

# Magnus type integrators for nonlinear parabolic problems

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# Outline

## **Exponential methods for semilinear parabolic problems**

- Semilinear parabolic initial-boundary value problems
- Framework of sectorial operators and analytic semigroups
- Time-discretisation by exponential Runge-Kutta methods

## **Magnus integrators for non-autonomous semilinear problems**

- Interpolatory Magnus integrators for non-stiff problems
- Problem class and numerical discretisation
- Stability and convergence analysis
- Example and numerical experiment

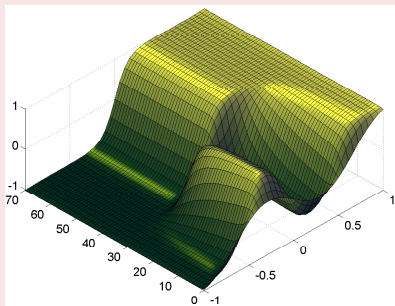
# Exponential methods for semilinear parabolic problems

# Allen-Cahn equation

Numerical solution of **Allen-Cahn equation**

$$\partial_t U(x, t) = c \cdot \partial_x^2 U(x, t) + U(x, t) \left(1 - U(x, t)^2\right), \quad c = 1/100,$$

by **exponential Runge-Kutta method**.

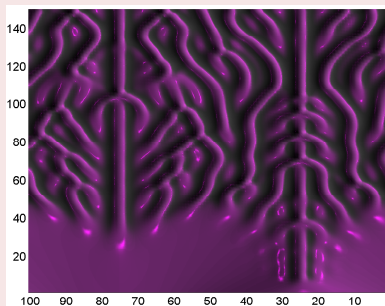


# Kuramoto-Sivashinsky equation

Numerical solution of Kuramoto-Sivashinsky equation

$$\partial_t U(x, t) = -\partial_x^4 U(x, t) - \partial_x^2 U(x, t) - U(x, t) \partial_x U(x, t)$$

by exponential Runge-Kutta method.



# Semilinear parabolic initial-boundary value problem

**General form.** Semilinear parabolic partial differential equation

$$\partial_t U(x, t) = \mathcal{A}(x) U(x, t) + B(x, t, U(x, t), \partial_x U(x, t))$$

involving strongly elliptic differential operator  $\mathcal{A}$  with smooth space-dependent coefficients and nonlinear part  $B$  of lower order. Additional boundary and initial condition.

**Abstract formulation.** Interpret partial differential equation as abstract differential equation for  $u(t) = U(\cdot, t)$

$$u'(t) = Au(t) + b(t, u(t)).$$

## Abstract framework of sectorial operators

Abstract initial value problem on Banach space  $(X, \|\cdot\|_X)$

$$u'(t) = Au(t) + b(t, u(t)), \quad 0 < t \leq T, \quad u(0) \text{ given.}$$

### Hypothesis

- Linear operator  $A: D \rightarrow X$  is *sectorial*. It holds

$$\|(\lambda I - A)^{-1}\|_{X \leftarrow X} \leq \frac{M}{|\lambda - a|}, \quad \lambda \in \mathbb{C} \setminus S_\phi(a),$$

where  $S_\phi(a) = \{\lambda \in \mathbb{C} : |\arg(a - \lambda)| \leq \phi\} \cup \{a\}$  with  $\phi \in (0, \pi/2)$ .

- Graph norm of  $A$  and norm in  $D$  are equivalent.

Define linear operator  $e^{tA}: X \rightarrow X$  by integral formula of Cauchy

$$e^{tA} = \frac{1}{2\pi i} \int_\Gamma e^\lambda (\lambda I - tA)^{-1} d\lambda, \quad t > 0, \quad e^{tA} = I, \quad t = 0.$$

# Analytic semigroup & Variation-of-constants formula

Fundamental relations for **analytic semigroup**  $(e^{tA})_{t \geq 0}$  generated by **sectorial operator**  $A: D \rightarrow X$

$$e^{(s+t)A} = e^{sA} e^{tA}, \quad s, t \geq 0, \quad \frac{d}{dt} e^{tA} = A e^{tA}, \quad t > 0,$$
$$\|e^{tA}\|_{X \leftarrow X} + \|e^{tA}\|_{D \leftarrow D} + \|t e^{tA}\|_{D \leftarrow X} \leq M, \quad 0 \leq t \leq T.$$

**Homogeneous equation.**

$$x'(t) = Ax(t),$$
$$x(t) = e^{tA} x(0).$$

**Inhomogeneous equation.**

$$y'(t) = Ay(t) + b(t),$$
$$y(t) = e^{tA} y(0) + \int_0^t e^{(t-\tau)A} b(\tau) d\tau.$$

## Intermediate spaces & Semilinear parabolic problem

**Intermediate spaces.** Norm in  $D = X_1 \subset X_\vartheta \subset X = X_0$  fulfills

$$\|x\|_{X_\vartheta} \leq K \|x\|_D^\vartheta \|x\|_X^{1-\vartheta}, \quad x \in D, \quad 0 \leq \vartheta \leq 1.$$

Bounds for analytic semigroup follow

$$\left\| e^{tA} \right\|_{X_\vartheta \leftarrow X_\vartheta} + \left\| t^\vartheta e^{tA} \right\|_{X_\vartheta \leftarrow X} + \left\| t^{1-\vartheta} e^{tA} \right\|_{D \leftarrow X_\vartheta} \leq M, \quad 0 \leq t \leq T.$$

**Semilinear problem.** Abstract differential equation

$$u'(t) = Au(t) + b(t, u(t)), \quad 0 < t \leq T, \quad u(0) \text{ given.}$$

### Hypothesis

For some  $0 \leq \beta < 1$  it holds  $b: [0, T] \times X_\beta \rightarrow X: (t, v) \mapsto b(t, v)$ .

Variation-of-constants formula **well-defined** in  $X_\beta$

$$u(t) = \underbrace{e^{tA} u(0)}_{\in X_\beta} + \int_0^t \underbrace{e^{(t-\tau)A}}_{X_\beta \leftarrow X} \underbrace{b(\tau, u(\tau))}_{\in X} d\tau.$$

## Example (Semilinear parabolic problem)

Parabolic initial-boundary value problem for  $U : [0, L] \times [0, T] \rightarrow \mathbb{R}$

$$\partial_t U(x, t) = \mathcal{A}(x) U(x, t) + B(x, t, U(x, t), \partial_x U(x, t)),$$

$$U(0, t) = 0 = U(L, t), \quad U(x, 0) = U_0(x), \quad 0 \leq x \leq L, \quad 0 \leq t \leq T,$$

$$\mathcal{A}(x) = \alpha(x) \partial_x^2 + \beta(x) \partial_x + \gamma(x) I,$$

as abstract initial value problem for  $u : [0, T] \rightarrow X : t \mapsto u(t) = U(\cdot, t)$

$$u'(t) = Au(t) + b(t, u(t)), \quad u(0) \text{ given.}$$

Here, let  $(Av)(x) = \mathcal{A}(x)v(x)$  and  $(b(t, v))(x) = B(x, t, v(x), \partial_x v(x))$ .

Problem fits into analytical framework for

$$X = L^2(0, L), \quad D = H^2(0, L) \cap H_0^1(0, L), \quad X_\beta = X_{1/2} = H_0^1(0, L).$$

# Exponential Runge-Kutta methods

**Problem.** Numerical discretisation of semilinear equation

$$u'(t) = Au(t) + b(t, u(t)), \quad 0 < t \leq T, \quad u(0) \text{ given.}$$

**Presumption.** Efficient calculation of  $e^{tA}$  and related functions

$$\varphi_j(tA) = \frac{1}{t^j} \int_0^t \tau^{j-1} e^{(t-\tau)A} d\tau, \quad t > 0, \quad \varphi_j(tA) = \frac{1}{j} I, \quad t = 0,$$

feasible, see HOCHBRUCK & LUBICH, 1997.

**Exponential Runge-Kutta methods.** Explicit one-step methods of high order constructed in HOCHBRUCK & OSTERMANN, 2004.

## Examples (Exponential Runge-Kutta methods)

**Exact solution.** Representation by variation-of-constants formula

$$u(t_{n+1}) = e^{hA} u(t_n) + \int_0^h e^{(h-\tau)A} b(t_n + \tau, u(t_n + \tau)) d\tau, \quad h > 0.$$

**Idea.** Replace  $b$  by **interpolation polynomial** and integrate.

**Exponential forward Euler method.** Approximation  $u_n \approx u(nh)$  by

$$u_{n+1} = e^{hA} u_n + h \varphi_1(hA) b(t_n, u_n), \quad \varphi_1(hA) = \frac{1}{h} \int_0^h e^{(h-\tau)A} d\tau.$$

**Explicit 2nd-order method.** Based on **exponential midpoint rule**

$$\begin{aligned} u_{n+1/2} &= e^{h/2A} u_n + h/2 \varphi_1(h/2A) b(t_n, u_n), \\ u_{n+1} &= e^{hA} u_n + h \varphi_1(hA) b(t_n + h/2, u_{n+1/2}). \end{aligned}$$

# Magnus integrators for non-autonomous semilinear problems

# Non-autonomous semilinear parabolic problem

Semilinear equation involving **time-dependent** sectorial operator

$$u'(t) = A(t)u(t) + b(t, u(t)), \quad 0 < t \leq T, \quad u(0) \text{ given.}$$

## Hypothesis

- *Linear operator  $A(t)$  is uniformly sectorial for  $t \in [0, T]$ .*
- *Intermediate space  $D \subset X_{1+\vartheta} \subset D(A(t)^2)$  is independent of  $t \in [0, T]$  for some  $0 \leq \vartheta < 1$ .*
- *Operator family  $A: [0, T] \rightarrow L(D, X)$  is Hölder-continuous with respect to  $t$  for some  $0 < \alpha \leq 1$*

$$\|A(t) - A(s)\|_{X_\vartheta \leftarrow X_{1+\vartheta}} \leq M(t-s)^\alpha, \quad 0 \leq s \leq t \leq T.$$

# Objectives

**Problem.** Non-autonomous semilinear evolution equation

$$u'(t) = A(t)u(t) + b(t, u(t)), \quad 0 < t \leq T, \quad u(0) \text{ given.}$$

**Question.** How to construct numerical scheme?

**Idea.** Combine

- Magnus integrator for linear part
- Exponential Runge-Kutta method for nonlinear part

# Interpolatory Magnus integrators

**Problem.** Linear non-autonomous equation with  $A: [0, T] \rightarrow \mathbb{R}^{n \times n}$

$$y'(t) = A(t)y(t), \quad t_n \leq t \leq t_n + h, \quad y(t_n) \text{ given.}$$

**Aim.** Approximation  $y_{n+1} \approx y(t_{n+1})$  at time  $t_{n+1} = t_n + h$ .

**Approach** (MAGNUS, 1954). Write solution in form

$$y(t_n + s) = e^{\Omega(s)} y(t_n), \quad 0 \leq s \leq h,$$

with  $\Omega(s) \in \mathbb{R}^{n \times n}$  given by **Magnus expansion**

$$\Omega(s) = \int_0^s A(t_n + \tau) d\tau - \frac{1}{2} \int_0^s \left[ \int_0^\tau A(t_n + \sigma) d\sigma, A(t_n + \tau) \right] d\tau + \dots$$

**Interpolatory Magnus integrators.** Truncate expansion and approximate integrals by quadrature rule.

## Second-order Magnus integrator

**Magnus expansion.** Representation of **exact solution**

$$y(t_n + s) = e^{\Omega(s)} y(t_n), \quad 0 \leq s \leq h,$$
$$\Omega(s) = \int_0^s A(t_n + \tau) d\tau - \frac{1}{2} \int_0^s \left[ \int_0^\tau A(t_n + \sigma) d\sigma, A(t_n + \tau) \right] d\tau + \dots$$

**Second-order Magnus integrator.** Truncate Magnus expansion after **first term** and approximate integral by **midpoint rule**

$$\Omega(h) \approx \int_0^h A(t_n + \tau) d\tau \approx hA(t_n + h/2).$$

Obtain **numerical approximation**  $y_{n+1} = e^{hA(t_n + h/2)} y_n.$

# Second-order Magnus integrator

**Second-order Magnus integrator.** Numerical approximation

$$y_{n+1} = e^{hA(t_n+h/2)} y_n.$$

**Error behaviour?** Scheme of **order 2**.

- **Non-stiff case** studied in ISERLES & NØRSETT, 1999.
- Time-dependent **Schrödinger type equations** analysed in HOCHBRUCK & LUBICH, 2003.
- Linear non-autonomous **parabolic problems** considered in GONZÁLEZ, OSTERMANN & TH., 2004.

# Magnus type integrator for semilinear equation

**Motivation.** Set  $A_{n+1/2} = A(t_n + h/2)$  and rewrite right-hand side of **non-autonomous semilinear equation**

$$\begin{aligned}u'(t) &= A(t)u(t) + b(t, u(t)) \\ &= A_{n+1/2} u(t) + b(t, u(t)) + (A(t) - A_{n+1/2})u(t),\end{aligned}$$

Apply **variation-of-constants formula**

$$\begin{aligned}u(t_{n+1}) &= e^{hA_{n+1/2}} u(t_n) + \int_0^h e^{(h-\tau)A_{n+1/2}} b(t_n + \tau, u(t_n + \tau)) d\tau \\ &\quad + \int_0^h e^{(h-\tau)A_{n+1/2}} (A(t_n + \tau) - A_{n+1/2})u(t_n + \tau) d\tau.\end{aligned}$$

# Magnus type integrator for semilinear equation

Representation by **variation-of-constants formula**

$$u(t_{n+1}) = e^{hA_{n+1/2}} u(t_n) + \int_0^h e^{(h-\tau)A_{n+1/2}} b(t_n + \tau, u(t_n + \tau)) d\tau \\ + \int_0^h e^{(h-\tau)A_{n+1/2}} (A(t_n + \tau) - A_{n+1/2}) u(t_n + \tau) d\tau.$$

## Basic idea.

- Omit (small) term  $(A(t_n + \tau) - A_{n+1/2}) u(t_n + \tau)$ .
- Replace  $b(t_n + \tau, u(t_n + \tau))$  with  $b(t_n + h/2, u_{n+1/2})$ .
- First-order approximation  $u_{n+1/2} \approx u(t_n + h/2)$ .

## Numerical scheme for semilinear equation

**Problem.** Non-autonomous semilinear evolution equation

$$u'(t) = Au(t) + b(t, u(t)), \quad 0 < t \leq T, \quad u(0) \text{ given.}$$

**Numerical method.** Combine second-order Magnus integrator and exponential midpoint rule. Auxiliary first-order approximation.

$$u_{n+1/2} = e^{h/2 A_{n+1/2}} u_n + h/2 \varphi_1(h/2 A_{n+1/2}) b(t_n, u_n),$$

$$u_{n+1} = e^{h A_{n+1/2}} u_n + h \varphi_1(h A_{n+1/2}) b(t_n + h/2, u_{n+1/2}), \quad n \geq 0.$$

**Special features.**

- Nonlinear part is integrated **explicitly**.
- Good **stability properties** due to exponential.
- Employ **relations**  $e^{h A_{n+1/2}} = e^{h/2 A_{n+1/2}} e^{h/2 A_{n+1/2}}$  and

$$\varphi_1(h A_{n+1/2}) = 1/2 (I + e^{h/2 A_{n+1/2}}) \varphi_1(h/2 A_{n+1/2}).$$

# Stability and convergence analysis

## Theorem (Stability)

*Under the above hypotheses with  $\vartheta = \mu$  the estimate*

$$\left\| \prod_{j=m}^n e^{hA_{j+1/2}} \right\|_{X_\nu \leftarrow X_\mu} \leq M (t_{n+1} - t_m)^{-\nu+\mu}, \quad 0 \leq t_m < t_n \leq T,$$

*is valid for  $0 \leq \mu \leq \nu < 1$  with constant  $M > 0$  independent of  $n$  and  $h$ .*

Main techniques of proof.

- Telescopic identity.
- Auxiliary estimates for  $(e^{hA_{j+1/2}} - e^{hA_{m+1/2}})e^{(t_j-t_m)A_{m+1/2}}$ .
- Gronwall inequality (weakly singular kernel).

## Convergence result

**Notation.** Define  $r_n, s_n : [t_n, t_{n+1}] \rightarrow X$  for  $n \geq 0$  by

$$r_n = (A - A(t_n))u + b(\cdot, u) - b(t_n, u(t_n)),$$

$$s_n = (A - A(t_n + h/2))u + b(\cdot, u) - b(t_n + h/2, u(t_n + h/2)).$$

Further set  $\|r\|_{X,\infty} = \max\{\|r_j(t)\|_X, t_j \leq t \leq t_{j+1}, 0 \leq j \leq n-1\}$ .

### Theorem (Convergence)

*Under the above hypotheses with  $\alpha = 1$  and  $\vartheta = \gamma$  for  $0 \leq \gamma \leq \beta < 1$  the following error estimate*

$$\|u_n - u(t_n)\|_{X_\beta} \leq C h^{2-\beta+\gamma} \left( \|r'\|_{X_\gamma,\infty} + (1 + |\log h|) \|s'\|_{X_\gamma,\infty} \right)$$

$$+ C h^2 \left( \|r''\|_{X,\infty} + \|s''\|_{X,\infty} \right), \quad 0 \leq t_n \leq T,$$

*is valid with constant  $C > 0$  independent of  $n$  and  $h$ .*

## Strategy

- Suitable **representation for global error**  $e_n = u_n - u(t_n)$ .
  - Defects of numerical solution  $u_n$  and internal stage  $u_{n+1/2}$ .
  - Smoothness of data  $A, b$  and exact solution  $u$ .
  - Taylor series expansions and integration.
- Extended **stability estimates**.
- Gronwall type inequality.

## Example (Parabolic initial-boundary value problem)

Parabolic initial boundary value problem for  $U: [0, 1] \times [0, 1] \rightarrow \mathbb{R}$

$$\partial_t U(x, t) = \alpha(x, t) \partial_x^2 U(x, t) + \beta(x, t) U(x, t) \partial_x U(x, t) + g(x, t, U(x, t)),$$

$$U(0, t) = 0 = U(1, t), \quad U(x, 0) = U_0(x), \quad 0 \leq x \leq 1, \quad 0 \leq t \leq 1,$$

as abstract initial value problem for  $u: [0, 1] \rightarrow X: t \mapsto u(t) = U(\cdot, t)$

$$u'(t) = A(t)u(t) + b(t, u(t)), \quad 0 < t \leq 1, \quad u(0) \text{ given.}$$

Here, let  $(A(t)v)(x) = \alpha(x, t) \partial_x^2 v(x)$  and further set

$$b(t, v)(x) = \beta(x, t) v(x) \partial_x v(x) + g(x, t, v(x)).$$

Problem fits into abstract framework for

$$X = L^2(0, 1), \quad D = H^2(0, 1) \cap H_0^1(0, 1), \quad X_\beta = X_{1/2} = H_0^1(0, 1).$$

Expected fractional **convergence order** in  $X_\beta$

$$\kappa = 2 - \beta + \gamma, \quad \beta = 1/2, \quad 0 \leq \gamma < 1/4.$$

# Numerical experiment

Initial-boundary value problem with **solution**  $U(x, t) = x(1-x)e^{-t}$

$$\partial_t U(x, t) = (1 + e^{-t}) \partial_x^2 U(x, t) - U(x, t) \partial_x U(x, t) + g(x, t, U(x, t)),$$
$$U(0, t) = 0 = U(1, t), \quad U(x, 0) = x(1-x), \quad 0 \leq x \leq 1, \quad 0 \leq t \leq 1.$$

Symmetric **finite differences** of spatial grid length  $\Delta x = (M+1)^{-1}$ .  
**Magnus type integrator** with time-step  $h$  (**Fourier techniques**).

$h \setminus M$	200	400	600	800
$2^{-3}$	1.7988	1.7987	1.7987	1.7987
$2^{-4}$	1.7504	1.7503	1.7502	1.7502
$2^{-5}$	1.7499	1.7496	1.7496	1.7496
$2^{-6}$	1.7498	1.7493	1.7493	1.7492

Table: Numerically observed temporal **convergence order** in discrete  $H_0^1$ -norm. Expected value  $\kappa = 2 - \beta + \gamma \approx 1.75$ .

## Related and future projects

- Numerical scheme based on Magnus integrators for **quasilinear parabolic equations**

$$u'(t) = A(u(t))u(t) + b(t, u(t)).$$

- **Commutator free methods** of higher order for linear problems

$$u'(t) = A(t)u(t) + b(t).$$

Approximation of homogeneous part  $u_{n+1} = e^{\frac{h}{2}\mathcal{A}_{n2}} e^{\frac{h}{2}\mathcal{A}_{n1}} u_n.$

- **Exponential linear multistep methods** for autonomous and non-autonomous problems.