Lie group and exponential integrators: Theory, implementation, and applications

PhD-thesis

Håvard Berland

Department of Mathematical Sciences, NTNU

September 14, 2006

Thesis overview

This thesis concerns the numerical solution of differential equations.

- Focus on time-integration

Aims:

- Construct and analyze schemes for numerical integration
- Measure in terms of computational speed and numerical quality

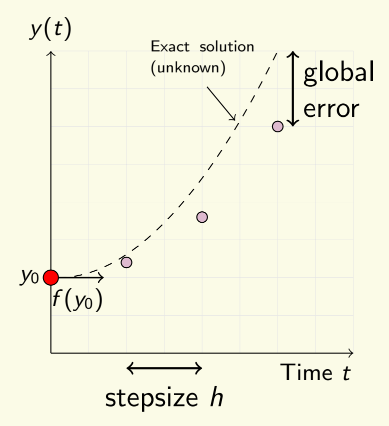
Numerical analysis for ordinary differential equations

A differential equation

$$y'(t) = f(y(t)), \qquad y_0 = y(0)$$

describes the time evolution of a quantity y, given

- its initial state y_0
- a function f describing how the solution y changes



One aim of numerical analysis

Design methods to minimize error while maximizing stepsize h

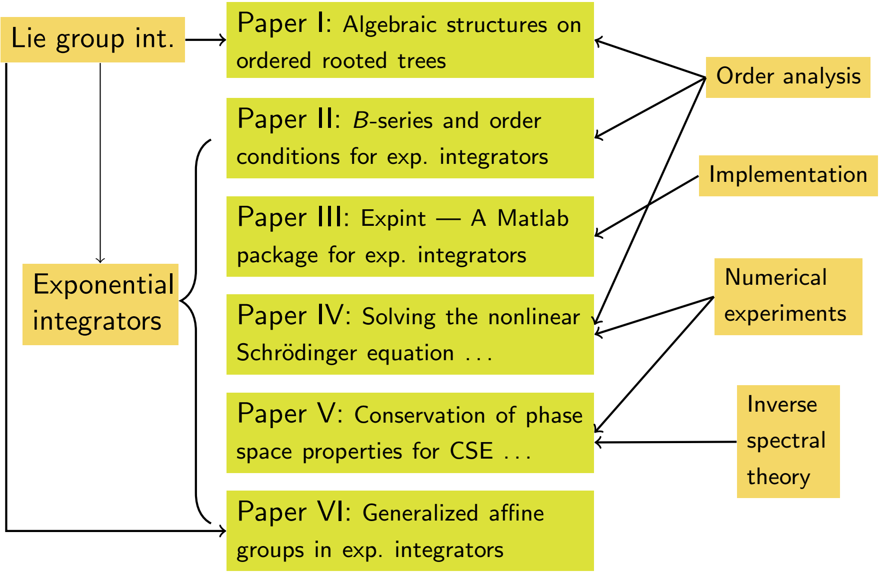
Applications

The solution we search for may be any quantity.

Some important examples are

- Weather forecasting
- Modeling of oil flow in reservoirs
- Modeling of ocean currents
- Evolution of water waves
- Planet positions in solar system

Overview of papers

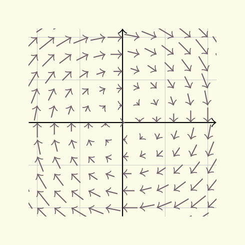


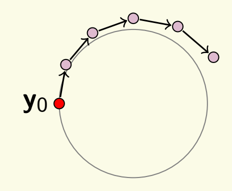
Lie group integrator, example

An equation in $\mathbf{R}^2$, (rotational vector field):

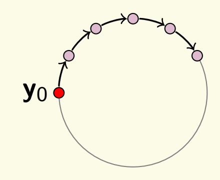
$$\dot{y}_1 = y_2$$
$$\dot{y}_2 = -y_1$$

$\frac{d}{dt}\|\mathbf{y}(t)\| = 0$, so $\|\mathbf{y}(t)\|$ is constant.





- Classical numerical integrators move in straight lines.



- Lie group integrators tailored for S^1-problems move along the solution manifold.

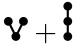
Order analysis using trees

Order analysis

Expand the exact and numerical solution in Taylor series in h, and compare term by term

$$\dot{y} = f(y) \sim$$ 

$$\ddot{y} = f'(y)\dot{y} = f'(y)f(y) \sim$$ 

$$y^{(3)} = f''(y)\dot{y}^2 + f'(y)\ddot{y} = f''(y)f(y)^2 + (f'(y))^2 f(y) \sim$$ 

Revolutionary trick by Butcher (1972):

- Work with trees instead of tedious expressions (number of terms in $y^{(i)}$ increase exponentially)

Hopf algebras and applications

Hopf algebras → Runge–Kutta analysis (Butcher 1972/Dür 1986)

Hopf algebras → Noncommutative geometry (Connes 1998)

Hopf algebras → Renormalization, quantum physics (Kreimer 1998)

- Brouder (2000) showed that these three Hopf algebras were equivalent.

The Leibniz rule

$$(fg)' = f'g + fg'$$

is the essential part of the entire structure!

Paper I

- We describe how Hopf algebra structures can be applied to a general class of Lie group integrators, extending the work of Butcher on classical Runge–Kutta integrators.
- Two relevant and connected Hopf algebra structures are presented.
- Backward error analysis explicitly computed using a logarithm map. Important for further analysis and construction of new schemes, where symplecticity and/or volume preservation is essential, as found in Chartier, Murua and Faou 2006.

Exponential integrators, format

A differential equation

$$y'(t) = f(y(t))$$

can be solved using a Runge–Kutta scheme given a previously computed value y_n,

$$\begin{aligned} Y_i &= y_n + h\sum_{j=1}^{s} a_{ij} f(Y_j), \quad i = 1, \ldots, s \\ y_{n+1} &= y_n + h\sum_{i=1}^{s} b_i f(Y_j). \end{aligned}$$

Order analysis specifies what values can be used for the coefficients a_{ij} and b_i.

Exponential integrators, format

The differential equation can be split into two parts

$$y'(t) = f(y(t)) = Ly(t) + N(y)$$

and can be solved by an exponential integrator given a previously computed value y_n,

$$\begin{aligned} Y_i &= \mathrm{e}^{c_i hL} y_n + h \sum_{j=1}^{s} a_{ij}(hL) N(Y_j), \quad i = 1, \dots, s \\ y_{n+1} &= \mathrm{e}^{hL} y_n + h \sum_{i=1}^{s} b_i(hL) N(Y_j). \end{aligned}$$

The coefficient functions $a_{ij}(hL)$ and $b_i(hL)$ must at least satisfy classical Runge–Kutta conditions for $L \to 0$.

Why exponential integrators

For systems of differential equations ($y(t)$ is vector-valued), *explicit* Runge–Kutta schemes may experience an upper limit on the timestep h, depending on the eigenvalues of the system.

Increasing spatial resolution in a PDE problem typically reduces the limit on h, sometimes unacceptable.

Two possible solutions to remedy stepsize restrictions:

- Use implicit Runge–Kutta schemes. Expensive evaluation of Y_i at each stage (nonlinear systems of equations).
- Use exponential explicit Runge–Kutta schemes. One needs to compute exponentials of L, but it is hopefully less expensive than implicit Runge–Kutta.

Exponential integrators

From the scheme format, there will be two immediate analytical features of exponential integrators of Runge–Kutta-format:

- If $N(y) = 0$ the scheme will yield the exact solution
- If $L = 0$ the scheme will reduce to the *underlying RK-scheme*

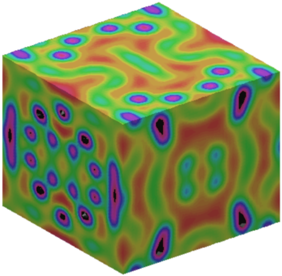
Paper II:

- Classical order analysis using bicolored trees
- Provides a procedure for constructing exponential integrators
- Convergence is more subtle for stiff problems, as discussed in Hochbruck and Ostermann 2005

Paper III, MATLAB package for exponential integrators

A MATLAB package for modular implementation of exponential integrators

- Easy implementation and comparison of more than 30 exponential integrators
- Numerous examples of discretizations of common PDEs
- Written for *exponential general linear methods*, of which exponential Runge–Kutta-integrators are a subset



Exponential integrators, φ functions

A frequently used class of exponential-like functions used in exponential integrators are the

φ functions

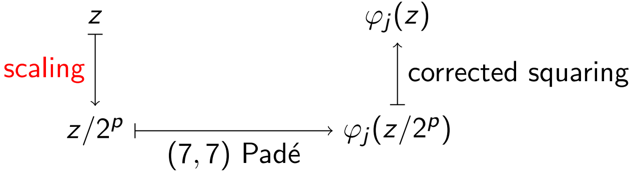
$$\varphi_j(z) = \frac{1}{(j-1)!}\int_0^1 \mathrm{e}^{(\theta-1)z}\theta^{j-1}\,\mathrm{d}\theta, \qquad j = 1, 2, \ldots,$$

for $j = 1, 2, 3$ (and for $z \neq 0$),

$$\varphi_1(z) = \frac{\mathrm{e}^z - 1}{z}, \quad \varphi_2(z) = \frac{\mathrm{e}^z - z - 1}{z^2},$$
$$\text{and} \quad \varphi_3(z) = \frac{\mathrm{e}^z - z^2/2 - z - 1}{z^3}.$$

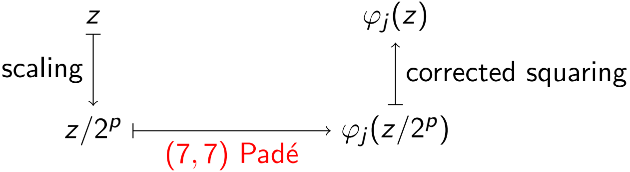
- *Numerical issues when z near* 0.

Scaling and squaring of φ functions (Paper III)



- p is chosen such that $\|z/2^p\|_\infty \leq 1$.

Scaling and squaring of φ functions (Paper III)



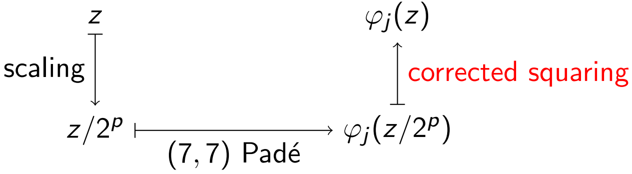
(d, d)-Padé approximation of φ_j:

$\varphi_j(z) = N_d^j(z)/D_d^j(z) + \mathcal{O}(z^{2d+1})$ where

$$N_d^j(z) = \frac{d!}{(2d+j)!} \sum_{i=0}^{d} \left[\sum_{k=0}^{i} \frac{(2d+j-k)!(-1)^k}{k!(d-k)!(j+i-k)!} \right] z^i$$

$$D_d^j(z) = \frac{d!}{(2d+j)!} \sum_{i=0}^{d} \frac{(2d+j-i)!}{i!(d-i)!} (-z)^i$$

Scaling and squaring of φ functions (Paper III)



Theorem (Paper VI)

$$\varphi_j(2\alpha) = \frac{1}{2^j}\left(e^{\alpha}\varphi_j(\alpha) + \sum_{k=1}^{j}\frac{1}{(j-k)!}\varphi_k(\alpha)\right)$$

(compare to $e^{2z} = e^z e^z$)

Exponential integrators for nonlinear Schrödinger

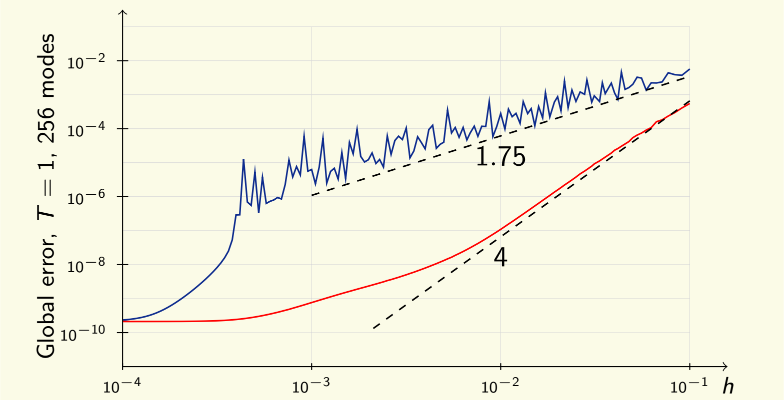
What are the important criteria for a "good integrator"?

- Local error, predicted by order analysis (Paper II)
- Global error, sometimes known analytically from local error, sometimes only observed numerically (Paper IV)
- Preservation of conservation quantities (Paper V)
- Processor/memory demands

Exp. integrators for nonlinear Schrödinger (Paper IV)

Analytical and observed global error. Periodic BC.
$iu_t = -u_{xx} + (V(x) + |u|^2)u$
Regularity is decay of Fourier coeff.

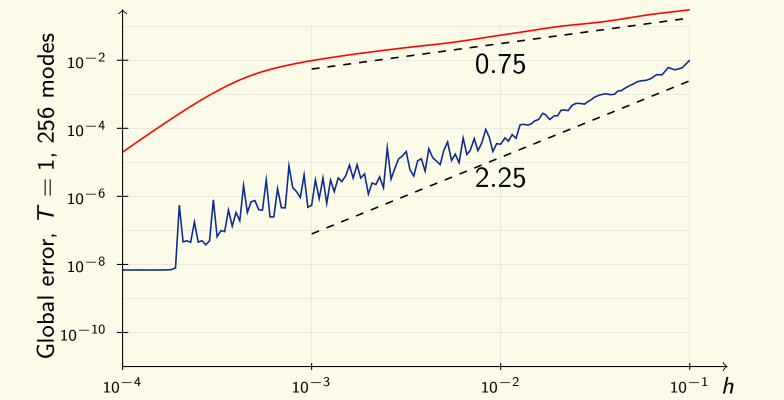
IC	Pot	LAWSON4	ETD4RK
∞	2	1.75	4
2	∞	2.25	0.75
2	2	1.75	0.75
∞	∞	4	4



Exp. integrators for nonlinear Schrödinger (Paper IV)

Analytical and observed global error. Periodic BC.
$\mathrm{i}u_t = -u_{xx} + (V(x) + |u|^2)u$
Regularity is decay of Fourier coeff.

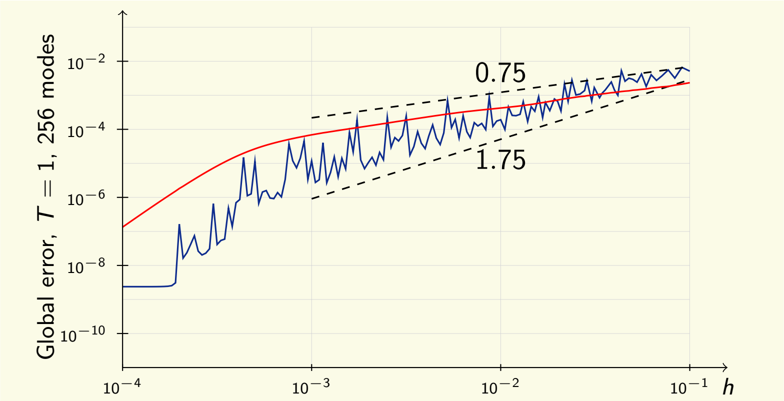
IC	Pot	LAWSON4	ETD4RK
∞	2	1.75	4
2	∞	2.25	0.75
2	2	1.75	0.75
∞	∞	4	4



Exp. integrators for nonlinear Schrödinger (Paper IV)

Analytical and observed global error. Periodic BC.
$iu_t = -u_{xx} + (V(x) + |u|^2)u$
Regularity is decay of Fourier coeff.

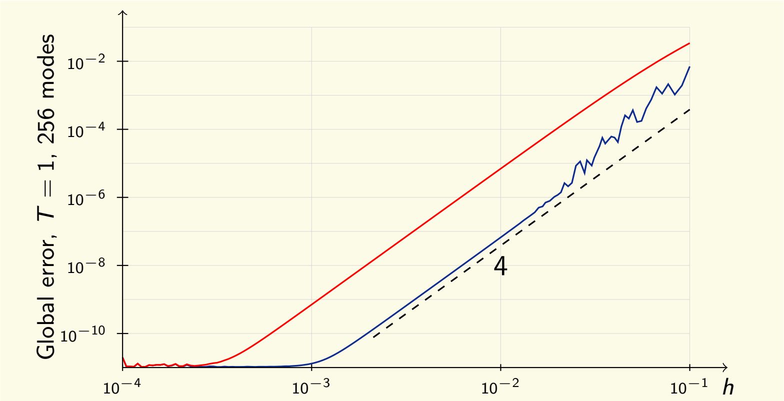
IC	Pot	LAWSON4	ETD4RK
∞	2	1.75	4
2	∞	2.25	0.75
2	2	1.75	0.75
∞	∞	4	4



Exp. integrators for nonlinear Schrödinger (Paper IV)

Analytical and observed global error. Periodic BC.
$iu_t = -u_{xx} + (V(x) + |u|^2)u$
Regularity is decay of Fourier coeff.

IC	Pot	LAWSON4	ETD4RK
∞	2	1.75	4
2	∞	2.25	0.75
2	2	1.75	0.75
∞	∞	4	4



Exp. integrators for nonlinear Schrödinger (Paper V)

$$u_t = \mathrm{i} u_{xx} + 2\mathrm{i}|u|^2 u \qquad (\star)$$

- Aim: Assess "goodness" of numerical integrator by monitoring preservation of conserved quantities over long time-scales.

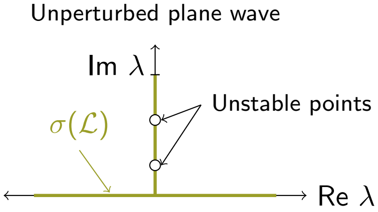
Lax pair for $(\star)$

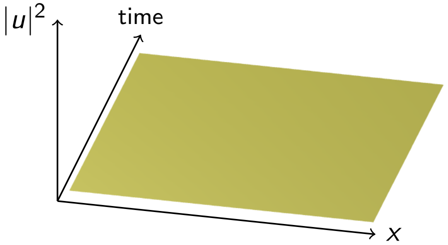
$$\mathcal{L} = \begin{pmatrix} \mathrm{i}\frac{\partial}{\partial x} & u^* \\ u & \mathrm{i}\frac{\partial}{\partial x} \end{pmatrix} \qquad \mathcal{A} = \begin{pmatrix} -\mathrm{i}|u|^2 & u_x^* \\ -u_x & \mathrm{i}|u|^2 \end{pmatrix}$$

The spectrum $\sigma(\mathcal{L})$ is *invariant* in time if *u is a solution of* $(\star)$.

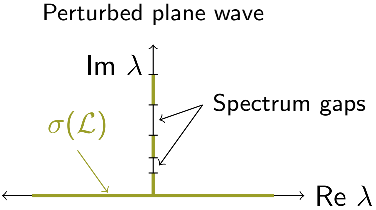
- Initial condition is a perturbation of an unstable plane wave solution (periodic boundary conditions).

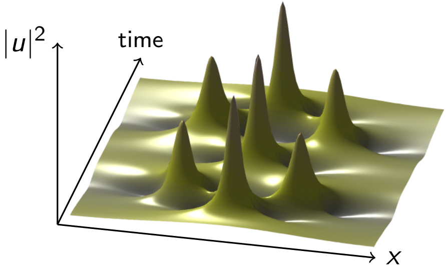
Spectrum preservation (Paper V)

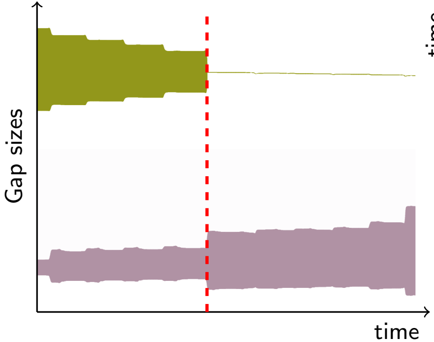


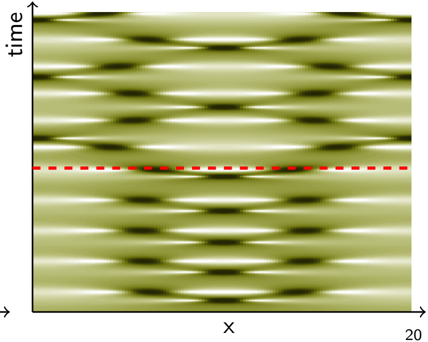


Spectrum preservation (Paper V)









Paper V conclusions

- Exponential integrators preserve the spectrum better and are faster than the split-step schemes which are most prominent in the literature for this problem.
- CFREE4 preserves the spectrum for the longest time, slightly better than LAWSON4 (possibly related to stiff order)
- A multisymplectic scheme (order 2 and implicit) was slower and less able to preserve the spectrum compared to the other schemes.

Thanks

Thanks to co-authors:

- Brynjulf Owren (Paper I, II, IV)
- Bård Skaflestad (Paper II, III, IV)
- Will Wright (Paper III)
- Constance Schober and Alvaro Islas (Paper V)

Thanks for your attention!