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

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based on joint works with
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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 $\quad y_{n+1} = y_n + hf\left(\frac{y_n + y_{n+1}}{2}\right).$

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

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

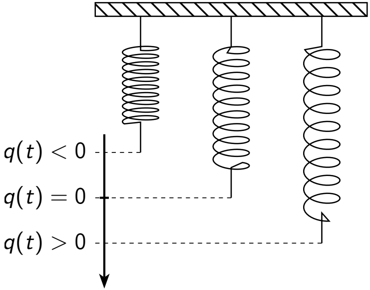
the Hamiltonian $H(p, q)$ is a first integral: $H(p(t), q(t)) = const$.

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: →anim.

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.

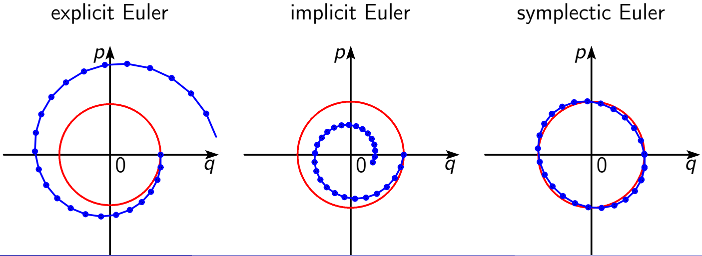
$$H(p_{n+1}, q_{n+1}) = (1 + kh^2)H(p_n, q_n).$$

- 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) $\qquad y_n = z(nh)$

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.

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.

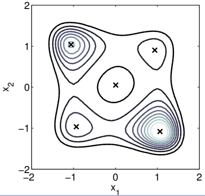
Itô integral: for $f(t)$ a (continuous and adapted) stochastic process,

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

Example in 2D

A quartic potential V (see level curves):

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



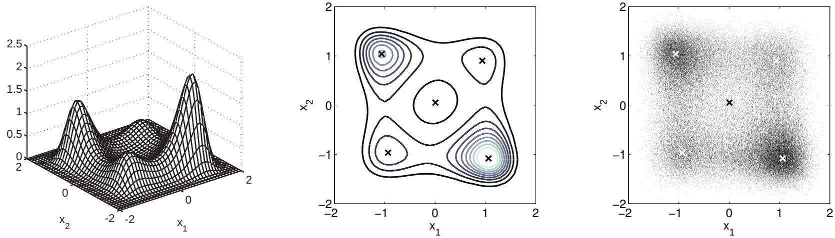
Example: Overdamped Langevin equation (Brownian dynamics)

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

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



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

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

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 $T = Nh$,

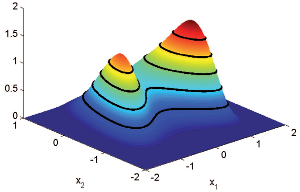
$$\frac{1}{N+1}\sum_{k=0}^{N} \phi(X_k) \simeq \int_{\mathbb{R}^d} \phi(y)d\mu_\infty(y), \qquad \text{error } \mathcal{O}(h^p + T^{-1/2}),$$

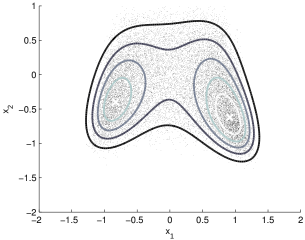
- Compute many trajectories $\{X_n^i\}$ of length of length $t = Nh$,

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

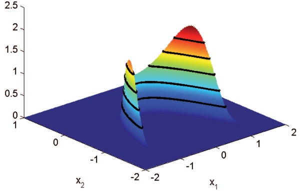
Example: stiff and nonstiff Brownian dynamics.

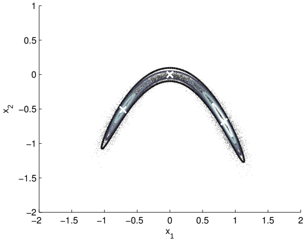
Gibbs density $\rho_\infty(x) = Ze^{-\frac{2}{\sigma^2}V(x)}$.





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: Parabolic SPDE case

Consider a semilinear parabolic stochastic PDE:

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

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

$$\begin{aligned} du(t) &= Au(t)dt + f\big(u(t)\big)dt + dW(t)\ ,\ \ t>0 \\ u(0) &= u_0. \end{aligned}$$

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.

Aim

Construct efficient high order time integrators with favorable stability properties for stiff nonlinear stochastic problems,

$$dX(t) = f(X(t))dt + \sum_{r=1}^{m} g^r(X(t))dW_r(t), \qquad X(0) = X_0 \in \mathbb{R}^d.$$

Main difficulties:

- Avoid computing derivatives (using Runge-Kutta type schemes) with a reduced number of function evaluations (independent of the dimension of the system).
- high weak order r, multi-d, general non-commutative noise,

$$\left|\mathbb{E}\big(\phi(X(t_n))\big) - \mathbb{E}\big(\phi(X_n)\big)\right| \leq Ch^r, \qquad \text{for all } t_n = nh \leq T.$$

- high strong order q, $\mathbb{E}\big(|X(t_n) - X_n|\big) \leq Ch^q$.
- Long time behavior for ergodic SDEs (and SPDEs): high order p.

Remark: in general $p \geq r \geq q$.

Plan of the talk

1. Order conditions for the invariant measure
2. Postprocessed integrators for ergodic SDEs and SPDEs
3. Optimal explicit stabilized integrator
4. An algebraic framework based on exotic aromatic Butcher-series

Order conditions for the invariant measure

1. Order conditions for the invariant measure
2. Postprocessed integrators for ergodic SDEs and SPDEs
3. Optimal explicit stabilized integrator
4. An algebraic framework based on exotic aromatic Butcher-series

- 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.

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*

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

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

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

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

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.

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

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

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

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 in the torus $\mathbb{T}^d$ (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 (Abdulle, V., Zygalakis)

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 the modified SDE

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

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.

Postprocessed integrators for ergodic SDEs and SPDEs

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

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 (V.)

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

$$A_j^* \rho_\infty = 0 \quad j < p, \quad \textit{(order } p \textit{ for the invariant measure)},$$

and

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

then (order $p+1$ for the invariant measure)

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

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)

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

The SPDE case: 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:

$$\begin{aligned} v_{n+1} &= v_n + hAv_{n+1} + hF(v_n) + \sqrt{h}\xi_n^Q \\ &= J_1 v_n + hJ_1 F(v_n) + \sqrt{h} J_1 \xi_n^Q, \end{aligned}$$

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

with

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

Analysis of the postprocessed Euler method

Theorem (Bréhier, V.)

- *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,*

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

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

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

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

Numerical experiments (stochastic heat equation)

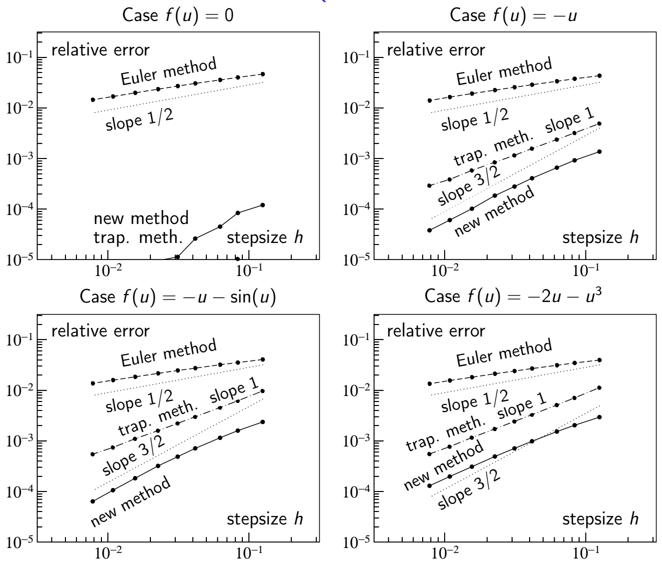
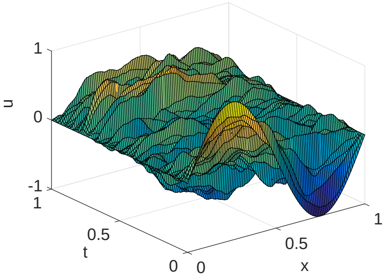


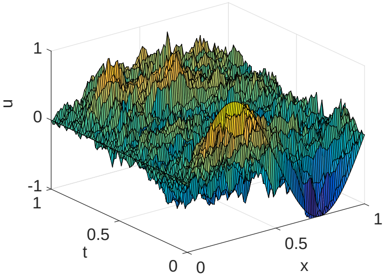
Figure: Orders of convergence, test function $\varphi(u) = \exp(-\|u\|^2)$.

Qualitative behavior

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



standard Euler method



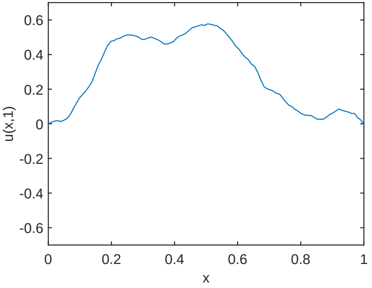
postprocessed method

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.

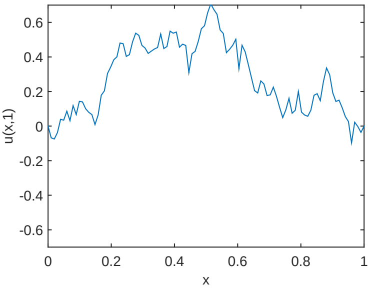
Related work: Chong and Walsh, 2012 (regularity study of the $\theta = 1/2$ stochastic method).

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).

Optimal explicit stabilized integrator for stiff and ergodic SDEs

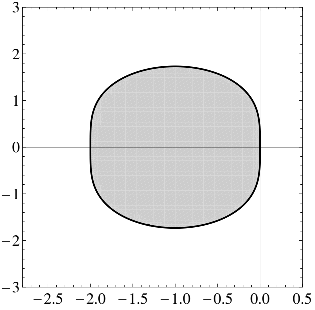
A. Abdulle, I. Almuslimani, G. V., *Optimal explicit stabilized integrator of weak order one for stiff and ergodic stochastic differential equations*, *SIAM JUQ*, 2018.

Stability analysis of (deterministic) integrators

Stability function. Consider $y'(t) = \lambda y(t),\ y(0) = 1$.
A Runge-Kutta method with stepsize h yields $y_{n+1} = R(h\lambda) y_n$.

$$\text{Stability domain} \qquad \mathcal{S} := \{z \in \mathbb{C}; |R(z)| \leq 1\}.$$

Stiff integrators. If $\mathbb{C}^- \subset \mathcal{S}$, the method is called *A*-stable.
If in addition $R(\infty) = 0$, the method is called *L*-stable.



Example: the Heun method (explicit)
$y_{n+1} = y_n + \frac{h}{2} f(y_n) + \frac{h}{2} f\big(y_n + hf(y_n)\big)$.
$R(z) = 1 + z + \frac{z^2}{2}$.
The stability condition $-2 \leq h\lambda \leq 0$ becomes for diffusion problems $h\Delta x^{-2} \leq C$ (severe stepsize restriction).

Example: the θ-method for the heat equation

$$\partial_t u = \partial_{xx} u, \quad t > 0, x \in (0,1)$$

with Dirichlet boundary conditions: $u(0,t) = u(1,t) = 0$.

Discretization.

Spatial discretization with finite differences, with $\Delta x = 1/100$.
Time discretization: θ-method with $\Delta t = 0.01$.

$$U_{n+1} = U_n + (1-\theta)\Delta t A U_n + \theta \Delta t A U_{n+1}.$$

Comparison of $\theta = 1/2$ (A-stable, not L-stable) or $\theta = 1$ (L-stable), with initial condition $u(x,0) = \sin(2\pi x)$ or $u(x,0) = \sin(2\pi x) + 1$.

Remark.

If $\theta = 0$ (Forward Euler), severe timestep restriction $\Delta t \leq 0.0002$.

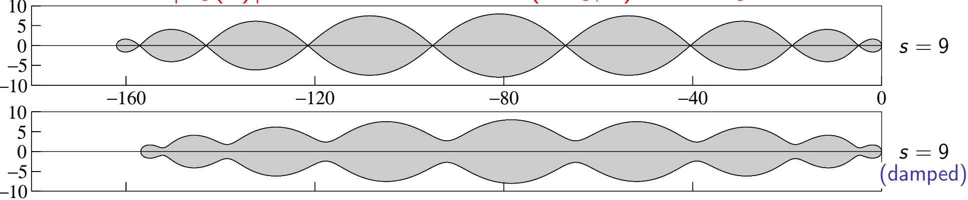
Example: first order Chebyshev methods

An s-stage Runge-Kutta method $y_0 \mapsto y_1$.

$$
\begin{aligned}
K_1 &= y_0 + \frac{h}{s^2} F(y_0), \qquad K_0 = y_0, \\
K_j &= \frac{2h}{s^2} F(K_{j-1}) + 2K_{j-1} - K_{j-2}, \; j = 2, \ldots, s \\
y_1 &= K_s
\end{aligned}
$$

Stability function given by $R_s(z) = T_s\left(1 + \frac{z}{s^2}\right)$ where $T_s(\cos x) = \cos(sx)$ are the Chebyshev polynomials.

It satisfies $|R_s(z)| \le 1$ for all real $z \in (-d_s, 0)$, with $d_s = 2s^2$.



Explicit stabilized integrators (Chebyshev methods)

Yuan'Chzao Din (1958), Franklin (1959), Guillou, Lago (1960)...

- 1. RKC: Methods based on three-term recurrence relation (non-optimal) with $d_s \simeq 0.66 \cdot s^2$
  van der Houwen, Shampine, Sommeijer, Verwer (RKC, IMEX extension IRKC, 1980-2007), Zbinden (PRKC 2011)
- 2. Methods based on composition (no-recurrence relation)
  Bogatyrev, Lebedev, Skvorstov, Medovikov (DUMKA 1976-2004), Jeltsch, Torrilhon 2007
- 3. ROCK methods (close to optimal stability for second order)
  Abdulle, Medovikov (ROCK2 2000-02) with $d_s \simeq 0.81 \cdot s^2$
  Abdulle (ROCK4 2002-05) with $d_s \simeq 0.35 \cdot s^2$
- 4. Extension to stiff stochastic problems: S-ROCK methods
  Weak order 1: Abdulle, Cirilli, Li, Hu (S-ROCK 2007-2009,τ-ROCK methods 2010) with $d_s \simeq 0.33 \cdot s^2$
  Weak order 2: Abdulle, Vilmart, Zygalakis (S-ROCK2 SIAM SISC 2014) with $d_s \simeq 0.43 \cdot s^2$

Classical S-ROCK method [Abdulle and Li, 2008]

The classical S-ROCK $X_0 \mapsto X_1$ is defined as:

$$
\begin{aligned}
K_0 &= X_0 \\
K_1 &= X_0 + \mu_1 h f(X_0) \\
K_i &= \mu_i h f(K_{i-1}) + \nu_i K_{i-1} + \kappa_i K_{i-2}, \quad i = 2, \ldots, s, \\
X_1 &= K_s + \sum_{r=1}^{m} g^r(K_s) \Delta W_j
\end{aligned}
$$

Remarks

- In the stochastic case for the classical S-ROCK method, the damping is chosen as $\eta = \eta_s$ where $\eta_s \gg 1$.
- Stability domain size $d_s \simeq 0.33 \cdot s^2$.

New stochastic Chebyshev method (SK-ROCK)

The new S-ROCK method, denoted SK-ROCK (for stochastic second kind orthogonal Runge-Kutta-Chebyshev method) is defined as

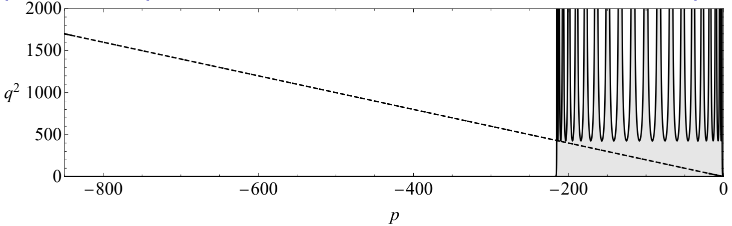
$$
\begin{aligned}
K_0 &= X_0 \\
K_1 &= X_0 + \mu_1 h f(X_0 + \nu_1 Q) + \kappa_1 Q \\
K_i &= \mu_i h f(K_{i-1}) + \nu_i K_{i-1} + \kappa_i K_{i-2}, \quad i = 2, \ldots, s. \\
X_1 &= K_s,
\end{aligned}
$$

where $Q = \sum_{r=1}^{m} g^r(X_0)\Delta W_j$.

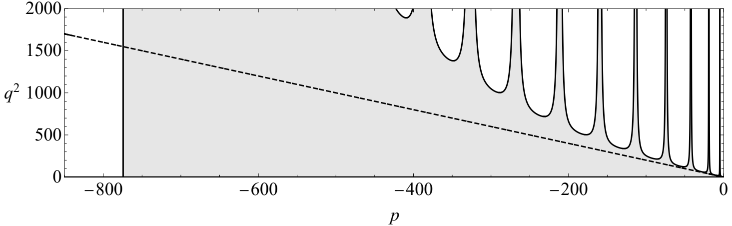
Remarks

- Analogously to the deterministic method, the damping parameter η is fixed to a small value (typically $\eta = 0.05$).
- Without noise ($g^r = 0$), we recover the standard deterministic Chebyshev method.
- Stability domain size $d_s \geq (2 - \frac{4}{3}\eta)s^2$.

New optimal explicit stabilized scheme for MS stiff problems



standard S-ROCK method (Abdulle and Li, 2008, $s = 20$, $\eta = 6.95$)
stability domain size $d_s \simeq 0.33 \cdot s^2$.



new SK-ROCK method ($s = 20$, $\eta = 0.05$)
stability domain size $d_s \geq (2 - \frac{4}{3}\eta)s^2$.

First and second kind Chebyshev polynomials

- First kind $T_s(\cos\theta) = \cos(s\theta)$,

$$T_j(p) = 2pT_{j-1}(p) - T_{j-2}(p),$$

where,

$$T_0(p) = 1,\ T_1(p) = p$$

- Second kind $\sin\theta\ U_s(\cos\theta) = \sin((s+1)\theta)$,

$$U_j(p) = 2pU_{j-1}(p) - U_{j-2}(p),$$

where,

$$U_0(p) = 1,\ U_1(p) = 2p.$$

Notice that the relation $T_s'(p) = sU_{s-1}(p)$ between first and second kind Chebyshev polynomials will be repeatedly used in our analysis.

Construction of SK-ROCK

Lemma

Let $s \geq 1$ and $\eta \geq 0$. Applied to the linear scalar test equation $dX = \lambda X dt + \mu X dW$, the new SK-ROCK yields

$$X_{n+1} = R(\lambda h, \mu\sqrt{h}, \xi_n) X_n$$

where $p = \lambda h, q = \mu\sqrt{h}$, $\xi_n \sim \mathcal{N}(0,1)$ is a Gaussian variable and

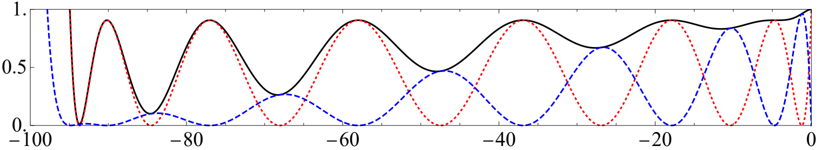
$$R(p,q,\xi) = \frac{T_s(\omega_0 + \omega_1 p)}{T_s(\omega_0)} + \frac{U_{s-1}(\omega_0 + \omega_1 p)}{U_{s-1}(\omega_0)}(1 + \frac{\omega_1}{2} p) q \xi.$$

Theorem

There exist $\eta_0 > 0$ and s_0 such that for all $\eta \in [0, \eta_0]$ and all $s \geq s_0$, for all $p \in [-2\omega_1^{-1}, 0]$ and $p + \frac{1}{2}|q|^2 \leq 0$, we have $\mathbb{E}(|R(p,q,\xi)|^2) \leq 1$.

New optimal explicit stabilized schemes:

Main idea: we use second kind Chebyshev polynomials
$U_{s-1}(x) = s^{-1} T_s'(x)$, and $T_s(x)^2 + (1-x^2) U_{s-1}(x)^2 = 1$.



$\mathbb{E}(|R(p,q,\xi)|^2) = A(p)^2 + B(p)^2 q^2$ as a function of p ($q^2 = -2p$).

Features of the new optimal second kind explicit Chebyshev methods:

- Coincides with the optimal deterministic Chebyshev method of order one ($d_s \geq (2 - \frac{4}{3}\eta) \cdot s^2$) for deterministic problems and inherits its optimal stability domain size.
- A postprocessor of order two is constructed for Brownian dynamics (for invariant measure sampling).

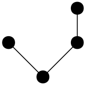
An algebraic framework based on exotic aromatic Butcher-series

A. Laurent, G. V., *Exotic aromatic B-series for the study of long time integrators for a class of ergodic SDEs*, *ArXiv, submitted*, 2017.

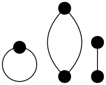
Aromatic Butcher-series

Stochastic case: Tree formalism for strong and weak errors on finite time: Burrage K., Burrage P.M., 1996; Komori, Mitsui, Sugiura, 1997; Rößler, 2004/2006, ...
Here we focus of the accuracy for the invariant measure (long time).

We rewrite high-order differentials with trees. We denote $F(\gamma)(\phi)$ the elementary differential of a tree γ.

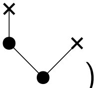
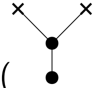
$F(\bullet)(\phi) = \phi$, $F($$)(\phi) = \phi' f$, $F($$)(\phi) = \phi''(f, f'f)$

Aromatic forests: introduced for deterministic geometric integration by Chartier, Murua, 2007 (See also Bogfjellmo, 2015)

$F($$)(\phi) = \mathrm{div}(f) \times \left(\sum \partial_i f_j \partial_j f_i\right) \times \phi' f$

New exotic aromatic B-series: using lianas

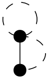
Grafted aromatic forests: a random vector $\xi \sim \mathcal{N}(0, I_d)$ is represented by crosses (in the spirit of P-series)

$F($  $)(\phi) = \phi''(f'\xi, \xi)$ and $F($  $)(\phi) = \phi' f''(\xi, \xi)$.

We also introduce lianas in our forests called exotic aromatic forests:

$F($  $) = \sum_i \phi''(f' e_i, e_i) = \mathbb{E}(\phi''(f'\xi, \xi))$.

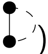
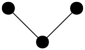
$F($  $) = \sum_i \phi''(e_i, e_i) = \Delta\phi = \mathbb{E}(\phi''(\xi, \xi))$.

$F($  $) = \sum_{i,j} \phi''(e_i, f'''(e_j, e_j, e_i)) = \sum_i \phi''(e_i, (\Delta f)'(e_i))$.

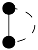
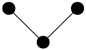
Integration by parts using trees: examples

$$\int_{\mathbb{R}^d} F\Big($$  $$\Big)(\phi)\rho_\infty dy = \sum_{i,j} \int_{\mathbb{R}^d} \frac{\partial^3 \phi}{\partial x_i \partial x_j \partial x_j} f_i \rho_\infty dy$$

$$= -\sum_{i,j} \left[\int_{\mathbb{R}^d} \frac{\partial \phi}{\partial x_i \partial x_j} \frac{\partial f_i}{\partial x_j} \rho_\infty dy + \int_{\mathbb{R}^d} \frac{\partial \phi}{\partial x_i \partial x_j} f_i \frac{\partial \rho_\infty}{\partial x_j} dy \right]$$

$$= -\int_{\mathbb{R}^d} F\Big($$  $$\Big)(\phi)\rho_\infty dy - \frac{2}{\sigma^2} \int_{\mathbb{R}^d} F\Big($$  $$\Big)(\phi)\rho_\infty dy.$$

We obtain:

 $\sim -$  $- \frac{2}{\sigma^2}$  .

Remark: the new exotic aromatic B-series satisfy an isometric equivariance property (see related work on characterizing affine equivariant maps by McLachlan, Modin, Munthe-Kaas, Verdier, 2016)

Order conditions for the invariant measure

$$Y_i^n = X_n + h\sum_{j=1}^{s} a_{ij} f(Y_j^n) + d_i \sigma \sqrt{h}\xi_n, \qquad i = 1, \dots, s,$$
$$X_{n+1} = X_n + h\sum_{i=1}^{s} b_i f(Y_i^n) + \sigma\sqrt{h}\xi_n,$$

Theorem (Laurent, V., Conditions for order p)

Order	*Tree* τ	$F(\tau)(\phi)$	*Order condition*
1		$\phi' f$	$\sum b_i = 1$
2		$\phi' f' f$	$\sum b_i c_i - 2\sum b_i d_i = -\frac{1}{2}$
		$\phi' \Delta f$	$\sum b_i d_i^2 - 2\sum b_i d_i = -\frac{1}{2}$
3		$\phi' f' f' f$	$\sum b_i a_{ij} c_j - 2\sum b_i a_{ij} d_j + \sum b_i c_i - (\sum b_i d_i)^2 = 0$
	$\dots$	$\dots$	$\dots$

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 ($\bar{s}+1$ instead of $\bar{s}$ for linearized Euler) for sampling the invariant distribution of parabolic SPDEs

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

  (proof in a simplified linear case).
- study of algebraic structures with exotic aromatic Butcher trees.

Current works:

- analysis of the order of convergence in the general semilinear SPDE case.
- combination with Multilevel Monte-Carlo strategies.