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Innovation and Creativity

Exponential integrators

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Abstract

We give an introduction to exponential integrators, starting with a motivation for their use. A format for describing exponential integrators as an extension of general linear schemes (including RK-schemes and multistep-schemes), and order conditions in this setup are developed. Stiff order conditions are relevant for parabolic problems and are also described. A Matlab package has been developed to ease the implementation and testing of most known exponential integrators, we describe this package and end with some numerical examples using it.

(50 minute talk)

Overview

1. Motivation, splitting of the equation
2. Format for exponential integrators
3. Stiff order conditions
4. φ functions
5. Numerical results
6. A brief history
7. References

Motivation

We want to solve semilinear problems, typically PDEs,

$$u_t = \mathcal{L}u + \mathcal{N}(u, t), \qquad u(x, 0) = u_0(x)$$

- The linear operator $\mathcal{L}$ is typically unbounded, yielding, after space discretization, a system of ODEs that normally would have to be solved by an implicit integrator.
- The nonlinear operator is assumed to be nonstiff in the sense that it can be approximated by an explicit method.
- This is typically the case when $\mathcal{N}$ does not depend on spatial derivatives.

Motivation, cont.

A space-discretization yields a system of ODEs,

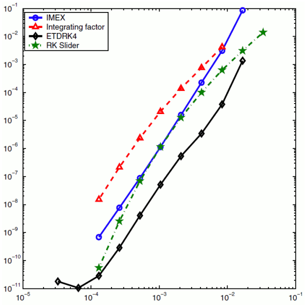
$$\dot{y} = Ly + N(y, t), \qquad y(0) = y_0$$

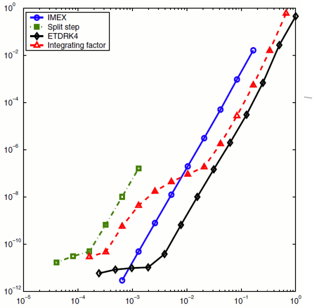
where L is now a matrix.

— This splitting is not unique for a given differential equation
— L is better kept time-independent, for computational reasons.

The strategy is to treat the linear part exactly, and the nonlinear part in an explicit manner.

Example, expints vs other types





Kuramoto–Sivashinsky, global error vs. timestep. 512-point spectral discretization.

Allen–Cahn, global error vs. timestep. 80-point Chebyshev spectral discretization.

(plots taken from Kassam and Trefethen, 2005)

Exponential integrator

Definition

An exponential integrator has the following properties

1. If $L = 0$ the scheme reduces to a standard general linear method (the *underlying scheme*).
2. If $N(y, t) = 0$ for all y and t, the scheme reproduces the exact solution of $\dot{y} = Ly + N(y, t)$.

General linear methods are a generalization of both Runge–Kutta and multistep schemes.

A simple example

Take the equation

$$\dot{y} = Ay + b$$

where A and b are constants as an example.

The numerical integrator

$$y_{n+1} = e^{hA} y_n + \frac{e^{hA} - 1}{hA} hb$$

will solve this equation (let it be scalar or vector) exactly.

It is an exponential integrator in the sense just defined. In the limit $A \to 0$, we recover the Euler scheme.

Derivation of an exponential integrator

Let $\dot{y} = Ly + N(y,t)$. Premultiply with e^{-tL} (integrating factor)

$$\mathrm{e}^{-tL}\dot{y} = \mathrm{e}^{-tL}Ly + \mathrm{e}^{-tL}N(y,t)$$

integrate,

$$\int_{t_n}^{t_n+h} \frac{\mathrm{d}}{\mathrm{d}\tau}\left(\mathrm{e}^{-\tau L}y(\tau)\right)\,\mathrm{d}\tau = \int_{t_n}^{t_n+h} \mathrm{e}^{-\tau L}N(y,\tau)\,\mathrm{d}\tau$$

$$\mathrm{e}^{-(t_n+h)L}y(t_n+h) - \mathrm{e}^{-t_nL}y(t_n) = \int_{t_n}^{t_n+h} \mathrm{e}^{-\tau L}N(y,\tau)\,\mathrm{d}\tau$$

$$y(t_n+h) = \mathrm{e}^{hL}y(t_n) + \mathrm{e}^{(t_n+h)L}\int_{t_n}^{t_n+h} \mathrm{e}^{-\tau L}N(y,\tau)\,\mathrm{d}\tau$$

Derivation cont.

Substitute $\tau = t_n + \theta h$ in the integral,

$$y(t_n + h) = \mathrm{e}^{hL} y(t_n) + h \int_0^1 \mathrm{e}^{(1-\theta)hL} N(y(t_n + \theta h), t_n + \theta h)\, \mathrm{d}\theta$$

which is still an exact representation of the solution.

— Exponential Time Differencing (ETD) schemes now arise from approximating $N(y(\tau), \tau)$ by a polynomial $p(\theta)$ and then integrating exactly.

— Approximating by a constant at $\theta = 0$ is the simplest choice, and it leads to ETD-Euler

$$y_{n+1} = \mathrm{e}^{hL} y_n + h\varphi_1(hL) N(y(t_n), t_n)$$

Building the polynomial

For building the polynomial $p(\theta)$ approximating $N(y, t)$ when integrating from t_n to t_{n+1} there are two approaches,

— Intermediate stages, find lower order approximations Y_i of y at points within $t_n < t < t_{n+1}$ and use $N(Y_i)$ in some quadrature rule. This is the Runge–Kutta approach.

— Use the approximate values of y at earlier time-steps. This leads to multistep-schemes (Adams–Bashforth).

— Combining these two approaches, we get general linear methods.

ETD-schemes

Formalizing the above framework, we note the following lemma

Lemma

The exact solution of the initial value problem

$$\dot{y}(t) = Ly(t) + N(y(t)), \qquad y(0) = y_0$$

has the expansion

$$y(t) = e^{tL} y_0 + \sum_{\ell=1}^{\infty} \varphi_\ell(tL) t^\ell N^{(\ell-1)}(y_0).$$

where

$$\varphi_\ell(z) = \frac{1}{(\ell-1)!} \int_0^1 e^{(1-\theta)z} \, \theta^{\ell-1} \, d\theta.$$

Lawson schemes

An alternative to the ETD-approach which also leads to exponential integrators was developed by Lawson in 1967.

1. Change of variables: $z(t) = \mathrm{e}^{-(t-t_n)L} y(t)$ yielding in the system $\dot{z}(t) = \mathrm{e}^{-(t-t_n)L} N(\mathrm{e}^{(t-t_n)L} z(t))$.
2. Apply a general linear scheme to the system in z, updating z_n to z_{n+1}.
3. Calculate $y_{n+1} = \mathrm{e}^{hL} z_{n+1}$.

The Lawson–Euler scheme is

$$y_{n+1} = \mathrm{e}^{hL} y_n + h\mathrm{e}^{hL} N(y_n, t)$$

The same methodology is also found in the PDE-literature as the

Integrating Factor method, reported to work well on convection-dominated problems.

General format for exp. integrators

Our exponential integrators (RK-type) can be written in a general framework, let

$$Y_i = h \sum_{j=1}^{s} a_{ij}(hL) N(Y_j, t_n + c_j h) + e^{c_i hL} y_n, \quad i = 1, \ldots, s$$

$$y_{n+1} = h \sum_{i=1}^{s} b_i(hL) N(Y_j, t_n + c_j h) + e^{hL} y_n.$$

where $a_{ij}(hL) = a_{ij}(z)$ and $b_i(z)$ are now analytic coefficient *functions* of $z = hL$.

— We require that these functions fulfill classical order conditions in the limit $z \to 0$.

— We will do general linear methods in a moment.

— Classical order analysis is straightforward.

Tableau of coefficients

The coefficient functions are conveniently grouped in an extended Butcher tableau

$$
\begin{array}{c|ccc|c}
c_1 & a_{11}(z) & \cdots & a_{1s}(z) & e^{c_1 z} \\
\vdots & \vdots & & \vdots & \vdots \\
c_s & a_{s1}(z) & \cdots & a_{ss}(z) & e^{c_s z} \\
\hline
 & b_1(z) & \cdots & b_s(z) & e^{z}
\end{array}
$$

Lawson–Euler:

$$y_n = \exp(hL)y_{n-1} + \exp(hL)N(y_{n-1}, t_{n-1})$$

$$
\begin{array}{c|c|c}
0 & 0 & 1 \\
\hline
 & e^z & e^z
\end{array}
$$

ETD-Euler:

$$y_n = \exp(hL)y_{n-1} + \varphi_1(hL)N(y_{n-1}, t_{n-1})$$

$$
\begin{array}{c|c|c}
0 & 0 & 1 \\
\hline
 & \varphi_1(z) & e^z
\end{array}
$$

Lawson schemes

Given coefficients of a Runge–Kutta scheme,

$$\tilde{a}_{ij}, \quad \tilde{b}_i \quad \text{and} \quad c_j,$$

the corresponding Lawson scheme is given by the coefficient functions

$$a_{ij}(z) = \tilde{a}_{ij} \mathrm{e}^{(c_i - c_j)z} \quad \text{and} \quad b_i(z) = \tilde{b}_i \mathrm{e}^{(1-c_i)z}.$$

Lawson, 4th order

The most common integrator of the Lawson type, based on Kutta's classical order 4 scheme is

$$
\begin{array}{c|cccc}
0 & & & & \\
\frac{1}{2} & \frac{1}{2}e^{z/2} & & & \\
\frac{1}{2} & & \frac{1}{2} & & \\
1 & & & e^{z/2} & \\
\hline
 & \frac{1}{6}e^{z} & \frac{1}{3}e^{z/2} & \frac{1}{3}e^{z/2} & \frac{1}{6}
\end{array}
$$

- Easy and relatively cheap to implement.
- Does not preserve fixed points.
- Performs well on NLS.
- Stiff order 1.

ETD RK-schemes

A fourth order ETD of Runge–Kutta type, common in recent literature,

$$
\begin{array}{c|cccc}
0 & & & & \\
\frac{1}{2} & \frac{1}{2}\varphi_1(z/2) & & & \\
\frac{1}{2} & & \frac{1}{2}\varphi_1(z/2) & & \\
1 & \varphi_1(z/2)(e^{z/2}-1) & & \varphi_1(z/2) & \\
\hline
 & \varphi_1 - 3\varphi_2 + 4\varphi_3 & 2\varphi_2 - 4\varphi_3 & 2\varphi_2 - 4\varphi_3 & -\varphi_2 + 4\varphi_3
\end{array}
$$

— Due to Cox and Matthews 2002.

— Stiff order 2.

Exponential general linear schemes

The currently best-performing exponential integrators are in the family of Exponential general linear schemes.

Define a vector of quantities passed from step to step:

$$Y^{[n]} = \begin{bmatrix} y_1^{[n]} & \cdots & y_r^{[n]} \end{bmatrix}^T$$

the write the scheme as

$$Y_i = h \sum_{j=1}^{s} a_{ij}(z) N(Y_j) + \sum_{j=1}^{r} u_{ij}(z) y_j^{[n]}$$

$$y_i^{[n+1]} = h \sum_{j=1}^{s} b_{ij}(z) N(Y_j) + \sum_{j=1}^{r} v_{ij}(z) y_j^{[n]}$$

The coefficient functions are typically grouped in four matrix-valued functions, $A(z)$, $B(z)$, $U(z)$ and $V(z)$.

Exponential general linear schemes

Tableau

$$\begin{array}{c|c|c} c & A(z) & U(z) \\ \hline & B(z) & V(z) \end{array}$$

Schemes in this talk rely on the following structure of the quantities passed from step to step:

$$y^{[n]} = \begin{bmatrix} y_n & hN_{n-1} & hN_{n-2} & \dots & hN_{n-r+1} \end{bmatrix}^T$$

where $N_{n-i} = N(y_{n-i}, t_{n-i})$. This choice enables both ETD Adams–Bashforth and Generalized Lawson schemes to be easily represented. As a starting procedure, exponential Runge–Kutta can be used.

Example scheme, ABNørsett3

This is a third order ETD Adams–Bashforth scheme, classical order 3, stiff order 3.

$$
\begin{array}{c|cc|ccc}
0 & & & 1 & 0 & 0 \\
1 & \varphi_1 + \frac{3}{2}\varphi_2 + \varphi_3 & & \varphi_0 & -2\varphi_2 - 2\varphi_3 & \frac{1}{2}\varphi_2 + \varphi_3 \\
\hline
 & \varphi_1 + \frac{3}{2}\varphi_2 + \varphi_3 & 0 & \varphi_0 & -2\varphi_2 - 2\varphi_3 & \frac{1}{2}\varphi_2 + \varphi_3 \\
 & 1 & 0 & 0 & 0 & 0 \\
 & 0 & 0 & 0 & 1 & 0
\end{array}
$$

where $\varphi_0(z) = e^z$.

Example scheme, GenLawson42

Classical order 4, stiff order 3

$$
\begin{array}{c|cccc|cc}
0 & & & & & 1 & 0 \\
\frac{1}{2} & \frac{1}{2}\varphi_{1,2} + \frac{1}{4}\varphi_{2,2} & & & & \varphi_{0,2} & -\frac{1}{4}\varphi_{2,2} \\
\frac{1}{2} & \frac{1}{2}\varphi_{1,2} + \frac{1}{4}\varphi_{2,2} - \frac{3}{4} & \frac{1}{2} & & & \varphi_{0,2} & -\frac{1}{4}\varphi_{2,2} + \frac{1}{4} \\
1 & \varphi_1 + \varphi_2 - \frac{3}{2}\varphi_{0,2} & & \varphi_{0,2} & & \varphi_0 & -\varphi_2 + \frac{1}{2}\varphi_{0,2} \\
\hline
 & \varphi_1 + \varphi_2 - \varphi_{0,2} - \frac{1}{3} & \frac{1}{3}\varphi_{0,2} & \frac{1}{3}\varphi_{0,2} & \frac{1}{6} & \varphi_0 & -\varphi_2 + \frac{1}{3}\varphi_{0,2} + \frac{1}{6} \\
 & 1 & 0 & 0 & 0 & 0 & 0
\end{array}
$$

where $\varphi_{i,j}(z) = \varphi_i(c_j z)$.

Stiff order conditions

If $\mathcal{L}$ (the original differential operator) is unbounded, one cannot expect $\|hL\| \to 0$ in computations or analysis, independently of the spatial discretization parameter. Classical order analysis relies on this.

For semilinear parabolic problems, one is able to prove that although $\mathcal{L}$ is unbounded, the functions φ can be bounded, and thereby bounding the coefficient functions. Then one gets convergence proofs, see Hochbruck and Ostermann 2005.

This requires a set of stricter order conditions generalizing classical order conditions, denoted *“stiff order conditions”*.

Stiff order, preservation of fixed points

For fixed points we have $Ly = -N(y)$ and we require the integrator to give $y_1 = y_0$. Inserting this in the format of an expontial RK-scheme, one obtains the requirement

$$y_0 = -\sum_{i=1}^{s} b_i(z)z + e^z y_0 \quad \Rightarrow \quad \sum_{i=1}^{s} b_i(z) = \varphi_1(z)$$

and for the inner stages we get the requirements

$$\sum_{j=1}^{s} a_{ij}(z) = c_i \varphi_1(c_i z) \quad \text{for each } i$$

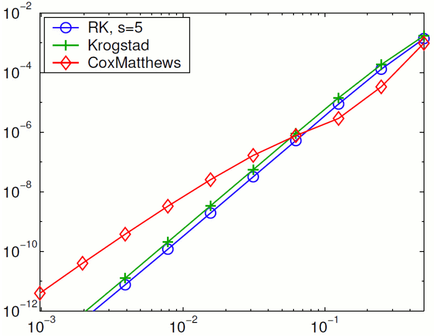
These are two examples of stiff order conditions. Schemes of stiff order 2 and higher preserve fixed points.

Example, order reduction

A nonlinear heat equation,

$$u_t = u_{xx} + \frac{1}{1+u^2} + \Phi(x,t)$$

where $\Phi(x,t)$ is such that the exact solution is $e^t(1-x)x$.



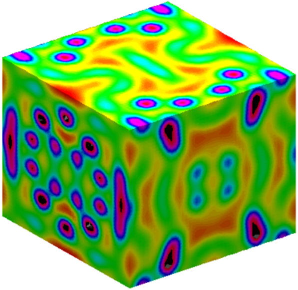
global error vs. timestep

200 grid points, homogeneous Dirichlet BC. “CoxMatthews” is ETD4RK, and has order 3 in this plot. Krogstad is a Generalized Lawson scheme.

Plot taken from Hochbruck and Ostermann 2005.

MATLAB package

For testing, there is a MATLAB package, EXPINT, featuring:

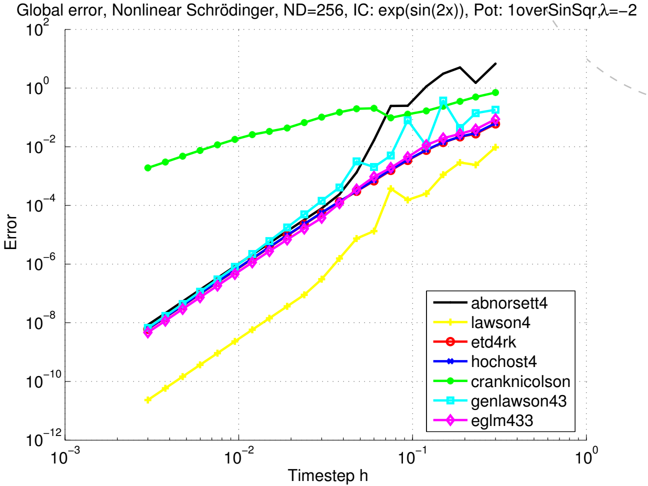


- Easy implementation and comparison of exponential integrators (47 schemes right now).
- Numerous examples of discretizations of common PDEs.
- φ functions computed by (7,7)-Padé-approximations together with scaling and corrected squaring.

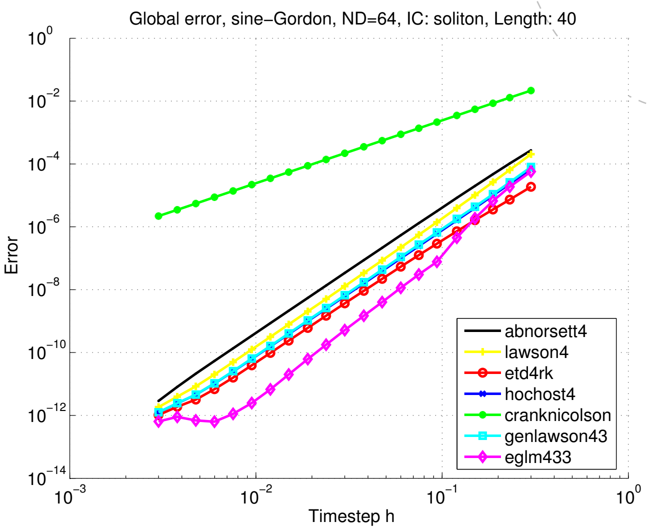
The EXPINT-package and an accompanying technical report may be downloaded from

`http://www.math.ntnu.no/num/expint/`

Example, nonlinear Schrödinger



Example, sine-Gordon equation



φ functions

Crucial to ETD-schemes are the evaluation of the φ functions,

$$\varphi_\ell(z) = \frac{1}{(\ell-1)!}\int_0^1 e^{(1-\theta)z}\theta^{\ell-1}\,d\theta, \qquad \ell = 1, 2, \ldots.$$

For small values of ℓ and $z > 0$, these are

$$\varphi_\ell(0) = \frac{1}{\ell!}$$

$$\varphi_1(z) = \frac{e^z - 1}{z}$$

$$\varphi_2(z) = \frac{e^z - z - 1}{z^2}$$

$$\varphi_3(z) = \frac{e^z - z^2/2 - z - 1}{z^3}$$

Defining $\varphi_0(z) = e^z$ the functions

obey the recurrence

$$\varphi_{\ell+1}(z) = \frac{\varphi_\ell(z) - \frac{1}{\ell!}}{z}, \quad \ell = 0, 1, \ldots$$

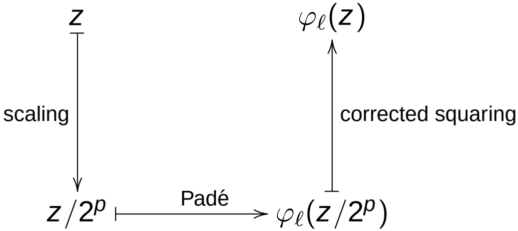
φ functions cont.

Evaluation of these functions has numerical issues.
Possible approaches:

- Taylor series for small z, direct formula for non-small (Cox and Matthews 2002).
- Contour integral, works well for suitable chosen radius of contour (Kassam and Trefethen 2005).
- Scaling, Padé and (corrected) squaring (next slides).
- Krylov subspace approximation (Hochbruck, Selhofer, Lubich 1998).

φ functions, scaling, Padé and corrected squaring

The procedure for evaluation is:



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

φ functions, Padé approximation

The general form of the (d,d)-Padé approximant of φ_ℓ is

$$\varphi_\ell(z) = \frac{N_d^\ell(z)}{D_d^\ell(z)} + \mathcal{O}(z^{2d+1})$$

where the unique polynomials N_d^ℓ and D_d^ℓ are

$$\begin{aligned} N_d^\ell(z) &= \frac{d!}{(2d+\ell)!} \sum_{i=0}^{d} \left[\sum_{j=0}^{i} \frac{(2d+\ell-j)!(-1)^j}{j!(d-j)!(\ell+i-j)!} \right] z^i \\ D_d^\ell(z) &= \frac{d!}{(2d+\ell)!} \sum_{i=0}^{d} \frac{(2d+\ell-i)!}{i!(d-i)!} (-z)^i \end{aligned} \tag{1}$$

φ functions, corrected squaring

Squaring the exponential function is easy, $e^{2z} = e^z e^z$. But for φ functions, we need correctional terms,

$$\varphi_{2\ell}(2z) = \frac{1}{2^{2\ell}} \left[\varphi_\ell(z)\varphi_\ell(z) + \sum_{j=\ell+1}^{2\ell} \frac{2}{(2\ell - j)!} \varphi_j(z) \right],$$

$$\varphi_{2\ell+1}(2z) = \frac{1}{2^{2\ell+1}} \left[\varphi_\ell(z)\varphi_{\ell+1}(z) + \sum_{j=\ell+2}^{2\ell+1} \frac{2}{(2\ell + 1 - j)!} \varphi_j(z) \right.$$
$$\left. + \frac{1}{\ell!} \varphi_{\ell+1}(z) \right].$$

A brief history

— Certaine 1960
  ETD2 and ETD3 based on Adams–Moulton methods
— Lawson 1967
  Generalized RK processes (Lawson schemes), A-stability
— Nørsett 1969
  ETD based on Adams–Bashforth schemes, A-stability
— Verwer and van der Houwen 1974
  ETD linear multistep methods
— Friedli 1978
  ETD based on explicit RK schemes, order conditions
— Strehmel and Weiner 1982
  Adaptive RK schemes, order theory, B-stability

A brief history

- Hochbruck, Lubich and Selhofer 1998
  Exponential integrators (exp4) with inexact Jacobian
- Beylkin, Keiser and Vozovoi 1998
  ETD methods of Adams type
- Cox and Matthews 2002
  ETDRK methods of order 3 and 4
- Celledoni, Owren and Martinsen 2003
  Commutator-free Lie group methods
- Krogstad 2005
  Generalized Lawson methods
- Hocbruck and Ostermann 2005
  Stiff order conditions, convergence proof

Credits

Credits are due to my collaborators

- Prof. Brynjulf Owren, Norwegian University of Science and Technology, Trondheim, Norway
- Dr. Will Wright, La Trobe University, Melbourne, Australia.
- Bård Skaflestad, Norwegian University of Science and Technology, Trondheim, Norway.

Future work

Some ideas:

- More analysis on evaluation of φ functions.
- Exponential integrators preserving multisymplecticity?
- Conservation of invariants.

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