Numerical Instabilities in the Accelerated Orbit Following Monte-Carlo Method

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Abstract

Analytic results on the propagation of the numerical errors in the accelerated orbit following Monte-Carlo (AOFMC) method are exposed. A simple trick that reduces the programming complexity is suggested. The structure of a code for a second order stochastic Runge-Kutta integrator is presented.

1. On the sampling errors in the orbit following method

Consider the Fokker-Planck equation that describes the gyro-averaged particle motion in axial symmetric tokamak magnetic field configuration in the full phase space. Its general form (at the collision time scale) is

$$\partial_t F(t,\mathbf{x}) = \partial_i[(V^i(\mathbf{x})/\varepsilon + U^i(\mathbf{x},t))F + \partial_i(D^{i,j}(\mathbf{x},t)\partial_j F);\ \varepsilon << 1 \quad (1.1)$$

where we denoted ($\partial_i = \partial/\partial x_i$). Typically $\mathbf{x}=\{p_1,q_1, p_2,q_2, p_3,q_3\}$ with gyro-angle q_3 and toroidal angle q_1. The vector field $V^i(x)$ represents an integrable Hamiltonian system. The terms $\boldsymbol{U}$ and $\boldsymbol{D}$ are related to collisions, ripple and RF heating. The variables $\mathbf{p}=\{p_1,p_2,p_3\}$ are invariants. The phase space is foliated by tori labeled by $\mathbf{p}$. The MC update in the case of R.F heating was studied in refs.[1-3]. *Consider only the case without resonance, with incommensurable frequencies. Then the unperturbed motion (due to V) is ergodic when restricted to the invariant tori*. The frequency of the (unperturbed) motion in the variables $\mathbf{q}=\{q_1, q_2, q_3\}$, related to the motion on the invariant tori, is large compared to the collision frequency. Consequently the following sequence of updates will give an approximation of the MC method performed with the **exact orbit averaged** $\boldsymbol{U}$ and $\boldsymbol{D}$, in the 3 D space of invariants.

Denote $S^i = U^i + \partial_j D^{ij}$. Follow the trajectory on a single bounce period and memorize the positions. Because the toroidal frequency is much larger, the points of the trajectory are approximately uniformly distributed (in the angle variable) on the invariant torus. Denote the positions $\mathbf{x}_a$,, at N time step t_i on a bounce period. These time steps can be random or deterministic uniform. Compute the update $\mathbf{x}\to\mathbf{x}+\boldsymbol{\delta x}$ (corresponding to orbit averaged movement) where

$$\delta x^i = N^{-1/2}\sum_{a=1}^{N}(S^i(x_a)\Delta t + \Delta w^i{}_a) \quad (1.2)$$

where $\boldsymbol{\Delta t}$ is a small time step compared to the collision time, $\Delta w^i{}_a$. are. centered Gaussian variables with covariance $<\Delta w^i{}_a.\ \Delta w^j{}_b.> = \Delta t\ \delta_{a,b}\ D^{i,j}$. This update corresponds to one accelerated time step. In the backward Kolmogorov equation appears at each update step an approximate orbit averaged diffusion coefficient and drift. Also a statistical error of order $N^{-1/2}$ appears whose effect will be studied, in the following analytic simplified models.

2.The numerical instabilities induced by sampling errors in orbit following method

In order to study the effect of the approximation of the orbit averaging, with random errors at each accelerated step, we consider a simplified model of the numerical process. For solubility reasons we consider the space of the invariants is one-dimensional. The stochastic differential equation (SDE), that describes the evolution of the invariant $\boldsymbol{x}$ has the form $dx=v(x)\,dt+\sigma(x)\,dw(t)$, where $w(t)$ is a standard Wiener process, and $v(x)$ is the orbit averaged drift. The orbit averaged diffusion coefficient is modeled by $D(x)=\sigma(x)^2$. In the AOFMC estimation there are statistical fluctuations in the drift and the diffusion coefficient, consequently the real evolution of the results of the Monte-Carlo simulation is described by the SDE $dx=[v(x)+\Delta v(t)]\,dt+[\sigma(x)+\Delta\sigma(t)]\,dw(t)$. Here Δv_1 and $\Delta\sigma_1$ are respectively the statistical fluctuations of the drift and of the diffusion coefficient in the process of numerical Monte-Carlo approximation of the orbit-averaged values. Ornstein-Uhlenbeck process models the fluctuations of the velocity and diffusion coefficient:

$$\Delta v(t) = \delta_v y_1(t);\ \Delta\sigma(t) = \delta_\sigma\, y_2(t)$$

$$dy_i(t) = y_i(t)\,dt/\tau_i + (2/\tau_i)^{1/2}dw_i(t),\ i=\overline{1,2}$$

The symbols δ_v *and* δ_σ denotes the intensity of the numerical noises that perturb the drift and the diffusion coefficient. The standard Wiener processes dw, dw_1 and dw_2 are independent. The amplitude of the processes $y_1(t)$ and $y_2(t)$ are normalized to unit. Their correlations times are τ_1 respectively τ_2 .

2.1 The linearized approximation

We approximate locally the drift and dispersion by linear functions

$$v(x) = v_0 + v_1 x;\ \sigma(x) = \sigma_0 + \sigma_1 x$$

The resulting equation describes a random walk on the one-dimensional affine group

$$dx(t) = (v_1 dt + \sigma_1 dw(t))\,x + du(t)$$

$$du(t) = (v_0 + \delta_v y_1(t))dt + dw(t)(\sigma_0 + y_2(t)\,\delta_\sigma)$$

In the framework of this approximation, **in the case $v_1 < 0$** (that is a deterministically stable system) the resulting model is a particular case of the stochastic models of the parametric instability, studied in the works [4-7]. The resulting equation describes the evolution of a subcritical stochastic system that randomly crosses the instability threshold, due to the term $\sigma_1 x$. **Without noise, when $\sigma_1=0$,** in the stationary state the random variable $x(t)$ has an approximate Gaussian distribution near the equilibrium state, with half width Γ that can be approximated by

$$\Gamma^2 = {\sigma_m}^2/(2v_1)\text{ , where we denoted}$$

$${\sigma_m}^2 = {\delta_v}^2\tau_1 + {\sigma_0}^2 + {\delta_\sigma}^2$$

In the general case, when $\sigma_1\neq 0$, the probability distribution of the random variable $x(t)$ in the stationary state is less concentrated. According to the results from refs. [4, 6] for large amplitudes it has the following asymptotic decay

$$prob(|x(t)|>X) \propto X^{-2-\beta}$$

The exponent β is given by

$$\beta = 2v_1/{\sigma_1}^2$$

The half-width of the distribution near the equilibrium point is given by $\Gamma=\sigma_m/\sigma_1$. The main effect is the destabilization: instead of the Gaussian distribution we have power law decay. **The numerical errors have a power law distribution instead of a Gaussian one, even in the deterministic stable case.**

2.2.The effect of sample errors in the orbit averaged drift term.

Consider the exact orbit averaged Fokker-Planck equation for the distribution function $f(P_1,P_2,P_3)$ of the invariants ($\partial_i = \partial/\partial P_i$)

$$\partial_t f + g^{-1/2}\partial_i(g^{1/2}V_i f) = g^{-1/2}\partial_i(g^{1/2}D_{i,j}\partial_j f) \quad (2.1)$$

The corresponding stochastic differential equation in the Ito formalism is

$$dP_i = U_i dt + a_{i,m}dw_m \text{ where } D_{i,j} = a_{i,m}\,a_{j,m}/2 \text{ and}$$

$$U_i = V_i + g^{-1/2}\partial_i(g^{1/2}D_{i,j}) \quad (2.2)$$

Suppose that only the drift term V_i is subjected to numerical errors along simulation, caused by an estimation of the orbit averaged drift term by N samples. Correlated white noises $dW_i^{(N)}$ will approximate these errors. Then the stochastic differential equation has this new term:

$$dP_i = U_i dt + dW_i^{(N)} + a_{i,m}dw_m$$

where $\left\langle \Delta W_i^{(N)}(t,t+\Delta t)\Delta W_j^{(N)}(t,t+\Delta t)\right\rangle = \Delta t d_{i,j}^{(N)}$

Consequently, from the simulations results an evolution with an increased diffusion coefficient

$$D_{i,j}^{(N)} = D_{i,j} + d_{i,j}^{(N)}/2 = D_{i,j} + O(N^{-1/2})$$

The same estimation results by approximating the errors in the second term in (2.2) by white noise.

2.3. The effect of sample errors in the diffusion term.

Contrary to the errors in the drift term, the following analysis proves that the fluctuations in the orbit averaged diffusion term do not produce instabilities.

The effect of the noise on the diffusion coefficient will be modeled by a dichotomous symmetric random Poisson process with time constant $\lambda>0$. Denote ± the states of the two state random variable $\eta=\pm 1$ and by $f_\pm(P,t)$ the distribution function in the corresponding states, by $a^\pm_{i,m}$ the random terms in these states. Neglecting the drift terms we have the stochastic differential equations

$$dP_i = (a^+{}_{i,m}(1+\eta)/2 + a^-{}_{i,m}(1-\eta)/2)dw_m$$

The equation for the distribution function is ($\partial_i = \partial/\partial P_i$)

$$\partial_t f_\pm = g^{-1/2}\partial_i(g^{1/2}D^\pm{}_{i,j}\partial_j f_\pm) \pm \lambda(f_- - f_+) \quad (2.3)$$

The main result is: **The bistable noise does not induce instabilities**. For a more precise formulation observe that the Eq.(2.3) can be rewritten in a matrix form

$$\begin{pmatrix}\partial_t f_+\\ \partial_t f_-\end{pmatrix} = \begin{pmatrix}-A_+ - \lambda & \lambda\\ \lambda & -A_- - \lambda\end{pmatrix}\begin{pmatrix}f_+\\ f_-\end{pmatrix} := -\hat{\mathbf{B}}_\lambda\begin{pmatrix}f_+\\ f_-\end{pmatrix}$$

where $\boldsymbol{A_\pm}$ are positive symmetric second order differential operators in a Hilbert space $\mathbf{H}$. This Hilbert space is defined by the norm

$$\|\psi\|^2 = \int g^{1/2}(P)|\psi(P)|^2 dP$$

The operator $\boldsymbol{B_\lambda}$, is defined in the extended Hilbert space of the couple of functions $(f_+, f_-)^T$ with the norm

$$\left\|(f_+,f_-)^T\right\|^2 = \int g^{1/2}(|f_+|^2 + |f_+|^2)dP$$

By using this formalism we have the following:

Proposition

The evolution of the system perturbed by dichotomous noise, that models the fluctuations of the diffusion coefficients in the Fokker-Planck equation Eq.(2.1) is stable, in the sense that

$$\lim_{t\to\infty}\left\|\exp(-B_\lambda t)\psi\right\| = 0$$

For the largest relaxation time T of the perturbed system and the relaxation times $T_\pm$ of the system in states ±, we have: $min(T_+,T_-)\le T\le max(T_+,T_-)$. To each pair of eigenvalues $(a^+{}_m, a^-{}_n)$ of the operators (A^+, A^-) , the operator B has a pair of eigenvalues $(b_{m,n}^{(1)}, b_{m,n}^{(2)})$ such that $\min(a^+{}_m, a^-{}_n) \le b_{m,n}^{(1)} \le \max(a^+{}_m, a^-{}_n) \le b_{m,n}^{(2)}$. For $\lambda\to\infty$ (when the noise approaches the white noise) we have $b_{m,n}^{(1)} \to (a^+{}_m + a^-{}_n)/2$.

3. Numerical methods

3.1. Simplified programming with stochastic Euler method

The use of the analytical form of the derivatives Eq.(2.2) in the Monte-Carlo simulation of the traiectories can be avoided by using the two step modification of the Euler-Maruyama scheme. Consider the Ito stochastic differential equation with standard independent Wiener processes dw_m

$$dx_i = a_i(x,t)dt + b_{i,m}(x,t)dw_m(t);\quad 1\le i\le \dim x; 1\le m\le \dim w \quad (3.1)$$

and the following updates, after the increments dw_m were generated

$$\delta x_i = a_{i,m}(x,t)dw_m(t);$$

$$dx_i = v_i(x,t)dt + a_{i,m}(x+\delta x,t)dw_m(t)$$

Then [8], the Fokker-Planck equation for the probability density *f(x,t)has the form* Eq. (2.1).

3.2 Weak order 2 stochastic integrator for general system of SDE

Contrary to the deterministic case, in the case of the system of SDE it is difficult to construct higher order integrators without subroutines that gnenerates numerically the derivatives. The integrator from Ref.[8], page 487-487 was adapted. The prototype of the integrator is: *void SDEintegrator1(int dimx, int dimw, int dimobs, StochDiffEq* pSDE, double xstart[], double dt, double Ntraject, double tobs, double tfin, double mobs[], double error[]);*

The integers dimx, dimw has the meaning from Eq.(3.1), dim x the minimal dimension of the array xstart[], that gives the initial position . The parameter dimobs is the number of observables whose mean values and errors are in the arrays mobs[] and error[]. The integrator computes the time averages (from tobs to tfin) and averages over several trajectories (*double Ntraject*). The explicit form of the system of SDE is given by the pointer *StochDiffEq* pSDE*. This pointer specifies the class that generates the functions $a_i(x,t)$ and $b_{i,m}(x,t)$ from Eq.(3.1). In the *class StochDiffEq{}* there are functions that returns the values of the observables, whose mean values are computed. The random variables $dw_m(t)$ are generated by the public accessible functions from the *class RandVariable{}*, that contains generators for the exact Gaussian (by polar method), as well as more rapid discrete normalized variables, accessed from the interior of the function SDEintegrator(.). The integrator was tested by using exact results from refs.[4-6].

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