2}. \tag{12}$$

If we suppose that ε plays the same part as Δx we find the same stability criterion as for the classical time-explicit finite difference scheme (see [13]):

$$\sigma\frac{\Delta t}{\Delta x^2}<\frac{1}{2}.$$

Consider the example,

$$\begin{aligned}&\frac{\partial f}{\partial t}-\frac{\partial^2 f}{\partial x^2}=0,\\&f(0)=f_0,\\&(x,t)\in[-10,10]\times[0,0.5],\end{aligned} \tag{13}$$

with

$$\begin{aligned}&f_0(x)=1, && |x|\leqslant 2,\\&f_0(x)=0, && \text{otherwise}.\end{aligned}$$

Numerical experimentation with this example confirms the part played by parameters ε and Δt, as provided for by criterion (12). On the other hand, we observe that parameter N does not affect the stability of the method.

We can refer to Figs. 1 and 2 on which the exact solution,

$$f(x,t)=\frac{1}{\sqrt{4\pi t}}\int_R e^{-|(x-u)/4t|^2}f_0(u)\,du,$$

and the approximated solution of Eq. (13) are being compared. The influence of the shape function ζ_ε and its derivative is discussed in [10, 14].

2.4. *Symmetrization*

We have been working so far on the entire space, or at least on an interval $[-L, L]$ such that f is zero or negligible between $-L$ and L. Let us consider a

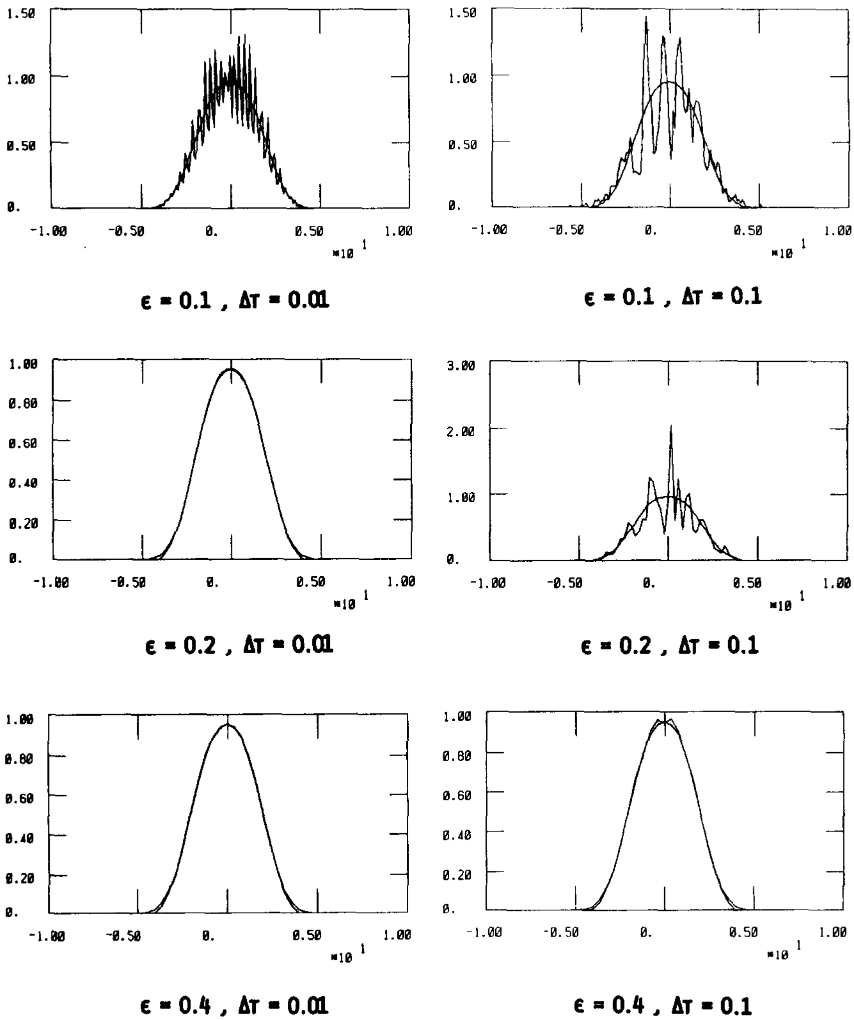


FIG. 1. Heat diffusion equation—effect of Δt and ε ($N = 50$ particles per ε, $T = 0.5$).

diffusion equation on a bounded interval such that f is not zero at the boundaries of the interval, for example,

$$\begin{aligned} &\frac{\partial f}{\partial t} - \sigma \frac{\partial}{\partial x}\left((1-x^2)\frac{\partial f}{\partial x}\right) = 0, \\ &f(x, 0) = f_0(x), \\ &(x, t) \in [-1, 1] \times [0, T], \end{aligned} \tag{14}$$

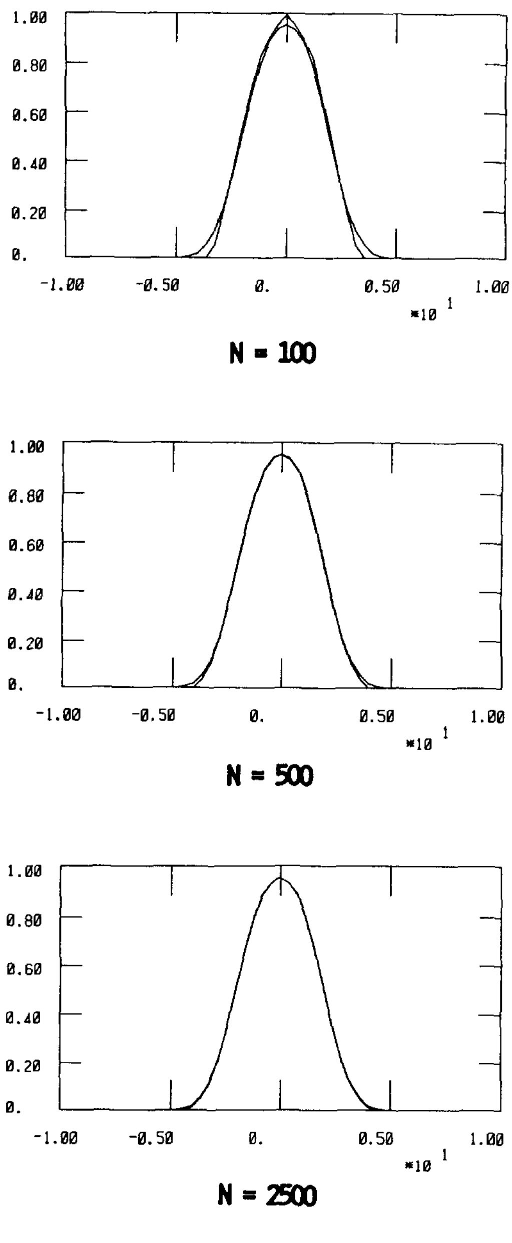


FIG. 2. Heat diffusion equation—effect of N ($\varepsilon = 0.4$, $\Delta t = 0.01$, $T = 0.5$).

with $f_0 = 1$ (in which case $f = 1$). The particle approximation of this equation yields

$$\hat{f}(x, t) = \sum_{j=1}^{N} \omega_j f_0(\xi_j) \zeta_\varepsilon(x - x_j(t)),$$

where $x_j(t)$ is the solution of the differential equation

$$\dot{x}_j(t) = \sigma(1 - x_j^2(t)) \frac{\partial}{\partial x} \left(\operatorname{Log} \frac{1}{f(x_j(t), t)} \right),$$
$$x_j(0) = \xi_j;$$

i.e., in an approximated form:

$$\frac{x_j^{n+1} - x_j^n}{\Delta t} = \sigma(1 - (x_j^n)^2) \frac{\hat{f}'(x_j^n)}{\hat{f}(x_j^n)}.$$

A sufficient condition for the stability of the method clearly remains

$$\sigma \frac{\Delta t}{\varepsilon^2} < \frac{1}{2}.$$

If satisfied, this condition guarantees that for any j,

$$x_j^{n+1} \in [-1 - \varepsilon, 1 + \varepsilon].$$

If $x_j^{n+1} > 1$ (resp. $x_j^{n+1} < -1$) we assign to this particle the new position:

$$\bar{x}_j^{n+1} = 2 - x_j^n \qquad (\text{resp. } \bar{x}_j^{n+1} = -2 - x_j^n).$$

We are then sure that all particles remain within the interval $[-1, 1]$. It then remains to correctly estimate the values $\hat{f}'(x_j^{n+1})$ and $\hat{f}(x_j^{n+1})$ in the neighborhood of -1 and 1. For example, let us consider the neighborhood of 1 and let

$$\mathcal{N}_{n+1} = \{x_k^{n+1}, 1 - \varepsilon < x_k^{n+1} \leqslant 1\}.$$

If $x_j^{n+1} \in \mathcal{N}_{n+1}$ we define

$$\begin{aligned} \hat{f}(x_j^{n+1}) &= \sum_{k=1}^{N} \omega_k f_0(\xi_k) \zeta_\varepsilon(x_j^{n+1} - x_k^{n+1}) + \sum_{k \in \mathcal{N}_{n+1}} \omega_k f_0(\xi_k) \zeta_\varepsilon(x_j^{n+1} + x_k^{n+1} - 2), \\ \hat{f}'(x_j^{n+1}) &= \sum_{k=1}^{N} \omega_k f_0(\xi_k) \zeta'_\varepsilon(x_j^{n+1} - x_k^{n+1}) + \sum_{k \in \mathcal{N}_{n+1}} \omega_k f_0(\xi_k) \zeta'_\varepsilon(x_j^{n+1} + x_k^{n+1} - 2), \end{aligned} \tag{15}$$

In particular, we notice:

$$\hat{f}(1, (n+1)\,\Delta t) = 2 \sum_{k \in \mathcal{N}_{n+1}} \omega_k f_0(\xi_k) \zeta_\varepsilon(1 - x_j^{n+1}),$$
$$\hat{f}'(1, (n+1)\,\Delta t) = 0.$$

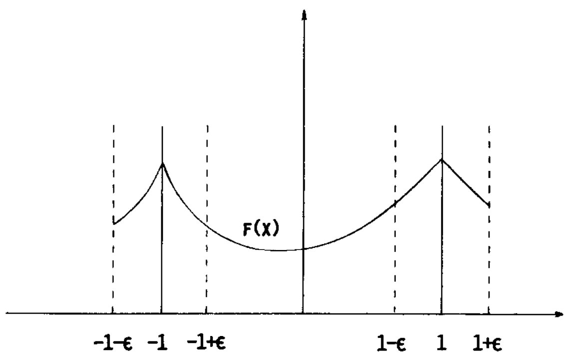
Similarly let $\mathcal{N}_{n+1} = \{x_k^{n+1}, -1 \leqslant x_k^{n+1} \leqslant -1+\varepsilon\}$. If $x_j^{n+1} \in \mathcal{N}_{n+1}$ we define

$$\hat{f}(x_j^{n+1}) = \sum_{k=1}^{N} \omega_k f_0(\xi_k)\, \zeta_\varepsilon(x_j^{n+1} - x_k^{n+1}) + \sum_{k \in \mathcal{N}_{n+1}} \omega_k f_0(\xi_k)\, \zeta_\varepsilon(x_j^{n+1} + x_k^{n+1} + 2),$$
$$\hat{f}'(x_j^{n+1}) = \sum_{k=1}^{N} \omega_k f_0(\xi_k)\, \zeta'_\varepsilon(x_j^{n+1} - x_k^{n+1}) + \sum_{k \in \mathcal{N}_{n+1}} \omega_k f_0(\xi_k)\, \zeta'_\varepsilon(x_j^{n+1} + x_k^{n+1} + 2). \quad (16)$$

This manner of proceeding produces f symmetrically in the neighborhood of -1 and 1:

$$\forall x \in [-1-\varepsilon, -1], \qquad f(x) = f(-2-x),$$
$$\forall x \in [1, 1+\varepsilon], \qquad f(x) = f(2-x).$$

This leads to



Numerical experimentation on Eq. (14) confirms the need for these boundary processings: if corrections (15) and (16) are not made, particles accumulate in the neighborhood of -1 and 1 with the course of time, and the approximated solution tends to infinity with t in the neighborhood or -1 and 1!

Solving a diffusion equation on a bounded area with nondegenerate boundary conditions of the Dirichlet or Neumann type has not been dealt with yet.

3. Fast Ion Transport: Fokker–Planck Equation

3.1. *Introduction*

We now contemplate investigating fast ion transport in a background plasma. Each particle species k is characterized by its mass m_k, its charge $q_k = Z_k e$, its energy $E_k(x)$ and its density $n_k(x)$. Index k refers to fast ions ($k = \alpha$), electrons ($k = e$), and ions ($k = i$) of the background plasma. Variable x indicates the location within a 1-dimensional plasma.

Let $f = f(x, v, \mu, t)$ be the distribution function of fast ions in plane geometry ($v = (v_x^2 + v_y^2 + v_z^2)^{1/2}$, $\mu = \mathbf{x} \cdot \mathbf{v}(\|\mathbf{x}\| \; \|\mathbf{v}\|)$. The action of Coulombian collisions between fast ions and background plasma electrons and ions is modelled, in the absence of a signifiant electromagnetic field, by the Fokker–Planck equation [15],

$$\frac{\partial f}{\partial t} + \mu v \frac{\partial f}{\partial x} - \frac{1}{v^2}\left[\frac{\partial}{\partial v}(a(x, v) f) + \frac{\partial}{\partial v}\left(b(x, v)\frac{\partial f}{\partial v}\right) + \frac{\partial}{\partial \mu}\left((1-\mu^2)\, c(x, v)\frac{\partial f}{\partial \mu}\right)\right] = 0$$

where a, b, c are functions depending on the physical characteristics of the background plasma. Let: $g = v^2 f$. This equation can be written in a conservative form,

$$\frac{\partial g}{\partial t} + \frac{\partial}{\partial x}(\mu v g) + \frac{\partial}{\partial v}(A(x, v)\, g) + \frac{\partial}{\partial v}\left(B(x, v)\frac{\partial g}{\partial v}\right) + \frac{\partial}{\partial \mu}\left((1-\mu^2)\, C(x, v)\frac{\partial g}{\partial \mu}\right) = 0, \tag{17}$$

with

$$A(x, v) = -\frac{1}{v^2} a(x, v) + \frac{2}{v^3} b(x, v),$$

$$B(x, v) = -\frac{1}{v^2} b(x, v),$$

$$C(x, v) = -\frac{1}{v^2} C(x, v).$$

Similarly, in spherical geometry ($r = (x^2 + y^2 + z^2)^{1/2}$, $v = (v_x^2 + v_y^2 + v_z^2)^{1/2}$, $\mu = \mathbf{r} \cdot \mathbf{v}_r / \|\mathbf{r}\| \; \|\mathbf{v}_r\|$), the Fokker–Planck equation can be written

$$\frac{\partial g}{\partial t} + \frac{\partial}{\partial r}(\mu v g) + \frac{\partial}{\partial v}(A(x, v)\, g) + \frac{\partial}{\partial \mu}\left((1-\mu^2)\frac{v}{r} g\right)$$
$$+ \frac{\partial}{\partial v}\left(B(x, v)\frac{\partial g}{\partial v}\right) + \frac{\partial}{\partial \mu}\left((1-\mu^2)\, C(x, v)\frac{\partial g}{\partial \mu}\right) = 0, \tag{18}$$

with $g = r^2 v^2 f$.

For density- and energy-homogeneous plasmas and for fast-ion energy E_α such that

$$\frac{m_\alpha}{m_i} E_i \ll E_\alpha \ll \frac{m_\alpha}{m_e} E_e,$$

we can suppose as a first approximation that

$$A(x, v) = A(v) \simeq -\alpha_e v - \alpha_i v^{-2},$$

$$B(x, v) \simeq 0,$$

$$C(x, v) = C(v) \simeq -\gamma_e v^{-2} - \gamma_i v^{-3},$$

where α_e, α_i, γ_e, γ_i are coefficients depending on the physical characteristics of the background plasma (see below).

Two typical examples of such situations are exhibited in [11]:

(a) slowing down of 1-MeV protons in a boron–deuterium–tritium (BDT) plasma such that $n_e = 2.5 \times 10^{23}\ \text{cm}^{-3}$, $n_i = 7.14 \times 10^{22}\ \text{cm}^{-3}$, and $E_e = E_i = 50$ KeV,

(b) slowing down of 3.5 MeV α-particles in a deuterium–tritium (DT) plasma such that $n_e = n_i = 2.5 \times 10^{26}\ \text{cm}^{-3}$ and $E_e = E_i = 50$ KeV.

Let v_0 be the initial velocity of fast ions. Let λ_{de}, λ_{di} be the electronic and ionic Debye lengths in the background plasma:

$$\lambda_{de} = \left(\frac{E_e}{4\pi n_e e^2}\right)^{1/2},$$

$$\lambda_{di} = \left(\frac{E_i}{4\pi n_i Z_i^2 e^2}\right)^{1/2}.$$

Let $\log \Lambda_e$, $\log \Lambda_i$ be the electronic and ionic Coulomb logarithms:

$$\log \Lambda_e = \log\left(\frac{m_\alpha}{m_\alpha + m_e} \frac{\lambda_{de}\lambda_{di}}{(\lambda_{de}^2 + \lambda_{di}^2)^{1/2}} \frac{2E_e}{Z_\alpha e^2}\right),$$

$$\log \Lambda_i = \log\left(\frac{m_\alpha}{m_\alpha + m_i} \frac{\lambda_{de}\lambda_{di}}{(\lambda_{de}^2 + \lambda_{di}^2)^{1/2}} \frac{m_i v^2}{Z_\alpha Z_i e^2}\right).$$

Let t_E be the energy relaxation time for scattering from electrons [15]:

$$t_E = \frac{3}{8\sqrt{2\pi}} \frac{m_\alpha E_e^{3/2}}{n_e m_e^{1/2} Z_\alpha e^4 \log \Lambda_e}.$$

Let us take t_E, $v_0 t_E$, and v_0 as time, length, and velocity units. Then we obtain the following values of coefficients α_e, α_i, γ_e, γ_i in both physical situations described above:

	α_e	α_i	γ_e	γ_i
Situation (a) ($\log \Lambda_i \simeq 12$)	0.05	0.1452	0.0125	0.576
Situation (b) ($\log \Lambda_i \simeq 10$)	0.05	0.206	0.0035	0.0619

3.2. *Particle Approximation*

Under the previous physical hypothesis the Fokker–Planck equation in plane geometry can be written ($g = v^2 f$):

$$\frac{\partial g}{\partial t} + \frac{\partial}{\partial x}(\mu v g) - \frac{\partial}{\partial v}((\alpha_e v + \alpha_i v^{-2})\, g) - \frac{\partial}{\partial \mu}\left((1-\mu^2)(\gamma_e v^{-2} + \gamma_i v^{-3}) \frac{\partial g}{\partial \mu}\right) = 0. \quad (19)$$

The generalization of the method described in Section 2 leads to this equation in the form:

$$\frac{\partial g}{\partial t}+\frac{\partial}{\partial x}(\mu v g)-\frac{\partial}{\partial v}\left[(\alpha_e v+\alpha_i v^{-2})\, g\right]-\frac{\partial}{\partial \mu}\left[\left((1-\mu^2)(\gamma_e v^{-2}+\gamma_i v^{-3})\frac{1}{g}\frac{\partial g}{\partial \mu}\right) g\right]=0.$$

The function $g_0=v^2 f_0$ is approximated by a sum of tensor products of regularized Dirac functions:

$$g_0=\frac{1}{N}\sum_{j=1}^{N}\zeta_{\varepsilon_x}(x-x_j^0)\,\zeta_{\varepsilon_v}(v-v_j^0)\,\zeta_{\varepsilon_\mu}(\mu-\mu_j^0).$$

An approximated solution of Eq. (19) can then be written

$$\hat{g}(x, v, \mu, t)=\frac{1}{N}\sum_{j=1}^{N}\zeta_{\varepsilon_x}(x-x_j(t))\,\zeta_{\varepsilon_v}(v-v_j(t))\,\zeta_{\varepsilon_\mu}(\mu-\mu_j(t)), \tag{20}$$

where, for any j, $x_j(t)$, $v_j(t)$, and $\mu_j(t)$ are solutions of the characteristic differential equations

$$\begin{aligned}&\dot{x}_j(t)=\mu_j(t)\, v_j(t),\\ &x_j(0)=x_j^0;\end{aligned} \tag{21}$$

$$\begin{aligned}&\dot{v}_j(t)=-\alpha_e v_j(t)-\alpha_i v_j^{-2}(t),\\ &v_j(0)=v_j^0;\end{aligned} \tag{22}$$

$$\begin{aligned}\dot{\mu}_j(t)=&-(1-\mu_j^2(t))(\gamma_e v_j^{-2}(t)+\gamma_i v_j^{-3}(t))\\ &\frac{1}{\hat{g}(x_j(t), v_j(t), \mu_j(t))}\frac{\partial \hat{g}}{\partial \mu}(x_j(t), v_j(t), \mu_j(t)),\\ \mu_j(0)=&\ \mu_j^0.\end{aligned} \tag{23}$$

Thus, according to (20) we obtain

$$\begin{aligned}\dot{\mu}_j(t)=&-(1-\mu_j^2(t))(\gamma_e v_j^{-2}(t)+\gamma_i v_j^{-3}(t))\\ &\times\left(\frac{\sum_{k=1}^{N}\zeta_{\varepsilon_x}(x_j(t)-x_k(t))\,\zeta_{\varepsilon_v}(v_j(t)-v_k(t))\,\zeta'_{\varepsilon_\mu}(\mu_j(t)-\mu_k(t))}{\sum_{k=1}^{N}\zeta_{\varepsilon_x}((x_j(t)-x_k(t))\,\zeta_{\varepsilon_v}(v_j(t)-v_k(t))\,\zeta_{\varepsilon_\mu}(\mu_j(t)-\mu_k(t))}\right).\end{aligned}$$

Coupled equations (21), (22), (23) are approximated by a classical explicit Euler scheme. We observe that Eq. (22) directly integrates; we obtain

$$v_j(t)=\left(\left((v_j^0)^3+\frac{\alpha_i}{\alpha_e}\right)e^{-3\alpha_e t}-\frac{\alpha_i}{\alpha_e}\right)^{1/3}. \tag{24}$$

In spherical geometry the Fokker–Planck equation can be written in the form ($g = r^2 v^2 f$):

$$\frac{\partial g}{\partial t} + \frac{\partial}{\partial r}(\mu v g) - \frac{\partial}{\partial v}((\alpha_e v + \alpha_i v^{-2})\, g)$$
$$+ \frac{\partial}{\partial \mu}(1-\mu^2)\left[\frac{v}{r} - (\gamma_e v^{-2} + \gamma_i v^{-3})\frac{1}{g}\frac{\partial g}{\partial \mu}\right] g = 0.$$

An approximated solution can then be written

$$\hat{g}(r, v, \mu, t) = \frac{1}{N}\sum_{j=1}^{N} \zeta_{\varepsilon_r}(r - r_j(t))\, \zeta_{\varepsilon_v}(v - v_j(t))\, \zeta_{\varepsilon_\mu}(\mu - \mu_j(t)),$$

where, for any j, $r_j(t)$, $v_j(t)$, and $\mu_j(t)$ are solutions to the following characteristic differential equations:

$$\dot{r}_j(t) = \mu_j(t)\, v_j(t),$$
$$r_j(0) = r_j^0;$$
$$\dot{v}_j(t) = -\alpha_e v_j(t) - \alpha_i v_j^{-2}(t),$$
$$v_j(0) = v_j^0;$$
$$\dot{\mu}_j(t) = (1 - \mu_j^2(t))\left(\frac{v_j(t)}{r_j(t)} - (\gamma_e v_j^{-2}(t) + \gamma_i v_j^{-3}(t))\right.$$
$$\left.\times\left(\frac{\sum_{k=1}^{N} \zeta_{\varepsilon_r}(r_j(t) - r_k(t))\, \zeta_{\varepsilon_v}(v_j(t) - v_k(t))\, \zeta'_{\varepsilon_\mu}(\mu_j(t) - \mu_k(t))}{\sum_{k=1}^{N} \zeta_{\varepsilon_r}(r_j(t) - r_k(t))\, \zeta_{\varepsilon_v}(v_j(t) - v_k(t))\, \zeta_{\varepsilon_\mu}(\mu_j(t) - \mu_k(t))}\right)\right)$$
$$\mu_j(0) = \mu_j^0.$$

From Eq. (24), we deduce that the modulus $v(t)$ of fast ion velocity decreases with time until it reaches the thermal velocity $V_{thi} = (2E_i/m_i)^{1/2}$ of background plasma ions. At that point, the fast ions are thermalized and Eq. (19) is not valid any more. A simple calculation shows that this thermalization takes place for $t \simeq 0.99\, t_E$ and $v \simeq 0.0793\, v_0$ in situation (a) (resp. $t \simeq 0.81\, t_E$ and $v \simeq 0.154\, v_0$ in situation (b)).

Let us assume that at initial time, the fast ions are uniformly spread between $-0.1\,\lambda_0$ and $0.1\,\lambda_0$. Let us assume, moreover, that $v = v_0$ and the values of μ are uniformly spread between -1 and 1. Without restriction to generality, we may assume that $0 \leqslant x \leqslant 0.1\,\lambda_0$. The fast ions that escape the box on the left side with a negative velocity are "reflected" and re-enter the box with a velocity of the same modulus but with positive sign. If $\mu_j^{n+1} < -1$ or $\mu_j^{n+1} > 1$, we proceed as stated for the model equation in Section 2.4.

We assume that the box is sufficiently wide, so that no fast ions can reach the right side of the box during the simulation.

Figures 3–6 show the distribution of particles in phase space (x, μ) with the course of time. We can very clearly observe the effect of the diffusion term in μ,

$$-\frac{\partial}{\partial\mu}\left((1-\mu^2)(\gamma_e v^{-2}+\gamma_i v^{-3})\frac{\partial g}{\partial\mu}\right),$$

which is more important in situation (a) than in situation (b), as expected, due to the values γ_e and γ_i.

3.3. *Energy Depositions*

By definition, the rate of the energy density deposited by fast ions in background plasma is written

$$\mathscr{E}(x, t) = \int_0^\infty \int_{-1}^1 v^2 \frac{\partial}{\partial v}((\alpha_e v + \alpha_i v^{-2})\, g)\, dv\, d\mu.$$

An integration by parts provides

$$\mathscr{E}(x, t) = -2\int_0^\infty \int_{-1}^1 (\alpha_e v^2 + \alpha_i v^{-1})\, g\, dv\, d\mu.$$

Using the weak approximation $\tilde{g}$ of g,

$$\tilde{g}(x, v, \mu, t) = \frac{1}{N}\sum_{j=1}^N \delta(x - x_j(t))\, \delta(v - v_j(t))\, \delta(\mu - \mu_j(t)),$$

we obtain the following approximation of $\mathscr{E}$

$$\tilde{\mathscr{E}}(x, t) = -\frac{2}{N}\sum_{j=1}^N (\alpha_e v_j^2(t) + \alpha_i v_j^{-1}(t))\, \delta(x - x_j(t)).$$

Hence, after regularization,

$$\hat{\mathscr{E}}(x, t) = -\frac{2}{N}\sum_{j=1}^N (\alpha_e^2 v_j(t) + \alpha_i v_j^{-1}(t))\, \zeta_{\varepsilon_x}(x - x_j(t)).$$

The density of the energy lost by fast ions at time $n\,\Delta t$ in background plasma is therefore written

$$\mathscr{E}^n(x) \simeq \int_0^{n\,\Delta t} \hat{\mathscr{E}}(x, u)\, du.$$

The trapezoidal integration formula provides

$$\mathscr{E}^n(x) \simeq \Delta t \sum_{k=1}^{n-1} \hat{\mathscr{E}}(x, k\,\Delta t) + \frac{1}{2}\hat{\mathscr{E}}(x, n\,\Delta t)).$$

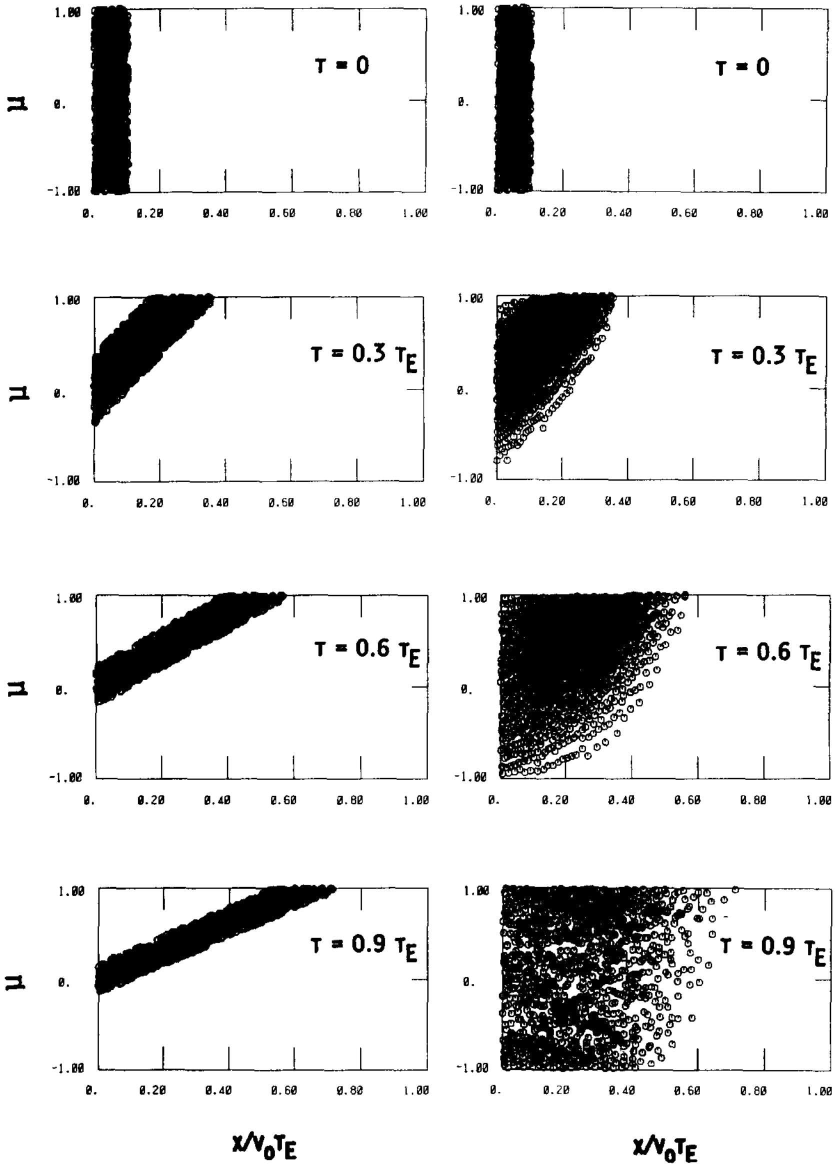


FIG. 3. 1 MeV protons in a 50 KeV BDT plasma (x, μ) phase space (plane geometry): Left without diffusion; right with diffusion; $\Delta t = 0.01\ t_E$; $\varepsilon_x = 0.025\ v_0 t_E$; $\varepsilon_v = 0.025\ v_0$; $\varepsilon_\mu = 0.2$; $N = 1000$.

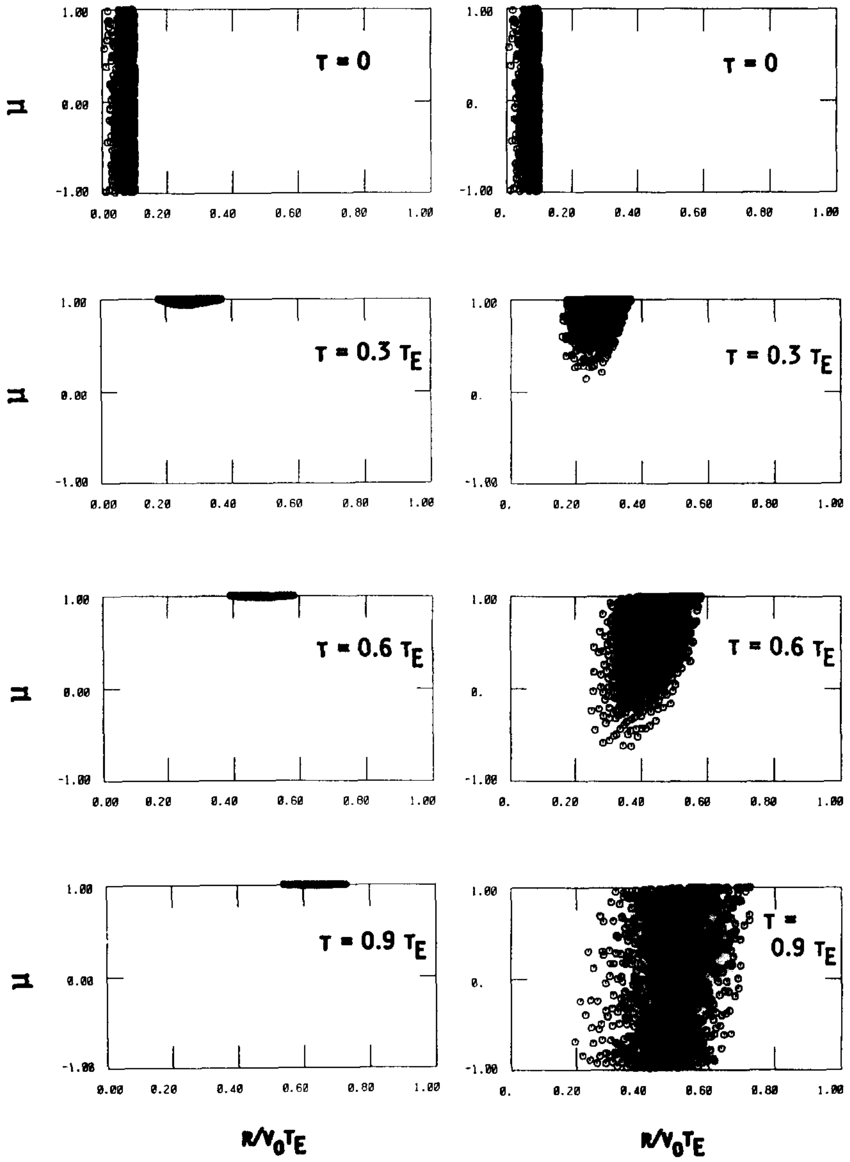


FIG. 4. 1 MeV protons in a 50 KeV BDT plasma (r, μ) phase space (spherical geometry): Left without diffusion; right with diffusion; $\Delta t = 0.01\ t_E$; $\varepsilon_x = 0.025\ v_0 t_E$; $\varepsilon_v = 0.025\ v_0$; $\varepsilon_\mu = 0.2$; $N = 1000$.

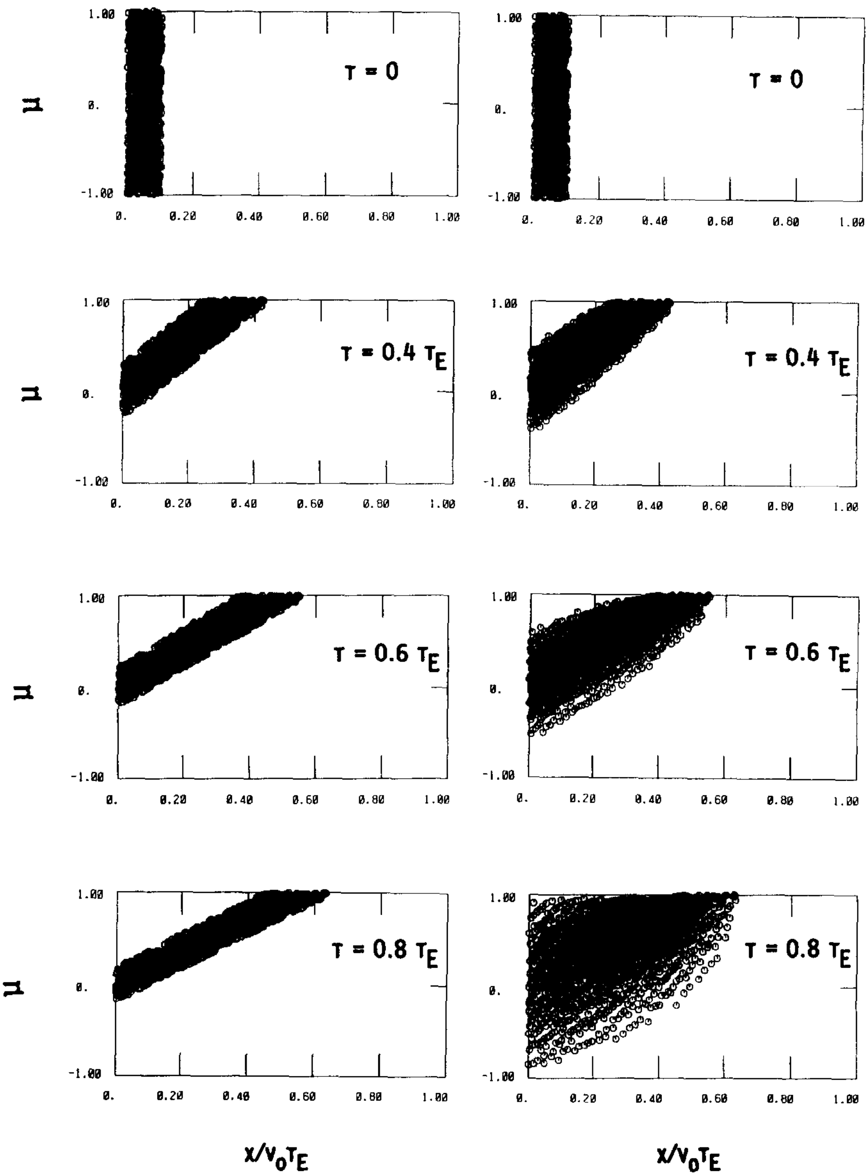


FIG. 5. 3.5 MeV α-particles in a 50 KeV DT plasma (x, μ) phase space (plane geometry): Left without diffusion; right with diffusion; $\Delta t = 0.01\ t_E$; $\varepsilon_x = 0.025\ v_0 t_E$; $\varepsilon_v = 0.025\ v_0$; $\varepsilon_\mu = 0.2$; $N = 1000$.

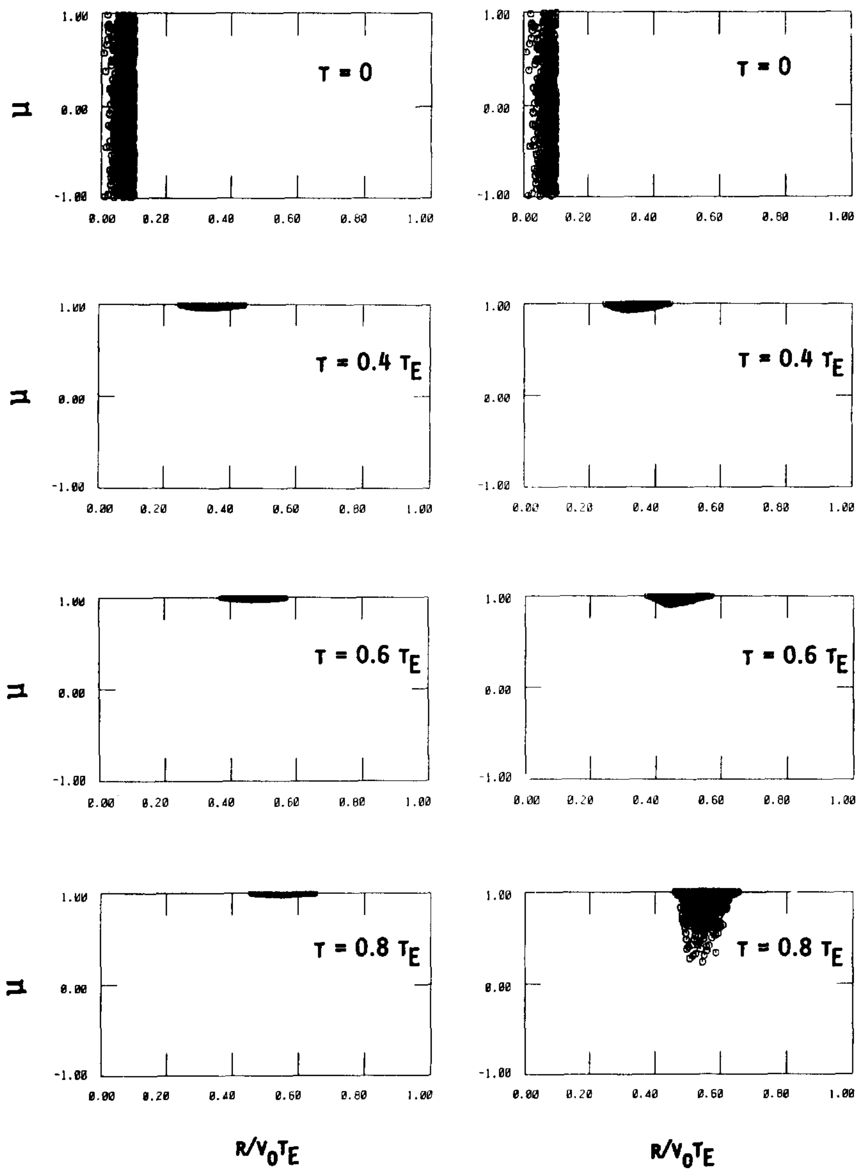


FIG. 6. 3.5 MeV α-particles in a 50 KeV DT plasma (r, μ) phase space (spherical geometry): Left without diffusion; right with diffusion; $\Delta t = 0.01\, t_E$; $\varepsilon_r = 0.025\, v_0 t_E$; $\varepsilon_v = 0.025\, v_0$; $\varepsilon_\mu = 0.2$; $N = 1000$.

The density of the energy lost by fast ions at time $n\,\Delta t$ on background plasma electrons is written

$$\mathscr{E}_e^n(x) \simeq \Delta t\left(\sum_{k=1}^{n-1} \hat{\mathscr{E}}_e(x, k\,\Delta t)+\frac{1}{2}\hat{\mathscr{E}}_e(x, n\,\Delta t)\right),$$

with

$$\hat{\mathscr{E}}_e(x, t) = -\frac{2}{N}\alpha_e \sum_{j=1}^{N} v_j^2(t)\zeta_{\varepsilon_x}(x-x_j(t)).$$

For the background plasma ions we obtain

$$\mathscr{E}_i^n(x) \simeq \Delta t\left(\sum_{k=1}^{n-1} \hat{\mathscr{E}}_i(x, k\,\Delta t)+\frac{1}{2}\hat{\mathscr{E}}_i(x, n\,\Delta t)\right),$$

with

$$\hat{\mathscr{E}}_i(x, t) = -\frac{2}{N}\alpha_i \sum_{j=1}^{N} v_j^{-1}(t)\,\zeta_{\varepsilon_x}(x-x_j(t)).$$

Figures 7 and 8 exhibit the functions $\hat{\mathscr{E}}_e^n$ and $\hat{\mathscr{E}}_i^n$ for both physical examples as described above. They can be compared with the results previously obtained with other methods such as [11, 16].

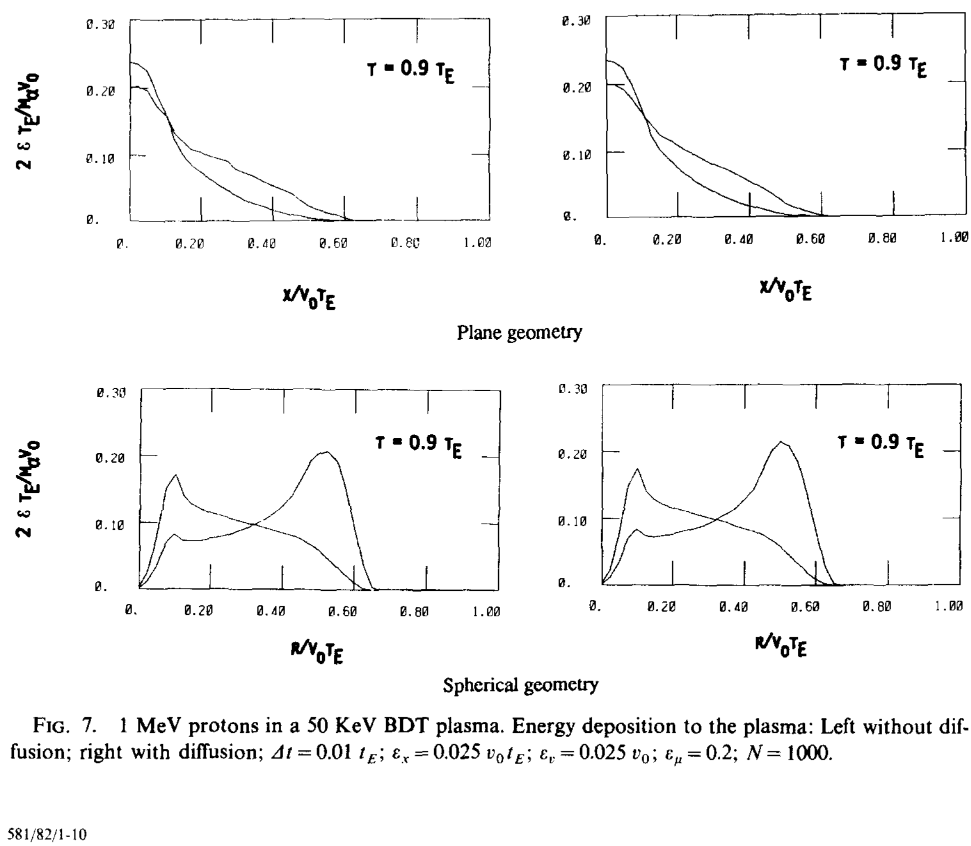


FIG. 7. 1 MeV protons in a 50 KeV BDT plasma. Energy deposition to the plasma: Left without diffusion; right with diffusion; $\Delta t = 0.01\ t_E$; $\varepsilon_x = 0.025\ v_0 t_E$; $\varepsilon_v = 0.025\ v_0$; $\varepsilon_\mu = 0.2$; $N = 1000$.

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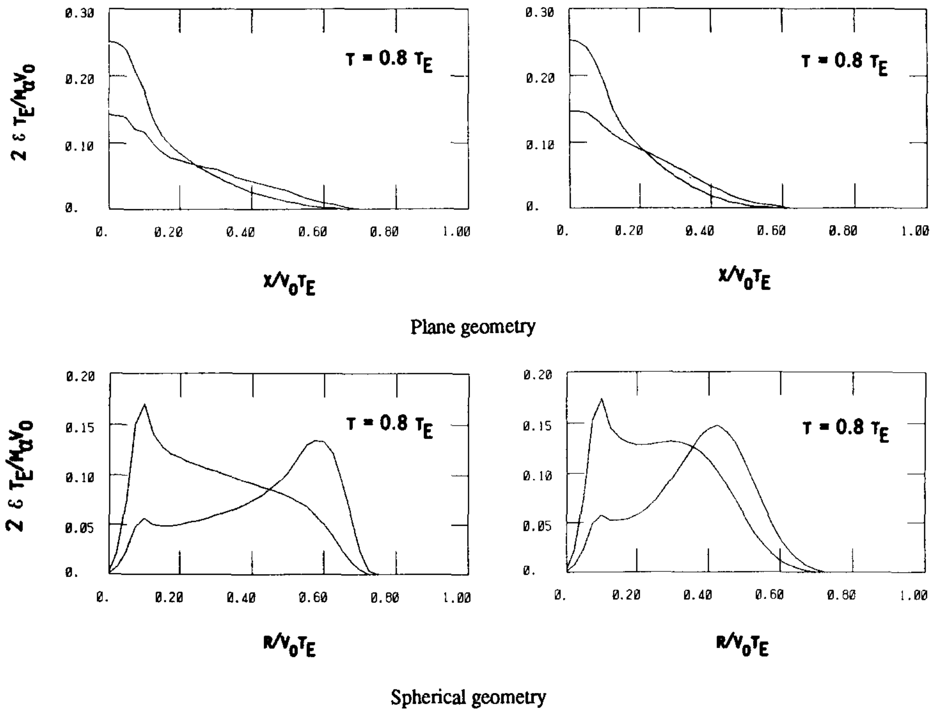

FIG. 8. 3.5 MeV α-particles in a 50 KeV DT plasma. Energy deposition to the plasma: Left without diffusion; right with diffusion; $\Delta t = 0.01\ t_E$; $\varepsilon_x = 0.025\ v_0 t_E$; $\varepsilon_v = 0.025\ v_0$; $\varepsilon_\mu = 0.2$; $N = 1000$.

4. IMPLEMENTATION

The main cost of this method lies in the calculation of sums of terms of the type

$$\zeta_{\varepsilon_x}(x_j - x_k)\,\zeta_{\varepsilon_v}(v_j - v_k)\,\zeta_{\varepsilon_\mu}(\mu_j - \mu_k) \tag{25}$$

or

$$\zeta_{\varepsilon_x}(x_j - x_k)\,\zeta_{\varepsilon_v}(v_j - v_k)\,\zeta'_{\varepsilon_\mu}(\mu_j - \mu_k), \tag{26}$$

which are involved for each particle x_j, v_j, μ_j at each time step. We use a classical data processing procedure as described in [1, p. 277], referring to the calculation of interparticle forces at short range. Each particle is set in a cell with a size of $\varepsilon_x \varepsilon_v \varepsilon_\mu$. Since terms (25) or (26) equal zero for $|x_j - x_k| \leqslant \varepsilon_x$, $|v_j - v_k| \leqslant \varepsilon_v$, or $|\mu_j - \mu_k| \leqslant \varepsilon_\mu$, only particles (x_k, v_k, μ_k) contained in the same cell as (x_j, v_j, μ_j) or in an adjacent one can contribute to the sums of terms (25) or (26).

On a computer of the type CRAY-1S we observed CPU times in the region of 10^{-4} s per time step and per particle in a nonvectorized code.

5. Conclusions

As we recently described [17] a deterministic particle method is available to manage transport-diffusion equations. The application of this method to the Fokker–Planck equation gives good results, with reasonable computing times, though the code is not vectorized. The benefits of this method are of several types:

(1) It is versatile, since it covers transport problems as well as transport-diffusion problems.

(2) It offers an easy and natural way to deal with the effect of a force field acting on particles. It is in fact sufficient to add the contribution of this force field to the motion of the particles in phase space and to resolve the transformed motion equations.

(3) It avoids the need for using Monte Carlo methods, which often lead to noisy results.

(4) One can always assign the same "weight" to all particles, without this weight being modified during the simulation.

(5) Because the problem is 3-dimensional (x, v, μ variables), and that we use "few" particles, the cost of this method is still reasonable.

(6) The constraint imposed on the time step to ensure stability is very similar to the condition obtained for the classical explicit finite difference method.

Notice that this method, which consists in the simulation of a physical medium by means of a set of "numerical" particles mutually interacting at least within a certain neighborhood, is very close to the methods used in molecular dynamics. It presently has two drawbacks:

(1) The solution of the problem dealt with must be strictly positive (however, see [14]).

(2) It is not easy to take boundary conditions into account, such as Dirichlet or Neumann, especially if the boundary at which these conditions must be applied is geometrically "complicated."

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