

NUMERICAL ALGORITHM BASED ON THE PDE METHOD FOR THE SOLUTION OF THE FOKKER PLANCK EQUATION *

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Abstract

This paper discusses a fast and accurate algorithm for the numerical solution of the Fokker-Planck equation (FPE) based on the PDE (Partial Differential Equation) method. The PDE concepts and methods are largely used in computer simulation of fluid-dynamical systems. This method can be used for studies of stochastic beam dynamics in one dimensional phase space in a storage rings. The performances of the PDE-method are calculated using the stochastic cooling process in the CR storage ring [1].

INTRODUCTION

We describe an algorithm for numerical solution of the Fokker-Planck Equation (FPE). The numerical solution of the FPE in general is interesting for a number of stochastic physics problems. This problem, especially if variable coefficients are included in the model, is computationally very expensive. The solution of FPE often takes a long time even with today's high-speed computers. The algorithm described here makes the calculation of the cumulative distribution functions for the predicted process computationally much less expensive. This improvement is achieved by solving the Kolmogorov backward equation numerically instead of employing the previously used closed form solution. The resulting method is shown to be notably faster than the standard method for the probability function calculation.

The FPE is a second order partial differential equation; it can be put in the form

$$\frac{\partial \psi(t, z)}{\partial t} = \left(\frac{\partial}{\partial z} F(t, z) - \frac{1}{2} \frac{\partial^2}{\partial z^2} D(t, z) \right) \psi(t, z) \quad (1)$$

where $F(t, z)$ and $D(t, z)$ are known functions which may depend, in principle, on time, and $\psi(t, z)$ represents the unknown solution. It can be shown [2] that this solution corresponds to the z -coordinate probability distribution of a mass less particle whose dynamics is described by the Langevin equation.

The algorithm described here involves the numerical solution of parabolic Partial Differential Equations (PDE) (1). Solving PDEs numerically is a well-established topic both in mathematics and in applied areas. There exists a vast literature and there are also many 'black box' PDE solvers available (e.g. the PDE toolbox of Matlab or Mathematic packages). Nevertheless, in order to keep the text as self-contained as possible, we give here a rough sketch of the numerical method. For a more detailed description we refer to the following text books [2-5].

PDE ALGORITHM

The key to the numerical solution of PDEs such as eq. (1) by using finite difference methods is to discretise 'space' z and time t , where the discrete set of Δz -values $\{0, \Delta z, 2\Delta z, \dots, N\Delta z\}$ (N - number of grid points) and the Δt -values $\{0, \Delta t, 2\Delta t, \dots\}$ are considered. The algorithm computes values ψ_{ij} which approximate the true solution ψ by $\psi_{ij} = \psi(i\Delta t, j\Delta z)$ for $i = 0, 1, 2, \dots$ and $j = 0, 1, \dots, N$. The accuracy of this approximation depends on the step sizes Δt and Δz . The algorithm works by considering a grid row with fixed time Δt , starting with an approximation of the initial condition: $(\psi_{00}, \dots, \psi_{0N})$. Then, in each step, the algorithm uses the approximation $(\psi_{i0}, \dots, \psi_{iN})$ for time $i\Delta t$ to compute an approximation for time $(i+1)\Delta t$. To simplify the presentation we consider the function $\psi(t, z)$.

Using numerical approximations for the partial derivatives we can then write the application of the differential operator

$$L = \frac{\partial}{\partial z} F(z, t) + \frac{1}{2} \frac{\partial^2}{\partial z^2} D(z, t) \quad (2)$$

as a matrix vector multiplication. Collecting all the terms we get

$$L \psi(n\Delta t, n\Delta z) = L^N \psi_n^n \quad n [1, \dots, N] \quad (3)$$

where L^N is the tri-diagonal matrix given by

$$L^N = \begin{pmatrix} d_1 & p_1 & 0 & 0 \\ r_2 & d_2 & p_2 & 0 \\ 0 & r_i & d_i & p_i \\ 0 & 0 & r_N & d_N \end{pmatrix}, \quad (4)$$

$$r_i = -\frac{F_i}{2\Delta z} + \frac{D_i}{2\Delta z^2}, \dots, i \in [2, N]; \quad d_i = -\frac{D_i}{\Delta z^2}, \dots, i \in [1, N];$$

$$p_i = \frac{F_i}{2\Delta z} + \frac{D_i}{2\Delta z^2}, \dots, i \in [1, N-1].$$

The approximations introduced above one suggest the following approximation to the PDE:

$$\frac{\psi^{n+1} - \psi^n}{\Delta t} = L^N (\theta \psi^{n+1} + (1-\theta) \psi^n), \quad (5)$$

where $\theta \in [0, 1]$ is a parameter of the method. For $\theta=0$ the derivative on the right hand side is evaluated only for the current approximation ψ^n . For all values $\theta>0$ the derivative is evaluated for a mixture of ψ^n and ψ^{n+1} . In these cases one has to solve a system of linear equations to compute ψ^{n+1} from ψ^n . By rearranging the terms in (5) we get

$$(I - \Delta t \theta L^N) \psi_i^{n+1} = (I - \Delta t (1-\theta) L^N) \psi_i^n, \quad (6)$$

where I is the $N \times N$ identity matrix. The choice of the parameter θ affects the stability of the method. Common choices are $\theta = 0$ (Euler scheme), $\theta = 1/2$ (Crank Nicolson scheme) and $\theta = 1$ (implicit Euler scheme).

SOLVER WITH THE PDE METHOD

Using the equations discussed previously the numerical calculation procedure is as follows. One has to construct the set of the linear algebraic equations following the equation (6). Taking into account the matrix of operators (4) the left side of the equation (6) is written as multiplication of the tri-diagonal matrix (4) on the vector ψ_i^{n+1} . The right side of eq.(6) can be written as a vector f_i , which is obtained by multiplying matrix $(I - \Delta t(1-\theta)L^N)$ by the known ψ_i^n . One gets

$$\begin{pmatrix} b_1 & c_1 & 0 & 0 \\ a_2 & b_2 & c_2 & 0 \\ 0 & a_i & b_i & c_i \\ 0 & 0 & a_N & b_N \end{pmatrix} \begin{pmatrix} \psi_1^{n+1} \\ \psi_2^{n+1} \\ \psi_i^{n+1} \\ \psi_N^{n+1} \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \\ f_i \\ f_N \end{pmatrix}, \quad (7)$$

$$a_i = -\frac{T}{2} \left(\frac{D_i}{\Delta z^2} + \frac{F_i}{\Delta z} \right); \quad b_i = 1 + T \frac{D_i}{\Delta z^2}; \quad c_i = -\frac{T}{2} \left(\frac{D_i}{\Delta z^2} - \frac{F_i}{\Delta z} \right);$$

$$f_i = \psi_i^n + \frac{W}{2} \left(-\frac{F_{i+1}\psi_{i+1}^n - F_{i-1}\psi_{i-1}^n}{\Delta z} + \frac{D_{i+1}\psi_{i+1}^n - 2D_i\psi_i^n + D_{i-1}\psi_{i-1}^n}{\Delta z^2} \right)$$

$W = \Delta t(1-\theta)$, $T = \Delta t\theta$. To solve a tri-diagonal system of equations (7) one can use so called the "tri-diagonal matrix algorithm" also known as the "Thomas algorithm" [6], which is a simplified form of Gauss elimination. With Thomas algorithm the solution can be obtained in N operations instead of N^3 required for Gaussian elimination.

SIMULATION EXAMPLES

For the PDE approach the discretisation step size in time Δt and the number N of steps in space Δz influence the accuracy and speed of the simulation. The parameter θ affects the stability of the method. Only the quality of the result and the time used to obtain it are of interest.

We performed two kinds of numerical simulations to compare accuracy and execution time of the proposed algorithm. In the first simulations we define the performance of computing time using an implementation of the PDE method. In the second simulations we define the performance of the PDE algorithm with respect to the accuracy of the method. For simulations the computer with a dual core Pentium 4 processor (2.8GHz) was used.

We apply the PDE method to calculate the stochastic cooling process in the CR [1] in the longitudinal phase space. In this case the z value in eq. (7) is the relative particle momentum spread ($\delta = \Delta p/p$). The function $\psi(t, z)$ is the particle density and can be written as $\psi(t, \delta) = \Delta N_0 / \Delta \delta$. To calculate the drift F and diffusion D coefficients we use formulae given in ref.[7]. The main

parameters of the beam and stochastic cooling system of the CR are given in Table 1.

Table 1: Main Parameters of the Stochastic Cooling System in the CR.

Total number of antiprotons, N_0	10^8
Beam energy, GeV	3
Frequency slip factor :	
Average over the ring	-0.017
Local: from pick-up to kicker	-0.041
Revolution frequency, MHz	1.315
Bandpass (f_{\min}, f_{\max}), GHz	1-2
Min/Max harmonic number	800 / 1600
Effective temperature of amplifier noise, K	73
Pick-up impedance, Z_p, Ω	720
Kicker-impedance, Z_c, Ω	2880
Number of pick-ups, n_p	2
Number of kickers, n_k	2
Gain	2×10^7
Initial rms momentum spread, δ_{rms}	0.0035

We are interested in the evolution of the distribution function $\psi(t, \delta)$ with time. The initial distribution $\psi(0, \delta)$ is parabolic. The *rms* value δ_{rms} of the $\psi(t, \delta)$ distribution is calculated at each time step. The accuracy is defined as difference of calculated integral of the $\psi(t, \delta)$ function at time t_{max} and $t=0$.

$$\varepsilon = \frac{1}{N_0} \left(\int_{-\delta_{max}}^{\delta_{max}} \psi(t_{max}, \delta) - \int_{-\delta_{max}}^{\delta_{max}} \psi(0, \delta) \right), \quad (8)$$

where N_0 is the total number of particles. In our simulation we assume a maximal cooling time $t_{max}=25$ s. The beam equilibrium (when the action of the diffusion and cooling terms are comparable) begins at 20 s. Obviously, during the further 5 s one should observe a stable value of δ_{rms} , which indicates the stability of the method. In Fig.1 we show the evolution of δ_{rms} for the different parameters θ .

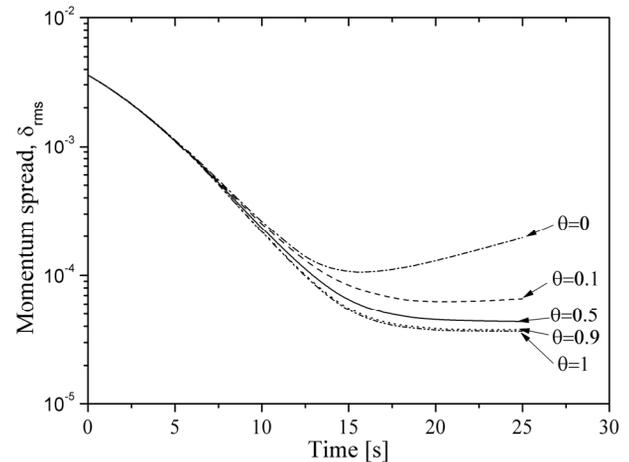


Figure 1: Evolution of the *rms* momentum spread depending on the parameter θ . $\Delta t=10^{-4}$, $N=400$.

The results shown in Fig.1 were obtained for the time step Δt of 10^{-4} s and number of grid points $N=400$. For these parameters the accuracy of the method, which changes during cooling, is shown in Fig.2. One can see that a stable solution and an accuracy of the method better than 2% are obtained when the parameter θ is in the range of 0.5 – 1.

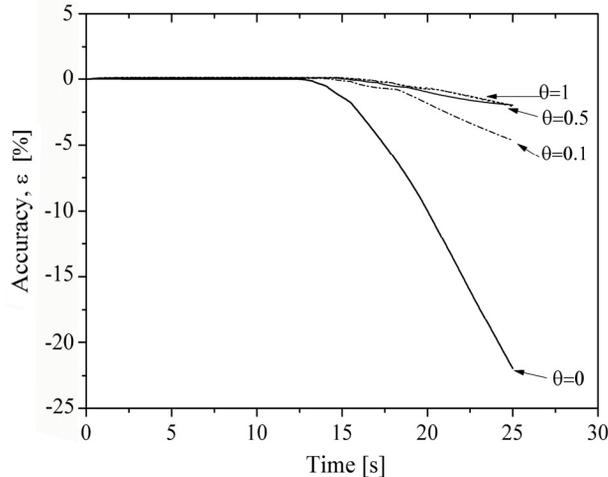


Figure 2: The accuracy of the PDE algorithm for different parameters of θ . $\Delta t=10^{-4}$, $N=400$.

In our next test simulations we compare the computation time and the accuracy of the PDE algorithm for a different time steps and number of grid points. Of course this leads to some difficulties, because some changes in the drift and diffusion coefficients cause large changes in the trade-off between the accuracy and computation time. To be self-consistent we fix all parameters included in the F and D coefficients according to the Table 1 and change only the time step and the number of grid points. In all our simulations we take the parameter $\theta = 0.5$. Fig. 3 shows the computation time as function of the number of grid points for different time steps. The calculated accuracy of the method is shown in Fig.4.

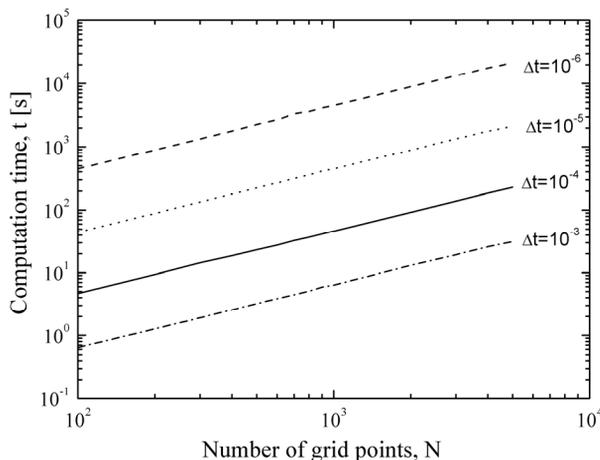


Figure 3: The computation time as a function of the number of grid points (Δt is the time step).

As it can be seen, for most parameter sets the PDE method is noticeably fast while yielding the acceptable accuracy. One should note that for an accuracy better than 2% one can choose the N in the range of 400 - 1000 and a time step of $\Delta t=10^{-3} - 10^{-4}$ having a fast computation time in the order of few seconds. The accuracy and stability of the PDE method becomes problematic for a time step larger than 0.001 s or for a number of the grid points less than 200.

In figure 4 we see that the accuracy of the PDE algorithm has a weak dependence on the time step, while the number of grid points affects it very strongly.

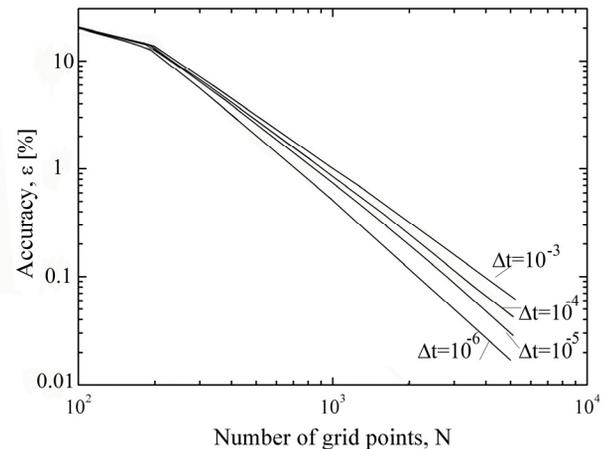


Figure 4: The accuracy of the PDE algorithm.

In the near future this work will be extended to higher dimensions, and it will be applied to more realistic parameters for studying the dynamics of particles in storage rings.

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