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

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based on joint works with

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Oberwolfach Workshop on GNI, March 2016

# 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,

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

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

Two standard approaches using an ergodic integrator of order $p$:

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

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

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

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

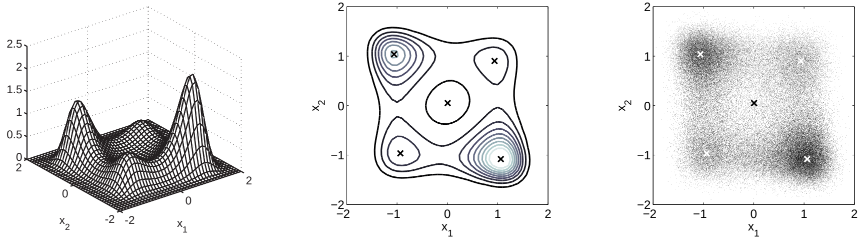
# Example: Overdamped Langevin equation (Brownian dynamics)

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

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

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

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



# Parabolic SPDE case

Example: Consider a semilinear parabolic stochastic PDE:

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

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

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

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 $\mu_\infty^h$ 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 $u(t,x) = \mathbb{E}\phi\big(X(t,x)\big)$,*

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

## High order approximation of the numerical invariant measure

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

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

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

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

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

## 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, V., Zygalakis)

Consider an ergodic integrator $X_n \mapsto X_{n+1}$ (with weak order $\geq 1$) 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

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

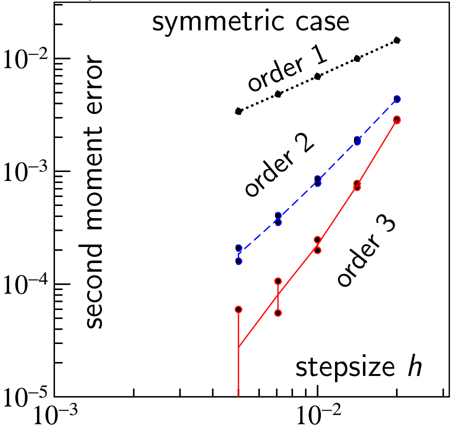
has order 3 for the invariant measure (assuming ergodicity).

Remark 1: the weak order of accuracy is only 1.

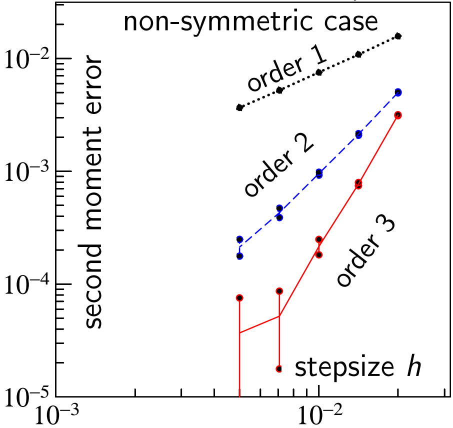
Remark 2: derivative free versions can also be constructed.

# Convergence of the modified Euler-Maruyama schemes

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




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




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

# 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*

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

*and*

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

*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)

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

# Postprocessed integrators for parabolic SPDEs

1. Order conditions for the invariant measure
2. Postprocessed integrators for ergodic SDEs
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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 $H$

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

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

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

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

- 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

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

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

# Numerical experiments (stochastic heat equation)

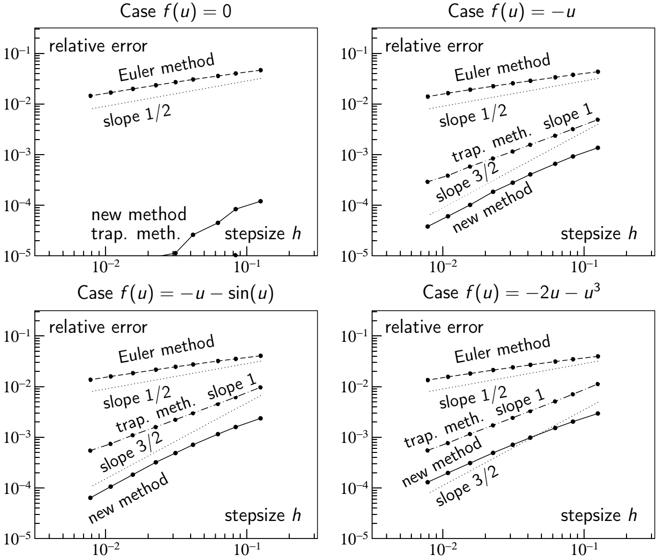
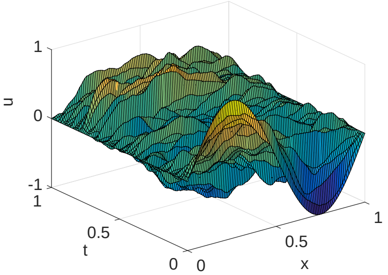


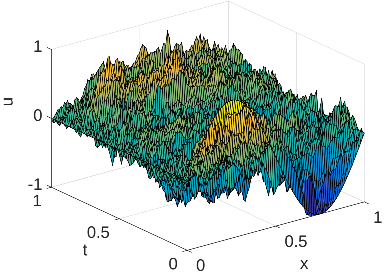

Figure: Orders of convergence, test function $\varphi(u) = \exp(-\|u\|^2)$.

# Qualitative behavior

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




standard Euler method



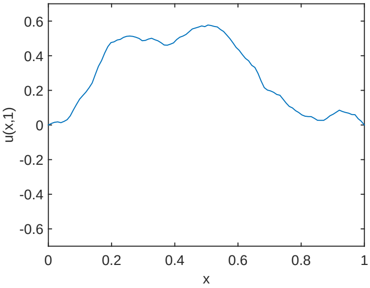

postprocessed method

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.

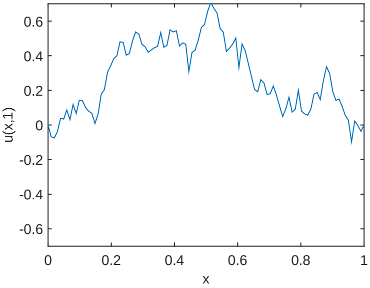
Related work: Chong and Walsh, 2012 (regularity study of the $\theta = 1/2$ stochastic method).

# Qualitative behavior

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




standard Euler method

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# 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.