High-order integrators for sampling the invariant distribution of stochastic ordinary and partial differential equations.

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based on joint works with
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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,

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

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

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

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

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*

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

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

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

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

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.

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

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,*

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

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

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

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)

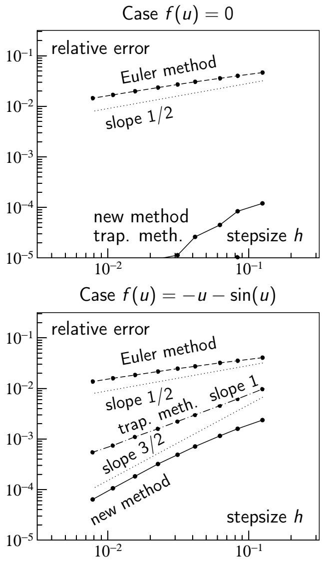

Figure: Orders of convergence, test function $\varphi(u) = \exp(-\|u\|^2)$.

Optimal explicit stabilized integrator for stiff and ergodic SDEs

1. Order conditions for the invariant measure
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4. An algebraic framework based on exotic aromatic Butcher-series

A. Abdulle, I. Almuslimani, G. V., *Optimal explicit stabilized integrator of weak order one for stiff and ergodic stochastic differential equations*, *ArXiv, submitted*, 2017.

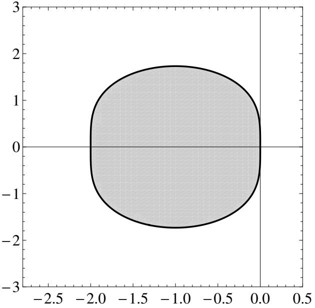
See the poster of Ibrahim Almuslimani today at 6 p.m. (Atrium).

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).

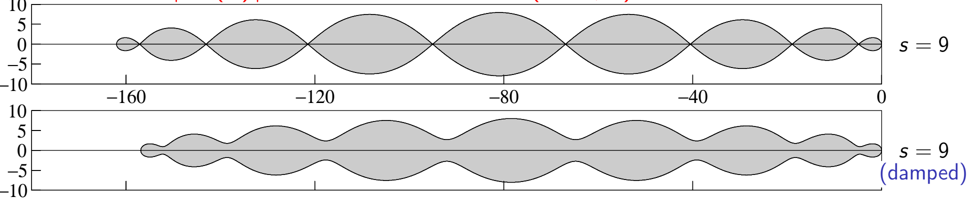
Example: first order Chebyshev methods

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

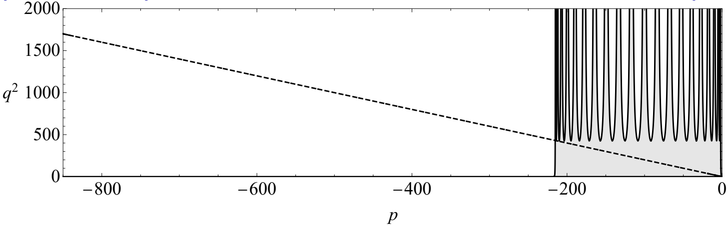


Explicit stabilized integrators (Chebyshev methods)

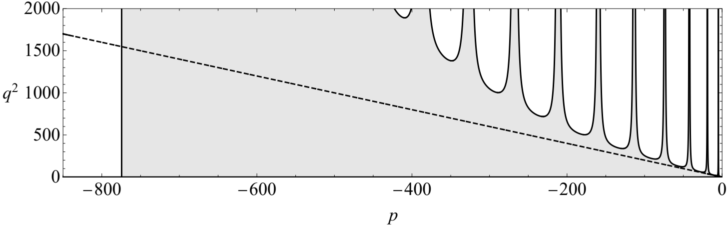
Yuan'Chzao Din (1958), Franklin (1959), Guillou, Lago (1960)...

- 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 preprint 2012) with $d_s \simeq 0.43 \cdot s^2$

New optimal explicit stabilized scheme for MS stiff problems



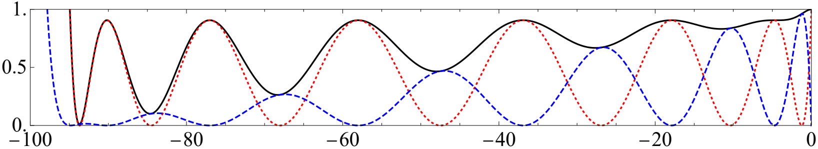
standard S-ROCK method (Abdulle and Li, 2008, $s = 20$, $\eta = 6.95$)
stability domain size $d_s \simeq 0.33 \cdot s^2$.



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

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

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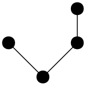
A. Laurent, G. V., *Exotic aromatic B-series for the study of long time integrators for a class of ergodic SDEs*, *ArXiv, submitted*, 2017.

See the poster of Adrien Laurent today at 6 p.m. (Atrium).

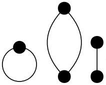
Aromatic Butcher-series

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.

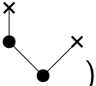
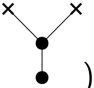
$F(\bullet)(\phi) = \phi,$ $F($  $)(\phi) = \phi' f,$ $F($  $)(\phi) = \phi''(f, f'f)$

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

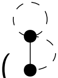
Grafted aromatic forests: a random vector $\xi \sim \mathcal{N}(0, I_d)$ is represented by crosses (in the spirit of P-series)

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

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

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

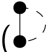
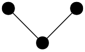
$F($  $) = \sum_i \phi''(e_i, e_i) = \Delta\phi = \mathbb{E}(\phi''(\xi, \xi))$.

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

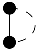
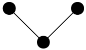
Integration by parts using trees: examples

$\int_{\mathbb{R}^d} F($$)(\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($$)(\phi)\rho_\infty dy - \frac{2}{\sigma^2} \int_{\mathbb{R}^d} F($$)(\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		$\phi' f' f' f$	$\sum b_i a_{ij} c_j - 2\sum b_i a_{ij} d_j$ $+\sum b_i c_i - (\sum b_i d_i)^2 = 0$
	...	...	...

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.