On superconvergence features of methods based on the Crank-Nicolson scheme in the context of diffusion PDEs (deterministic and stochastic)

Gilles Vilmart

Based on joint works with
Assyr Abdulle (Lausanne), Ibrahim Almuslimani (Rennes), Guillaume Bertoli (Geneva), Christophe Besse (Toulouse) and Charles-Edouard Bréhier (Lyon)

UNIVERSITÉ DE GENÈVE
FACULTÉ DES SCIENCES
Section de mathématiques

Contents

In this talk, we present two situations where the Crank-Nicolson method is surprisingly more accurate than one could expect:

1. In the context of splitting methods for parabolic PDEs

2. In the context of ergodic stochastic parabolic PDEs

Part 1

1. In the context of splitting methods for parabolic PDEs
2. In the context of ergodic stochastic parabolic PDEs

- G. Bertoli and V., Strang splitting method for semilinear parabolic problems with inhomogeneous boundary conditions: a correction based on the flow of the nonlinearity, SIAM J. Sci. Comput. 42 (2020), A1913-A1934.
- G. Bertoli, C. Besse, and V., Superconvergence of the Strang splitting when using the Crank-Nicolson scheme for parabolic PDEs with oblique boundary conditions, arXiv:2011.05178, submitted.

The Strang splitting method

For parabolic semilinear problems of the form

$$\begin{aligned} \partial_t u(x,t) &= Du(x,t) + f(x,u(x,t)) \;\; \text{in } \Omega \times (0,T], \\ Bu(x,t) &= b(x) \;\; \text{on } \partial\Omega \times (0,T], \\ u(x,0) &= u_0(x) \quad \text{in } \Omega, \end{aligned}$$

we consider time discretizations with splitting methods:

$$\phi_t^f : \qquad \partial_t u(x,t) = f(x,u(x,t)) \quad \text{in } \Omega \times (0,T],$$

$$\phi_t^D : \qquad \begin{array}{rcl} \partial_t u(x,t) & = & Du(x,t) \quad \text{in } \Omega \times (0,T], \\ Bu(x,t) & = & b(x) \text{ on } \partial\Omega \times (0,T]. \end{array}$$

For approximating $u(t_n,x) \simeq u_n(x)$, $t_n = n\tau$, the Strang splitting method writes

$$u_{n+1} = \phi^f_{\frac{\tau}{2}} \circ \phi^D_{\tau} \circ \phi^f_{\frac{\tau}{2}}(u_n),$$

Or alternatively, another version writes:

$$u_{n+1} = \phi^D_{\frac{\tau}{2}} \circ \phi^f_{\tau} \circ \phi^D_{\frac{\tau}{2}}(u_n).$$

The Crank-Nicolson method

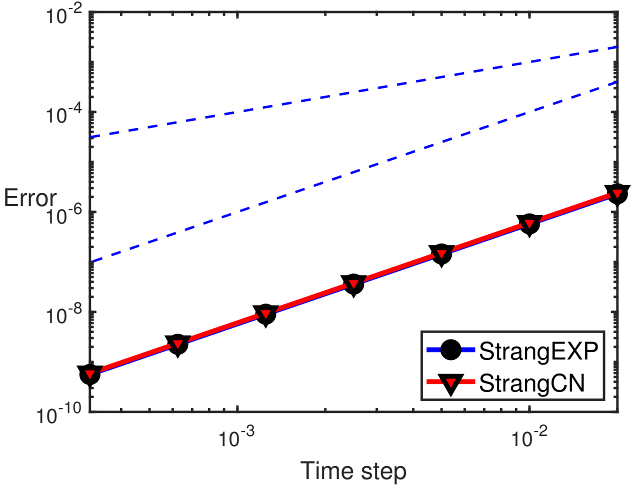
It is typical to approximate the exact flow of the diffusion part,

$$u(t) = \phi_t^D(u_0): \qquad \begin{array}{rcl} \partial_t u &=& Du \quad \text{in } \Omega \times (0,T], \\ Bu &=& b \quad \text{on } \partial\Omega \times (0,T], \end{array}$$

either with a Krylov method, or with a Runge-Kutta type method, such as the Crank-Nicolson method (formally of order two),

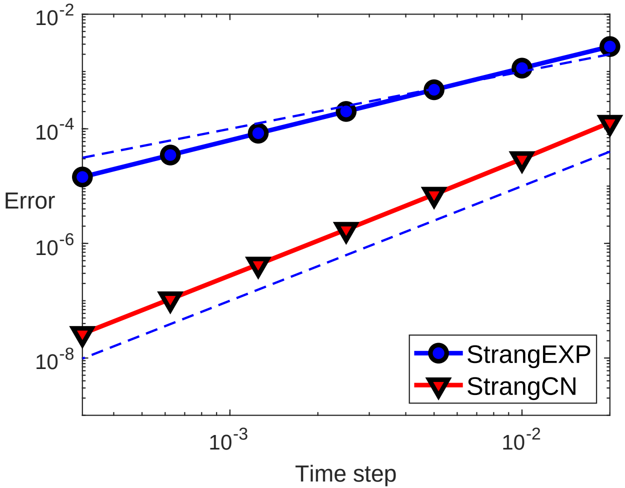
$$u_1 = \phi_\tau^{D,CN}(u_0): \qquad \begin{array}{rcl} \frac{u_1(x)-u_0(x)}{\tau} &=& D\frac{u_1(x)+u_0(x)}{2} \quad \text{in } \Omega, \\ B\frac{u_0(x)+u_1(x)}{2} &=& b(x) \quad \text{on } \partial\Omega. \end{array}$$

A numerical example on $\Omega = (0, 1)$



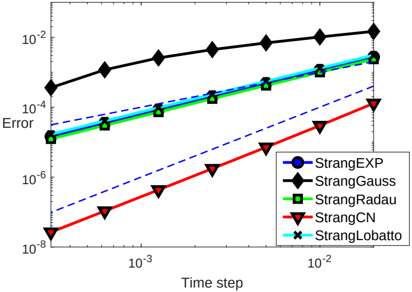
$$\partial_t u = \partial_{xx} u + e^{-x} \text{ on } \Omega, \quad \partial_x u + u = 1 \text{ on } \partial\Omega, \quad u(x, 0) = 1.$$

A numerical example: order reduction!

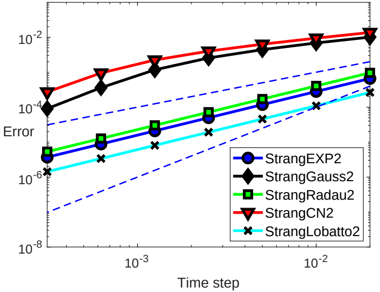


$$\partial_t u = \partial_{xx} u + 1 \text{ on } \Omega, \quad u = 1 \text{ on } \partial\Omega, \quad u(x,0) = 1.$$

With other approximations of the diffusion part?



$$u_{n+1} = \phi^f_{\frac{\tau}{2}} \circ \phi^D_{\tau} \circ \phi^f_{\frac{\tau}{2}}(u_n)$$



$$u_{n+1} = \phi^D_{\frac{\tau}{2}} \circ \phi^f_{\tau} \circ \phi^D_{\frac{\tau}{2}}(u_n)$$

$$\partial_t u = \partial_{xx} u + 1 \text{ on } \Omega, \quad u = 1 \text{ on } \partial\Omega, \quad u(x,0) = 1.$$

What happened?

An observation from (W. Hundsdorfer and J. Verwer. 1994): the reason of the order reduction is that $w = \phi_\tau^f(u_n)$ does not preserve the boundary conditions, i.e. $Bu_n = b \not\Longrightarrow Bw = b$ for $Bf(u) \neq 0$.

Possible remedies to order reduction in splitting methods:

- (L. Einkemmer and A. Ostermann, 2016) Modify the splitting as:

  $$u_{n+1} = \phi_{\frac{\tau}{2}}^{D+q_n} \circ \phi_\tau^{f-q_n} \circ \phi_{\frac{\tau}{2}}^{D+q_n}(u_n),$$

  where q_n is chosen such that $Bq_n = Bf(u_n) + \mathcal{O}(\tau)$ on $\partial\Omega$.
- (G. Bertoli and V., 2020) Consider a five step splitting method as

  $$u_{n+1} = \phi_{\frac{\tau}{2}}^{f} \circ \phi_{\frac{\tau}{2}}^{-q_n} \circ \phi_\tau^{D+q_n} \circ \phi_{\frac{\tau}{2}}^{-q_n} \circ \phi_{\frac{\tau}{2}}^{f}(u_n)$$

  where q_n is computed only using the source flow output $\phi_{\frac{\tau}{2}}^f(u_n)$ such that $w = \phi_{\frac{\tau}{2}}^{-q_n} \circ \phi_{\frac{\tau}{2}}^f(u_n)$ satisfies the boundary conditions $Bw = b$ up to $\mathcal{O}(\tau^2)$.

  This halves the number of evaluations of the diffusion part ϕ_τ^D.

Note: In this talk, we shall not use the above "repair" techniques.

Superconvergence of splitting with Crank-Nicolson

For the diffusion-reaction problem, consider the splitting method

$$u_{n+1} = \phi^f_{\frac{\tau}{2}} \circ \phi^{D,CN}_\tau \circ \phi^f_{\frac{\tau}{2}}(u_n).$$

Theorem (Bertoli, Besse, V., 2020) (order two for $f = f(x)$)

Let $u_0 \in W^{2,p}(\Omega)$ with $Bu_0 = b$ on $\partial\Omega$ and $f = f(x) \in L^p(\Omega)$. Then the global error $e_n = u_n - u(t_n)$ satisfies

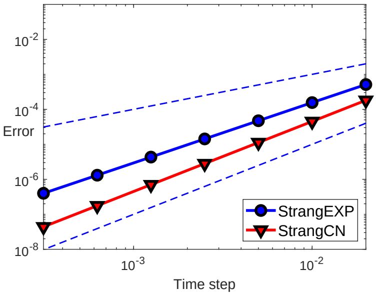
$$\|e_n\|_{L^p(\Omega)} \leq \frac{C\tau^2}{t_n}, \qquad e_n = \left(r(\tau A)^n - e^{n\tau A}\right) A^{-1}(Du_0 + f),$$

where A is the restriction of the operator D to the set of functions satisfying the homogeneous boundary condition $Bu(x) = 0$ on $\partial\Omega$, and $r(z) = \frac{1+\frac{z}{2}}{1-\frac{z}{2}}$ is the stability function of the CN scheme.

Remark. This result does not persist for $\phi^{D,CN}_{\frac{\tau}{2}} \circ \phi^f_\tau \circ \phi^{D,CN}_{\frac{\tau}{2}}$.

Homogeneous case: $A = D, f = 0, u_0 \in D(A)$, see A. Hansbo, 1999.

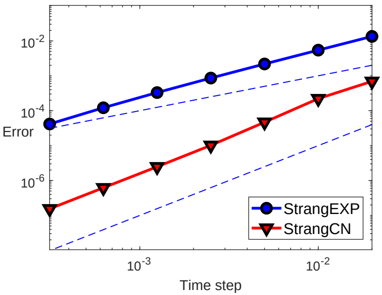
Numerical experiments on $\Omega = (0,1)^2$: nonlinear case



$$f(u) = u$$

Robin boundary conditions

$$u + \partial_n u = u_0 \text{ on } \partial\Omega$$



$$f(u) = u^2$$

Dirichlet + Neumann boundary conditions

$$\partial_t u = \Delta u + f(u) \text{ on } \Omega, \quad u(x,0) = u_0(x).$$

Part 2

1. In the context of splitting methods for parabolic PDEs

2. In the context of ergodic stochastic parabolic PDEs

- C.-E. Bréhier and V., High-order integrator for sampling the invariant distribution of a class of parabolic stochastic PDEs with additive space-time noise, SIAM J. Sci. Comput 38 (2016) A2283-A2306.
- A. Abdulle, I. Almuslimani, and V., Optimal explicit stabilized integrator of weak order one for stiff and ergodic stochastic differential equations, SIAM/ASA J. Uncertain. Quantif. 6 (2018), 937-964.
- A. Abdulle, C.-E. Bréhier, and V., Convergence analysis of explicit stabilized integrators for parabolic semilinear stochastic PDEs, arXiv:2102.03209, Submitted.

Parabolic stochastic PDE case

Consider e.g. the semilinear stochastic heat equation:

$$\begin{aligned} \partial_t u(t,x) &= \partial_{xx} u(t,x) + f\big(u(t,x)\big) + \dot{W}(t,x),\ t>0, x\in(0,1),\\ u(0,x) &= u_0(x),\ x\in(0,1),\\ u(t,x) &= 0,\ x\in\partial(0,1), \end{aligned}$$

or its abstract formulation on the Hilbert space H:

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

Ergodicity convergence properties,

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

The stochastic PDE case: the θ-method

$$du(t) = Au(t)dt + f\big(u(t)\big)dt + dW^Q(t), \quad u(0) = u_0 \in H.$$

- θ-method (linearized):

$$v_{n+1} = v_n + \theta\tau v_n + (1-\theta)\tau A v_{n+1} + \tau f(v_n) + \sqrt{\tau}\xi_n^Q$$

- $\theta = 1/2$ method ("Crank-Nicolson")
- $\theta = 1$ method ("Euler method"):

$$v_{n+1} = J_1 v_n + \tau J_1 f(v_n) + \sqrt{\tau} J_1 \xi_n^Q,$$

where $J_1 = \big(I - \tau A\big)^{-1}$ and $\sqrt{\tau}\xi_n^Q = W^Q\big((n+1)\tau\big) - W^Q\big(\tau h\big)$.
order of convergence is $\overline{s} - \varepsilon$ for all $\varepsilon > 0$ (see Bréhier 2014):

$$\overline{\mathrm{s}} = \sup\left\{\mathrm{s} \in (0,1)\ ;\ \mathrm{Trace}\Big((-\mathrm{A})^{-1+\mathrm{s}}\mathrm{Q}\Big) < +\infty\right\} > 0.$$

Example: for $A = \frac{\partial^2}{\partial x^2}$, $Q = I$ in dimension 1, we have $\overline{\mathrm{s}} = 1/2$.

Numerical experiments (stochastic heat equation)

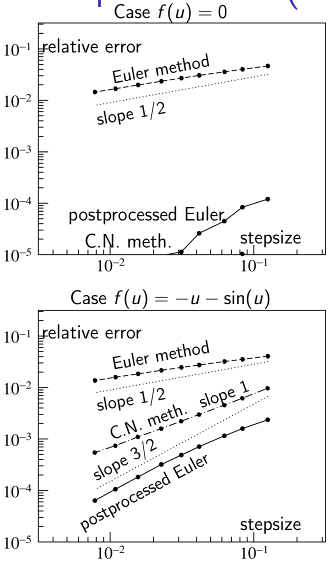


Figure: Orders of convergence, test function $\varphi(u) = \exp(-\|u\|^2)$.

Quadratic one-dimensional 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 $z = \lambda\tau$, $\xi_n \sim \mathcal{N}(0,1)$,

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

$\overline{X}_n$ 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 (Crank-Nicolson):
$A(z) = \frac{1+z/2}{1-z/2}$, $B(z) = \frac{1}{1-z/2}$ (see Chong, Walsh, 2012).
Remark: Impossible to be exact (without postprocessing) for an explicit Runge-Kutta method or an L-stable method ($A(\infty) = 0$).

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: $dX(t) = -\nabla V(X(t))dt + \sigma dW(t)$.

$$X_{n+1} = X_n - \tau \nabla V \left(X_n + \frac{1}{2}\sigma\sqrt{\tau}\xi_n \right) + \sigma\sqrt{\tau}\xi_n, \qquad \overline{X}_n = X_n + \frac{1}{2}\sigma\sqrt{\tau}\xi_n.$$

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,

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

Quadratic one-dimensional case (Ornstein-Uhlenbeck)

Proposition: invariant measure preservation

For a postprocessed integrator where $z = \lambda\tau$, $\xi_n \sim \mathcal{N}(0,1)$,

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

$\overline{X}_n$ 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 the order two method from Leimkhuler, 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).

Quadratic one-dimensional 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 by explicit stabilized methods (Abdulle, Almuslimani, V., 2018)

For all $s \geq 1$, the family of polynomials

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

satisfy the invariant mesure preservation condition

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

For $s = 1$, we recover the scheme of Leimkhuler, Matthews, 2013.
Related work for MCMC: Vargas, Pereyra, Zygalakis (2020).

Analysis of the postprocessed Euler method

Theorem (Bréhier, V., 2016)

- *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,*

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

Remark: No such estimate $\mathcal{O}(e^{-ct_n})$ *for Crank-Nicolson.*

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

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

Remark: error for the standard Euler: $\mathcal{O}\left(\tau^{\mathrm{s}}\right)$, $\mathrm{s} \in (0, \bar{\mathrm{s}})$.

Strong convergence of explicit stabilized methods

$$u_{n+1}^h = A_s(\tau\Lambda_h)u_n^h + B_s(\tau\Lambda_h)P_h(\tau F(u_n^h) + \Delta W_n^Q).$$

Remark: the stage s is chosen s.t. $\tau\lambda_{max,h} \leq L_s$, i.e. $\tau C h^{-2} \simeq s^2$.

Theorem (Abdulle, Bréhier, V., 2021)

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 $\alpha \in (0, \overline{\alpha})$,

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

where $C_{T,\alpha}$ is independent of h, τ, α.

Stability functions for the SK-ROCK method

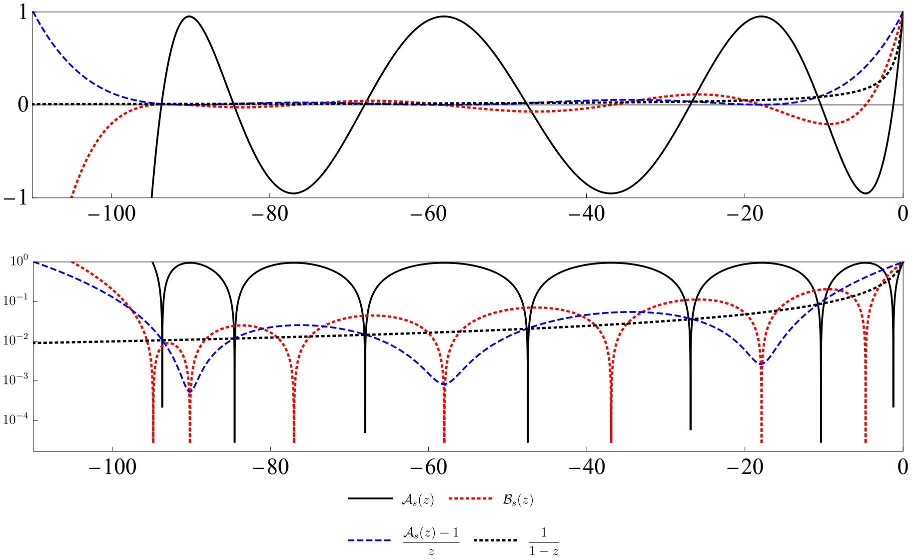


Figure: Stability functions,degree $s = 7$, damping parameter $\eta = 0.05$.

Concluding remarks

- Surprisingly, the Crank-Nicolson scheme (not L-stable) performs better that the exact solution in the Strang splitting method, avoiding order reduction phenomena.
- This seems specific to the Crank-Nicolson scheme, and it does not persist for dispersive problems, e.g.

$$i\partial_t u = \partial_{xx} u + 1 \text{ on } \Omega, \quad u = 1 \text{ on } \partial\Omega, \quad u(x,0) = 1.$$

- In the context of ergodic stochastic dynamics, L-stability is a desirable property and high order for the invariant measure can be achieved in spite of the low regularity of the solution.

Current related works:

- deterministic: Analysis for nonlinear $f(u)$? Case of absorbing boundary conditions?
- stochastic: study of algebraic structures with exotic aromatic Butcher trees, accelerating the convergence to equilibrium using reversible perturbations (Stratonovitch noise).