Exponential integrators – construction, analysis, implementation and applications

Marlis Hochbruck

Heinrich-Heine Universität Düsseldorf

October 2009

Outline

Motivation

Exponential integrators

Highly oscillatory problems

Applications in laser plasma dynamics

Chemical reaction

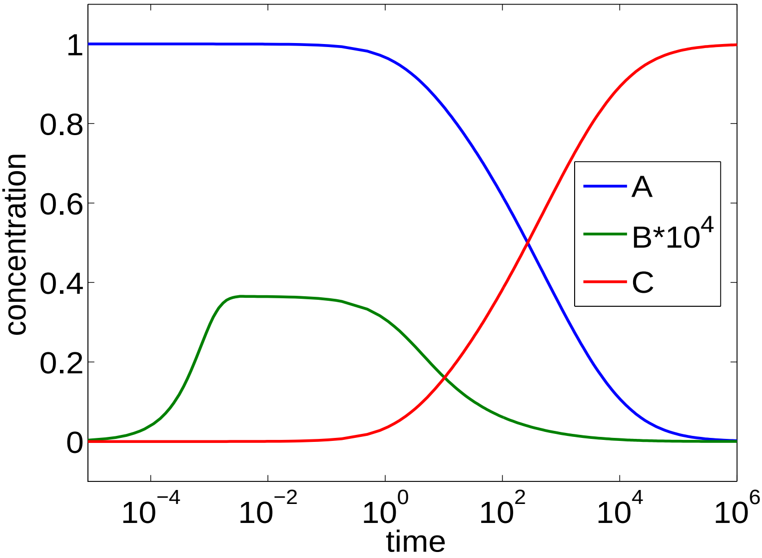
$$\begin{array}{cccc} A & \xrightarrow{0.04} & B & \text{(slow)} \\ B+B & \xrightarrow{3\cdot 10^7} & C+B & \text{(very fast)} \\ B+C & \xrightarrow{10^4} & A+C & \text{(fast)} \end{array}$$

system of odes

$$\begin{array}{lllllll} A: & y_1' & = & -0.04y_1 & + & 10^4 y_2 y_3 & & \\ B: & y_2' & = & 0.04y_1 & - & 10^4 y_2 y_3 & - & 3\cdot 10^7 y_2^2 \\ C: & y_3' & = & & & & & 3\cdot 10^7 y_2^2 \end{array}$$

initial condition $y_1(0) = 1, \quad y_2(0) = 0, \quad y_3(0) = 0$

Concentrations



Statistics

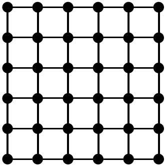
standard scheme including step size control (until $T = 100$ sec)

	explicit	implicit
number of steps	106 173	57
rejected steps	18 121	7
$f(y)$	745 765	114
$f'(y)$	–	4
LU decompositions	–	21
CPU time (in sec)	58.9	0.05

Reaction-diffusion equation

so far reaction equation $y = y(t)$
diffusion added: $y = y(t, x)$

$$\begin{array}{llcll} A: & y_1' & = & -0.04y_1 + 10^4 y_2 y_3 & +\mu\Delta y_1 \\ B: & y_2' & = & \dots & +\mu\Delta y_2 \\ C: & y_3' & = & \dots & +\mu\Delta y_3 \end{array}$$



3 odes per grid point
$\longrightarrow$ very large problems
$\longrightarrow$ implicit methods inefficient

Dreams and reality

dream of ...

- few steps which are cheap

sadly have ...

	problem	stable for	implementation requires
explicit	non stiff	$h \sim L^{-1}$	f
implicit	stiff	–	f, f' solution of $F(y) = 0$ LU decomposition

Dreams and reality

dream of ...

- few steps which are cheap

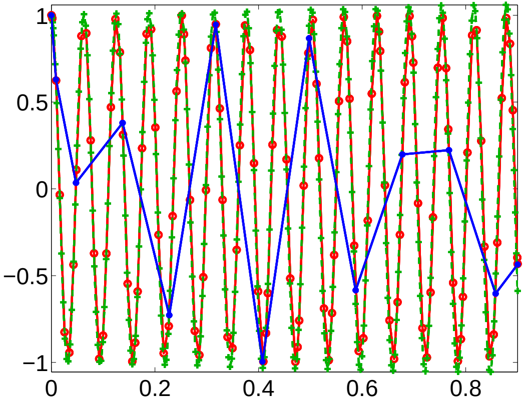
sadly have ...

	problem	stable for	implementation requires
explicit	non stiff	$h \sim L^{-1}$	f
implicit	stiff	–	f, f' solution of $F(y) = 0$ LU decomposition

if could be even worse ...

Highly oscillatory toy problem

$$y'' = -\omega^2 y + \sin(y), \qquad \omega = 100, \qquad y(0) = y'(0) = 1$$



	steps	$f(y)$
expl.	72	433
impl.	144	641
expo.	12	48

Philosophy

solve stiff or oscillatory ivp

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

principles of construction of exponential integrators

- identify most important properties of problem
- choose prototype of equation (stiff or oscillatory)
- solve prototype exactly
- use exact solution of prototype in numerical scheme

Construction of exponential integrators

problem	$y'(t) = f(y(t)),$	$y(0) = y_0$
linearization	$y' = Ay + g(y),$	$y(0) = y_0$
prototype	$u' = Au + g,$	$u(0) = y_0$
exact solution	$u(t) = y_0 + t\varphi(tA)(Ay_0 + g)$	
	$\varphi(tA) = \dfrac{1}{t} \displaystyle\int_0^t \mathrm{e}^{(t-\tau)A} g \,\mathrm{d}\tau$	
approximation	$y(h) \approx y_0 + h\varphi(hA) f(y_0)$	

exponential Euler scheme

Exponential Rosenbrock methods

$$y'(t) = f(y(t)), \qquad y_n \approx y(t_n), \qquad J_n = f'(y_n)$$

general explicit scheme

$$Y_{ni} = y_n + c_i h_n \varphi_1(c_i h_n J_n) f(y_n) + h_n \sum_{j=2}^{i-1} a_{ij}(h_n J_n) D_{nj},$$

$$D_{ni} = f(Y_{ni}) - f(y_n), \qquad i = 2, \dots, s$$

$$y_{n+1} = y_n + h_n \varphi_1(h_n J_n) f(y_n) + h_n \sum_{i=2}^{s} b_i(h_n J_n) D_{ni}.$$

coefficients b_i, a_{ij} are *linear combinations* of *bounded* operators

$$\varphi_k(hA) = \frac{1}{h^k} \int_0^h \mathrm{e}^{(h-\tau)A} \frac{\tau^{k-1}}{(k-1)!} \, \mathrm{d}\tau, \qquad k = 1, \dots, \ell$$

H., Ostermann, Schweitzer, SINUM 2009

old idea ...

- Certaine, 1960
- Gautschi, 1961
- Pope, 1963
- Lawson, 1967
- Nørsett, 1969
- Ehle, Lawson, 1975
- Lambert, Sigurdsson, 1972
- Verwer, 1975
- Friedli, 1978
- Nauts and Wyatt, 1983
- Park and Light, 1986
- Strehmel, Weiner, 1987
- ...

this old idea has been regarded as *not practical* because of the matrix functions involved

Implementation

exponential integrators require approximation of

$$\varphi(hA)b$$

numerical linear algebra enters the game

- diagonalization of A
  - e.g. by FFT
- approximation of $\varphi(z)$ by rational functions (Padé approximations or uniform approximations)
  - requires solution of linear systems $(A - \gamma I)x = v$
- Krylov subspace methods
  - require Ax

Druskin, Knizhnerman 1989, 1995; H., Lubich, 1997, ...

"Nineteen dubious ways to compute the exponential of a matrix, twenty-five years later" (Moler, Van Loan 2003)

Recent contributions

new work (integrators) ...

- H., Lubich, Selhofer, 1998
- Cox, Matthews, 2002
- Krogstad, 2005
- Kassam, Trefethen, 2005
- H., Ostermann, 2005, 2006
- H., Ostermann, Schweitzer, 2009
- ...

---

many papers in numerical linear algebra

Highly oscillatory problems

- Newtonian equations of motion
  (molecular dynamics, astrophysics, ...)

$$q'' = f(q), \qquad f(q) = -\nabla V(q)$$

  V potential (w.l.o.g. mass matrix $M = I$)
- Störmer-Verlet-leapfrog method, $f_n = -\nabla V(q_n)$

$$\begin{aligned} q'_{n+1/2} &= q'_n + \frac{1}{2} h f_n, \\ q_{n+1} &= q_n + h q'_{n+1/2}, \\ q'_{n+1} &= q'_{n+1/2} + \frac{1}{2} h f_{n+1} \end{aligned}$$

  - symmetric and symplectic, order 2
  - linear stability: $h\omega < 2$, ω^2 max. eigenvalue of $\nabla^2 V$

Multiple time scales

$$q'' = f(q), \qquad f(q) = -\nabla V(q)$$

- many applications contain multiple time scales

$$V(q) = W(q) + U(q), \qquad \|\nabla^2 W(q)\| \gg \|\nabla^2 U(q)\|$$

- fast forces $f_{\text{fast}}(q) = -\nabla W(q)$
  (cheap)
- slow forces $f_{\text{slow}}(q) = -\nabla U(q)$
  (expensive, only one evaluation per time step)
- splitting

$$q'' = f_{\text{fast}}(q) + f_{\text{slow}}(q)$$

Multiple time stepping

$$q'' = f_{\mathrm{fast}}(q) + f_{\mathrm{slow}}(q)$$

- given q_n, q'_n, compute averaged position

  $$\overline{q}_n = a(q_n)$$

  and solution of

  $$u'' = f_{\mathrm{fast}}(u) + f_{\mathrm{slow}}(\overline{q}_n) \quad \text{with} \quad u(0) = q_n,\ u'(0) = q'_n$$

  forwards from 0 to h and backwards from 0 to $-h$
- compute q_{n+1} and q'_{n+1} via

  $$q_{n+1} - 2q_n + q_{n-1} = u(h) - 2u(0) + u(-h)$$
  $$q'_{n+1} - q'_{n-1} = u'(h) - u'(-h)$$

- symmetric scheme

H., Lubich, 1999

History

special case of quadratic potentials

$$W(q) = \frac{1}{2} q^T \Omega^2 q, \qquad \Omega \text{ sym., pos. semi-def.}$$

- Gautschi 1961 ($\Omega = \omega I$, $\omega \gg 1$)
- Deuflhard 1979

- Grubmüller et. al., 1991: impulse method
- Tuckerman, Berne, Martyna, 1992

- García-Archilla, Sanz-Serna, Skeel, 1999
  mollified impulse method
- H., Lubich, 1999: Gautschi type method

Gautschi type method for $q'' + \Omega^2 q = g(q)$

variation-of-constants formula: exact solution satisfies

$$\begin{bmatrix} q(t+h) \\ q'(t+h) \end{bmatrix} = R(h\Omega) \begin{bmatrix} q(t) \\ q'(t) \end{bmatrix} + \int_t^{t+h} \begin{bmatrix} \Omega^{-1} \sin(t+h-s)\Omega \\ \cos(t+h-s)\Omega \end{bmatrix} g\big(q(s)\big)\, ds$$

motivates numerical scheme

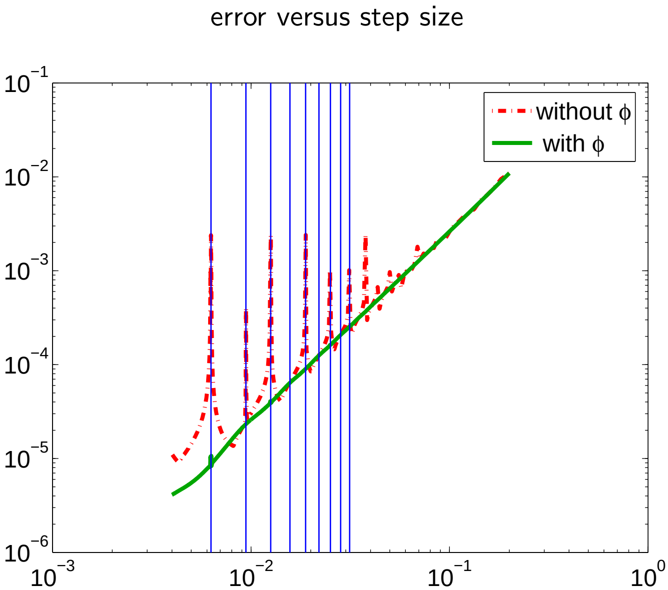
$$\begin{bmatrix} q_{n+1} \\ q'_{n+1} \end{bmatrix} = R(h\Omega) \begin{bmatrix} q_n \\ q'_n \end{bmatrix} + \begin{bmatrix} \frac{1}{2} h^2 \Psi(h\Omega) g_n \\ \frac{1}{2} h \Big(\Psi_0(h\Omega) g_n + \Psi_1(h\Omega) g_{n+1} \Big) \end{bmatrix},$$

where $g_n = g(\Phi(h\Omega) q_n)$ and

$$R(h\Omega) := \begin{bmatrix} \cos h\Omega & \Omega^{-1} \sin h\Omega \\ -\Omega \sin h\Omega & \cos h\Omega \end{bmatrix}$$

Hairer, Lubich, Wanner, GNI, 2002, 2006, Gautschi: $\phi \equiv 1$

Effect of filter functions



Assumptions on filter functions

- $\phi(0) = \psi(0) = \psi_0(0) = \psi_1(0) = 1$
- $\max_{\xi \geq 0} |\chi(\xi)| \leq M_1, \qquad \chi = \phi,\ \psi, \psi_0,\ \psi_1$
- $\max_{\xi \geq 0} \left| \dfrac{\phi(\xi) - 1}{\xi} \right| \leq M_2.$
- $\max_{\xi \geq 0} \left| \dfrac{1}{\sin \frac{\xi}{2}} \left(\operatorname{sinc}^2 \dfrac{\xi}{2} - \psi(\xi) \right) \right| \leq M_3$
- $\max_{\xi \geq 0} \left| \dfrac{1}{\xi \sin \frac{\xi}{2}} \left(\operatorname{sinc} \xi - \chi(\xi) \right) \right| \leq M_4, \qquad \chi = \phi,\ \psi_0,\ \psi_1$

$$\begin{bmatrix} q_{n+1} \\ q'_{n+1} \end{bmatrix} = R(h\Omega) \begin{bmatrix} q_n \\ q'_n \end{bmatrix} + \begin{bmatrix} \frac{1}{2} h^2 \Psi g_n \\ \frac{1}{2} h \Big(\Psi_0 g_n + \Psi_1 g_{n+1} \Big) \end{bmatrix}, \quad g_n = g(\Phi q_n)$$

Theorem (Grimm, H., 2006)

assumptions

- exact solution q satisfies finite energy condition

$$\frac{1}{2}\|q'\|^2 + \frac{1}{2}q^T\Omega^2 q \leq \frac{1}{2}K$$

- above assumptions on filter functions satisfied

then

$$\|q(t_n) - q_n\| \leq h^2 C, \qquad t_0 \leq t_n = t_0 + nh \leq t_0 + T,$$

where C depends on $T, K, M_1, \dots, M_4$, $\|g\|, \|g_q\|$ and $\|g_{qq}\|$ (but *not* on $q^{(k)}$, $k > 1$ or $\|\Omega\|$)

- additional assumptions on filter functions satisfied

$$\|q'(t_n) - q_n'\| \leq hC', \qquad t_0 \leq t_n = t_0 + nh \leq t_0 + T$$

Sketch of proof

- insert exact solution into numerical scheme $\longrightarrow$ defects
- derive expressions for defects
- subtract numerical solution, obtain error recursion, solve recursion by discrete variation-of-constants formula)
- take explicit expressions for defects to bound all sums which occur
- apply Gronwall lemma

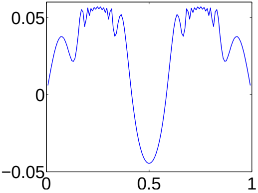
---

no higher temporal derivatives of solution

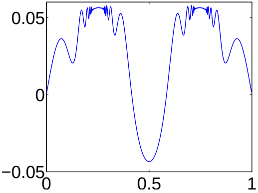
Example: $u'' = u_{xx} - \sin u$

Störmer-Verlet-leapfrog method, $h = 0.02$

128 Fourier modes

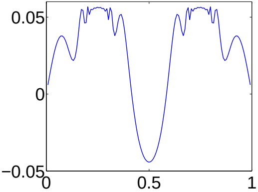


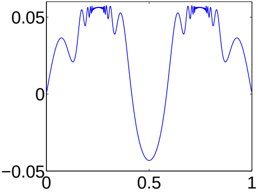
512 Fourier modes

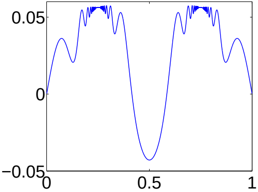


2048 Fourier modes

Gautschi type exponential integrator, $h = 0.02$







Summary – theory

	problem	stable for	implementation requires
explicit	non stiff	$h \sim L^{-1}$	f
implicit	stiff	–	f, f', solution of $F(y) = 0$, LU decomposition
exponential	stiff, oscillatory	–	f, f', $\varphi(hf')v$

Applications

Relativistic laser-plasma dynamics

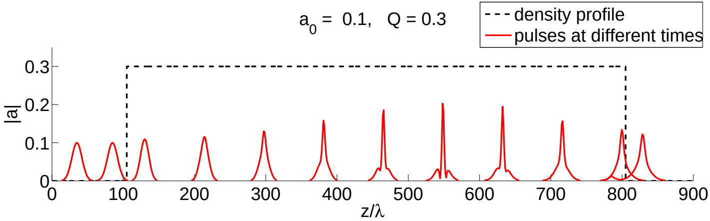
Düsseldorf, Jena, München

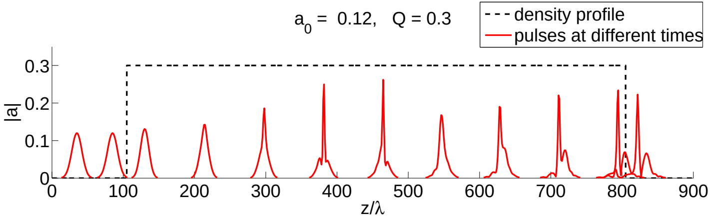
Project B3

joint work with

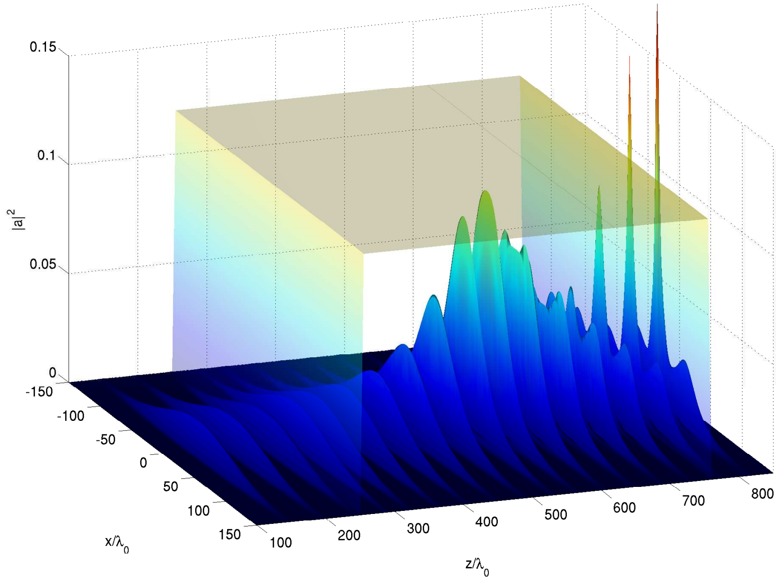
Christoph Karle, Julia Schweitzer, Karl-Heinz Spatschek

Laser plasma interaction, 1d model

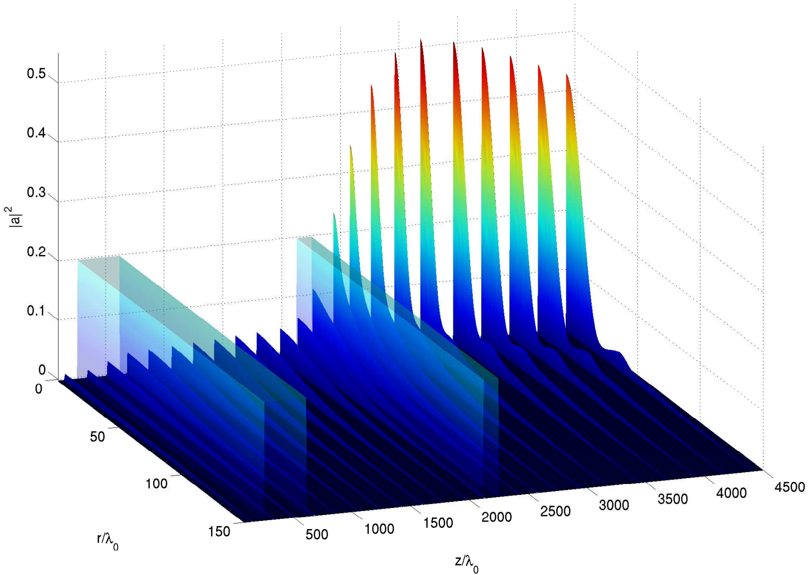




Laser plasma interaction, 2d model



Plasma lens (cylindrical coordinates)



Physical model

nonlinear wave equation (vector potential ansatz for Maxwell equations) with linearized density equation

$$\frac{\partial^2}{\partial t^2} a - \Delta a = -Q \frac{n_e + \delta n}{\gamma} a$$

$$\frac{\partial^2}{\partial t^2} \delta n + Q n_e \delta n = -n_e \Delta \gamma$$

$$\gamma^2 = 1 + |a|^2 \qquad \text{relativistic factor}$$

- a vector potential
- n_e density profile
- δn density variation
- Q density factor

Simulation

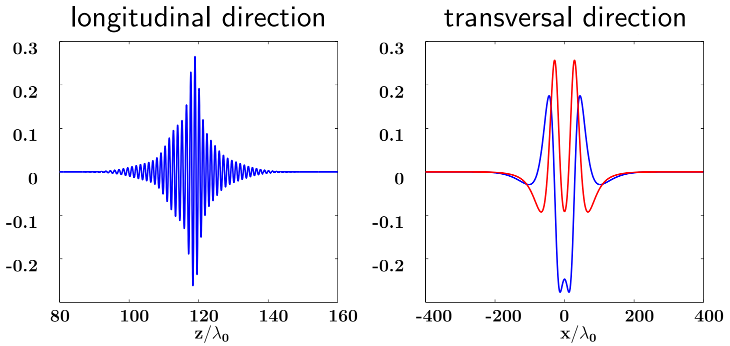
in vacuum

- linear wave equation, Gautschi type integrator
  $\longrightarrow$ arbitrarily large time steps
- matrix functions via 2d fft
  (expensive and hard to parallelize)

in plasma

- nonlinear equations
- time steps smaller
- 2d fft too expensive

Plasma simulation

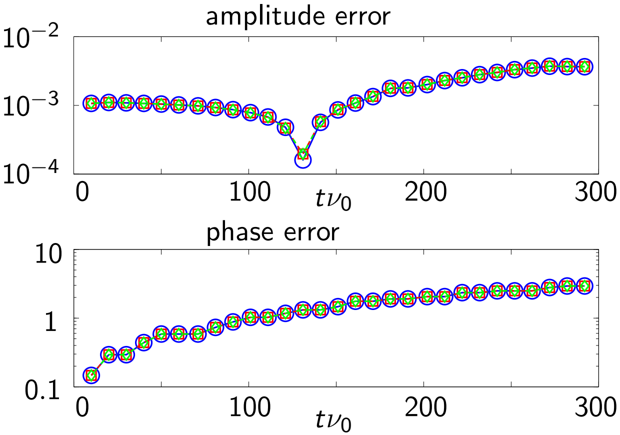


splitting:

$$\Omega^2 \approx -\frac{\partial^2}{\partial z^2}\ , \qquad g(a) \rightarrow g(a) + \frac{\partial^2}{\partial x^2} a$$

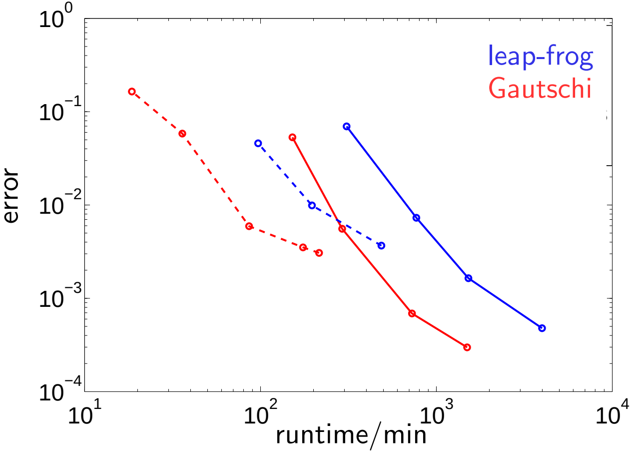
- longitudinal direction ⇒ pseudo spectral method and Gautschi type integrator (1d ffts)
- transversal direction ⇒ finite differences, treat as nonlinear part (easy to parallelize)

Splitting error



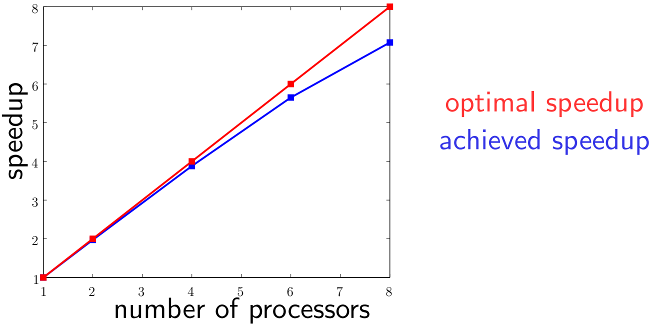
- without splitting
- splitting, pseudo spectral method
- splitting, finite differences

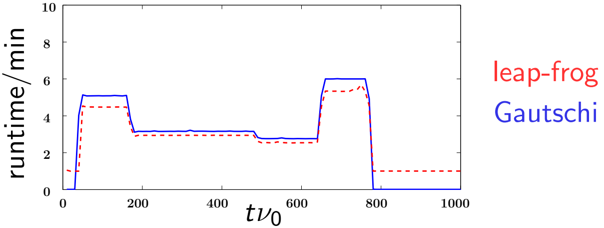
Runtimes 2d



dashed: low resolution, solid: high resolution

Parallelization





Summary

exponential integrators

- construction
- general concept
- “black box” integrator for “smooth” problems
- convergence analysis for highly oscillatory problems
- efficient for special problems (plasma physics) with problem adapted evaluation of matrix functions