High-order sampling of the invariant distribution of ergodic stochastic dynamics: preconditioning and postprocessing

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based on joint works with
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Milstein's method: 50 years on, Nottingham, June 2025

Long time accuracy for ergodic stochastic problems

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

Under standard ergodicity assumptions,

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

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

Different types of convergence as $h \to 0$:

- strong order q (fixed finite time T),

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

- weak order r (fixed finite time T),

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

- order p for the invariant measure (long time behavior): in general $p \geq r \geq q$.

Long time accuracy for ergodic stochastic problems

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

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 $t = Nh$,

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

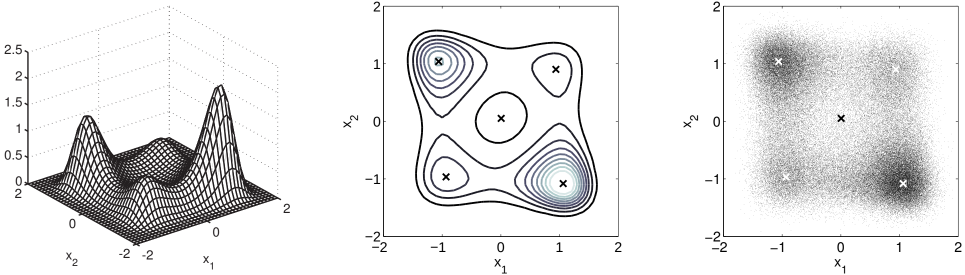
Example: Overdamped Langevin equation (Brownian dynamics)

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

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

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

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



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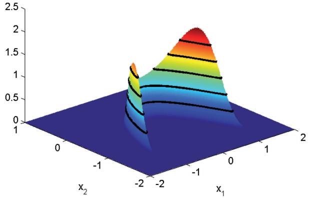
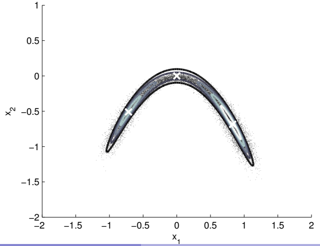
Example ($d = 2$), Stiff case:

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



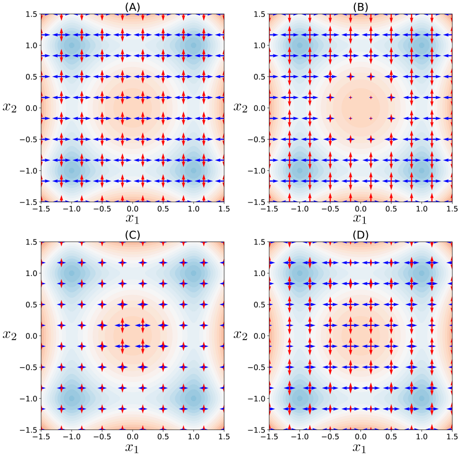


Variable diffusion case: preconditioning the ergodic dynamics

$$dX = \left(-D^T D(X)\nabla V(x) + \mathrm{div}(D^T D)(X)\right)dt + \sqrt{2}D(X)dW, \qquad (\text{variable } D(x) \in \mathbb{R}^{d\times d})$$

$$D_A(x) = \begin{pmatrix} 2 & 0 \\ 0 & 1.5 \end{pmatrix}$$

$$D_B(x) = \frac{1}{1+5e^{-\|x\|^2/0.18}} I$$



$$D_C(x) = (1 + 5e^{-\|x\|^2/0.18})I$$

$$D_D(x) = I - \frac{xx^T}{2\|x\|^2+1}$$

Quadruple well potential $V(x) = \sqrt{\frac{17}{16} - 2x_1^2 + x_1^4} + \sqrt{\frac{17}{16} - 2x_2^2 + x_2^4}$.

Variable diffusion case: preconditioning the ergodic dynamics

Consider the Langevin dynamics with smooth variable diffusion $D(x) \in \mathbb{R}^{d\times d}$ symmetric and uniformly positive definite (same invariant measure with $\rho_\infty(x) = Ze^{-\frac{\sigma^2}{2}V(x)}$),

$$dX = F(X)dt + \sigma D(X)dW, \qquad F(x) = -D^2(x)\nabla V(x) + \frac{\sigma^2}{2}\mathrm{div}(D^2)(x).$$

The Leimkuhler-Matthews (2013) scheme:

$$X_{n+1} = X_n + hF(X_n) + \sigma D\frac{\xi_n + \xi_{n+1}}{2}, \qquad \xi_n \sim \mathcal{N}(0, I) \text{ i.i.d.}$$

Challenge: generalization of the Leimkhuler-Matthews in the variable diffusion case?

- For $D(x) = I$ (identity matrix), it yields order two for the invariant measure.
- For $D(x) = D$ (constant matrix), it yields order two for the invariant measure.
- For $D(x)$, variable, it is not consistent in general. The modified version

$$X_{n+1} = X_n + hF(X_n) + \frac{h}{4}\frac{\sigma^2}{2}\mathrm{div}(D^2)(x) + \sigma D\frac{\xi_n + \xi_{n+1}}{2},$$

has order one in the one-dimensional case $d = 1$, but is not consistent in general.

Plan of the talk

1. Part 1: High order for the invariant measure and postprocessors
   - Weak order condition and order conditions sampling for the invariant measure
   - Postprocessors for sampling for the invariant measure
2. Part 2: High-order in the variable diffusion case
   - New generalization of the Leimkuhler-Matthews Scheme
   - Bias analysis based on exotic aromatic Butcher-series

1. Part 1: High order for the invariant measure and postprocessors
   - Weak order condition and order conditions sampling for the invariant measure
   - Postprocessors for sampling for the invariant measure

- Abdulle, V., Zygalakis, *High order numerical approximation of ergodic SDE invariant measures*, *SIAM SINUM*, 2014.
- Abdulle, V., Zygalakis, *Long time accuracy of Lie-Trotter splitting methods for Langevin dynamics*, *SIAM SINUM*, 2015.
- G. V., *Postprocessed integrators for the high order integration of ergodic SDEs*, *SIAM SISC*, 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*

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

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

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

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

$$= \int_0^{+\infty}\int_{\mathbb{R}^d} u(t,x)(A_p)^*\rho_\infty(x)dxdt.$$

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)

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

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

Order conditions for the invariant measure sampling

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

Theorem (Laurent, V., 2020, Conditions for order p for the invariant measure)

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		$\phi' f' f' f$	$\sum b_i a_{ij} c_j - 2\sum b_i a_{ij} d_j$ $+\sum b_i c_i - (\sum b_i d_i)^2 = 0$
	$\dots$	$\dots$	$\dots$

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).

First derived as a non-Markovian method by Leimkuhler, Matthews (2013), see Leimkuhler, Matthews, Tretyakov (2014),

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

Postprocessed integrators for ergodic SDEs: nonlinear case

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., 2015)

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

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

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

Related: Bréhier, V., SIAM SISC 2016, order improved by $+1$ for the stochastic heat eq.

Part 2: High-order in the variable diffusion case

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- Laurent, V., *Exotic aromatic B-series for the study of long time integrators for a class of ergodic SDEs*, *Math. Comp.*, 2020.
- Laurent, V., *Order conditions for sampling the invariant measure of ergodic stochastic differential equations on manifolds*, *FoCM*, 2022.
- Bronaco, Leimkuhler, Phillips, V.. Order two scheme for the invariant measure sampling of Langevin dynamics with variable diffusion, submitted, 2025.

New generalization of the Leimkuhler-Matthews Scheme

Consider the Langevin dynamics with smooth variable diffusion $D(x) \in \mathbb{R}^{d\times d}$ symmetric and uniformly positive definite (same invariant measure with $\rho_\infty(x) = Ze^{-\frac{2}{\sigma}V(x)}$),

$$dX = F(X)dt + \sigma D(X)dW, \qquad F(x) = -D^2(x)\nabla V(x) + \frac{\sigma^2}{2}\mathrm{div}(D^2)(x).$$

The new postprocessed scheme has the form

$$X_{n+1} = X_n + hF(\overline{X}_n) + \hat{\Phi}_h^D\Big(X_n + \frac{h}{4}F(\overline{X}_{n-1})\Big),$$
$$\overline{X}_n = X_n + \frac{1}{2}\sigma\sqrt{h}D(X_n)\xi_n,$$

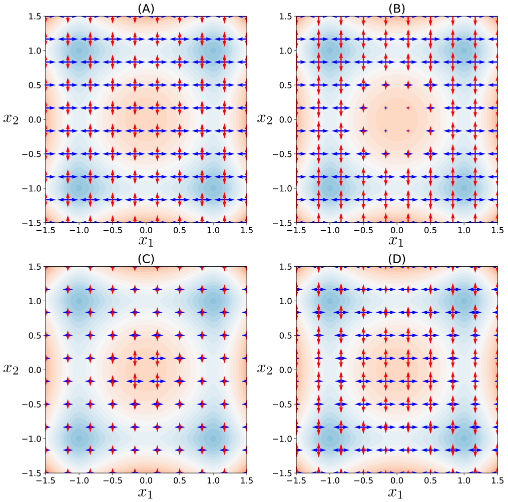
where $I + \hat{\Phi}_h^D$ is a weak order 2 integrator of $dX = \sigma D(X)dW$.

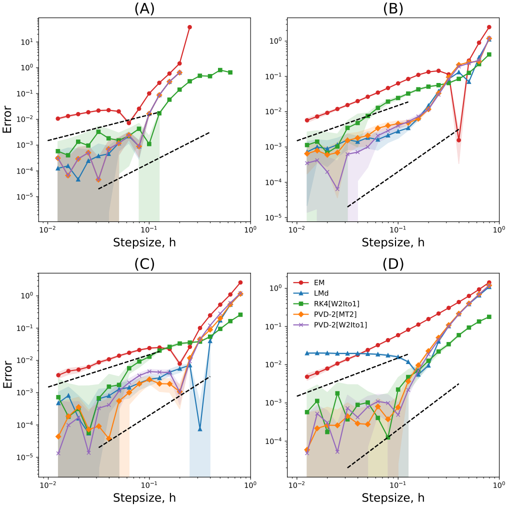
Theorem (Bronasco, Leimkuhler, Phillips, and V., 2025, submitted)

The postprocessed method with $\overline{X}_n$ above is second-order for sampling the invariant measure and has only one evaluation of ∇V per step.

Numerical experiments: Quadruple well potential

$$dX = \left(-D^2(X)\nabla V(x) + \mathrm{div}(D^2)(X)\right)dt + \sqrt{2}D(X)dW, \qquad (\text{symmetric } D(x) \in \mathbb{R}^{d\times d})$$

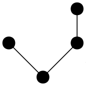




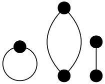
Aromatic Butcher-series

Deterministic B-series: Hairer & Wanner, 1972, using Butcher's seminal work (1960s).
Link with Hopf algebras of trees in quantum physics (Connes, Kreimer, 1980s).
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 $F(\gamma)(f)$ the elementary differential of a tree γ.

For deterministic B-series: $F(\bullet)(f) = f$, $F($$)(f) = f'f$, $F($$)(f) = f''(f, f'f)$

Aromatic forests: introduced for deterministic geometric integration for the study of volume preservation independently by Chartier, Murua, 2007, and Iserles, Quispel, Tse, 'K-loops' 2007 (see algebra structures in Bogfjellmo, 2015, Laurent, McLachlan, Munthe-Kaas, Verdier, 2024)

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

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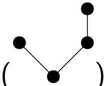
For S-series (Murua, 1999) : $F(\bullet)(\phi) = \phi$, $F($$)(\phi) = \phi' f$, $F($$)(\phi) = \phi''(f, f'f)$

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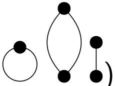
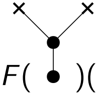
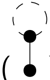
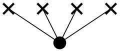
$F($$)(\phi) = \text{div}(f) \times \left(\sum \partial_i f_j \partial_j f_i\right) \times \phi' f$

Computing the expectation using lianas: examples

Grafted aromatic forests (like P-series): $\xi \sim \mathcal{N}(0, I_d)$ is represented by crosses.

$\mathbb{E}[F($  $)(\phi)] = \mathbb{E}[\phi'(f''(\xi,\xi))] = \sum_{i,j,k=1}^{d} \partial_i\phi\partial_{jk}f_i\mathbb{E}[\xi_j\xi_k] = \sum_{i,j=1}^{d} \partial_i\phi\partial_{jj}f_i = \phi'\Delta f = F($  $)(\phi)$,

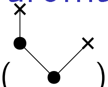
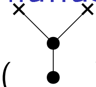
$\mathbb{E}[F($  $)(\phi)] = \mathbb{E}[\phi^{(4)}(\xi,\xi,\xi,\xi)] = \sum_{i,j,k,l} \partial_{i,j,k,l}\phi\mathbb{E}[\xi_i\xi_j\xi_k\xi_l]$

$= \sum_{i} \partial_{i,i,i,i}\phi\mathbb{E}[\xi_i^4] + 3\sum_{\substack{i,j\\ i\neq j}} \partial_{i,i,j,j}\phi\mathbb{E}[\xi_i^2]\mathbb{E}[\xi_j^2]$

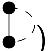
$= 3\sum_{i,j} \partial_{i,i,j,j}\phi = 3\Delta^2\phi = 3F($  $)(\phi)$.

Idea of the proof for general trees: L. Isserlis' theorem (Wick's probability theorem).

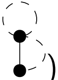
New exotic aromatic B-series: using lianas

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

We introduce lianas in our trees, now called exotic aromatic trees and forests:

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

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

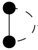
$F($  $) = \sum_{i,j} \phi''(e_i, f'''(e_j, e_j, e_i)) = \sum_i \phi''(e_i, (\Delta f)'(e_i))$.

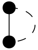
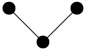
Related algebraic structures: E. Bronasco, Exotic B-series and S-series, 2024.
Study of affine equivariant property by McLachlan, Modin, Munthe-Kaas, Verdier, 2016 and orthogonal equivariant maps by Laurent, Munthe-Kaas, 2023.

Integration by parts using exotic aromatic trees: example

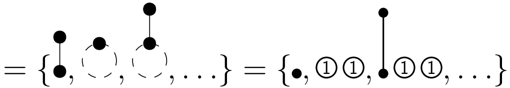
$$\int_{\mathbb{R}^d} F($$  $$)(\phi)\rho_\infty dy = \int_{\mathbb{R}^d} (\Delta\phi)' f \phi \rho_\infty dy = \sum_{i,j} \int_{\mathbb{R}^d} \frac{\partial^3 \phi}{\partial x_i \partial x_j \partial x_j} f_i \rho_\infty dy$$

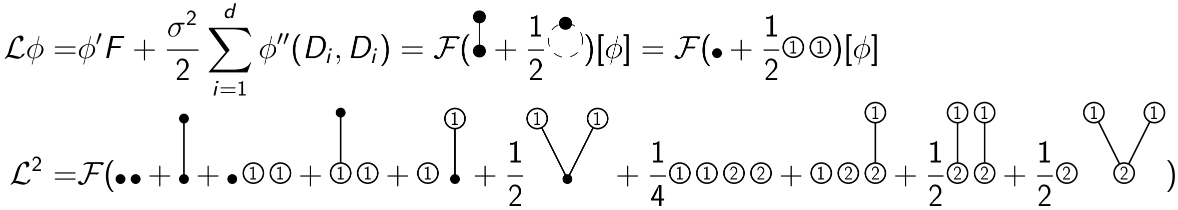
$$= -\sum_{i,j} \left[\int_{\mathbb{R}^d} \frac{\partial \phi}{\partial x_i \partial x_j} \frac{\partial f_i}{\partial x_j} \rho_\infty dy + \int_{\mathbb{R}^d} \frac{\partial \phi}{\partial x_i \partial x_j} f_i \frac{\partial \rho_\infty}{\partial x_j} dy \right]$$

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

where we used $\nabla \rho_\infty = f \rho_\infty$. We obtain:  $\sim -$  $-$  .

Convergence analysis in the variable diffusion case

New notation for exotic aromatic trees: $EAT =$ 



Theorem (Bronasco, 2024, Bronasco, Leimkuhler, Phillips, and V., submitted 2025)

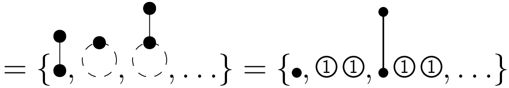
We can use integration by parts denoted by $\sim$ to modify $\mathcal{A}_k$ without changing the value of $A_k^*\rho_\infty$. The order p condition becomes

$$(a \circ A)(\tau) = 0, \quad \text{for all } \tau \in EAT, |\tau| \leq p,$$

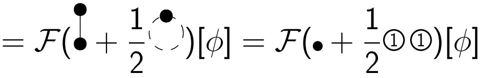
where A is an adjoint operation of the integration by parts.

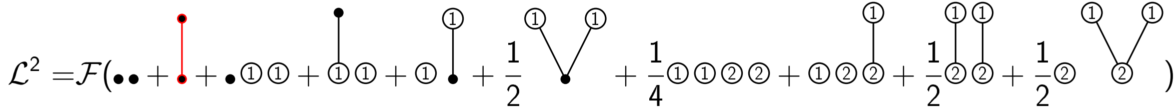
Convergence analysis in the variable diffusion case

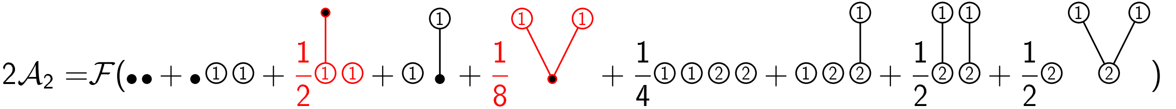
New notation for exotic aromatic trees: *EAT* =



$$\mathcal{L}\phi = \phi' F + \frac{\sigma^2}{2}\sum_{i=1}^{d} \phi''(D_i, D_i) =$$

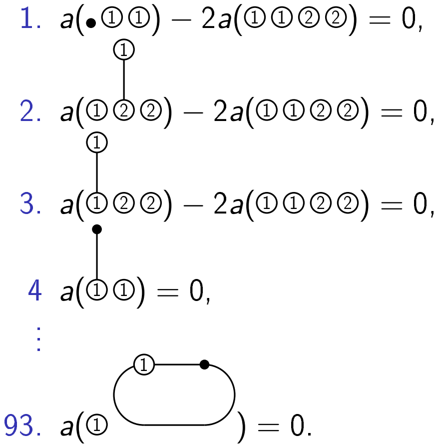




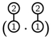


List of order conditions for the variable diffusion case

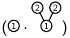
There are 93 order conditions for order 2 for the invariant measure sampling!



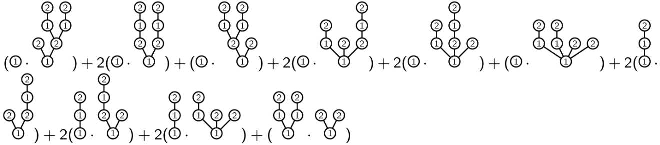
```
> f1 = [PT 1 [PT 2 []], PT 1 [PT 2 []]]
> display $ vector f1
```



```
> f2 = [PT 1 [], PT 1 [PT 2 [], PT 2 []]]
> display $ vector f2
```



```
> display $ graftFF f1 f2
```



Ongoing work: design of a systematic symbolic manipulation package in Haskel for exotic trees and forests (with E. Bronasco and J.L. Falcone).

Conclusion

- preconditioning for ehancing the convergence to equilibrium of ergodic dynamics.
- postprocessing allows to increase the order of accuracy for sampling the invariant measure without increasing the number of force evaluations (same as the simplest Euler-Maruyama method).
- construction in the stochastic context inspired by geometric numerical integration.

Related ongoing work:

- preconditioned integrators for SPDEs, stochastic heat equation (with A. Debussche, C.-E. Bréhier, and A. Laurent).
- design of a systematic symbolic manipulation package in Haskel for exotic trees and forests (with E. Bronasco and J.L. Falcone).
- accelerating the convergence to equilibrium using reversible perturbations (Stratonovitch noise), with G. Pavliotis.

Papers and preprints available at: `www.unige.ch/~vilmart`

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.

Theorem (Abdulle, V., Zygalakis, 2015)

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 exists a modified equation

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

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).

Related work on modified equations for SDEs: Shardlow (2006, strong), Zygalakis, (2011, weak) , Debussche & Faou, (2011, ergodic problems), Abdulle Cohen, V., Zygalakis (2013, weak), Bronasco, Laurent (2024, ergodic, algebraic structures).

Example of high order integrator for the invariant measure (Brownian dynamics)

Theorem (Abdulle, V., Zygalakis, 2015)

For $p \geq 1$ and Brownian dynamics $dX = f(X)dt + \sigma dW$, $f = -\nabla V$, the Euler-Maruyama scheme $X_{n+1} = X_n + hf(X_n) + \sigma \Delta W_n$ applied to the modified SDE

$$\begin{aligned} dX &= (f + hf_1 + h^2 f_2 + \ldots + h^{p-1} f_{p-1})(X)dt + \sigma dW \\ f_1 &= -\tfrac{1}{2} f'f - \tfrac{\sigma^2}{4} \Delta f, \\ f_2 &= -\tfrac{1}{2} f'f'f - \tfrac{1}{6} f''(f,f) - \tfrac{1}{3}\sigma^2 \textstyle\sum_{i=1}^d f''(e_i, f'e_i) - \tfrac{\sigma^2}{4} f'\Delta f - \tfrac{\sigma^4}{6}(\Delta f)'f - \tfrac{\sigma^4}{24}\Delta^2 f, \\ &\ldots \end{aligned}$$

has order p for the invariant measure of $dX = f(X)dt + \sigma dW$ (assuming ergodicity).

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

Remark 2: derivative free versions can also be constructed.

Related: algebraic structures based on exotic aromatic trees and forests (Laurent, V., 2020, Bronasco, 2024, Bronasco, Laurent, 2024).