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Numerical solution of two dimensional Fokker–Planck equations

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Abstract

We present a robust finite difference scheme for the integration of the Fokker–Planck (FP) equation with two variables plus time. The scheme is checked with problems where analytical solutions exist and it is compared with finite element codes, as well as with simulations of the associated Stochastic Differential Equation (SDE). The precision and stability of the scheme are verified.

Keywords: Nonlinear beam dynamics; Stochastic processes; Fokker–Planck equation; Finite difference scheme; Operator splitting method

1. Introduction

It is well known that Markovian diffusion processes can be described with the Fokker–Planck (FP) equation. The FP equation is a partial differential equation for the probability density and the transition probability of these stochastic processes. Furthermore, it can be shown that diffusion processes are the solution of Stochastic Differential Equations (SDE) with Gaussian white noise [1].

SDE are an important tool in dynamics and are used extensively for modelling single particle dynamics in accelerators under the influence of noise [2]. The sources of noise are for instance random fields, random ground motion or quantum fluctuations of the radiation.

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The physical questions one wants to answer are: what is the longtime behaviour of the dynamics, what is the probability for the particle to hit the vacuum chamber and then be lost (first mean passage time), what are the average fluctuations of the particle around the periodic design orbit of the accelerator (moments) and what is the time evolution of the probability density?

In order to solve these questions one can follow two ways:

- one way is to consider the SDE directly, as it is described in [3–5]. With the SDE each initial condition must be studied through an ensemble of realizations. For higher dimensions and because of the huge number of realizations this approach requires a large amount of CPU time,
- an alternative way is to investigate the FP equation. Since only few exact solutions are available for this type of partial differential equation, especially in higher dimensions, one has to develop powerful and fast numerical schemes.

In this paper we describe a finite difference scheme to solve the FP equation with two phase space variables plus time. Extensive numerical simulations for this problem have been performed by Bergman and Spencer, using finite elements for the FP integration, and Monte Carlo simulation for the SDE. For further reading see [6]. Here we concentrate on the finite difference scheme because of its simple implementation, its flexibility with respect to different boundary conditions, the straightforward extension to higher dimensional problems, its efficiency concerning CPU time and because it is easy to understand the physical meaning of each term in the scheme.

The present paper is organized as follows. In Section 2 the scheme is presented with its linear stability analysis. Section 3 offers some examples: the damped harmonic oscillator, where we check the accuracy by comparison with the exact solution, and the Duffing problem, where we compare the results with a finite element integrator of the equation as well as with the results obtained by the numerical simulation of the SDE. Section 4 summarizes the main results of this work.

2. The difference scheme and the stability analysis

Typical differential equations one finds in accelerator physics are:

$$\begin{aligned} \dot{x} &= v, \\ \dot{v} &= -a_1(x) - a_2(x, v) + \sqrt{2\sigma}\eta(t), \end{aligned} \tag{1}$$

where $\eta(t)$ is a Gaussian white noise. Here we study two cases:

An harmonic oscillator with damping and noise

$$\begin{aligned} \dot{x} &= v, \\ \dot{v} &= -Kx - \gamma v + \sqrt{2\sigma}\eta(t). \end{aligned} \tag{2}$$

And the stochastic Duffing oscillator, a nonlinear oscillator, with damping, multiplicative noise and additive noise

$$\begin{aligned} \dot{x} &= v, \\ \dot{v} &= -\omega^2[(\alpha + \sqrt{2D_{11}}\eta_1(t))x + \epsilon x^3] - 2\tau\omega\dot{x} + \sqrt{2D_{22}}\eta_2(t), \end{aligned} \tag{3}$$

with the corresponding FP equations

$$\frac{\partial \rho}{\partial t} = \left(-\frac{\partial v}{\partial x}\right)\rho + \left(\frac{\partial}{\partial v}(\gamma v + Kx) + \sigma\frac{\partial^2}{\partial v^2}\right)\rho, \tag{4}$$

$$\frac{\partial \rho}{\partial t} = -\frac{\partial(v\rho)}{\partial x} + \frac{\partial}{\partial v}[(a_1(x) + a_2(x,v))\rho] + \frac{1}{2}\frac{\partial^2}{\partial v^2}(2D\rho), \tag{5}$$

($a_1(x) = \omega^2 x(\alpha + \epsilon x^2)$, $a_2(x_1 v) = 22\omega v, D = D_{11}\omega^4 x^2 + D_{22}$) respectively. Eqs. (2) and (3) constitute simple examples for the particle oscillations around the periodic design trajectory of a storage ring (betatron oscillations).

The FP equation is a partial differential equation for the evolution of the *transition probability* $p(x, v, t|x_0, v_0, t_0)$ and the *density function* $\rho(x, v, t) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} p(x, v, t|x_0, v_0)\rho_0 \, dx_0 \, dv_0$ where ρ_0 is the initial condition. Eqs. (4) and (5) can be written in the form of two fluxes, one in x and one in v, such that

$$\frac{\partial \rho}{\partial t} = \frac{\partial(F_1)}{\partial x} + \frac{\partial(F_2)}{\partial v}$$

a form which suggests to employ an operator splitting method (see [7]). We evaluate first implicitly the v derivative and then also implicitly the x derivative with a tridiagonal scheme:

$$\frac{\rho_{i,j}^{n+1/2} - \rho_{i,j}^{n}}{\Delta t} = \frac{F_{i,j+1/2}^{n+1/2} - F_{i,j-1/2}^{n+1/2}}{\Delta v}, \tag{6}$$

$$F_{i,j+\frac{1}{2}} = D\frac{\rho_{i,j+1} - \rho_{i,j}}{\Delta v} + (a_1(x) + a_2(x, v + \Delta v))\frac{\rho_{i,j+1} + \rho_{i,j}}{2}, \tag{7}$$

$$\frac{\rho_{i,j}^{n+1} - \rho_{i,j}^{n+1/2}}{\Delta t} = -v\frac{\rho_{i+1,j}^{n+1} - \rho_{i-1,j}^{n+1}}{2\Delta x}. \tag{8}$$

If we make the von Neuman analysis of stability of the finite difference scheme for this problem, we find that the amplification factors for the two steps of the schemes (6) and (8) are

$$g_{\mathrm{I}} = \frac{1}{1 + A\,\sin^2(q\,\Delta v/2) - ia_{(x,v+(\Delta v/2))}(\Delta t/\Delta v)\sin(q\,\Delta v)}$$

and

$$g_{\mathrm{II}} = \frac{1}{1 + iv(\Delta t/\Delta v)\sin(k\,\Delta x)},$$

respectively. With $A = (\Delta t/\Delta v^2)D$ and $a_{(x,v-(\Delta v/2))} \simeq a_{(x,v-(\Delta v/2))}$. Therefore

$$|g| \leq 1 \tag{9}$$

and the scheme is *unconditionally stable*. The scheme is second-order accurate in Δt, Δx and Δv.

3. Numerical results

We apply the scheme to the solution of the problems listed above, at first to the damped harmonic oscillator of Eq. (2), with the corresponding FP equation [8]

$$\frac{\partial \rho}{\partial t} = \left(-\frac{\partial v}{\partial x}\right)\rho + \left(\frac{\partial}{\partial v}\left(\gamma v + Kx + \sigma\frac{\partial}{\partial v}\right)\rho\right).$$

The exact solution, for a delta initial condition $\delta(x - x_0, v - v_0)$ is

$$\rho = \frac{e^{\gamma t}\exp[-[a(\xi - \xi_0)^2 + 2h(\xi - \xi_0)(\eta - \eta_0) + b(\eta - \eta_0)^2]/2\Delta]}{2\pi\Delta^{1/2}}, \tag{11}$$

where

$$a = 2\sigma\int_0^t \exp(-2\mu_1 t)\,dt = \frac{\sigma}{\mu_1}[1 - \exp(-2\mu_1 t)],$$

$$b = 2\sigma\int_0^t \exp(-2\mu_2 t)\,dt = \frac{\sigma}{\mu_2}[1 - \exp(2\mu_2 t)],$$

$$h = -2\sigma\int_0^t \exp(-(\mu_1 + \mu_2)t)\,dt = \frac{-2\sigma}{(\mu_1 + \mu_2)}[1 - \exp(-(\mu_1 + \mu_2)t)],$$

$$\Delta = ab - h^2,$$

and

$$\xi = (x\mu_1 - v)\exp(-\mu_2 t), \qquad \eta = (x\mu_2 - v)\exp(-\mu_1 t)$$

with

$$\mu_1 = -\frac{\gamma}{2} + \sqrt{\frac{\gamma^2}{4} - K}, \qquad \mu_2 = -\frac{\gamma}{2} - \sqrt{\frac{\gamma^2}{4} - K}\ .$$

The time evolution of the probability density consists of a drift due to the deterministic part of the motion and a diffusion due to the noise (see Fig. 1).

In order to evaluate the accuracy of the finite difference scheme we calculated first the norm of the error between the numerical solution and the exact solution defined by

$$\|e\| = \sqrt{\frac{1}{N}\left(\sum(\rho_{i,j}^{\text{num}} - \rho_{i,j}^{\text{exact}})^2\right)},$$

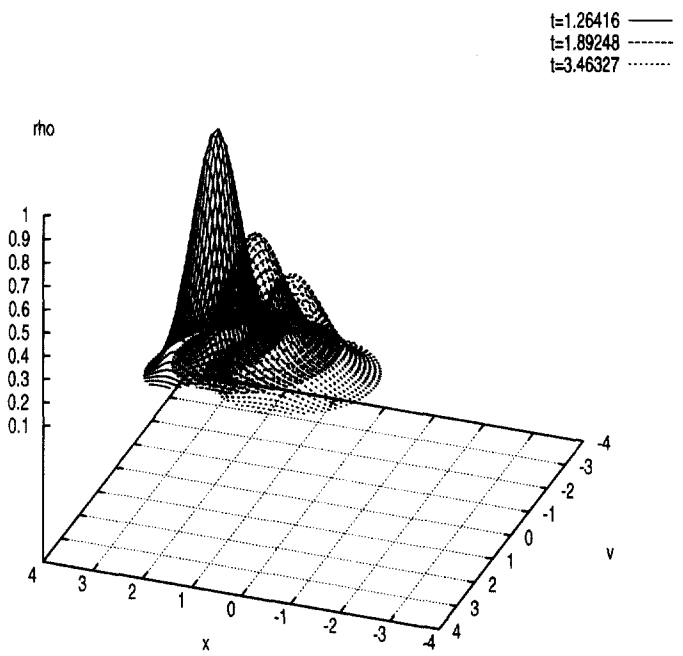

Fig. 1. Density evolution in the damped linear harmonic oscillator equation, drift and diffusion resulting from the stochastic excitation.

where the sum is extended over all the grid points and N is the total number of points in such a grid. Alternatively, the accuracy of the scheme is checked by comparison of the second order moments.

These calculations were performed for the strongly damped oscillator with strong diffusion $K = 1$, $\gamma = 2.1$, $\sigma = 0.8$ and with a grid of 80×80 and $\Delta x = \Delta y = 0.1$, $\Delta t = \pi/1000$. As initial condition the exact solution (11) at time $t = 0.95$ was chosen.

The *error norm* found after 800 times steps of integration on a HP9000-735 workstation, with double precision was $\|e\| = 0.000529$ and with single precision $\|e\| = 0.000530$ (which agrees with the order of the error in the moments). In Table 1 we summarize the calculations of the moments for $t = 3.46327$ (the numerical results for single and double precision are coincident up to this order). A typical solution run of $t \simeq 3$ (1000 times steps) takes around 2 min of computational time.

Next we analyze the nonlinear problem (3). The SDE includes additive and multiplicative noise. The drift term will be obtained following the Ito rule in order to have an exact comparison with the studies of [6]. The FP equation corresponding to the stochastic Duffing oscillator is

Table 1
The calculations of moments for $t = 3.46327$

Moment	Numerical	Exact
E[XX]	0.01037	0.01035
E[XV]	−0.00297	−0.00296
E[VV]	0.00793	0.00795

$$\frac{\partial p}{\partial t} = -\frac{\partial (vp)}{\partial x} + \left(\frac{\partial}{\partial v} \left[2\tau\omega v + \omega^2 x(\alpha + \epsilon x^2) + \frac{1}{2}\frac{\partial}{\partial} 2D \right] p \right), \tag{12}$$

where $D = D_{11}\omega^4 x^2 + D_{22}$.

For means of comparison we have performed numerical simulations of the SDE with the Heun scheme [3]:

$$x_i(t+h) = x_i + \frac{h}{2}(f_i(x_i(t)) + f_i(\hat{x}_i(h))) + g_{ij}(x_i(t)) \cdot \hat{W}_j(h), \tag{13}$$

$$\hat{x}_i(h) = x_i(t) + f_i(x_i(t)) \cdot h + g_{ij}(x_i(t)) \cdot \hat{W}_j(h), \tag{14}$$

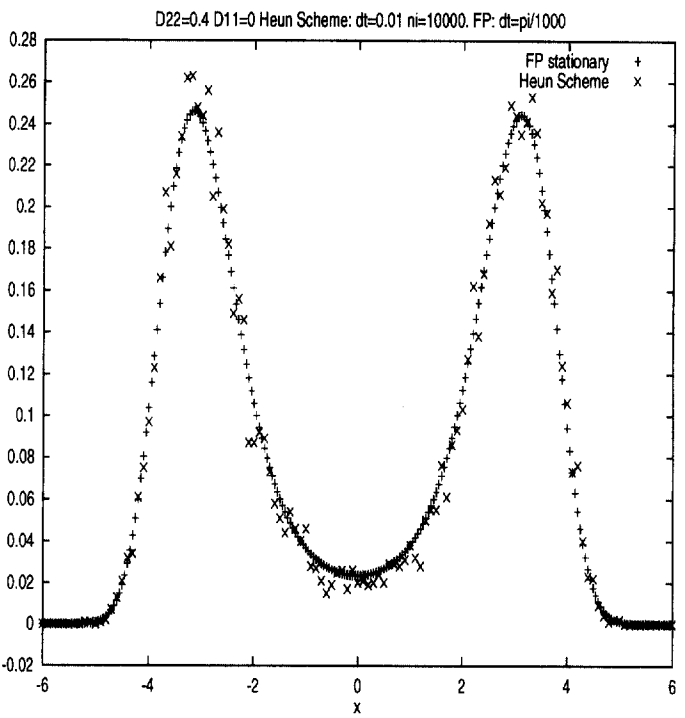

Fig. 2. Stationary solution of the additive noise case, calculated with 10 000 realizations of the SDE with i.c. (0, 0) compared with our integrated FP equation for the same i.c.

where $\hat{W}_j(h)$ is a random vector with the same first. moments as the normally distributed $W_j(h) = \int_t^{t+h} \mathrm{d}s\, \eta_j(s)$ (with $\eta(s)$ Gaussian white noise). That means $\langle \hat{W}_j(h) \rangle = 0$, $\langle \hat{W}_i(h) \hat{W}_j(h) \rangle = h\delta_{ij}$. It can be simulated by setting $\hat{W}_j(h) = \sqrt{12}(r_j - 0.5)$ with r_j being an independent uniformly distributed random number.

We follow the evolution of 10 000 samples with a time step of $h = 0.01$. In order to calculate the density we group the samples into cells of $\Delta x = 0.1 = \Delta v$. The noise parameters are $D_{11} = 0$, $D_{22} = 0.4$ (only additive noise). Fig. 2 shows the conditional probability (integrated over v) of the stationary solution calculated from both the SDE and FP equation. The initial condition in this case is $(x_0 = 0, v_0 = 0)$. Our FP integrator is in agreement with the simulation of the SDE within the statistical error.

Integrating the SDE with a non-delta initial condition will be always very CPU time consuming. We should remark that even when one is able to integrate the SDE there still remains the problem of averaging the solution for an extended set of initial conditions. Namely besides performing n samples for each initial condition, one has to weight them according to the initial condition distribution and plot the results in histograms.

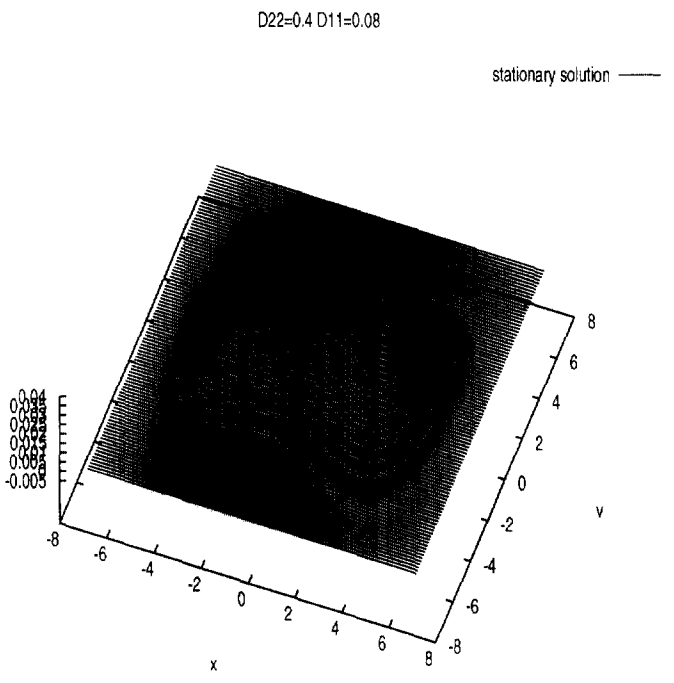

Fig. 3. $D_{22} = 0.4$, $D_{11} = 0.08$, view of the stationary density in phase space ($\mathrm{d}t = \pi/1000$). Finite difference integration.

Next we compare our results with other codes for the FP equation. We have set the parameters to $D_{11} = 0.08$, $D_{22} = 0.4$ and $D_{11} = 0.24$, $D_{22} = 0.4$ in order to compare our scheme with the finite element integration [6]. In the work by Bergman et al. [6], a noise-induced transition was observed. For more information about noise-induced transitions, see [9]. In the additive noise case, the system has two stable points (see Fig. 2) just like the deterministic system. Under multiplicative noise the probability at the origin grows (see Fig. 3). Further increasing the strength of the multiplicative noise changes the stability of the origin, *the origin becomes a stable point* Fig. 4. The finite element integrator takes approximately 3 min for integrating 3 s of the system, whereas our finite difference method took approximately 2 min.

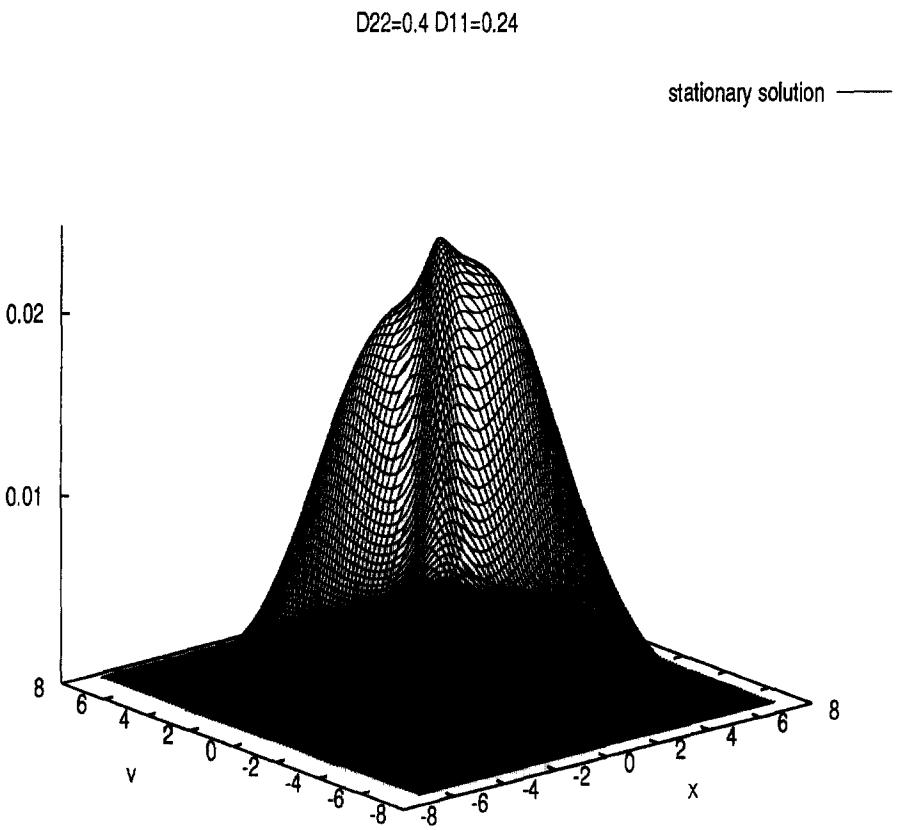

Fig. 4. $D_{22} = 0.4$, $D_{11} = 0.24$, view of the stationary density in phase space ($dt = \pi/1000$). Finite difference integration.

4. Conclusions

In this paper, we report the successful implementation of a robust finite difference scheme for the solution of Fokker–Planck equations in two dimensions plus time. We have checked the integrator with some exactly solvable problems, with a finite element integrator of the equation as well as with the results obtained by the numerical simulation of the SDE.

Because of the wide applicability of FP equations in dynamics it is important to find a reliable numerical procedure for FP equations. According to the successful calibration, this scheme is a good candidate to simulate some more complicated and realistic cases: higher dimensional problem, non-Gaussian white noise (Ornstein–Uhlenbeck) and time dependent coefficients.

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