Postprocessed integrators for the high order sampling of the invariant distribution of stiff SDEs and SPDEs.

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joint work with

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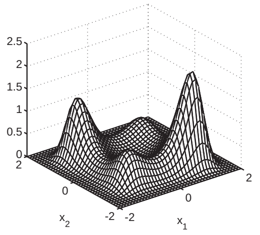
Example: Overdamped Langevin equation (Brownian dynamics)

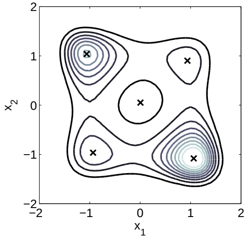
$$dX(t) = -\nabla V(X(t))dt + \sqrt{2}dW(t).$$

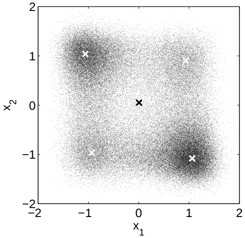
$W(t)$: standard Brownian motion in $\mathbb{R}^d$.
Ergodicity: invariant measure μ has density $\rho(x) = Ce^{-V(x)}$,

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

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







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,

$$\begin{aligned} \lim_{T\to\infty} \frac{1}{T}\int_0^T \phi(X(t)) &= \int_{\mathbb{R}^d} \phi(y)d\mu(y) \\ \left|\mathbb{E}(\phi(X(t))) - \int_{\mathbb{R}^d} \phi(x)\mu(x)dx\right| &\leq K(x,\phi)e^{-ct}, \quad \text{for all } t \geq 0. \end{aligned}$$

Two standard approaches using an ergodic integrator of order p:

- Compute a single long trajectory $\{X_n\}$ of length $T = Nh$,
$$\frac{1}{N+1}\sum_{k=0}^{N} \phi(X_k) \simeq \int_{\mathbb{R}^d} \phi(y)d\mu(y), \qquad \text{error } \mathcal{O}(h^p + T^{-1/2}),$$
- Compute many trajectories $\{X_n^i\}$ of length of length $t = Nh$,
$$\frac{1}{M}\sum_{i=1}^{M} \phi(X_N^i) \simeq \int_{\mathbb{R}^d} \phi(y)d\mu(y), \qquad \text{error } \mathcal{O}(e^{-ct} + h^p + M^{-1/2}).$$

Parabolic SPDE case

Example: Consider a semilinear parabolic stochastic PDE:

$$\frac{\partial u(t,x)}{\partial t} = \frac{\partial^2 u(t,x)}{\partial x^2} + f\big(u(t,x)\big) + \dot{W}(t,x)\ ,\ \ t \in (0,+\infty), x \in \Omega$$
$$u(0,x) = u_0(x)\ ,\ \ x \in \Omega$$
$$u(t,x) = 0\ ,\ \ x \in \partial\Omega,$$

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

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

Under appropriate assumptions, $\big(u(t)\big)_{t\in\mathbb{R}^+}$ is an ergodic process.
Aim: design an efficient high order integrator for sampling the invariant distribution.

Plan of the talk

1. Order conditions for the invariant measure
2. Postprocessed integrators for ergodic SDEs
3. Postprocessed integrators for parabolic SPDEs

Order conditions for the invariant measure

1. Order conditions for the invariant measure
2. Postprocessed integrators for ergodic SDEs
3. Postprocessed integrators for parabolic SPDEs

- 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

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

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

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

$$\begin{aligned} \lambda_p &= \int_0^{+\infty} \int_{\mathbb{R}^d} \Big(A_p - \frac{\mathcal{L}^{p+1}}{(p+1)!}\Big) u(t,x)\rho(x) dx dt \\ &= \int_0^{+\infty} \int_{\mathbb{R}^d} u(t,x) \big(A_p\big)^* \rho(x) dx dt. \end{aligned}$$

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

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

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

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, G.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

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

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

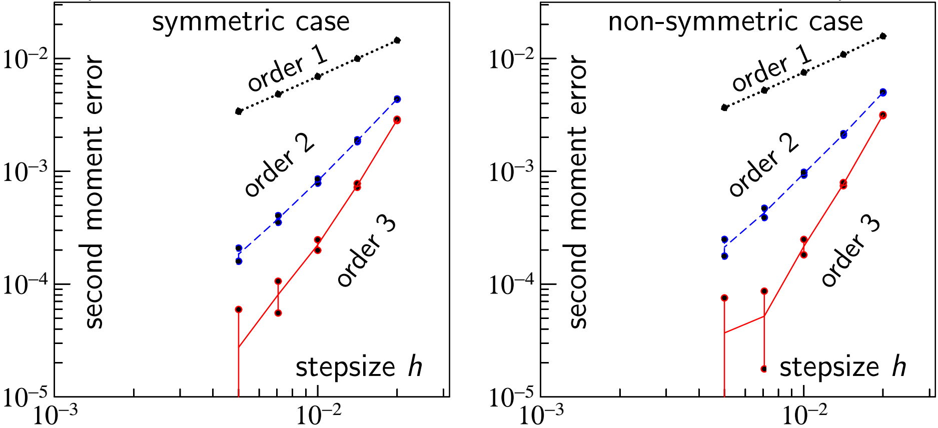
has order 3 for the invariant measure (assuming ergodicity).

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 $T = 10^8$).



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

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*

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

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

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

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

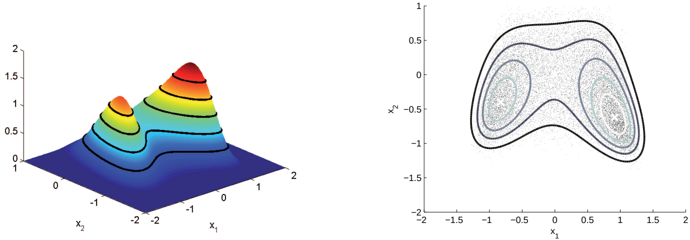
The matrix J_n^{-1} is the inverse of $J_n = I - hf'(X_n + a\sigma\sqrt{h}\xi_{n-1})$.

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

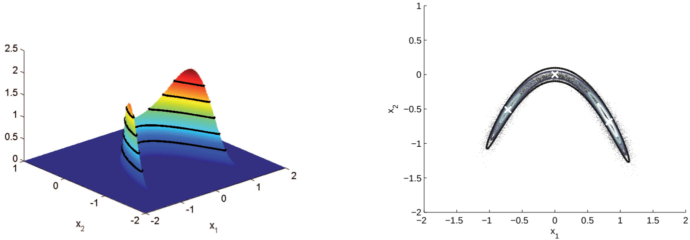
$$\overline{X}_n = X_n - hb\nabla V(\overline{X}_n) + c\sigma\sqrt{h}\xi_n, \quad b = \sqrt{2}/2, \quad c = \sqrt{4\sqrt{2}-1}\Big/2.$$

Example: stiff and nonstiff Brownian dynamics.

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

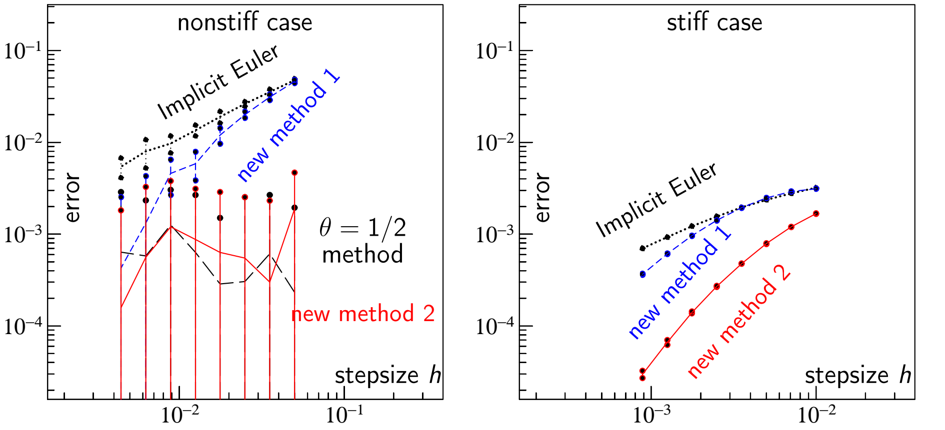


Nonstiff case $V(x) = (1-x_1^2)^2 + x_2^4 - x + x_1\cos(x_2) + (x_2 + x_1^2)^2$



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: stiff and nonstiff Brownian dynamics.



Error in $\int_{\mathbb{R}^d} (x_2 + x_1^2)^2 \rho(x) dx$ 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*, *preprint*.

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
$$Ae_k = -\lambda_k e_k$$
$$\big(e_k\big)_{k\in 1,\dots} \text{ complete orthonormal system of } H$$
$$0 < \lambda_1 \leq \ldots \leq \lambda_k \underset{k\to+\infty}{\to} +\infty$$
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:

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

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:

$$v_{n+1} = J_1 v_n + hJ_1 F(v_n) + \sqrt{h} J_1 \xi_n^Q.$$

New postprocessed scheme

$$\begin{aligned} u_{n+1} =& J_1\Big(u_n + hF\Big(u_n + \frac{1}{2}\sqrt{h} J_2 \xi_n^Q\Big) + \frac{\sqrt{2}-1}{2} J_2 \sqrt{h}\xi_n^Q\Big) \\ &+ \frac{3-\sqrt{2}}{2}\sqrt{h} J_2 \xi_n^Q \end{aligned}$$

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

with

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

Idea of the contruction

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,*

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

- *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: $\mathcal{O}\left(h^{\mathrm{s}}\right)$, $\mathrm{s} \in (0, \overline{\mathrm{s}})$.

Analysis in infinite dimension (linear case)

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

Numerical scheme and spectral decomposition: $u_n = \sum_{p=1}^{+\infty} u_n(p)e_p$

$$u_{n+1}(p) = \mathcal{A}(-\lambda_p h, -b_p h)u_n(p) + \sqrt{h}\sqrt{q_p}\mathcal{B}(-\lambda_p h, -b_p h)\xi_{n,p}$$
$$\overline{u}_n(p) = \mathcal{C}(-\lambda_p h)u_n(p) + \sqrt{h}\sqrt{q_p}\mathcal{D}(-\lambda_p h)\xi_{n,p},$$

with

$$\mathcal{A}(z,\beta) = \frac{1+\beta}{1-z}, \quad \mathcal{B}(z,\beta) = \frac{1+\frac{\beta}{2} - \frac{3-\sqrt{2}}{2}z}{(1-z)(1-\frac{3-\sqrt{2}}{2}z)},$$
$$\mathcal{C}(z) = 1, \quad \mathcal{D}(z) = \frac{1}{2(1-z/2)^{1/2}}.$$

Analysis in infinite dimension (linear case)

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

Exact and numerical Gaussian invariant distributions:
$\mu_\infty = \mathcal{N}(0, Q_\infty)$ and $\overline{\mu}^h_\infty = \mathcal{N}(0, \overline{Q}^h_\infty)$ with

$$Q_\infty e_p = \frac{q_p}{2(\lambda_p + b_p)} e_p$$

$$\overline{Q}^h_\infty e_p = \lim_{n\to+\infty} \mathbb{E}|\overline{u}_n(p)|^2 e_p = \frac{q_p}{2(\lambda_p + b_p)} \overline{\mathcal{R}}(-\lambda_p h, -b_p h) e_p,$$

where

$$\overline{\mathcal{R}}(z,\beta) = \mathcal{C}(z)^2 \mathcal{R}(z,\beta) - 2(z+\beta)\mathcal{D}(z)^2$$

$$\mathcal{R}(z,\beta) = \frac{-2(z+\beta)\mathcal{B}(z,\beta)^2}{1-\mathcal{A}(z,\beta)^2}$$

Analysis in infinite dimension (linear case)

Key identity:

$$\left|1-\overline{\mathcal{R}}(z,\beta)\right| \leq |z\beta| \frac{C}{(1-z)^2}.$$

This is better than for the Euler scheme:

$$\left|1-\mathcal{R}_E(z,\beta)\right| = \frac{z+\beta}{2-z-\beta}.$$

Let $\varphi \in \mathcal{C}^2(H,\mathbb{R})$. Thanks to a Taylor expansion:

$$\begin{aligned}
\Big|\int_H \varphi d\mu_\infty - \int_H \varphi d\overline{\mu}_\infty^h\Big| &\leq C(\varphi)\Big|\sum_{p=1}^{+\infty} \left|\langle\left(Q_\infty - \overline{Q}_\infty^h\right)e_p, e_p\rangle\right| \\
&\leq C(\varphi)\sum_{p=1}^{+\infty} \frac{q_p}{2(\lambda_p+b_p)}\left|1-\overline{\mathcal{R}}(-\lambda_p h, -b_p h)\right| \\
&\leq C(\varphi)\sum_{p=1}^{+\infty} \frac{q_p}{\lambda_p^{1-\mathrm{s}}}\frac{(\lambda_p h)^{1-\mathrm{s}}}{(1+\lambda_p h)^2} h^{1+\mathrm{s}}.
\end{aligned}$$

Numerical experiments (stochastic heat equation)

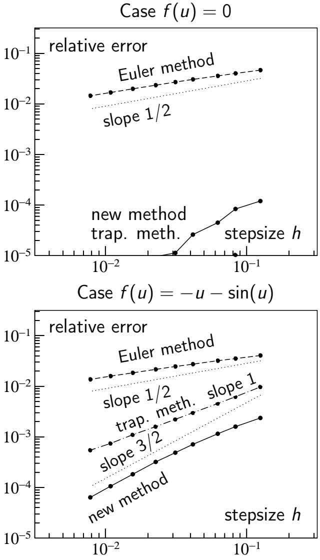
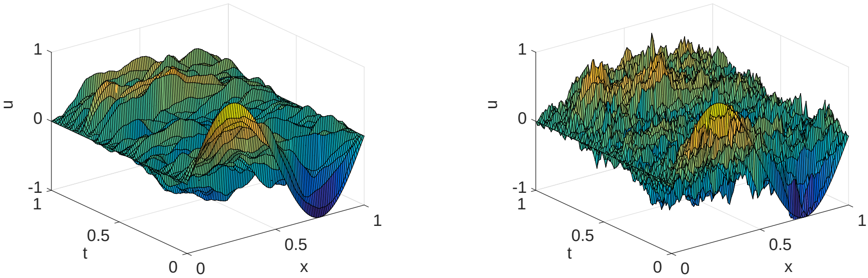


Figure: Orders of convergence, test function $\varphi(u) = \exp -(\|u\|^2)$.

Qualitative behavior

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



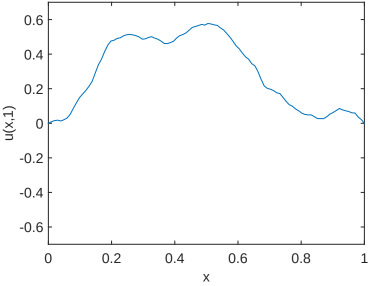
standard Euler method　　　　postprocessed method

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

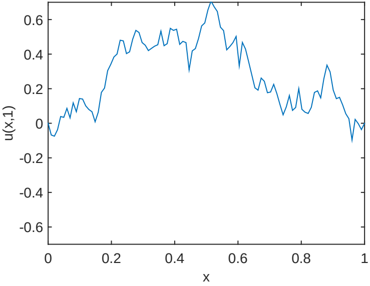
Related work: Chong and Walsh, 2012 (regularity study of the $\theta = 1/2$ stochastic method).

Qualitative behavior

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



standard Euler method



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

Summary

- 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

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

  Features:
  - exponential convergence,
  - exact sampling if $F = 0$,
  - analysis of the improved order of convergence for linear F,
  - correct spatial regularity.

Open question: analysis of the order of convergence in the general semilinear SPDE case.