Numerics for Mean-Square Dissipative Stochastic Differential Equations

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Sharing ideas, sharing lives



The numerics of preserving structures



Geometric numerical integration

- The denomination recalls the approach to geometry formulated by Felix Klein in his Erlangen program (1893);
- geometry = the study of invariants under certain transformations;
- geometric numerical methods launched to retain peculiar features of dynamical systems under discretizations;
- Arnold (2002), speech addressed to the participants of the International Congress of Mathematicians in Beijing:

"The design of stable discretizations of systems of PDEs often hinges on capturing subtle aspects of the structure of the system in the discretization. This new geometric viewpoint has provided a unifying understanding of a variety of innovative numerical methods developed over recent decades";

Geometric numerical integration (ctd.)

- subtle connection with the so-called *geometric integration theory* by Hassler Whitney (1957);
- Arnold shows that the function spaces introduced by Whitney (the so-called Whitney elements) represent what is required for a geometric discretization of many PDEs.
- Douglas N. Arnold, Differential complexes and numerical stability, Proceedings of the ICM, Beijing 2002, vol. 1, 137–157 (2002).
- R. McLachlan, Featured Review: Geometric Numerical Integration: Structure-Preserving Algorithms for Ordinary Differential Equations. SIAM Review 45(4), 817–821 (2003).
- **E**. Hairer, C. Lubich, G. Wanner, Geometric numerical integration. Structure-preserving algorithms for ordinary differential equations, Second edition, Springer Series in Computational Mathematics 31, Springer-Verlag, Berlin (2006).
 - E. Hairer, C. Lubich, G. Wanner, Geometric numerical integration illustrated by the Störmer-Verlet method, Acta Numer. 12, 399–450 (2003).

Geometric numerical integration (ctd.)

A famous method: leapfrog method, also known as Störmer-Verlet method. This method, for the discretization of the second order problem

$$\ddot{q} = f(q),$$

is given by

$$q_{n+1} - 2q_n + q_{n-1} = h^2 f(q_n).$$

Extensively used in many fields, such as celestial mechanics and molecular dynamics.

- First due to Störmer (1907), a variant of this scheme to compute the motion of ionized particles in the Earth's magnetic field (aurora borealis);
- above formulation due to Verlet (1967) for the computer simulation of molecular dynamics models;
- interested in the history of science, he discovered that his scheme was previously used by several authors: for instance, by Newton in his Principia (1687), to prove Kepler's second law.

Geometric numerical integration (ctd.)

- Seminal contribution by De Vogelaere (1956), "a marvellous paper, short, clear, elegant, written in one week, submitted for publication and never published";
- examples of numerical methods (such as the symplectic Euler method) retaining the symplecticity of Hamiltonian problems;
- still regarding Hamiltonian problems, successive contributions by Ruth (1983) and Kang (1985);
- 1988 starting year for the establishment of a theory of conservative numerics for Hamiltonian problems: criterion for the numerical conservation of the symplecticity via Runge-Kutta methods independently by Lasagni, Sanz-Serna, Suris, depending on a similar condition discovered by Cooper (1987) for the numerical conservation of quadratic first integrals.

R. D'Ambrosio, Numerical approximation of differential problems, Springer, to appear.

Stochastic differential equations

Itō problem:

$$\mathrm{d}X(t) = f(X(t))\mathrm{d}t + g(X(t))\mathrm{d}W(t), \quad t \ge 0,$$

 $f: \mathbb{R}^d \to \mathbb{R}^d \text{ (drift)}, \, g: \mathbb{R}^d \to \mathbb{R}^{d \times m} \text{ (diffusion)},$

W(t) *m*-dimensional Wiener process. Integral form:

$$X(t) = X(0) + \int_0^t f(X(s))ds + \underbrace{\int_0^t g(X(s))dW(s)}_{\text{Itō integral}^*}.$$

*On a uniform grid $\{0 < t_1 < t_2 < \cdots \leq t_n\}$, it is defined as

$$\lim_{n \to \infty} \sum_{j=1}^{n} g(X(t_j))(W(t_{j+1}) - W(t_j)).$$

Wiener increments are $\sqrt{h} \cdot \mathcal{N}(0, 1) - distributed$, where $h = t_{j+1} - t_j$.

Stochastic geometric numerical integration



Stochastic geometric numerical integration

- Invariance of asymptotic laws in the discretization of linear systems (Schurz, 1999);
- stochastic oscillators (Melbo, Higham, 2004; Burrage, Lythe, 2007, 2009; Vilmart, 2014; Welfert, 2017; D'Ambrosio, Moccaldi, Paternoster, 2018; Laurent, Vilmart, 2020; D'Ambrosio, Scalone, 2020, 2021);
- stochastic Hamiltonian (Burrage 2012, 2014) and Poisson problems (Cohen, Vilmart, 2021);
- invariant measure of **ergodic SDEs** (Abdulle, Vilmart, Zygalakis, 2014; Laurent, Vilmart, 2021);
- energy-preserving methods for **stochastic Hamiltonians**.
- C. Chen, D. Cohen, R. D'Ambrosio, A. Lang, *Drift-preserving numerical integrators for stochastic Hamiltonian systems*, Adv. Comput. Math. (2020).
 - R. D'Ambrosio, G. Giordano, B. Paternoster, A. Ventola, *Perturbative analysis of stochastic Hamiltonian problems under time discretizations*, Appl. Math. Lett. (2021).
 - R. D'Ambrosio, S. Di Giovacchino, Long-term analysis of stochastic Hamiltonian problems under time discretizations, submitted.

Outline of the talk

Mean-square dissipation



- R. D'Ambrosio, S. Di Giovacchino, *Mean-square contractivity of stochastic theta-methods*, Comm. Nonlin. Sci. Numer. Simul. (2021).
- R. D'Ambrosio, S. Di Giovacchino, Nonlinear stability issues for stochastic Runge-Kutta methods, Comm. Nonlin. Sci. Numer. Simul. (2021).

Stochastic Hamiltonian problems

- C. Chen, D. Cohen, R. D'Ambrosio, A. Lang, *Drift-preserving numerical integrators for stochastic Hamiltonian systems*, Adv. Comput. Math. (2020).
- R. D'Ambrosio, G. Giordano, B. Paternoster, A. Ventola, *Perturbative analysis of stochastic Hamiltonian problems under time discretizations*, Appl. Math. Lett. (2021).



Outline of the talk





Memorandum on nonlinear deterministic equations

Consider a nonlinear test problem

$$\begin{cases} y'(t) = \varphi(t, y(t)), & t \ge 0, \\ y(0) = y_0, \end{cases}$$

with $\varphi:\mathbb{R}\times\mathbb{R}^m\to\mathbb{R}^m$ satisfying a one-sided Lipschitz condition

$$\left(\varphi(t,y_1) - \varphi(t,y_2)\right)^{\mathsf{T}}(y_1 - y_2) \le 0, \qquad (\star)$$

for all $t \ge 0$ and $y_1, y_2 \in \mathbb{R}^m$. Denote by y(t) and $\tilde{y}(t)$ two solutions with initial conditions y_0 and \tilde{y}_0 , respectively. Condition (*) implies the contractivity of the trajectories

$$||y(t_2) - \tilde{y}(t_2)|| \le ||y(t_1) - \tilde{y}(t_1)||,$$

for $0 \le t_1 \le t_2$, where $\|\cdot\|$ is any norm in \mathbb{R}^m , and the corresponding problem is said to be dissipative. Contractive numerical solutions for dissipative problems: AN-stability, G-stability, algebraic stability, ... (pioneered by Dahlquist, 1975).

Stochastic contractivity

Nonlinear Itō problem:

 $dX(t) = f(X(t))dt + g(X(t))dW(t), \quad t \in [0,T]$

Assumptions

- (i) C^1 -continuity of drift and diffusion;
- (ii) one-sided Lipschitz condition for the drift

$$\langle x-y, f(x)-f(y) \rangle \leq \mu \|x-y\|^2, \quad \forall x, y \in \mathbb{R}^n;$$

(iii) global Lipschitz for the diffusion

$$\|g(x) - g(y)\|^2 \le L \|x - y\|^2, \quad \forall x, y \in \mathbb{R}^n.$$

Stochastic contractivity (ctd.)

Theorem (Higham, Kloeden, 2005)

Assume (i) – (iii) hold. Then, two solutions X(t) e Y(t) of an Itō SDE with $\mathbb{E}||X_0||^2 < \infty$ and $\mathbb{E}||Y_0||^2 < \infty$ satisfy

$$\mathbb{E} \|X(t) - Y(t)\|^2 \le \mathbb{E} \|X_0 - Y_0\|^2 e^{\alpha t},$$

where

$$\alpha = 2\mu + L.$$

 $\alpha < 0$ provides mean-square contractivity.

D.J. Higham, P.E. Kloeden, Numerical methods for nonlinear stochastic differential equations with jumps, Numer. Math. (2005).



R. D'Ambrosio, S. Di Giovacchino Mean-square contractivity of stochastic θ -methods, Comm. Nonlinear Sci Numer. Simul. (2021).

R. D'Ambrosio, S. Di Giovacchino Nonlinear stability issues of stochastic Runge-Kutta methods, Comm. Nonlinear Sci Numer. Simul. (2021).

Stochastic θ -methods

$\theta\text{-}\mathrm{Maruyama}$

$$X_{n+1} = X_n + (1-\theta)\Delta t f(X_n) + \theta \Delta t f(X_{n+1}) + g(X_n)\Delta W_n,$$

$\theta\text{-Milstein}$

$$X_{n+1} = X_n + (1-\theta)\Delta t f(X_n) + \theta\Delta t f(X_{n+1}) + g(X_n)\Delta W_n$$
$$+ \frac{1}{2}g'(X_n)g(X_n)(\Delta W_n^2 - \Delta t),$$

Nonlinear stability analysis:



R. D'Ambrosio, S. Di Giovacchino Mean-square contractivity of stochastic θ -methods, Commun. Nonlinear Sci. Numer. Simul. (2021).

θ-Maruyama

Theorem

Under the assumptions (i)–(iii), any two θ -Maruyama numerical solutions X_n and Y_n , $n \ge 0$, satisfy the inequality

$$\mathbb{E} |X_n - Y_n|^2 \le \mathbb{E} |X_0 - Y_0|^2 e^{\nu(\theta, \Delta t)t_n},$$

where

$$\nu(\theta, \Delta t) = \frac{1}{\Delta t} \ln \beta(\theta, \Delta t), \quad \beta(\theta, \Delta t) = 1 + \frac{\alpha + (1 - \theta)^2 M \Delta t}{1 - 2\theta \mu \Delta t} \Delta t,$$

with

$$M = \sup_{t \in [0,T]} \mathbb{E} |f'(X(t))|^2.$$

Theorem

For any fixed value of $\theta \in [0,1]$, $|\nu(\theta, \Delta t) - \alpha| = \mathcal{O}(\Delta t)$.

θ -Milstein

Theorem

Under the assumptions (i)–(iii), any two θ -Maruyama numerical solutions X_n and Y_n , $n \ge 0$, satisfy the inequality

$$\mathbb{E} |X_n - Y_n|^2 \le \mathbb{E} |X_0 - Y_0|^2 e^{\epsilon(\theta, \Delta t)t_n},$$

where

$$\epsilon(\theta, \Delta t) = \frac{1}{\Delta t} \ln \gamma(\theta, \Delta t), \quad \gamma(\theta, \Delta t) = \beta(\theta, \Delta t) + \frac{\widetilde{M} \Delta t^2}{2(1 - 2\theta \mu \Delta t)},$$

with $\widetilde{M} = \sup_{t \in [0,T]} \mathbb{E} |h'(X(t))|^2, \quad h(X(t)) = g(X(t))g'(X(t)).$

Theorem

For any fixed value of
$$\theta \in [0,1]$$
, $|\epsilon(\theta, \Delta t) - \alpha| = \mathcal{O}(\Delta t)$.

Region of mean-square contractivity

Definition

For a nonlinear stochastic differential equation satisfying assumptions (i) - (iii), a θ -method is said to generate mean-square contractive numerical solutions in a region $\mathcal{R} \subseteq \mathbb{R}^+$ if, for a fixed $\theta \in [0, 1]$,

 $\nu(\theta, \Delta t) < 0, \quad \forall \Delta t \in \mathcal{R}$

for the θ -Maruyama,

$$\epsilon(\theta, \Delta t) < 0, \quad \forall \Delta t \in \mathcal{R}$$

for the θ -Milstein.

Definition

A stochastic θ -method is said unconditionally mean-square contractive if, for a given $\theta \in [0, 1]$, $\mathcal{R} = \mathbb{R}^+$.

Mean-square contractivity: θ -Maruyama

Mean-square contractivity holds true if

 $0<\beta(\theta,\Delta t)<1,$

for any $\Delta t \in \mathcal{R}$, i.e.

$$\mathcal{R} = \begin{cases} \left(0, \frac{|\alpha|}{(1-\theta)^2 M}\right), & \theta < 1, \\ \mathbb{R}^+, & \theta = 1. \end{cases}$$

The θ -Maruyama method with $\theta = 1$ (implicit Euler-Maruyama) is unconditionally mean-square contractive.

Mean-square contractivity: θ -Milstein

Mean-square contractivity holds true if

 $0<\gamma(\theta,\Delta t)<1,$

for any $\Delta t \in \mathcal{R}$, i.e.

$$\mathcal{R} = \begin{cases} \left(0, \frac{2|\alpha|}{2(1-\theta)^2 M + \widetilde{M}}\right), & \theta < 1, \\ \left(0, \frac{2|\alpha|}{\widetilde{M}}\right), & \theta = 1. \end{cases}$$

Parameter estimation as in global optimization algorithms.

Numerical tests: stochastic Ginzburg-Landau

$$f(X(t)) = -4X(t) - X(t)^3, \quad g(X(t)) = X(t), \quad X_0 = 1, Y_0 = 0.$$

For this problem L = 1 and $\mu = -4$, so $\alpha = -7 < 0$.

• stochastic trapezoidal method $(\theta = 1/2)$: $\mathcal{R} = (0, \frac{7}{4});$



Stochastic Ginzburg-Landau (ctd.)

• stochastic implicit Euler, unconditionally mean-square contractive;



Stochastic Ginzburg-Landau (ctd.)

• θ -Milstein method with $\theta = 1/2$: $\mathcal{R} = \left(0, \frac{14}{9}\right)$.



Numerical tests: nonlinear drift

$$f(X(t)) = -4 \begin{bmatrix} \sin(X_1(t)) \\ \sin(X_2(t)) \end{bmatrix}, \qquad g(X(t)) = \frac{1}{7} \begin{bmatrix} X_1(t) & \frac{3}{2}X_2(t) \\ \\ \frac{5}{2}X_1(t) & -\frac{1}{2}X_2(t) \end{bmatrix}$$

0

Initial data: $X_0 = \begin{bmatrix} 1 & 1 \end{bmatrix}^{\mathsf{T}}$ and $Y_0 = \begin{bmatrix} 0 & 0 \end{bmatrix}^{\mathsf{T}}$. For this problem the constants L and μ are estimated as L = 0.148 and $\mu = -3.56$, so $\alpha \approx -7.5 < 0$.

- Stochastic trapezoidal method: $\mathcal{R} = (0, 1.1875);$
- stochastic implicit Euler method, unconditionally mean-square contractive.

Numerical tests: nonlinear drift (ctd.)



Figure: Mean-square deviations over 2000 paths for the trapezoidal method.

Numerical tests: nonlinear drift (ctd.)



Figure: Mean-square deviations over 2000 paths for the implicit Euler method.

Outline of the talk



2 Stochastic Hamiltonian problems

Deterministic Hamiltonians: memorandum

$$\dot{y}(t) = J \nabla \mathcal{H}(y(t)), \quad t \ge 0, \\ y(0) = y_0, \qquad \qquad J = \begin{bmatrix} 0 & -I \\ I & 0 \end{bmatrix}.$$

• $y(t) = \begin{bmatrix} p(t) \\ q(t) \end{bmatrix} \in \mathbb{R}^{2d}$, generalized moments and coordinates;

• the Hamiltonian function

$$\mathcal{H}:\mathbb{R}^{2d}\to\mathbb{R}$$

is a first integral of the problem:

$$\mathcal{H}(y(t)) = \mathcal{H}(y_0), \qquad t \ge 0.$$

Indeed,

$$\frac{d}{dt}\mathcal{H}(y(t)) = \nabla \mathcal{H}(y(t))^{\mathsf{T}} \dot{y}(t) = \nabla \mathcal{H}(y(t))^{\mathsf{T}} J^{-1} \nabla \mathcal{H}(y(t)) = 0.$$

Conservative integrators

- **Symplectic Runge-Kutta** methods exactly preserve quadratic Hamiltonians;
- if the solution, computed by a Runge-Kutta method of order *p*, lays in a **compact set**, then

 $\mathcal{H}(y_n) = \mathcal{H}(y_0) + \mathcal{O}(h^p),$

over exponentially long times (Benettin-Giorgilli, 1994);

• nearly preserving **linear multistep methods** over long times (Hairer-Lubich, 2004);



• nearly preserving multivalue methods (Butcher, D'Ambrosio, 2017; D'Ambrosio, Hairer, 2013, 2014).

Stochastic Hamiltonian problems

For Hamiltonians of the form

$$\mathcal{H}(p(t),q(t)) = \frac{1}{2}p^{\mathsf{T}}p + V(q), \quad t \ge 0,$$

with $V\colon \mathbb{R}^d \to \mathbb{R}$ sufficiently smooth potential, we consider

$$dq(t) = p(t) dt,$$

$$dp(t) = -V'(q(t)) dt + \sum dW(t).$$

with $\Sigma \in \mathbb{R}^{d \times m}$.

Stochastic generalization of classical mechanics that reconciles

- Hamiltonian nature (canonical character of evolution equations)
- non-differentiability of Wiener process (stochastic effects visible, for instance, in the statistical independence of the future from the past, irreversibility of the time arrow, random effects exhibited by quantum mechanics in the context of the theory of diffusions).

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Invariance trace law (Burrage, 2014)

 $\mathbb{E}\left[\mathcal{H}(p(t), q(t))\right] = \mathbb{E}\left[\mathcal{H}(p(t_0), q(t_0))\right] + \frac{1}{2} \mathrm{Tr}\left(\Sigma^{\top} \Sigma\right) t$

Linear drift in the expected Hamiltonian.

Stochastic Hamiltonian problems

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Linear drift in the expected Hamiltonian.

Is this property naturally preserved along discretizations?

Numerical preservation of the trace law

In Burrage (2014), the experiments reveal that

- the stochastic perturbation of symplectic RK methods does not preserve the trace law;
- the same for energy-preserving schemes.

R. D'Ambrosio, G. Giordano, B. Paternoster, A. Ventola, *Perturbative analysis of stochastic Hamiltonian problems under time discretizations*, Appl. Math. Lett. 120, article number 107223 (2021).

Example: single Wiener process

$$dq(t) = p(t) dt$$

$$dp(t) = -V'(q(t)) dt + \sigma dW(t).$$

The linear part of the σ -expansions of p and q contains the secular term $\sigma\sqrt{t}$.

Numerical preservation of the trace law (ctd.)

C. Chen, D. Cohen, R. D'Ambrosio, A. Lang, Drift-preserving numerical integrators for stochastic Hamiltonian systems, Adv. Comp. Math. (2020).

$$\Psi_{n+1} = p_n + \Sigma \Delta W_n - \frac{h}{2} \int_0^1 V'(q_n + sh\Psi_{n+1}) ds,$$

$$q_{n+1} = q_n + h\Psi_{n+1},$$

$$p_{n+1} = p_n + \Sigma \Delta W_n - h \int_0^1 V'(q_n + sh\Psi_{n+1}) ds.$$

(*)

Theorem

If $V \in \mathcal{C}^1(\mathbb{R}^d)$, the scheme (\star) satisfies the trace law

$$\mathbb{E}\left[\mathcal{H}(p_n, q_n)\right] = \mathbb{E}\left[\mathcal{H}(p(t_0), q(t_0))\right] + \frac{1}{2} \mathrm{Tr}\left(\Sigma^{\top} \Sigma\right) t_n,$$

for any grid point $t_n = nh$.

Numerical test (stochastic pendulum)

-1

$$\mathcal{H}(p,q) = \frac{1}{2}p^2 - \cos(q), \quad \sigma = 0.25, \quad (p_0,q_0) = (1,\sqrt{2}).$$



Numerical test (double-well potential)

$$\mathcal{H}(p,q) = \frac{1}{2}p^2 + \frac{1}{4}q^4 - \frac{1}{2}q^2, \quad \sigma = 0.5, \quad (p_0,q_0) = (\sqrt{2},\sqrt{2}).$$



Numerical test (Hénon-Heiles with double noise)

$$\mathcal{H}(p,q) = \frac{1}{2} \begin{pmatrix} p_1^2 + p_2^2 \end{pmatrix} + \frac{1}{2} \begin{pmatrix} q_1^2 + q_2^2 \end{pmatrix} + \alpha \begin{pmatrix} q_1 q_2^2 - \frac{1}{3} q_1^3 \end{pmatrix},$$

$$\Sigma = \begin{pmatrix} 0.2 & 0 \\ 0 & 0.2 \end{pmatrix}, \quad p_0 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad q_0 = \begin{pmatrix} \sqrt{3} \\ 1 \end{pmatrix}, \quad \alpha = 1/16.$$



Spoiler: Stratonovich Hamiltonian problems

Stratonovich calculus obeys to the classical chain rule. Then, we have Hamiltonian conservation:

- $\mathcal{H}(q(t), p(t)) = \mathcal{H}(q(0), p(0)) := \mathcal{H}_0;$
- $\mathbb{E}\left[\mathcal{H}(q(t), p(t))\right] = \mathbb{E}\left[\mathcal{H}_0\right] = \mathcal{H}_0.$
- N. Milstein, YU. M. Repin, M.V. Tretyakov, Numerical Methods for Stochastic Systems Preserving Symplectic Structure, SINUM 2002.

Is this property naturally preserved along discretizations for long times?

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$$\mathbb{E}\left[\mathcal{H}(q_n, p_n)\right] = \mathcal{H}_0 + \mathcal{O}\left(\Delta t^{r+1}\right) + \mathcal{O}\left(\Delta t^r t_n\right) + \mathcal{O}\left(t_n \Delta t^r e^{C(\sigma)\Delta t^r t_n}\right),$$

where r is the weak order of the method.

Numerical test: double-well potential

$$V(q) = \frac{1}{4}q^4 - \frac{1}{2}q^2.$$

Stochastic perturbation of the energy-preseving scheme introduced (in the deterministic setting) by E. Celledoni *et al.* with r = 1:

$$\begin{split} q_{n+1} &= q_n + \xi_n \left[\frac{1}{6} p_n + \frac{2}{3} \left(\frac{p_n + p_{n+1}}{2} \right) + \frac{1}{6} p_{n+1} \right] = q_n + \frac{\xi_n}{2} \left(p_n + p_{n+1} \right), \\ p_{n+1} &= p_n - \xi_n \left[\frac{1}{6} V'(q_n) + \frac{2}{3} V'\left(\frac{q_n + q_{n+1}}{2} \right) + \frac{1}{6} V'(q_{n+1}) \right], \\ \text{where } \xi_n &= \Delta t + \sigma \Delta W_n. \end{split}$$

E. Celledoni, R. Mclachlan, D.I. Mclaren, B. Owren, G.R.W. Quispel, W.M. Wright, *Energy-preserving Runge-Kutta methods*, ESAIM: M2AN 2009.

We consider $\sigma = 1$ in next simulation.



Conclusions

- Structure-preservation in SDEs
- Long-term invariant (laws) preservation
- Avoid (when possible) the construction of new schemes
- Hidden properties given as conditional stability constraints



Thank you for your attention!