Explicit stabilized integrators for stiff problems: the interplay of geometric integration and stochastic integration

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based on joint works with

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Example of stiff problem: Solar atmosphere

Ongoing collaboration since 2022 with:

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A multi-fluid magnetohydrodynamic (MHD) model for the solar atmosphere:

Stiff source terms

Advection

$$\partial_t \rho_\alpha + \nabla\cdot(\rho_\alpha \mathbf{v}_\alpha) = m_\alpha \sum_{\beta\neq\alpha} \Gamma^{i,r}_{\alpha,\beta},\ \alpha,\beta \in \mathcal{H}^2$$

$$\partial_t(\rho_\alpha \mathbf{v}_\alpha) + \nabla\cdot\left(\rho_\alpha \mathbf{v}_\alpha \odot \mathbf{v}_\alpha - \overline{\overline{\tau_\alpha}} + P_\alpha \mathbb{I}\right) = n_\alpha q_\alpha(\mathbf{E} + \mathbf{v}_\alpha \times \mathbf{B}) + m_\alpha \sum_{\beta\neq\alpha}\left(\Gamma^{i,r}_{\alpha,\beta}\mathbf{v}_\alpha\right) + \sum_{\beta\neq\alpha} \mathbf{R}^{\alpha,\beta}_\alpha,\ \alpha,\beta \in \mathcal{H}^2$$

$$\partial_t e_\alpha + \nabla\cdot(e_\alpha \mathbf{v}_\alpha) + P_\alpha \nabla\cdot\mathbf{v}_\alpha = Q^\tau_\alpha + m_\alpha \sum_{\beta\neq\alpha}\Gamma^{i,r}_{\alpha,\beta} e_\alpha + \sum_{\beta\neq\alpha} Q^{\alpha,\beta}_\alpha,\ \alpha,\beta \in \mathcal{H}\times\mathcal{M}$$

$$\partial_t e_e + \nabla\cdot(e_e \mathbf{v_e}) + P_e \nabla\cdot\mathbf{v_e} = 0 + m_e \sum_{\beta\neq e}\Gamma^{i,r}_{e,\beta} e_e + \sum_{\beta\neq e} Q^{e,\beta}_e + \nabla\cdot(\kappa\nabla T_e),\ \alpha,\beta \in \{e\}\times\mathcal{M}$$

Parabolic terms

$$\partial_t \mathbf{B} - \nabla\times(\mathbf{v_e}\times\mathbf{B}) = \nabla\times\left(\frac{\nabla P_e}{n_e q_e}\right) - \nabla\times\left(\frac{\sum_{\beta\in\mathcal{H}}\mathbf{R}^{e,\beta}_e}{n_e q_e}\right)$$

$$\mathbf{v_e} = \sum_{\alpha\in\mathcal{H}} \frac{n_\alpha q_\alpha \mathbf{v}_\alpha}{n_e q_e} - \frac{\mathbf{J}}{n_e q_e},\ \mathbf{J} = \nabla\times\mathbf{B}/\mu_0$$

Example of an explicit stabilized method: PIROCK

PIROCK: integrator in time for stiff diffusion-advection-reaction systems (arising e.g. from a spatial discretization) of the form

$$\frac{dy(t)}{dt} = F(y) = F_D(y) + F_A(y) + F_R(y) + \text{Itô noise}, \quad y(0) = y_0.$$

We think of:

- $F_D(y)$ diffusion terms (spatial discretization of $\mathrm{div}(a\nabla\cdot)$), integrated with ROCK2 (order 2, explicit stabilized);
- $F_A(y)$ advection terms (spatial discretization of $b^T\nabla\cdot$), integrated with Runge-Kutta (order 3, explicit);
- $F_R(y)$, very stiff reaction terms, integrated with SDIRK method (order 2, L-stable, implicit).

A. Abdulle and V., PIROCK: a swiss-knife partitioned implicit-explicit orthogonal Runge-Kutta Chebyshev integrator for stiff diffusion-advection-reaction problems with or without noise, *JCP*, 2013.

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 $\quad y_{n+1} = y_n + hf(y_{n+1}),$
- θ-method $\quad y_{n+1} = y_n + \theta hf(y_n) + (1-\theta)hf(y_{n+1}),$
- 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.

$$m_i \ddot{q}_i(t) = -G \sum_{0 \le j \ne i \le 2} m_i m_j \frac{q_i(t) - q_j(t)}{\|q_i(t) - q_j(t)\|^3} \qquad (i = 0, 1, 2)$$

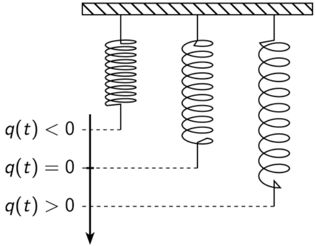
$q_i(t) \in \mathbb{R}^3$ positions, $p_i(t) = m_i \dot{q}_i(t)$ momenta, G, m_0, m_1, m_2 const.
This is a Hamiltonian system

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

with Hamiltonian (energy): $H(p, q) = T(p) + V(q)$

$$T(p) = \frac{1}{2} \sum_{i=0}^{2} \frac{1}{m_i} p_i^T p_i, \qquad V(q) = -G \sum_{i=1}^{2} \sum_{j=0}^{i-1} \frac{m_i m_j}{\|q_i - q_j\|}.$$

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, $m = 1$)

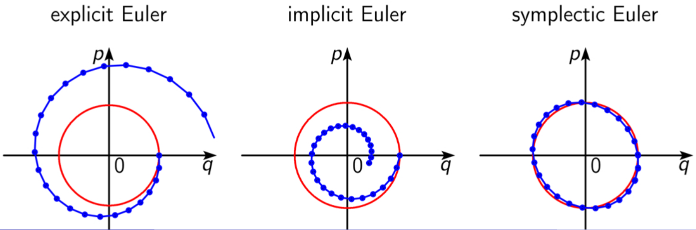
- Explicit Euler method: $q_{n+1} = q_n + hp_n, \qquad p_{n+1} = p_n - hkq_n.$

  energy amplification: $H(p_{n+1}, q_{n+1}) = (1 + kh^2)H(p_n, q_n).$
- Implicit Euler method: $q_{n+1} = q_n + hp_{n+1}, \qquad p_{n+1} = p_n - hkq_{n+1}.$

  energy damping: $H(p_{n+1}, q_{n+1}) = \frac{1}{1 + kh^2}H(p_n, q_n).$
- Symplectic Euler method: $q_{n+1} = q_n + hp_n, \qquad p_{n+1} = p_n - hkq_{n+1}.$

  exact conservation of a modified Hamiltonian energy $\tilde{H}_h(p, q) = H(p, q) + h\frac{kpq}{2}$

  satisfying $\tilde{H}_h(p_{n+1}, q_{n+1}) = \tilde{H}_h(p_n, q_n).$



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

$$\dot{z} = \widetilde{f}_h(z) = f(z) + hf_2(z) + h^2 f_3(z) + h^3 f_4(z) + \ldots, \quad z(0) = y_0$$

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, such as 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.

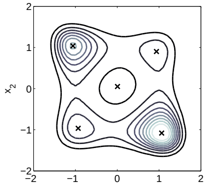
Itô integral: for $f(t)$ a (continuous and adapted) stochastic process,

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

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)

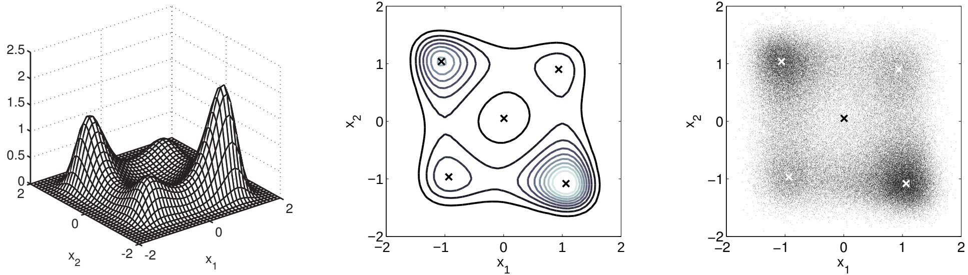
$$dX(t) = -\nabla V(X(t))dt + \sqrt{2}dW(t).$$

$W(t)$: standard Brownian motion in $\mathbb{R}^d$.

Ergodicity: invariant measure μ_∞ has Gibbs 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 ($d = 2$): $V(x) = (1 - x_1^2)^2 + (1 - x_2^2)^2 + \frac{x_1 x_2}{2} + \frac{x_2}{5}$.



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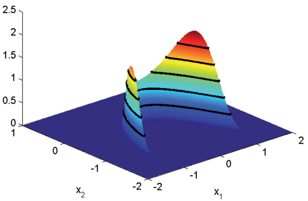
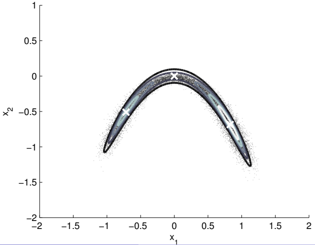
Example ($d = 2$), Stiff case:

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





Plan of the talk

1. Part 1: Stability of numerical integrators
   - Stability analysis for deterministic problems
   - Mean-square stability analysis for stochastic problems
   - Explicit stabilized methods
2. Part 2: 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
3. Part 3: Explicit stabilized integrators for stiff S(P)DEs
   - Optimal explicit stabilized integrators for stiff and ergodic SDEs
   - Explicit stabilized integrators for SPDEs

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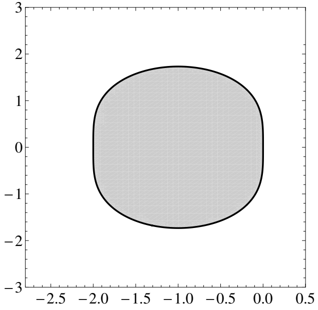
Stability analysis of (deterministic) integrators

Stability function. Consider $\frac{dy(t)}{dt} = \lambda y(t)$ (Dalquist test eq.).
A Runge-Kutta method with stepsize h yields $y_{n+1} = R(\lambda h) y_n$.

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

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



Example: the Heun method (explicit)

$$y_{n+1} = y_n + \frac{h}{2} f(y_n) + \frac{h}{2} f\left(y_n + hf(y_n)\right) = R(\lambda h) y_n$$

$$R(z) = 1 + z + \frac{z^2}{2}.$$

The stability condition $-2 \leq h\lambda \leq 0$ becomes for diffusion problems where $\lambda_{\max} = \mathcal{O}(\Delta x^{-2})$, $h \leq C\Delta x^2$ (severe CFL).

The case of mean-square stable stiff SDEs

A widely used test equation (Saito, Mitsui, 1996) to study stability

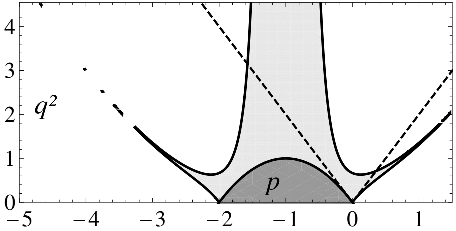
$$dX = \lambda X dt + \mu X dW(t), \quad \text{exact solution: } X(t) = e^{(\lambda - \frac{1}{2}\mu^2)t + \mu W(t)}$$

The mean-square stability domain for which $\mathbb{E}(|X(t)|^2) \to_{t\to\infty} 0$ is given by

$$\mathcal{S} = \{(\lambda, \mu) \in \mathbb{C}^2 \; ; \Re\lambda + \frac{1}{2}|\mu|^2 < 0\}.$$

Mean-square stability: A numerical integrator is called mean-square A-stable for the test equation if $\mathbb{E}(|X_n|^2) \to_{n\to\infty} 0$ for all $(\lambda, \mu) \in \mathcal{S}$.

Euler-Maruyama scheme (weak order 1)



$p = h\lambda$ (deterministic axis),
$q^2 = h\mu^2$ (stochastic axis).

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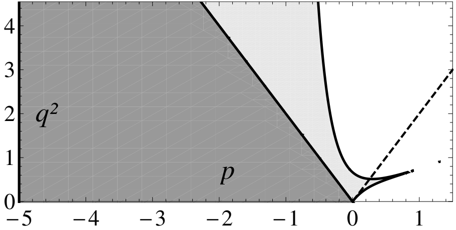
Drift-implicit θ-method (weak order 1)



$$y_{n+1} = y_n + (1-\theta) h f(y_n) + \theta h f(y_{n+1}) + g(y_n)\Delta W_n.$$

mean-square A-stable for $\theta \geq 1/2$ (Higham, 2000).

Explicit stabilized methods: first order Chebyshev methods

For fixed integer s, and a first order stability function of degree at most s of the form

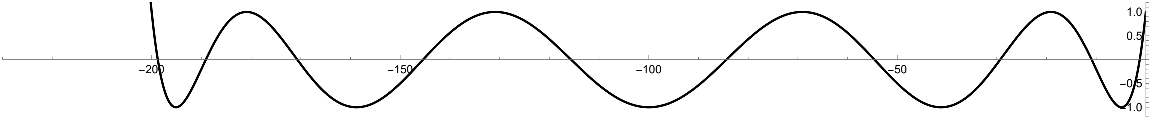
$$R_s(z) = 1 + z + a_2 z^2 + \ldots + a_s z^s,$$

find the coefficients $a_2, a_3, \ldots, a_s$ that maximize L_s where $L_s := \sup_{\ell \geq 0}(-\ell, 0) \subset \mathcal{S}$.

Theorem (Markoff, 1892, Yuan'Chzao Din, 1958, Franklin, 1959, Guillou, Lago, 1960)

For fixed integer s, the optimal solution that maximizes L_s is unique and 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 $z \in (-L_s, 0)$, with $L_s = 2s^2$.

Figure: $R_s(z)$ with $s = 10$ internal stages, $L_s = 200$.



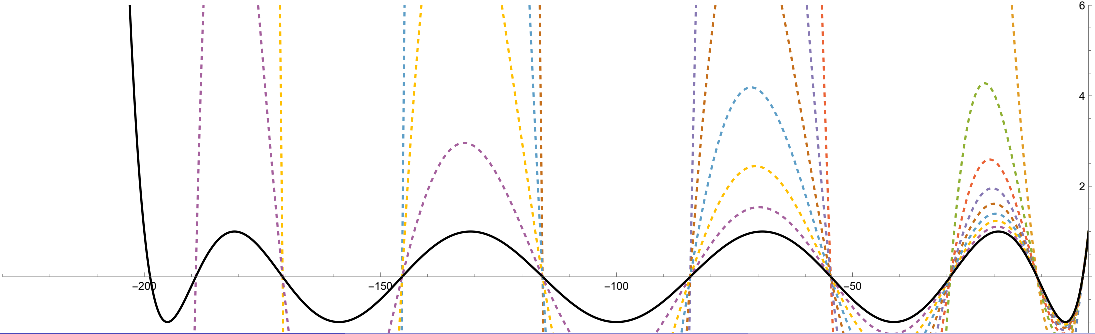
Example: first order Chebyshev methods, Naive implementation

Optimal stability function given by $R_s(z) = T_s\left(1 + \frac{z}{s^2}\right) = \prod_{j=1}^{s}(1 + \alpha_j z)$ with $\alpha_j = -1/\xi_j$

where $\xi_j, j = 1\ldots, s$ are the (all real) roots of $R_s(z)$ (Guillou-Lago, Saul'ev, 60', Lebedev, 70').
A naive implementation $y_0 \mapsto y_1$ is composing s explicit Euler steps:

$$K_0 = y_0, \qquad K_j = K_{j-1} + \alpha_j hF(K_{j-1}),\ j = 1, \ldots, s, \qquad y_1 = K_s.$$

Figure: stability polynomials for $K_j, j = 1\ldots, s$ with $s = 10$ internal stages.

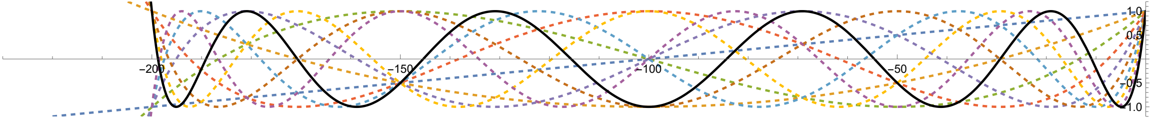


Example: first order Chebyshev methods, Stable implementation

An s-stage Runge-Kutta method $y_0 \mapsto y_1$ implemented using the Chebyshev recurrence relation $T_j(x) = 2xT_{j-1}(x) - T_{j-2}(x), \quad j \geq 2$ (Van der Houwen, Sommeijer, 80'):

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

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 $z \in (-L_s, 0)$, with $L_s = 2s^2$.



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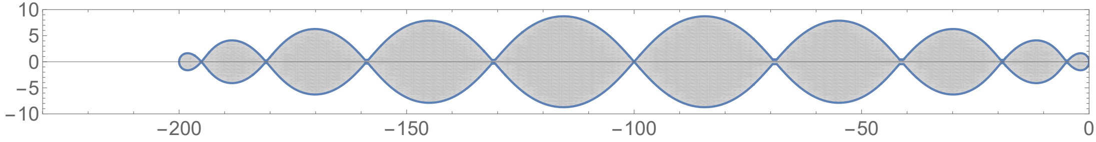


($s = 10$, no damping, $\eta = 0$)

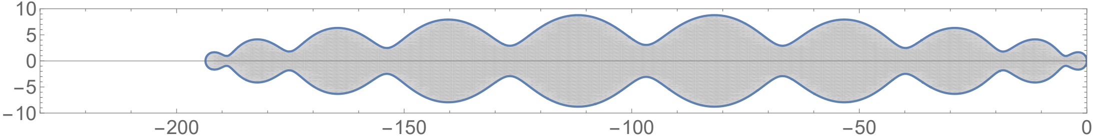
Example: first order Chebyshev methods, Stable implementation

Damped first order Chebyshev methods $y_0 \mapsto y_1$. Given $\eta > 0$,

$$\begin{aligned} K_1 &= y_0 + \mu_1 h f(y_0), \qquad K_0 = y_0, \\ K_i &= \mu_i h f(K_{i-1}) + \nu_i K_{i-1} + \kappa_i K_{i-2}, \quad i = 2, \ldots, s, \\ y_1 &= K_s \end{aligned}$$

$$R_s(z) = \frac{T_s(\omega_0 + \omega_1 z)}{T_s(\omega_0)}, \quad \omega_0 = 1 + \frac{\eta}{s^2}, \ \omega_1 = \frac{T_s(\omega_0)}{T_s'(\omega_0)}.$$

It satisfies $|R_s(z)| \leq 1$ for all $z \in (-L_s, 0)$, with $L_s = \left(2 - \frac{4}{3}\eta\right) s^2$.



($s = 10$, small damping with $\eta = 0.05$)

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$$R_s(z) = \frac{T_s(\omega_0 + \omega_1 z)}{T_s(\omega_0)}, \quad \omega_0 = 1 + \frac{\eta}{s^2}, \ \omega_1 = \frac{T_s(\omega_0)}{T_s'(\omega_0)}.$$

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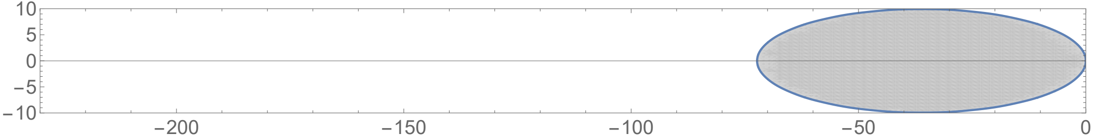


$(s = 10$,large damping with $\eta = 4)$

Classical S-ROCK method (Abdulle and Li, 2008)

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

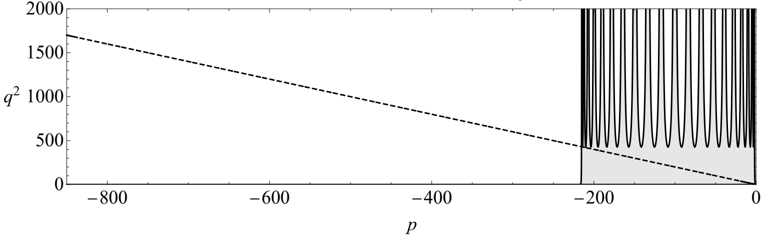
$$\begin{aligned} K_1 &= X_0 + \mu_1 h f(X_0), \qquad K_0 = X_0 \\ K_i &= \mu_i h f(K_{i-1}) + \nu_i K_{i-1} + \kappa_i K_{i-2}, \quad i = 2, \dots, s, \\ X_1 &= K_s + \sum_{r=1}^{m} g^r(K_s)\Delta W_j. \end{aligned}$$

$$R(p, q, \xi) = \frac{T_s(\omega_0 + \omega_1 p)}{T_s(\omega_0)}(1 + q\xi), \quad \omega_0 = 1 + \frac{\eta}{s^2}, \ \omega_1 = \frac{T_s(\omega_0)}{T_s'(\omega_0)}.$$

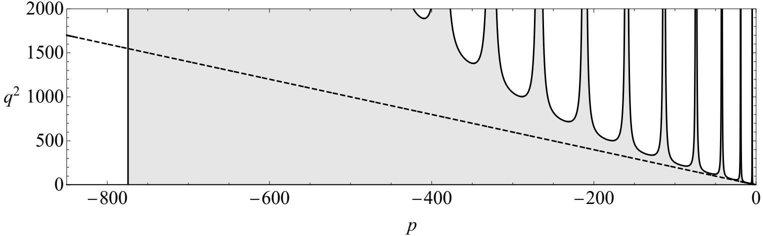
Remarks

- 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 $L_s \simeq 0.33 \cdot s^2$.

Optimal explicit stabilized scheme for MS stiff problems



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



SK-ROCK method (Abdulle, Almuslimani, V., 2018, $s = 20$, $\eta = 0.05$)
stability domain size $L_s \geq (2 - \frac{4}{3}\eta)s^2$, order two for the invariant measure.

Explicit stabilized integrators (Chebyshev methods)

Yuan'Chzao Din (1958), Franklin (1959), Guillou, Lago (1960), Bogatyrev, Lebedev, Skvorstov, Medovikov (DUMKA 1976-2004)...

- 1. RKC: based on three-term recurrence relation (non-optimal) with $L_s \simeq 0.66 \cdot s^2$ van der Houwen, Shampine, Sommeijer, Verwer (RKC, IMEX extension IRKC, 1980-2007), Zbinden (PRKC 2011), Almuslimani, V. (optimal control problems, 2020), multirate mRKC (Abdulle, Grote, Rosilho de Souza, 2021), stabilized gradient descent RKGD for optimisation with $\eta \gg 1$ (Eftekhari, Vandereycken, V., Zygalakis, 2021), stabilized leapfrog (Carle, Hochbruck, Sturm, 2020, Grote, Michel, Sauter, 2022).
- 2. ROCK methods (close to optimal stability for second order)
  Abdulle, Medovikov (ROCK2 2000-02), Abdulle, V. (PIROCK 2013) with $L_s \simeq 0.81 \cdot s^2$
  Abdulle (ROCK4 2002-05) with $L_s \simeq 0.35 \cdot s^2$.
- 3. Extension to stiff stochastic problems: S-ROCK methods
  Weak order 1: Abdulle, Cirilli, Li, Hu (2007-2009,2010)
  with $L_s \simeq 0.33 \cdot s^2$, Abdulle, Almuslimani, V. $L_s \simeq 2 \cdot s^2$ (SK-ROCK, 2018),
  Weak order 2: Abdulle, V., Zygalakis (S-ROCK2, 2014) $L_s \simeq 0.43 \cdot s^2$
  SPDE case: analysis of SK-ROCK by Abdulle, Brehier, V. (2023).

2. Part 2: 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.
- 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.

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,

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

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

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

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 $t = Nh$,

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

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

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

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

High order approximation of the numerical invariant measure

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

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

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.

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

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

$\ldots$

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).

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

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

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).

Back to stiff problems. Quadratic case (Ornstein-Uhlenbeck)

Consider the scalar OU process, with unique inv. measure $\mathcal{N}(0, \frac{\sigma^2}{2|\lambda|})$,

$$dX(t) = \lambda X(t)dt + \sigma dW(t), \qquad (\lambda < 0).$$

Proposition: invariant measure preservation

For a one-step integrator where $z = \lambda h$, $\xi_n \sim \mathcal{N}(0,1)$,

$$X_{n+1} = A(z)X_n + B(z)\sqrt{h}\sigma\xi_n,$$

$\overline{X}_n$ converges to the exact invariant measure iff $|A(z)| < 1$ and

$$\frac{-2zB(z)^2}{1 - A(z)^2} = 1.$$

For rational $A(z), B(z)$, this condition for all z implies $|A(\infty)| = 1$.

Example: $\theta = 1/2$ method: $A(z) = \frac{1+z/2}{1-z/2}$, $B(z) = \frac{1}{1-z/2}$ (see Chong, Walsh, 2012).

Remark: Impossible to be exact (without postprocessing) for an explicit Runge-Kutta method or an L-stable method ($A(\infty) = 0$).

Back to stiff problems. Quadratic case (Ornstein-Uhlenbeck)

Proposition: invariant measure preservation

For a postprocessed integrator (V. SISC 2015) where $z = \lambda h$, $\xi_n \sim \mathcal{N}(0,1)$,

$$X_{n+1} = A(z)X_n + B(z)\sqrt{h}\sigma\xi_n, \quad \overline{X}_n = C(z)X_n + D(z)\sqrt{h}\sigma\xi_n,$$

$\overline{X}_n$ converges to the exact invariant measure if $|A(z)| < 1$ and

$$\frac{-2zB(z)^2 C(z)^2}{1 - A(z)^2} - 2zD(z)^2 = 1.$$

- $\theta = 0$ meth., $A(z) = 1 + z$, $B(z) = 1 + \frac{z}{2}$, $C(z) = 1$, $D(z) = \frac{1}{2}$, (see Leimkuhler, Matthews, 2013).
- $\theta = 1$ method, $A(z) = B(z) = \frac{1}{1-z}$, $C(z) = 1$, $D(z) = \frac{1}{\sqrt{1-z/2}}$, (see Bréhier, V., 2016, order improved by +1 for the stochastic heat equation).

1. Part 1: Stability of numerical integrators

2. Part 2: High order for the invariant measure and postprocessors

3. Part 3: Explicit stabilized integrators for stiff S(P)DEs
   - Optimal explicit stabilized integrators for stiff and ergodic SDEs
   - Explicit stabilized integrators for SPDEs

- Abdulle, Almuslimani, V., *Optimal explicit stabilized integrator of weak order one for stiff and ergodic SDEs*, *SIAM JUQ*, 2018.
- Abdulle, Bréhier, V., *Convergence analysis of explicit stabilized integrators for parabolic semilinear SPDEs*, *IMAJNA*, 2023.

First and second kind Chebyshev polynomials

- First kind: $T_s(\cos\theta) = \cos(s\theta), s \geq 0,$

$$T_j(x) = 2xT_{j-1}(x) - T_{j-2}(x), \quad j \geq 2,$$

  where $T_0(x) = 1, T_1(x) = x.$

- Second kind: $\sin\theta \; U_s(\cos\theta) = \sin((s+1)\theta), s \geq 0,$

$$U_j(x) = 2xU_{j-1}(x) - U_{j-2}(x), \quad j \geq 2,$$

  where $U_0(x) = 1, U_1(x) = 2x.$

Useful properties:

$$T_s'(p) = sU_{s-1}(p), \qquad T_s(x)^2 + (1-x^2)U_{s-1}(x)^2 = 1, \qquad s \geq 1.$$

SK-ROCK Quadratic case (Ornstein-Uhlenbeck)

Consider the scalar OU process, with unique inv. measure $\mathcal{N}(0, \frac{\sigma^2}{2|\lambda|})$,

$$dX(t) = \lambda X(t)dt + \sigma dW(t), \qquad (\lambda < 0).$$

Theorem: invariant measure preservation by explicit stabilized methods (Abdulle, Almuslimani, V., 2018)

For all $s \geq 1$, the family of polynomials (involving first kind and second kind Chebyshev polynomials)

$$A(z) = T_s(1 + \tfrac{z}{s^2}), \quad B(z) = s^{-1} U_{s-1}(1 + \frac{z}{s^2})(1 + \frac{z}{2s}),$$

$$C(z) = 1, \qquad D(z) = \frac{1}{2s},$$

satisfies the invariant mesure preservation condition

$$\frac{-2zB(z)^2 C(z)^2}{1 - A(z)^2} - 2zD(z)^2 = 1.$$

SK-ROCK: optimal stability domain length (Abdulle, Almuslimani, V. 2018)

SK-ROCK (stochastic second kind orthogonal Runge-Kutta-Chebyshev method):

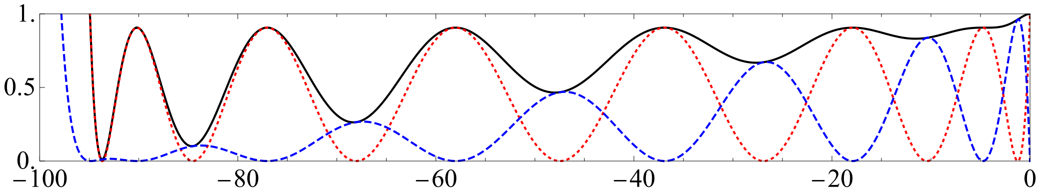
$$\begin{aligned} K_0 &= X_0 \\ K_1 &= X_0 + \mu_1 h f(X_0 + \nu_1 Q) + \kappa_1 Q \\ K_i &= \mu_i h f(K_{i-1}) + \nu_i K_{i-1} + \kappa_i K_{i-2}, \quad i = 2, \ldots, s. \\ X_1 &= K_s, \end{aligned}$$

where the noise increment is defined as $Q = \sum_{r=1}^{m} g^r(X_0)\Delta W_j$.

Features of SK-ROCK:

- 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.
- Theorem (Abdulle, Almuslimani, V. 2018): Stability domain size $L_s \geq (2 - \frac{4}{3}\eta)s^2$ and there is a postprocessor for order two for the invariant measure sampling.

SK-ROCK: optimal stability domain length (Abdulle, Almuslimani, V. 2018)

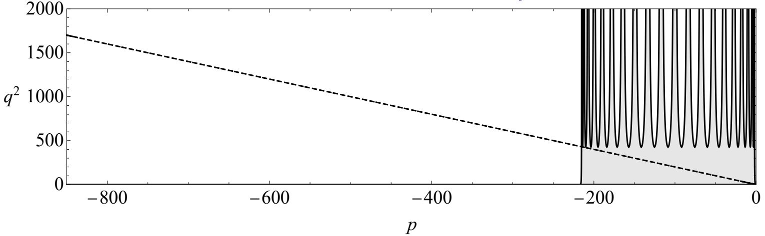


$\mathbb{E}(|R(p,q,\xi)|^2) = A(p)^2 + B(p)^2 q^2$ as a function of p ($q^2 = -2p$), $s = 10$ stages.

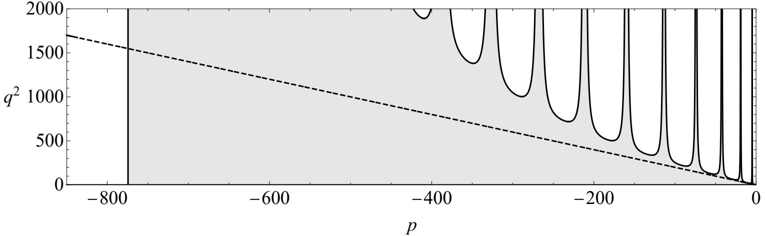
Features of SK-ROCK:

- 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.
- Theorem (Abdulle, Almuslimani, V. 2018): Stability domain size $L_s \geq (2 - \frac{4}{3}\eta)s^2$ and there is a postprocessor for order two for the invariant measure sampling.

Optimal explicit stabilized scheme for MS stiff problems



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



SK-ROCK method (Abdulle, Almuslimani, V., 2018, $s = 20$, $\eta = 0.05$)
stability domain size $L_s \geq (2 - \frac{4}{3}\eta)s^2$.

Convergence for parabolic SPDEs

- semilinear parabolic SPDE (F assumed Lipschitz):

$$du(t) = \Lambda u(t)dt + F(u(t))dt + \sigma dW^Q(t), \quad u(0) = u_0.$$

- Spatial discretization (finite elements with spatial mesh size Δx):

$$du^{\Delta x}(t) = \Lambda_{\Delta x} u^{\Delta x}(t)dt + P_{\Delta x} F(u^{\Delta x}(t))dt + \sigma P_{\Delta x} dW^Q(t), \quad u^{\Delta x}(0) = P_{\Delta x} u_0.$$

- Explicit stabilized integrator with timestep τ:

$$u_{n+1}^{\Delta x} = A_s(\tau\Lambda_{\Delta x}) u_n^{\Delta x} + B_s(\tau\Lambda_{\Delta x}) P_{\Delta x}(\tau F(u_n^{\Delta x}) + \sigma \Delta W_n^Q).$$

Remark: the stage parameter s is chosen such as

$$\tau \lambda_{max,\Delta x} \leq L_s, \qquad \text{i.e. } \tau C \Delta x^{-2} \simeq s^2.$$

Convergence for semilinear parabolic SPDEs

$$du(t) = \Lambda u(t)dt + F(u(t))dt + \sigma dW^Q(t), \quad u(0) = u_0.$$

with nonlinearity F assumed Lipschitz, $\overline{\alpha} = \sup\{s \in (0,1); \mathrm{Trace}\left((-\Lambda)^{-1+s} Q\right) < +\infty\}$.

Theorem (Abdulle, Bréhier, V., 2023) Strong convergence of order $\overline{\alpha}/2$.

Assume

$$A_s(0) = A_s'(0) = B_s(0) = 1, s \geq 1,$$

$$\sup_{s\geq 1, z\in[-L_s,0]} (1+|z|)|B_s(z)|^2 < \infty,$$

$$\sup_{s\geq 1, z\in[-L_s,-\delta]} |A_s(z)| < 1, \quad \text{for all } \delta \in (0,1],$$

$$\sup_{s\geq 1, |z|\leq\delta} (|A_s(z)| + |B_s(z)|) < \infty \quad \text{for some } \delta \in (0,1].$$

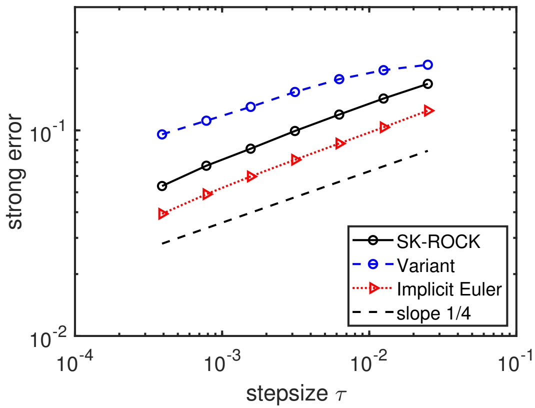
Then, for all $T > 0$, and all $\alpha \in (0, \overline{\alpha})$,

$$|\mathbb{E}\|u^{\Delta x}(n\tau) - u_n^{\Delta x}\|^2|^{1/2} \leq C_{T,\alpha}(1 + |u_0| t_n^{-\alpha/2})\tau^{\alpha/2},$$

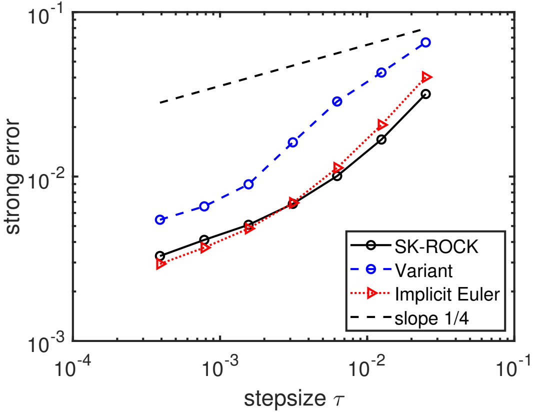
where $C_{T,\alpha}$ is independent of Δx, and τ assumed small enough.

Convergence plots for the semilinear SPDEs (1D)

$$\partial_t u(x,t) = \partial_{xx} u(x,t) + f(u(x,t)) + g(u(x,t))\partial_t W(x,t).$$



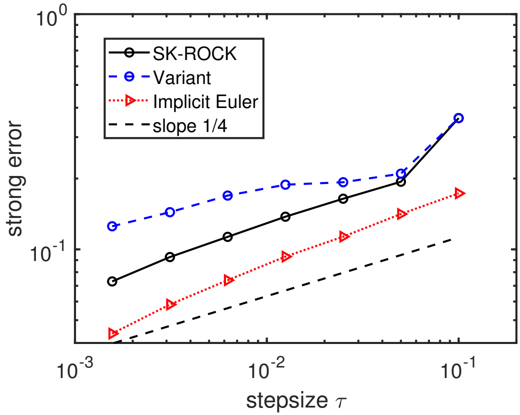
additive noise $g(u) = 1$



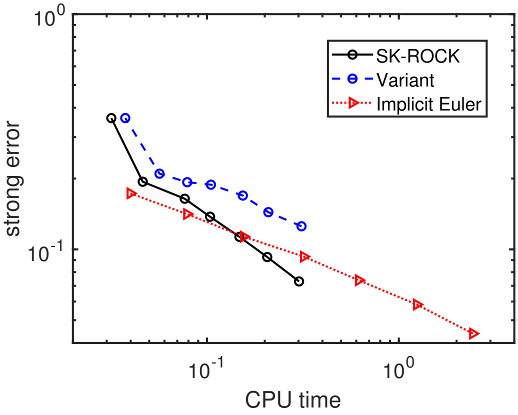
multiplicative noise $g(u) = u$

Convergence plots for the semilinear SPDEs (2D)

$$\partial_t u(x,y,t) = (\partial_{xx} + \partial_{yy})u(x,y,t) + f(u(x,y,t)) + \partial_t W(x,t).$$

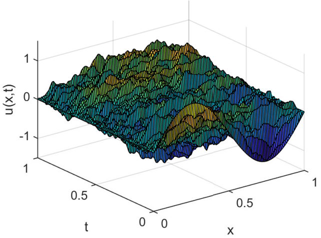


Error versus time stepsize

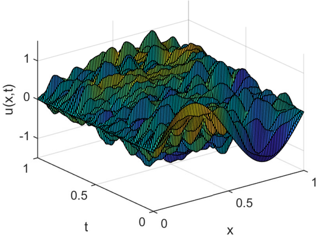


Error versus CPU time

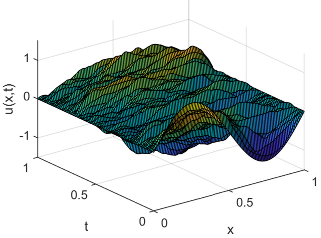
Qualitative behavior $\partial_t u = \partial_{xx} u - u - \sin(u) + \partial_t W, x \in (0,1)$, $(\Delta x = \tau = 1/100)$.



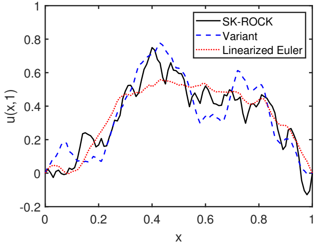
SK-ROCK method



variant method



Implicit Euler



Solution at $t = 1$

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

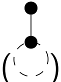
$$X_{n+1} = X_n + hF(\overline{X}_n) + \hat{\Phi}_h^D\Big(X_n + \frac{h}{4}F(\overline{X}_{n-1})\Big),$$
$$\overline{X}_n = X_n + \frac{1}{2}\sigma\sqrt{h}D(X_n)\xi_n,$$

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

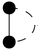
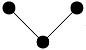
Theorem (Bronasco, Leimkuhler, Phillips, and V., 2024, in preparation)

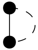
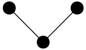
The postprocessed method with $\overline{X}$ above is second-order for sampling the invariant measure and has only one evaluation of ∇V per step.

Integration by parts using exotic aromatic trees: example

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

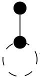
$$= -\sum_{i,j}\left[\int_{\mathbb{R}^d} \frac{\partial \phi}{\partial x_i \partial x_j}\frac{\partial f_i}{\partial x_j}\rho_\infty dy + \int_{\mathbb{R}^d} \frac{\partial \phi}{\partial x_i \partial x_j} f_i \frac{\partial \rho_\infty}{\partial x_j} dy\right]$$

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

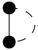
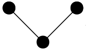
where we used $\nabla \rho_\infty = f \rho_\infty$. We obtain:  $\sim -$  $- \frac{2}{\sigma^2}$  .

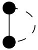
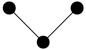
Deterministic B-series: Hairer & Wanner, 1972, using Butcher's seminal work (1960s).
Link with Hopf algebras of trees in quantum physics (Connes, Kreimer, 1980s).
Stochastic case: Tree formalism for strong and weak errors on finite time: Burrage K., Burrage P.M., 1996; Komori, Mitsui, Sugiura, 1997; Rößler, 2004/2006, ...

Integration by parts using exotic aromatic trees: example

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

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

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

where we used $\nabla\rho_\infty = f\rho_\infty$. We obtain:  $\sim -$  $- \frac{2}{\sigma^2}$  .

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.

Convergence analysis in the variable diffusion case

New notation for exotic aromatic trees: $EAT = \{ \cdots, \ldots \} = \{\bullet, \textcircled{1}\textcircled{1}, \bullet\textcircled{1}\textcircled{1}, \ldots\}$

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

$$\mathcal{L}^2 = \mathcal{F}(\bullet\bullet + \cdots + \bullet\textcircled{1}\textcircled{1} + \cdots\textcircled{1}\textcircled{1} + \textcircled{1}\cdots + \frac{1}{2}\cdots + \frac{1}{4}\textcircled{1}\textcircled{1}\textcircled{2}\textcircled{2} + \textcircled{1}\textcircled{2}\textcircled{2}\cdots + \frac{1}{2}\textcircled{2}\textcircled{2}\cdots + \frac{1}{2}\textcircled{2}\cdots\textcircled{2})$$

Theorem (Bronasco, 2024, Bronasco, Leimkuhler, Phillips, and V., in preparation)

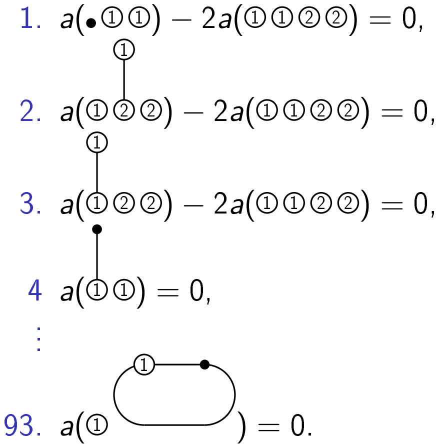
We can use integration by parts denoted by $\sim$ to modify $\mathcal{A}_k$ without changing the value of $A_k^*\rho_\infty$. The order p condition becomes

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

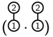
where A is an adjoint operation of the integration by parts.

List of order conditions for the variable diffusion case

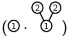
There are 93 order conditions for order 2 for the invariant measure sampling!



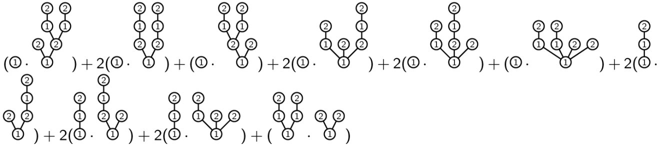

```
> f1 = [PT 1 [PT 2 []], PT 1 [PT 2 []]]
> display $ vector f1
```



```
> 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

- explicit stabilized methods: an efficient alternative to implicit methods for stiff dissipative problems (advantage: avoids preconditioners for linear algebra solvers, low memory usage, easier implementation, etc.).
- construction in the stochastic context inspired by geometric numerical integration.

Related ongoing work:

- collaboration with NASA affiliated lab. to apply explicit stabilized methods for solar atmosphere simulations.
- extension to high-order for Langevin dynamics with variable diffusion (with E. Bronasco, B. Leimkuhler, D. Phillips).
- preconditionned integrators (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.

Software codes available at: `www.unige.ch/~vilmart/software`