Numerical Stability Analysis in the Accelerated Orbit Following Monte-Carlo Method

G. Steinbrecher ,

University of Craiova, Association Euratom-MEdC, Romania

R. J. Dumont

CEA, IRFM, F-13108 Saint Paul Lez Durance, France.

Overview

- Motivation: numerical errors=>parametric noise
- Linear stochastic stability analysis
- Description of stochastic Runge-Kutta integrator

Motivation

- The Accelerated Orbit Following Monte-Carlo (AOFMC) Method [1-3] ⇔stochastic version of the perturbation theory of integrable Hamiltonian systems.(Neichstad theorems: V.I.Arnold,*Special Chapters on Differential Equations*, MIR, 1970)
- Numerical errors=>parametric noise
- Parametric noise destabilizes the stable linear systems [Steinbrecher, G.; Weyssow, B. Phys. Rev. Lett. 2004, 92, 125003-1 - 125003-4.]

The physical model, without numerical errors

- Hamiltonian integrable vector field $V^i(\mathbf{x})$.
- $\mathbf{x}=\{p_1,q_1, p_2,q_2, p_3,q_3\}$
- The Fokker-Planck equation for the gyro-averaged particle motion in axial symmetric tokamak magnetic field configuration in the **full 6D phase space**.

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

The unperturbed motion

- Hamilton equation: $dx^i/dt = V^i(x^1,\ldots,x^6)$

- Gyro-angle q_3 and toroidal angle q_1.
- Liouville-Arnold theorem [4]: all of the trajectories are on some 3D torus.
- The 6D phase space is foliated by these invariant tori[4].

The physical model

- The terms ***U*** and ***D*** are related to collisions, ripple and RF heating.
- The variables $\mathbf{p}=\{p_1,p_2,p_3\}$ are invariants;(magnetic momentum= $\mathbf{p_3}$)
- The phase space is foliated by tori labeled by **p**.
- Consider only the case without resonance, with incommensurable frequencies. Then the unperturbed motion (due to **V(x)**) is ergodic when restricted to the invariant tori.

ERGODICITY

- The fast motion on tori is ergodic. Slow perturbed motion of the invariants.
- Approximations: in deterministic case the Gauss averaging principle ⇔const. density on torus
- Stochastic approach: small parameter expansion $T_{bounce}/T_{collision}$
- Example: 2D square lattice (Oy, Ox), random resistor network. Shortcut along Oy<=>ergodicity
- 1 dim effective lattice.Averaging of conductivities in Oy direction .

Optimal AOFMC UPDATES
$\Delta t << T_{collision}$

- Denote: $S^i = U^i + \partial_i D^{i,j}$.
- Select positions $\mathbf{x}_{\mathbf{a}}$ at N time step t_i on a bounce period. Sampling points on torus.
- The update $\mathbf{x} \rightarrow \mathbf{x} + \delta\mathbf{x}$ is

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

Computing local **averaged** diffusion matrix and drift

- Method 1. Orbit following. Ergodicity
- Method 2. Monte-Carlo or deterministic integration on the torus, if the analytic form of the relation with action-angle variable is known
- At resonance (T_toroidal/T_bounce rational) problems.

The AOFMC update (2)

- Δw^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.
- Also a statistical error of order $N^{-1/2}$ *appears. It is a parametric noise, in the orbit averaged FP equation.*

Model 1: errors in drift term

- The exact orbit averaged Fokker-Planck equation. P_i = the invariants ($\partial_I = \partial/\partial P_i$)

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

- Denote $D_{i,j} = a_{i,m}a_{j,m}/2$
- The ITO SDE is

$$dP_i = (V_i + g^{-1/2}\partial_i(g^{1/2}D_{i,j}))dt + a_{i,m}dw_m$$

AOFMC approximation of OAMC

- The drift term V_i is subjected to sampling errors $dW_i^{(N)}$ along simulation, caused by an estimation of the orbit averaged drift term by N samples.
- Assume: $dW_i^{(N)}$ are Wiener processes:

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

The effect of sampling error on drift (1)

- The new SDE is

$$dP_i = (V_i + g^{-1/2}\partial_i(g^{1/2}D_{i,j}))dt + dW_i^{(N)} + a_{i,m}dw_m$$

The effect of sampling error on drift (2)

- From the simulations results an apparent evolution with an increased diffusion matrix.
- In this model no parametric destabilization appears. The new diffusion matrix is

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

Conclusion

- The effect of sampling errors in averaging the drift, produces an increase of the approximants of diffusion matrix of order $O(N^{-1/2})$.
- **Destabilization of linear stable points. (Random multiplicative process, parametric noise).**

Perturbations of the diffusion term. Modelling the effects of sample errors =**parametric noise**

- Two state Poisson process $\eta(t)$, time constant $\lambda > 0$. Random switching between $\eta(t) = \pm 1$ states.
- Balescu, R. Aspects of Anomalous Transport in Plasmas; I.O.P. Publishing, Bristol, 2005.
- Easy generalization to arbitrary N states, that approximates the real numerical noise
- Denote $f_{+}(P, t)$, $f_{-}(P, t)$ the distribution functions.

Perturbations of the diffusion term(=parametric noise)

- Model without drift. Standard normalised Wiener independent process $w_i(t)$:

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

- The diffusion matrix in *$\eta(t)=\pm 1$ states*

$$D^{\pm}_{i,j} = a^{\pm}_{i,m}\, a^{\pm}_{j,m} / 2$$

Perturbations of the diffusion term.

Equation for PDF

- Combination of Poisson and diffusion processes

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

- Notations: $-g^{-1/2}\partial_i (g^{1/2} D^{\pm}{}_{i,j}\partial_j f) := A_\pm f$

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

Perturbations of the diffusion term. Operator formalism

- The FP equation is

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

- $\boldsymbol{A}_{\pm}$ and $\boldsymbol{A}_{-}$ are positive symmetric second order differential operators in Hilbert space

Perturbations of the diffusion term. Hilbert space analysis

- The norm is

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

The operator $\mathbf{B}_{\lambda}$ is defined in the extended Hilbert space. The norm is

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

Results.

- If $\lambda > 0$ then $\mathbf{B}_{\lambda} > 0$
- **The evolution of the system is stable:**
- $$\lim_{t \to \infty} \left\| \exp(-B_{\lambda} t)\psi \right\| = 0$$
- *Denote: The largest relaxation time of the perturbed system=T*
- *The largest relaxation times of the system in states* $\pm$ *by* T_+ *,*T_-*.*
- *We have: min*$(T_+ ,T_-) \le T \le \max(T_+ ,T_-)$*.*

II. Numerical methods for SDE

- For SDE it is difficult to construct higher order Runge-Kutta algorithms. Subprograms that calculate the derivatives of the l.h.s. must be included. In simplest cases: Use MATHEMATICA to calculate the derivatives and to generate FORTRAN or C programs.
- Optimisation by hand these output programs

Useful tips

- Use exact Gaussian noise, instead of dichotomous noise. Computation of the terms of SDE is large, compared to Gaussian generator.
- Integrators with Gaussian noise can be combined with extrapolation. Are more stable at large time steps.

Simplified stochastic integrator for Fokker-Planck equation. Order 1/2, no need for subprograms for derivative

- The SDE for MC solution of the FP equation

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

is $$dx_i = U_i dt + a_{i,m} dw_m$$

- with $U_i = V_i + g^{-1/2}\partial_i (g^{1/2} D_{i,j})$ and $D_{i,j} = a_{i,m} a_{j,m}/2$

Weak first order approximation

- The updates are

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

$$\Delta x_i = v_i(x(t), t)\Delta t +$$

$$a_{i,m}(x(t) + \delta x, t)\Delta w_m(t)$$

$$x_i(t + \Delta t) = x_i(t) + \Delta x_i$$

Stochastic integrator without analytic derivatives

- Contrary to the deterministic case, in the case of the system of SDE it is difficult to construct higher order integrators without subroutines that generates numerically the derivatives. Few exceptions:
- The integrator from Ref.[8], page 487-487 was adapted.

Weak second order stochastic Runge-Kutta integrator

- This integrator solves the following system of stochastic differential equations

$$dx_i(t) = a_i(\mathbf{x}(t))dt + \sum_{a=1}^{m} b_{i,a}(\mathbf{x}(t))dw_a(t);\, 1 \le i \le d$$

- Notations $$y_i(t) := y_i,\, y_i(t + \Delta t)$$

Notations 1

- The driving noise:

$$\Delta w_i : normal, centered, dispersion = \Delta t$$

$$a_i := a_i(\mathbf{y}(t)); b_{i,a} := b_{i,a}(\mathbf{y}(t)); 1 \le i \le d, 1 \le a \le m$$

$$u_{\pm,i,a} = y_i \pm b_{i,a}\sqrt{\Delta t}$$

$$R_{\pm,i,a} = u_{\pm,i,a} + a_i \Delta t$$

Notations 2

- Condensed

$$u_{\pm,i,a} = \left(\mathbf{u}_{\pm,a}\right)_i$$

$$R_{\pm,i,a} = \left(\mathbf{R}_{\pm,a}\right)_i$$

$$z_i = y_i + a_i \Delta t + \sum_{a=1}^{m} b_{i,a} \Delta w_a$$

$$z_i = \left(\mathbf{z}\right)_i$$

Notations 3

- Random matrix $V_{a,b}$. Dimension: d**w**
- If b<a then **P(**$V_{a,b}$ =1**)= P(**$V_{a,b}$ =**-**1**)=1/2**
- **If b>a then** $V_{a,b}$ = **-**$V_{b,a}$
- $V_{a,a}$=1

Updates 1

$$c_{1,i} = \frac{1}{2}\left(a_i(\mathbf{z}) + a_i\right)\Delta t$$

$$c_{2,i} = \frac{1}{4}\sum_{a=1}^{m}\left(b_{i,a}(\mathbf{R}_{+,a}) + b_{i,a}(\mathbf{R}_{-,a}) + 2b_{i,a}\right)\Delta w_a$$

$$c_{3,i} = \frac{1}{4}\sum_{a=1}^{m}\sum_{\substack{r=1 \\ r\neq a}}^{m}\left(b_{i,a}(\mathbf{u}_{+,r}) + b_{i,a}(\mathbf{u}_{-,r}) - 2b_{i,a}\right)\Delta w_a$$

$$c_{4,i} = \frac{1}{4}\sum_{a=1}^{m}\left(b_{i,a}(\mathbf{R}_{+,a}) - b_{i,a}(\mathbf{R}_{-,a}) + 2b_{i,a}\right)\left[\left(\Delta w_a\right)^2 - (\Delta t)\right](\Delta t)^{-1/2}$$

Updates 2

$$c_{5,i} = \frac{1}{4}\sum_{a=1}^{m}\sum_{\substack{r=1\\ r\neq a}}^{m}\left(b_{i,a}(\mathbf{u}_{+,r}) - b_{i,a}(\mathbf{u}_{-,r})\right)\left[\Delta w_a \Delta w_r - V_{r,a}\Delta t\right](\Delta t)^{-1/2}$$

$$y_i(t + \Delta t) = y_i(t) + \sum_{k=1}^{5} c_{k,i}$$

Structure of the code 1

- 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 integrator computes the time averages (from tobs to tfin) and averages over several trajectories (*double Ntraject*).

Structure of the code 2

- 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 $b_{i,m}(x,t)$
- In the *class StochDiffEq{ }* there are functions that returns the values of the observables, whose mean values are computed.

The structure of the code 3

- 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 (2 state, 3 state).

Test of the code

- Exact results on the stationary PDF from refs[5-8] were used for test.

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