Long time numerical solution of stochastic differential equations: the interplay of geometric integration and stochastic integration

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based on joint work with

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July 2017, Sydney

Geometric integration

The aim of geometric integration is to study and/or construct numerical integrators for differential equations

$$\dot{y}(t) = f(y(t)), \qquad y(0) = y_0,$$

which share geometric structures of the exact solution.
In particular: symmetry, symplecticity for Hamiltonian systems, first integral preservation, Poisson structure, etc.

Examples of numerical integrators $y_n \simeq y(nh)$ (stepsize h):

- explicit Euler method $\quad y_{n+1} = y_n + hf(y_n).$
- implicit Euler method $\quad y_{n+1} = y_n + hf(y_{n+1}).$
- implicit midpoint rule $\quad y_{n+1} = y_n + hf\Big(\dfrac{y_n + y_{n+1}}{2}\Big).$

Example: simplified solar system (Sun-Jupiter-Saturn)

Universal law of gravitation (Newton)

Two bodies at distance D attract each others with a force proportional to $1/D^2$ and the product of their masses.

$$m_i \ddot{q}_i(t) = -G \sum_{0 \le j \ne i \le 2} m_i m_j \frac{q_i(t) - q_j(t)}{\|q_i(t) - q_j(t)\|^3} \quad (i = 0, 1, 2)$$

$q_i(t) \in \mathbb{R}^3$ positions, $p_i(t) = m_i \dot{q}_i(t)$ momenta, G, m_0, m_1, m_2 const.
This is a Hamiltonian system

$$\dot{q}(t) = \nabla_p H\big(p(t), q(t)\big), \qquad \dot{p} = -\nabla_q H\big(p(t), q(t)\big),$$

with Hamiltonian (energy): $H(p, q) = T(p) + V(q)$

$$T(p) = \frac{1}{2} \sum_{i=0}^{2} \frac{1}{m_i} p_i^T p_i, \quad V(q) = -G \sum_{i=1}^{2} \sum_{j=0}^{i-1} \frac{m_i m_j}{\|q_i - q_j\|}.$$

Conservation of first integrals

Energy conservation for Hamiltonian systems

For a Hamiltonian system

$$\dot{q}(t) = \nabla_p H\big(p(t), q(t)\big), \qquad \dot{p}(t) = -\nabla_q H\big(p(t), q(t)\big),$$

the Hamiltonian $H(p, q)$ is a first integral: $H(p(t), q(t)) = const$.

More generally, a quantity $C(y)$ is a first integral ($C(y(t)) = const$) of a general system $\dot{y} = f(y)$ if and only if

$$\nabla C(y) \cdot f(y) = 0, \qquad \text{for all } y.$$

Comparison of numerical methods: $\rightarrow$anim.

Example of a stochastic model: Langevin dynamics

It models particle motions subject to a potential V, linear friction and molecular diffusion:

$$\dot{q}(t) = p(t), \qquad \dot{p}(t) = -\nabla V(q(t)) - \gamma p(t) + \sqrt{2\gamma\beta^{-1}}\dot{W}(t).$$

$W(t)$: standard Brownian motion in $\mathbb{R}^d$,continuous, independent increments, $W(t+h) - W(t) \sim \mathcal{N}(0,h)$, a.s. nowhere differentiable.

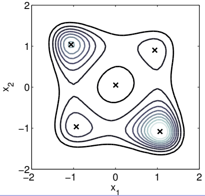
Itô integral: for $f(t)$ a (continuous and adapted) stochastic process,

$$\int_0^{t=t_N} f(s)dW(s) = \lim_{h\to 0} \sum_{n=0}^{N-1} f(t_n)(W(t_{n+1}) - W(t_n)), \qquad t_n = nh.$$

Example in 2D

A quartic potential V (see level curves):

$V(x) = (1-x_1^2)^2 + (1-x_2^2)^2 + \frac{x_1 x_2}{2} + \frac{x_2}{5}$.



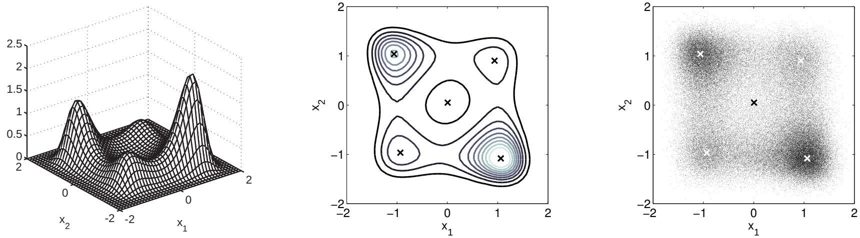
Example: Overdamped Langevin equation (Brownian dynamics)

$$dX(t) = -\nabla V(X(t))dt + \sqrt{2}dW(t).$$

$W(t)$: standard Brownian motion in $\mathbb{R}^d$.
Ergodicity: invariant measure μ_∞ has density $\rho_\infty(x) = Ce^{-V(x)}$,

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T \phi(X(s))ds = \int_{\mathbb{R}^d} \phi(y)d\mu_\infty(x), \quad a.s.$$

Example ($d=2$): $V(x) = (1-x_1^2)^2 + (1-x_2^2)^2 + \frac{x_1x_2}{2} + \frac{x_2}{5}$.



Long time accuracy for ergodic SDEs

$$dX(t) = f(X(t))dt + g(X(t))dW(t), \quad X(0) = x.$$

Under standard ergodicity assumptions,

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T \phi(X(t)) = \int_{\mathbb{R}^d} \phi(y)d\mu_\infty(y)$$

$$\left|\mathbb{E}(\phi(X(t))) - \int_{\mathbb{R}^d} \phi(y)d\mu_\infty(y)\right| \leq K(x,\phi)e^{-ct}, \quad \text{for all } t \geq 0.$$

Two standard approaches using an ergodic integrator of order p:

- Compute a single long trajectory $\{X_n\}$ of length $T = Nh$,

$$\frac{1}{N+1}\sum_{k=0}^{N} \phi(X_k) \simeq \int_{\mathbb{R}^d} \phi(y)d\mu_\infty(y), \qquad \text{error } \mathcal{O}(h^p + T^{-1/2}),$$

- Compute many trajectories $\{X_n^i\}$ of length of length $t = Nh$,

$$\frac{1}{M}\sum_{i=1}^{M} \phi(X_N^i) \simeq \int_{\mathbb{R}^d} \phi(y)d\mu_\infty(y), \qquad \text{error } \mathcal{O}(e^{-ct} + h^p + M^{-1/2}).$$

Parabolic SPDE case

Example: Consider a semilinear parabolic stochastic PDE:

$$\partial_t u(t,x) = \partial_{xx} u(t,x) + f\big(u(t,x)\big) + \dot{W}(t,x)\ ,\ \ t>0, x\in\Omega$$
$$u(0,x) = u_0(x)\ ,\ \ x\in\Omega$$
$$u(t,x) = 0\ ,\ \ x\in\partial\Omega,$$

or its abstract formulation in $L^2(\Omega)$:

$$du(t) = Au(t)dt + f\big(u(t)\big)dt + dW(t)\ ,\ \ t>0$$
$$u(0) = u_0.$$

Under appropriate assumptions, $\big(u(t)\big)_{t\geq 0}$ is an ergodic process.

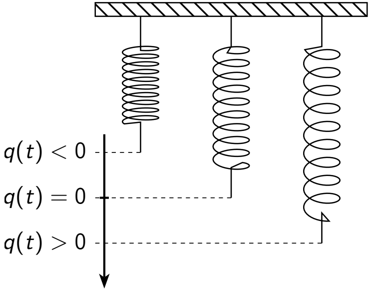
Aim: design an efficient high order integrator for sampling the SPDE invariant distribution.

Plan of the talk

1. Introduction: geometric numerical integration
2. Modified differential equations
3. Order conditions for the invariant measure
4. Postprocessed integrators for ergodic SDEs
5. Postprocessed integrators for parabolic SPDEs

S. Fiorelli Vilmart and G. V., *Computing the long term evolution of the solar system with geometric numerical integrators*, snapshots of modern mathematics from Oberwolfach, 2017.

A linear example: the harmonic oscillator



We consider the model of an oscillating spring, where $q(t)$ is the position relative to equilibrium at time t and $p(t)$ is the momenta.

$$\dot{q}(t) = \frac{1}{m}p(t), \qquad \dot{p}(t) = -kq(t)$$

The Hamiltonian energy of the system is

$$H(p,q) = \frac{1}{2m}p^2 + \frac{k}{2}q^2.$$

Comparison of energy conservations (harmonic oscillator, $m = 1$)

- Explicit Euler method: energy amplification.

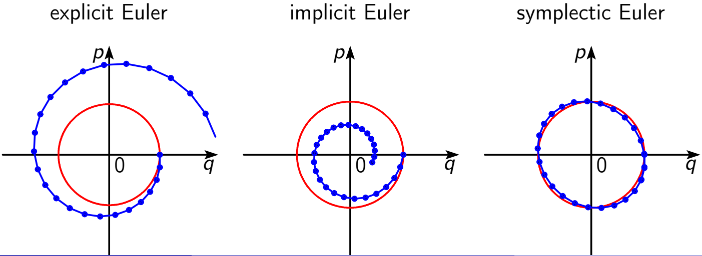
$$H(p_{n+1}, q_{n+1}) = (1 + kh^2) H(p_n, q_n).$$

- Implicit Euler method: energy damping.

$$H(p_{n+1}, q_{n+1}) = \frac{1}{1 + kh^2} H(p_n, q_n).$$

- Symplectic Euler method: exact conservation of a modified Hamiltonian energy $\tilde{H}_h(p, q) = H(p, q) + hkpq$.

$$\tilde{H}_h(p_{n+1}, q_{n+1}) = \tilde{H}_h(p_n, q_n)$$



What happened? Theory of backward error analysis

Given a differential equation

$$\dot{y} = f(y), \quad y(0) = y_0$$

and a one-step numerical integrator

$$y_{n+1} = \Phi_{f,h}(y_n)$$

we search for a modified differential equation

$$\dot{z} = \widetilde{f}_h(z) = f(z) + hf_2(z) + h^2 f_3(z) + h^3 f_4(z) + \dots, \quad z(0) = y_0$$

such that (formally) $\quad y_n = z(nh)$

Ruth (1983), Griffiths, Sanz-Serna (86), Gladman, Duncan, Candy (91), Feng (91), Sanz-Serna (92), Yoshida (93), Eirola (93), Hairer (94), Fiedler, Scheurle (96), ...

What happened? Energy conservation by symplectic integrators

$$\dot{q} = \nabla T(p), \qquad \dot{p} = -\nabla V(q).$$

Theorem (Benettin & Giorgilli 1994, Tang 1994)

For a symplectic integrator, e.g. the symplectic Euler method

$$q_{n+1} = q_n + h\nabla T(p_n), \qquad p_{n+1} = p_n - h\nabla V(q_{n+1}),$$

the modified differential equation remains Hamiltonian:

$$\dot{\widetilde{q}} = \widetilde{H}_p(\widetilde{p}, \widetilde{q}), \qquad \dot{\widetilde{p}} = -\widetilde{H}_q(\widetilde{p}, \widetilde{q})$$

$$\widetilde{H}(p,q) = H(p,q) + h\,H_2(p,q) + h^2 H_3(p,q) + \dots$$

Here $\widetilde{H}(q,p) = T(q) + V(p) - \frac{h}{2}\nabla T(q)^T \nabla V(p) + \frac{h^2}{12}\nabla V(p)^T \nabla^2 T(q) \nabla V(p) + \dots$.

Formally, the modified energy is exactly conserved by the integrator:

$$\widetilde{H}(p_n, q_n) = \widetilde{H}(\widetilde{p}(nh), \widetilde{q}(nh)) = \widetilde{H}(p_0, q_0) = const.$$

It allows to prove the good long time conservation of energy.

High order numerical integrators based on modified equations

Theorem (Chartier, Hairer, V., Math.Comp. 2007)

Given $y_{n+1} = \Phi_{f,h}(y_n)$, consider a suitable truncated modified equation

$$\dot{z} = f_h^{[r]}(z) = f(z) + hf_2(z) + \cdots + h^{r-1}f_r(z).$$

Then, the same integrator applied to the above modified equations,

$$z_{n+1} = \Phi_{f_h^{[r]},h}(z_n),$$

defines an integrator of order r for $\dot{y} = f(y)$.

Remark: The above modified equation is different but related to the one of backward error analysis. It can be viewed as a dual approach using the algebraic framework of B-series (Taylor-type series indexed by rooted trees), (Calaque, Ebrahimi-Fard, Manchon, 2008).

Example of a co-product of a Hopf algebra of trees:

Application: high-order modified implicit midpoint rule

Considering the modified implicit midpoint rule

$$y_{n+1} = y_n + hf_h^{[6]}\Big(\frac{y_n + y_{n+1}}{2}\Big),$$

applied to the modified differential equation

$$\dot{z} = f_h^{[6]} = f(z) + h^2 f_3(z) + h^4 f_5(z),$$

$$\begin{aligned}
f_3 &= \frac{1}{12}\Big(-f'f'f + \frac{1}{2}f''(f,f)\Big),\\
f_5 &= \frac{1}{120}\Big(f'f'f'f'f - f''(f,f'f'f) + \frac{1}{2}f''(f'f,f'f)\Big)\\
&+ \frac{1}{240}\Big(-\frac{1}{2}f'f'f''(f,f) + f'f''(f,f'f) + \frac{1}{2}f''(f,f''(f,f)) - \frac{1}{2}f^{(3)}(f,f,f'f)\Big)\\
&+ \frac{1}{80}\Big(-\frac{1}{6}f'f^{(3)}(f,f,f) + \frac{1}{24}f^{(4)}(f,f,f,f)\Big),
\end{aligned}$$

we obtain a method of order 6 for $\dot{y} = f(y)$.

Remarks: Connexion with Generating function symplectic integrators for Hamiltonian systems of Feng Kang (1986). It yields efficient integrators for specific problems (rigid body, Hairer, V. 2006).

Application: a high-order stochastic implicit midpoint rule

(Abdulle, Cohen, V., Zygalakis, SIAM SISC 2012).
The strategy of modified equations yields the integrator

$$X_{n+1} = X_n + hf_{h,1}\left(\frac{X_n + X_{n+1}}{2}\right) + g_{h,1}\left(\frac{X_n + X_{n+1}}{2}\right)\Delta W_n,$$

where $f_{h,1} = f + hf_1$ and $g_{h,1} = g + hg_1$ with

$$f_1 = \frac{1}{4}\left(\frac{1}{2}f''(g,g) - g'f'g\right) \qquad g_1 = \frac{1}{4}\left(\frac{1}{2}g''(g,g) - g'g'g\right),$$

Theorem

The modified stochastic implicit midpoint rule exactly conserves any quadratic first integral and has weak order 2: for all test function ϕ,

$$|\mathbb{E}(\phi(X_n) - \mathbb{E}(\phi(X(t_n))| \leq Ch^2, \qquad t_n = nh \leq T.$$

Note: the standard stochastic implicit midpoint rule has weak order 1.
The above methods have strong order 1/2 or 1: $\mathbb{E}(|X_n - t_n|) \leq Ch^{1/2}$.

Order conditions for the invariant measure

- A. Abdulle, G. V., K. Zygalakis, *High order numerical approximation of ergodic SDE invariant measures*, SIAM SINUM, 2014.
- A. Abdulle, G. V., K. Zygalakis, *Long time accuracy of Lie-Trotter splitting methods for Langevin dynamics*, SIAM SINUM, 2015.

A classical tool: the Fokker-Plank equation

$$dX(t) = f(X(t))dt + \sqrt{2}dW(t).$$

The density $\rho(x,t)$ of $X(t)$ at time t solves the parabolic problem

$$\partial_t \rho = \mathcal{L}^* \rho = -\mathrm{div}(f\rho) + \Delta\rho, \qquad t > 0, x \in \mathbb{R}^d.$$

For ergodic SDEs, for any initial condition $X(0) = X_0$, as $t \to +\infty$,

$$\mathbb{E}(\phi(X(t))) = \int_{\mathbb{R}^d} \phi(x)\rho(x,t)dx \longrightarrow \int_{\mathbb{R}^d} \phi(x)d\mu_\infty(x).$$

The invariant measure $d\mu_\infty(x) \sim \rho_\infty(x)dx$ is a stationary solution $(\partial_t \rho_\infty = 0)$ of the Fokker-Plank equation

$$\mathcal{L}^* \rho_\infty = 0.$$

Asymptotic expansions

Theorem (Talay and Tubaro, 1990, see also, Milstein, Tretyakov)

Assume that $X_n \mapsto X_{n+1}$ (weak order p) is ergodic and has a Taylor expansion $\mathbb{E}(\phi(X_1))|X_0 = x) = \phi(x) + h\mathcal{L}\phi + h^2 A_1\phi + h^3 A_2\phi + \dots$ If μ_∞^h denotes the numerical invariant distribution, then

$$\int_{\mathbb{R}^d} \phi d\mu_\infty^h - \int_{\mathbb{R}^d} \phi d\mu_\infty = \lambda_p h^p + \mathcal{O}(h^{p+1}),$$

where, denoting $u(t,x) = \mathbb{E}\phi\big(X(t,x)\big)$,

$$\lambda_p = \int_0^{+\infty}\int_{\mathbb{R}^d} \Big(A_p - \frac{\mathcal{L}^{p+1}}{(p+1)!}\Big) u(t,x)\rho_\infty(x)dxdt$$
$$= -\int_0^{+\infty}\int_{\mathbb{R}^d} u(t,x)\big(A_p\big)^*\rho_\infty(x)dxdt.$$

High order approximation of the numerical invariant measure

Assume that $X_n \mapsto X_{n+1}$ is ergodic with standard assumptions and

$$\mathbb{E}(\phi(X_1))|X_0 = x) = \phi(x) + h\mathcal{L}\phi + h^2 A_1\phi + h^3 A_2\phi + \dots$$

Standard weak order condition.

If $A_j = \frac{\mathcal{L}^j}{j!}$, $1 \leq j < p$, then (weak order p)

$$\mathbb{E}(\phi(X(t_n))) = \mathbb{E}(\phi(X_n)) + \mathcal{O}(h^p), \qquad t_n = nh \leq T.$$

Order condition for the invariant measure.

Theorem

If $A_j^* \rho_\infty = 0$, $1 \leq j < p$, then (order p for the invariant measure)

$$\lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} \phi(X_n) = \int_{\mathbb{R}^d} \phi d\mu_\infty + \mathcal{O}(h^p),$$

$$\mathbb{E}(\phi(X_n)) - \int_{\mathbb{R}^d} \phi d\mu_\infty = \mathcal{O}(\exp(-cnh) + h^p).$$

Application: high order integrator based on modified equations

It is possible to construct integrators of weak order 1 that have order p for the invariant measure.

This can be done inspired by recent advances in modified equations of SDEs (see Shardlow 2006, Zygalakis, 2011, Debussche & Faou, 2011, Abdulle Cohen, V., Zygalakis, 2013).

Theorem (Abdulle, V., Zygalakis)

Consider an ergodic integrator $X_n \mapsto X_{n+1}$ (with weak order ≥ 1) for an ergodic SDE (with technical assumptions),

$$dX = f(X)dt + g(X)dW.$$

Then, for all $p \geq 1$, there exist a modified equations

$$dX = (f + hf_1 + \ldots + h^{p-1}f_{p-1})(X)dt + g(X)dW,$$

such that the integrator applied to this modified equation has order p for the invariant measure of the original system $dX = fdt + gdW$ (assuming ergodicity).

Example of high order integrator for the invariant measure

Theorem

Consider the Euler-Maruyama scheme $X_{n+1} = X_n + hf(X_n) + \sigma \Delta W_n$ applied to Brownian dynamics ($f = -\nabla V$).
Then, the Euler-Maruyama scheme applied to

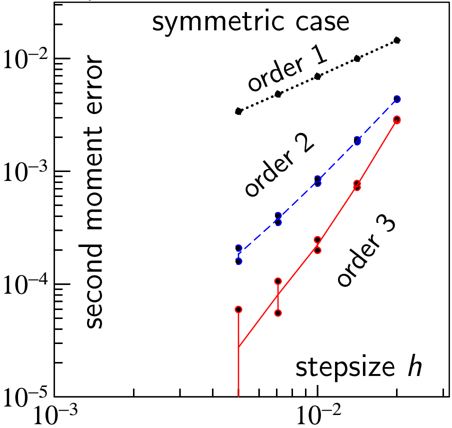
$$\begin{aligned} dX &= (f + hf_1 + h^2 f_2)dt + \sigma \Delta W_n \\ f_1 &= -\frac{1}{2} f' f - \frac{\sigma^2}{4} \Delta f, \\ f_2 &= -\frac{1}{2} f' f' f - \frac{1}{6} f''(f, f) - \frac{1}{3} \sigma^2 \sum_{i=1}^{d} f''(e_i, f' e_i) - \frac{1}{4} \sigma^2 f' \Delta f, \end{aligned}$$

has order 3 for the invariant measure (assuming ergodicity).

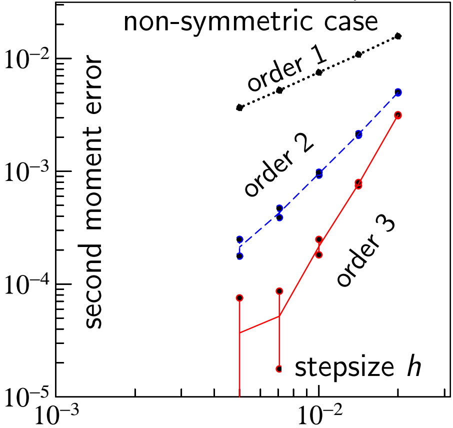
Remark 1: the weak order of accuracy is only 1.
Remark 2: derivative free versions can also be constructed.

Convergence of the modified Euler-Maruyama schemes

(double-well potential, long trajectories of length $T = 10^8$).



$V(x) = (1 - x^2)^2$



$V(x) = (1 - x^2)^2 - x/2.$

Postprocessed integrators for ergodic SDEs

G. V., *Postprocessed integrators for the high order integration of ergodic SDEs*, SIAM SISC, 2015.

Postprocessed integrators for ergodic SDEs

Idea: extend to the context of ergodic SDEs the popular idea of effective order for ODEs from Butcher 69',

$$y_{n+1} = \chi_h \circ K_h \circ \chi_h^{-1}(y_n), \qquad y_n = \chi_h \circ K_h^n \circ \chi_h^{-1}(y_0).$$

Example based on the Euler-Maruyama method

for Brownian dynamics: $dX(t) = -\nabla V(X(t))dt + \sigma dW(t)$.

$$X_{n+1} = X_n - h\nabla V\left(X_n + \frac{1}{2}\sigma\sqrt{h}\xi_n\right) + \sigma\sqrt{h}\xi_n, \qquad \overline{X}_n = X_n + \frac{1}{2}\sigma\sqrt{h}\xi_n.$$

X_n has order 1 of accuracy for the invariant measure.
$\overline{X}_n$ has order 2 of accuracy for the invariant measure (postprocessor).

This method was first derived as a non-Markovian method by [Leimkhuler, Matthews, 2013], see [Leimkhuler, Matthews, Tretyakov, 2014],

$$\overline{X}_{n+1} = \overline{X}_n + hf(\overline{X}_n) + \frac{1}{2}\sigma\sqrt{h}(\xi_n + \xi_{n+1}).$$

Postprocessed integrators

Postprocessing: $\overline{X}_n = G_n(X_n)$, with weak Taylor series expansion

$$\mathbb{E}(\phi(G_n(x))) = \phi(x) + h^p \overline{A}_p \phi(x) + \mathcal{O}(h^{p+1}).$$

Theorem

Under technical assumptions, assume that $X_n \mapsto X_{n+1}$ and $\overline{X}_n$ satisfy

$$A_j^* \rho_\infty = 0 \qquad j < p,$$

and

$$\left(A_p + [\mathcal{L}, \overline{A}_p]\right)^* \rho_\infty = 0,$$

(with $[\mathcal{L}, \overline{A}_p] = \mathcal{L}\overline{A}_p - \overline{A}_p\mathcal{L}$) then (order $p+1$ for the invariant measure)

$$\mathbb{E}(\phi(\overline{X}_n)) - \int_{\mathbb{R}^d} \phi \rho_\infty dx = \mathcal{O}\left(\exp\left(-cnh\right) + h^{p+1}\right).$$

Remark: the postprocessing is needed only at the end of the time interval (not at each time step).

New schemes based on the theta method

We introduce a modification of the $\theta = 1$ method:

$$X_{n+1} = X_n - h\nabla V(X_{n+1} + a\sigma\sqrt{h}\xi_n) + \sigma\sqrt{h}\xi_n, \quad a = -\frac{1}{2} + \frac{\sqrt{2}}{2},$$

A postprocessor of order 2

$$\overline{X}_n = X_n + c\sigma\sqrt{h}J_n^{-1}\xi_n, \quad c = \sqrt{2\sqrt{2}-1}\Big/2$$

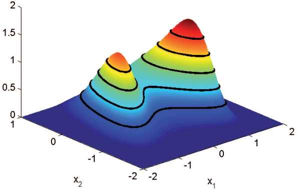
The matrix J_n^{-1} is the inverse of $J_n = I - hf'(X_n + a\sigma\sqrt{h}\xi_{n-1})$.

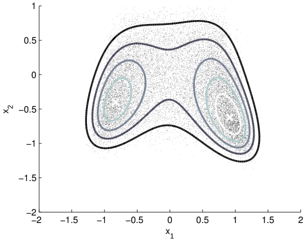
A postprocessor of order 2 (order 3 for linear problems)

$$\overline{X}_n = X_n - hb\nabla V(\overline{X}_n) + c\sigma\sqrt{h}\xi_n, \quad b = \sqrt{2}/2, \quad c = \sqrt{4\sqrt{2}-1}\Big/2.$$

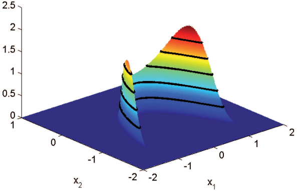
Example: stiff and nonstiff Brownian dynamics.

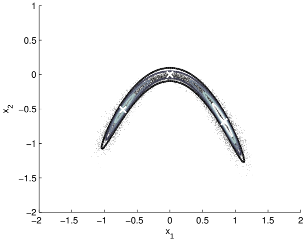
Gibbs density $\rho_\infty(x) = Z e^{-\frac{2}{\sigma^2} V(x)}$.





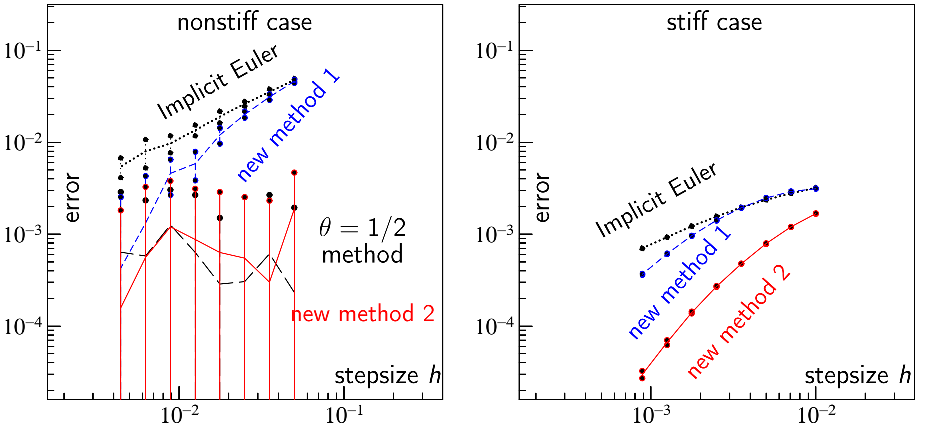
Nonstiff case $V(x) = (1 - x_1^2)^2 + x_2^4 - x + x_1 \cos(x_2) + (x_2 + x_1^2)^2$





Stiff case $V(x) = (1 - x_1^2)^2 + x_2^4 - x + x_3 \cos(x_2) + 100(x_2 + x_1^2)^2 + \frac{10^6}{2}(x_1 - x_3)^2$.

Example: stiff and nonstiff Brownian dynamics.



Error in $\int_{\mathbb{R}^d} (x_2 + x_1^2)^2 \rho_\infty(x) dx$ versus time stepsize h obtained using 10 trajectories on a long time interval of length $T = 10^5$.

Postprocessed integrators for parabolic SPDEs

C.-E. Bréhier and G. V., *High-order integrator for sampling the invariant distribution of a class of parabolic SPDEs with additive space-time noise*, SIAM SISC, 2016.

Abstract setting

Stochastic evolution equation on the Hilbert space H:

$$du(t) = Au(t)dt + F\big(u(t)\big)dt + dW^Q(t), \qquad u(0) = u_0 \in H.$$

- $A : D(A) \subset H \to H$ is a self-adjoint linear operator with

$$Ae_k = -\lambda_k e_k$$

$$\big(e_k\big)_{k\in 1,\ldots} \text{ complete orthonormal system of } H$$

$$0 < \lambda_1 \leq \ldots \leq \lambda_k \underset{k\to+\infty}{\to} +\infty$$

  Example: Laplace operator with homogeneous Dirichlet boundary conditions on a bounded domain $\mathcal{D} \subset \mathbb{R}^d$.

- $F : H \to H$ is a Lipschitz nonlinearity (with constant $\mathrm{L} < \lambda_1$), e.g. $F(u) = f \circ u$ with $f : \mathbb{R} \to \mathbb{R}$.

Abstract setting

Stochastic evolution equation on the Hilbert space H:

$$du(t) = Au(t)dt + F\big(u(t)\big)dt + dW^Q(t), \qquad u(0) = u_0 \in H.$$

- Noise: W^Q is a Q-Wiener process on H

$$W^Q(t) = \sum_{k \in \mathbb{N}^*} q_k^{1/2} \beta_k(t) \tilde{e}_k,$$

$$\big(\tilde{e}_k\big)_{k \in 1,\dots} \text{ complete orthonormal system of } H,$$

$$\beta_k, k \in \mathbb{N}^* \text{independent standard Wiener processes on } \mathbb{R},$$

$$Q\tilde{e}_k = q_k \tilde{e}_k, \quad q_k \geq 0, \quad \sup_k q_k < +\infty.$$

- Simplification:
  we assume that A and Q commute: $\tilde{e}_k = e_k$ for all k.

The linear implicit Euler scheme

Stochastic evolution equation on the Hilbert space H:

$$du(t) = Au(t)dt + F\big(u(t)\big)dt + dW^Q(t) \quad , \quad u(0) = u_0 \in H.$$

Euler scheme, with time-step size h:

$$\begin{aligned} v_{n+1} &= v_n + hAv_{n+1} + hF(v_n) + \sqrt{h}\xi_n^Q \\ &= J_1\Big(v_n + hF(v_n) + \sqrt{h}\xi_n^Q\Big), \end{aligned}$$

where $J_1 = \big(I - hA\big)^{-1}$ and $\sqrt{h}\xi_n^Q = W^Q\big((n+1)h\big) - W^Q\big(nh\big)$.

Order of convergence is $\overline{s} - \varepsilon$ for all $\varepsilon > 0$ (see Bréhier 2014):

$$\overline{\mathrm{s}} = \sup\Big\{\mathrm{s} \in (0,1)\ ;\ \mathrm{Trace}\Big((-\mathrm{A})^{-1+\mathrm{s}}\mathrm{Q}\Big) < +\infty\Big\} > 0.$$

Example: for $A = \frac{\partial^2}{\partial x^2}$, $Q = I$ in dimension 1, we have $\overline{\mathrm{s}} = 1/2$.

The postprocessed scheme

Linear Euler scheme:

$$v_{n+1} = J_1\Big(v_n + hF(v_n) + \sqrt{h}\xi_n^Q\Big).$$

New postprocessed scheme

$$u_{n+1} = J_1\Big(u_n + hF\Big(u_n + \frac{1}{2}\sqrt{h}J_2\xi_n^Q\Big) + \sqrt{h}\xi_n^Q\Big)$$

Postprocessing: $\overline{u}_n = u_n + \dfrac{1}{2}J_3\sqrt{h}\xi_n^Q,$

with

$$J_1 = (I - hA)^{-1}, \quad J_2 = (I - \frac{3-\sqrt{2}}{2}hA)^{-1}, \quad J_3 = (I - \frac{h}{2}A)^{-1/2}.$$

Idea of the construction

Construction as an IMEX (implicit-explicit) integrator for the SDE in $\mathbb{R}^d$:

$$dX(t) = \big(f_1(X(t)) + f_2(X(t))\big)dt + dW(t), \qquad X(0) = X_0.$$

with $f_0 = f_1 + f_2 = -\nabla V_0$.

Modified scheme with postprocessor:

$$\begin{aligned} X_{n+1} &= X_n + hf_1\left(X_{n+1} + a_1\sqrt{h}\xi_n\right) + hf_2(X_n + a_2\sqrt{h}\xi_n) \\ &\quad +(I + a_3 hf_1'(X_n))\sqrt{h}\xi_n \\ \overline{X}_n &= X_n + c\sqrt{h}\xi_n. \end{aligned}$$

Unknown coefficients: a_1, a_2, a_3, c, obtained using the order conditions.

Next, stabilization terms J_1, J_2, J_3 are added to guaranty the well-posedness in infinite dimension.

Analysis of the postprocessed Euler method

Theorem

- *The Markov chain* $\left(u_n, \overline{u}_{n-1}\right)_{n\in\mathbb{N}}$ *is ergodic, with unique invariant distribution, and for any test function* $\varphi : H \to \mathbb{R}$ *of class* $\mathcal{C}^2$*, with bounded derivatives,*

$$\left|\mathbb{E}(\varphi(\overline{u}_n)) - \int_H \varphi(y) d\overline{\mu}_\infty^h(y)\right| = \mathcal{O}\left(\exp(-\frac{(\lambda_1 - \mathrm{L})}{1+\lambda_1 h} nh)\right).$$

- *Moreover, for the case of a linear F, for any* $\mathrm{s} \in (0, \overline{\mathrm{s}})$,

$$\int_H \varphi(y) d\overline{\mu}_\infty^h(y) - \int_H \varphi(y) d\mu_\infty(y) = \mathcal{O}(h^{\mathrm{s}+1}).$$

Remark: error for the standard linear Euler: $\mathcal{O}(h^{\mathrm{s}})$, $\mathrm{s} \in (0, \overline{\mathrm{s}})$.

Numerical experiments (stochastic heat equation)

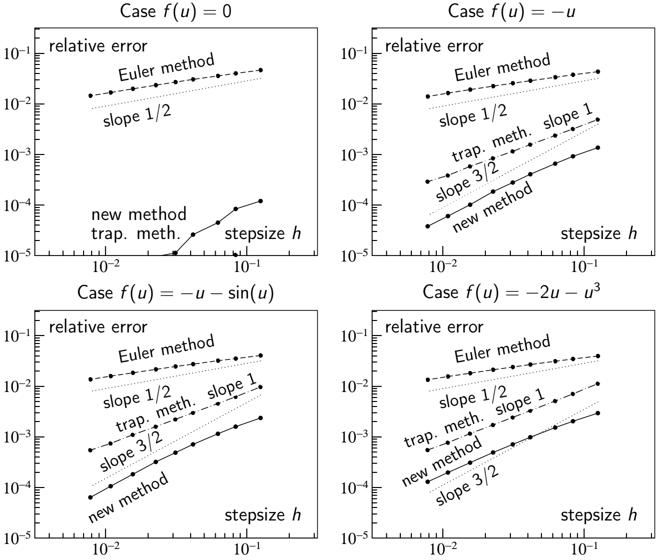
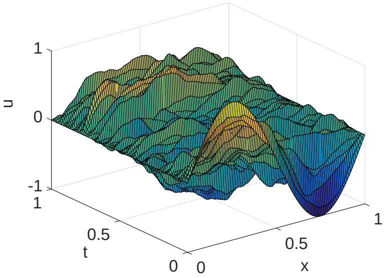


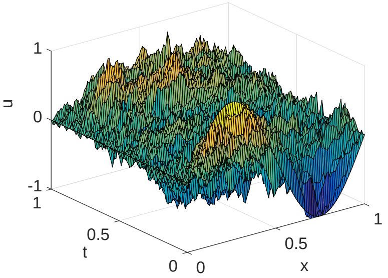
Figure: Orders of convergence, test function $\varphi(u) = \exp -(\|u\|^2)$.

Qualitative behavior

Data: $f(u) = -u - \sin(u)$, $Q = I$, $h = 0.01$.



standard Euler method



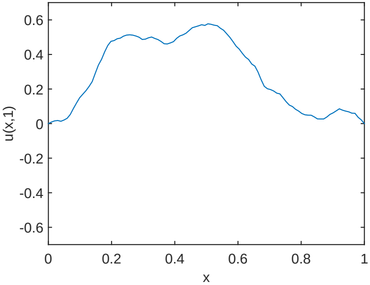
postprocessed method

Remark: the process $\left(\overline{u}_n\right)_{n\in\mathbb{N}}$ has the same spatial regularity as the continuous-time process $\left(u(t)\right)_{t\geq 0}$, while the Euler scheme $\left(v_n\right)_{n\in\mathbb{N}}$ is more regular.

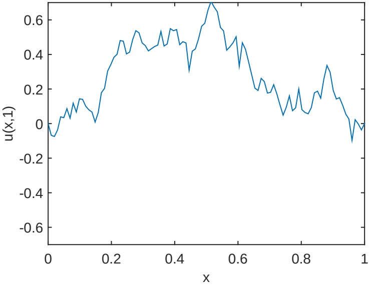
Related work: Chong and Walsh, 2012 (regularity study of the $\theta = 1/2$ stochastic method).

Qualitative behavior

Data: $f(u) = -u - \sin(u)$, $Q = I$, $h = 0.01$, $T = 1$.



standard Euler method



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Remark: the process $\left(\overline{u}_n\right)_{n\in\mathbb{N}}$ has the same spatial regularity as the continuous-time process $\left(u(t)\right)_{t\geq 0}$, while the Euler scheme $\left(v_n\right)_{n\in\mathbb{N}}$ is more regular.

Related work: Chong and Walsh, 2012 (regularity study of the $\theta = 1/2$ stochastic method).

Summary

- Using tools from geometric integration, we presented new order conditions for the accuracy of ergodic integrators, with emphasis on postprocessed integrators.
- In particular, high order in the deterministic or weak sense is not necessary to achieve high order for the invariant measure.
- A new high-order method for sampling the invariant distribution of parabolic semilinear SPDEs

$$du(t) = Au(t)dt + F\big(u(t)\big)dt + dW^Q(t),$$

with high-order of accuracy $\overline{s}+1$ instead of $\overline{s}$ (proof in a simplified linear case).

Current works:

- study of algebraic structures in stochastic modified equations.
- analysis of the order of convergence in the general semilinear SPDE case.
- combination with Multilevel Monte-Carlo strategies.