# Exponential Taylor methods: analysis and implementation

Antti Koskela
joint work with Alexander Ostermann
University of Innsbruck

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# Outline

Introduction

Exponential Taylor method

Implementation

Convergence results

Illustration: accumulation of errors

Example of state-independent inhomogeneity

# Outline

# The problem

We consider the time integration of stiff semilinear initial value problems

$$u'(t) = Au(t) + g(t, u(t)), \quad u(t_0) = u_0,$$

where $u(t) \in \mathbb{R}^d$, $A \in \mathbb{R}^{d \times d}$ ($d$ large),

$g$ is a nonlinear function with a moderate Lipschitz constant.

Specifically: problems arising from spatial semidiscretization of partial differential equations.

# Exponential integrators

Exponential integrators are based on the variation-of-constants formula

$$u(t) = \mathrm{e}^{(t-t_0)A} u_0 + \int_{t_0}^{t} \mathrm{e}^{(t-\tau)A} g(\tau, u(\tau)) \, \mathrm{d}\tau,$$

which gives the exact solution at time $t$.

Example: exponential Euler method

$$u_1 = \mathrm{e}^{hA} u_0 + h\varphi_1(hA) g(t_0, u_0)$$

where $h$ denotes the step size and $\varphi_1$ is the entire function

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

# Higher order exponential integrators

For the construction of high order exponential Runge–Kutta methods, and higher order exponential multistep methods, see:

M. Hochbruck and A. Ostermann:
Exponential integrators, Acta Numerica (2010).

These methods contain the entire functions

$$\varphi_k(z) = \int_0^1 \mathrm{e}^{(1-\theta)z} \frac{\theta^{k-1}}{(k-1)!} \, \mathrm{d}\theta, \quad k \geq 1.$$

For a matrix $A \in \mathbb{R}^{d \times d}$ and a vector $b \in \mathbb{R}^d$,
the evaluation of $\varphi_k(A)b$ is often costly.

# Outline

# Exponential Taylor method

Here, we consider multiderivative exponential integrators.
We replace the nonlinearity by its Taylor polynomial of degree $p-1$:

$$g(\tau, u(\tau)) \approx \sum_{k=0}^{p-1} \frac{(\tau - t_0)^k}{k!} \frac{\mathrm{d}^k}{\mathrm{d}t^k} g(t, u(t))\Big|_{t=t_0}.$$

Using the chain rule, we see that for $p = 4$
(when $g(t,u) = g(u)$)

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t} g(u) &= g'(u)u' \\
\frac{\mathrm{d}^2}{\mathrm{d}t^2} g(u) &= g''(u)(u', u') + g'(u)u'' \\
\frac{\mathrm{d}^3}{\mathrm{d}t^3} g(u) &= g'''(u)(u', u', u') + 3g''(u)(u'', u') + g'(u)u'''
\end{aligned}$$

# Exponential Taylor method

By using the known quantity $u_0$, we approximate

$$\frac{\mathrm{d}^{k-1}}{\mathrm{d}t^{k-1}} g(u(t))\Big|_{t=t_0} \approx w_k,$$

where $w_k$ is defined recursively by

$$u_0^{(k)} = A u_0^{(k-1)} + w_k, \quad k \geq 1$$

and

$$\begin{aligned} w_1 &= g(u_0) \\ w_2 &= g'(u_0)u_0' \\ w_3 &= g''(u_0)(u_0', u_0') + g'(u_0)u_0'' \\ w_4 &= g'''(u_0)(u_0', u_0', u_0') + 3g''(u_0)(u_0'', u_0') + g'(u_0)u_0''' \end{aligned}$$

# Exponential Taylor method

We insert the polynomial

$$g(\tau, u(\tau)) \approx \sum_{k=0}^{p-1} \frac{(\tau - t_0)^k}{k!} w_k$$

to the variation-of-constants formula

$$u(t) = \mathrm{e}^{(t-t_0)A} u_0 + \int_{t_0}^{t} \mathrm{e}^{(t-\tau)A} g(\tau, u(\tau)) \, \mathrm{d}\tau$$

to get the exponential Taylor method

$$u_1 = \mathrm{e}^{hA} u_0 + \sum_{k=1}^{p} h^k \varphi_k(hA) w_k.$$

# Exponential Taylor method

Here the functions $\varphi_k$ are as above:

$$\varphi_k(z) = \int_0^1 \mathrm{e}^{(1-\theta)z} \frac{\theta^{k-1}}{(k-1)!} \, \mathrm{d}\theta, \quad k \geq 1.$$

They satisfy $\varphi_k(0) = 1/k!$ and the recurrence relation

$$\varphi_{k+1}(z) = \frac{\varphi_k(z) - \varphi_k(0)}{z}, \quad \varphi_0(z) = \mathrm{e}^z.$$

# Linearized exponential Taylor method

For an autonomous problem

$$u'(t) = Au(t) + g(u(t)) = f(u(t)), \quad u(t_0) = u_0,$$

we linearize the differential equation at the numerical approximation $u_n$ at time $t_n$:

$$v'(t) = J_n v(t) + g_n(v(t)), \quad v(t_n) = u_n, \qquad (*)$$

where $J_n$ denotes the Fréchet derivative of $f$, and $g_n$ the remainder:

$$J_n = f'(u_n) = A + g'(u_n),$$
$$g_n(u) = f(u) - J_n u = g(u) - g'(u_n)u.$$

Applying an exponential Taylor method to (*) yields a so-called *linearized* exponential Taylor method.

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# Computational advantage

Computation of one time step done as follows:
(Al-Mohy and Higham 2010)

## Lemma

*Let* $A \in \mathbb{R}^{d \times d}$*,* $W = [w_p, w_{p-1}, \ldots, w_1] \in \mathbb{R}^{d \times p}, h \in \mathbb{R}$ *and*

$$\widetilde{A} = \begin{bmatrix} A & W \\ 0 & J \end{bmatrix} \in \mathbb{R}^{(d+p)\times(d+p)}, \quad J = \begin{bmatrix} 0 & I_{p-1} \\ 0 & 0 \end{bmatrix}, \quad v_0 = \begin{bmatrix} u_0 \\ e_p \end{bmatrix} \in \mathbb{R}^{d+p}$$

*with* $e_p = [0, \ldots, 0, 1]^\mathsf{T}$*. Then it holds*

$$\mathrm{e}^{hA} u_0 + \sum_{k=1}^{p} h^k \varphi_k(hA) w_k = \begin{bmatrix} I_d & 0 \end{bmatrix} \mathrm{e}^{h\widetilde{A}} v_0.$$

# Krylov approximation

To compute the appearing matrix exponential times vector product $\begin{bmatrix} I_d & 0 \end{bmatrix} e^{h\widetilde{A}} \begin{bmatrix} u_0 \\ e_p \end{bmatrix}$, Krylov methods are used.

The Arnoldi iteration produces an orthogonal basis $V_k \in \mathbb{R}^{d \times k}$ for the Krylov subspace

$$\mathcal{K}_k(A, b) = \mathrm{span}\{b, Ab, A^2 b, ..., A^{k-1} b\}.$$

and the Hessenberg matrix $H_k = V_k^{\mathsf{T}} A V_k \in \mathbb{R}^{k \times k}$.
Then the approximation

$$\mathrm{e}^{hA} b \approx V_k \mathrm{e}^{H_k} V_k^{\mathsf{T}} b = V_k \mathrm{e}^{H_k} e_1 \|b\|_2$$

is used.

# Krylov approximation

Numerically the convergence is found satisfying for $e^{h\widetilde{A}}\begin{bmatrix} u_n \\ e_p \end{bmatrix}$.

Example: here $A \in \mathbb{R}^{500\times 500}$ is symmetric, $\|hA\|_2 = 80$ and for $W \in \mathbb{R}^{500\times 5}$, $\|hW\|_2 \approx 2\cdot 10^5$.

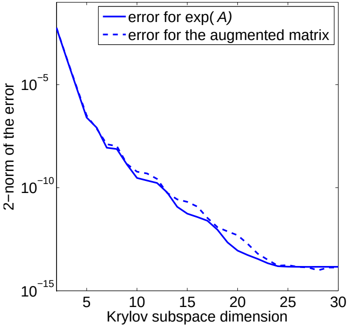


Figure: The errors of the Krylov approximations vs. the dimension of the Krylov subspace.

# Adaptive step sizes

An error control for the exponential Taylor integrator

$$u_1^{[p]} = \mathrm{e}^{hA} u_0 + \sum_{k=1}^{p} h^k \varphi_k(hA) w_k$$

can be obtained from the last term of the sum, since for small $h$ we may approximate

$$\|u(t_1) - u_1^{[p-1]}\|_2 \approx \|u_1^{[p]} - u_1^{[p-1]}\|_2 = \|h^p \varphi_p(hA) w_p\|_2.$$

$h^p \varphi_p(hA) w_p$ can be computed also using a single exponential of an augmented matrix.

# Computation of the derivatives

For autonomous nonlinearities $g(u)$, the vectors $w_i$ of the exponential Taylor method can be obtained by

$$
\begin{aligned}
w_1 &= g(u_0) \\
w_2 &= J^{(0)} f^{(0)}
\end{aligned}
$$

$$
i \geq 2 \quad \begin{cases} f^{(i-1)} = A f^{(i-2)} + w_i \\ w_{i+1} = \sum_{k=0}^{i-1} \binom{i-1}{k} J^{(i-1-k)} f^{(k)}, \end{cases}
$$

where

$$
f^{(k)} = \frac{\mathrm{d}^k}{\mathrm{d}t^k} f(u(t))\Big|_{u=u_n} \quad \text{and} \quad J^{(k)} = \frac{\mathrm{d}^k}{\mathrm{d}t^k} g'(u(t))\Big|_{u=u_n}.
$$

# Computation of the derivatives

References for the use of Automatic Differentiation:

- E.Hairer, S.Nørsett, G.Wanner, Solving Ordinary Differential Equations I. Nonstiff Problems, 2nd edition, Springer, Berlin, 1993.
- Griewank, Andreas: Evaluating Derivatives: Principles and Techniques of Algorithmic Differentiation (2008)
- G. F. Corliss, A. Griewank, P. Henneberger, G. Kirlinger, F. A. Potra and H. J. Stetter: High-order stiff ODE solvers via automatic differentiation and rational prediction (1997)

# Outline

# Assumptions

We assume that the involved matrix exponential satisfies the bound

$$\|\mathrm{e}^{tA}\| \leq C_0 \mathrm{e}^{\omega t}, \qquad t \geq 0$$

From this it also follows that

$$\|\varphi_k(tA)\| \leq \frac{C_0 \mathrm{e}^{\omega t}}{k!}, \qquad t \geq 0.$$

Using these, the convergence bounds depend only on the constants $C_0$ and $\omega$.

We also assume that the nonlinear term $g(t, u(t))$ sufficiently smooth.

# Convergence for linear equations

For the linear problem

$$u'(t) = Au(t) + g(t), \quad u(t_0) = u_0, \qquad t_0 \leq t \leq T$$

we have the following results

## Theorem

*Let the inhomogeneity $g$ be $p$ times differentiable with $g^{(p)} \in L^1(0, T)$. Then, the exponential Taylor method is convergent of order $p$.*

Proof: The exponential Taylor method gives:

$$u_{n+1} = \mathrm{e}^{hA} u_n + \sum_{k=1}^{p} h^k \varphi_k(hA) g^{(k-1)}(t_n), \quad n \geq 0,$$

# Convergence for linear equations

and we see that the error $e_{n+1} = u_{n+1} - u(t_{n+1})$ satisfies

$$e_{n+1} = \mathrm{e}^{hA} e_n - \delta_{n+1},$$

where

$$\delta_{n+1} = \int_0^h \mathrm{e}^{(h-\tau)A} \int_0^\tau \frac{(\tau - \xi)^{p-1}}{(p-1)!} g^{(p)}(t_n + \xi)\, \mathrm{d}\xi\, \mathrm{d}\tau.$$

which can be bounded using bound for $\|\varphi_k(tA)\|$.

Solving recursion for $e_n$ and bounding $\|\mathrm{e}^{tA}\|$ gives the result.

# Convergence for semilinear equation

For the semilinear equation

$$u'(t) = Au(t) + g(t, u(t)), \quad u(t_0) = u_0.$$

we have:

## Theorem

*Let the inhomogeneity* $\psi(t) = g(t, u(t))$ *be twice differentiable and* $\psi'' \in L^1(0, T)$*. Then, the exponential Taylor method is second order convergent.*

Proof. The Taylor scheme with $p = 2$ has the form

$$\begin{aligned} u_{n+1} = \mathrm{e}^{hA} u_n + h\varphi_1(hA) g(t_n, u_n) \\ + h^2 \varphi_2(hA)\big(g_t(t_n, u_n) + g_u(t_n, u_n)(Au_n + g(t_n, u_n))\big). \end{aligned}$$

# Convergence for semilinear equation

Expressing the exact solution with the second order Taylor polynomial, we get for the global error $e_n = u_n - u(t_n)$ the recursion

$$
\begin{aligned}
e_{n+1} = \mathrm{e}^{hA} e_n &+ h\varphi_1(hA)\big(g(t_n, u_n) - g(t_n, \widetilde{u}_n)\big) \\
&+ h^2\varphi_2(hA)\big(g_t(t_n, u_n) - g_t(t_n, \widetilde{u}_n)\big) \\
&+ h^2\varphi_2(hA) g_u(t_n, u_n)\big(Ae_n + g(t_n, u_n) - g(t_n, \widetilde{u}_n)\big) \\
&+ h^2\varphi_2(hA)\big(g_u(t_n, u_n) - g_u(t_n, \widetilde{u}_n)\big) u'(t_n) - \delta_{n+1},
\end{aligned}
$$

where

$$
\delta_{n+1} = \int_0^h \mathrm{e}^{(h-\tau)A} \int_0^\tau (\tau - \xi) \frac{\mathrm{d}^2 g}{\mathrm{d}t^2}\big(t, u(t)\big)\Big|_{t=t_n+\xi} \,\mathrm{d}\xi \,\mathrm{d}\tau.
$$

# Convergence for semilinear equation

Multiplying $e_{n+1}$ with $A$ and using $z\varphi_2(z) = \varphi_1(z) - 1$ we get respectively a recursion for $Ae_n$.

Combining these 2 recursions, and using standard Gronwall lemma, we obtain the estimate

$$\|e_n\| + h\|Ae_n\| \leq C \sum_{j=1}^{n} \Big( \|\mathrm{e}^{(n-j)hA}\delta_j\| + h\|A\mathrm{e}^{(n-j)hA}\delta_j\| \Big)$$

where $C$ is independent of $\|A\|$.

Bounding $\delta_j$ gives the result.

# Convergence for linearized scheme

When we apply the exponential Taylor method to the linearized equation

$$v'(t) = J_n v(t) + g_n(v(t)), \quad v(t_n) = u_n,$$

where

$$J_n = f'(u_n) = A + g'(u_n),$$
$$g_n(u) = f(u) - J_n u = g(u) - g'(u_n)u,$$

order three is possible. By construction,

$$g_n'(u_n) = 0.$$

and therefore the linearized exponential Taylor scheme for $p = 3$ has the form

$$\begin{aligned} u_{n+1} &= \mathrm{e}^{hJ_n} u_n + h\varphi_1(hJ_n) g_n(u_n) \\ &\quad + h^3 \varphi_3(hJ_n) g''(u_n)\big(J_n u_n + g_n(u_n), J_n u_n + g_n(u_n)\big) \\ &= u_n + h\varphi_1(hJ_n) f(u_n) + h^3 \varphi_3(hJ_n) f''(u_n)\big(f(u_n), f(u_n)\big). \end{aligned}$$

# Convergence for linearized scheme

**Theorem**

*Let the inhomogeneity $\psi(t) = g(u(t))$ be three times differentiable with $\psi''' \in L^1(0, T)$. Then, the linearized exponential Taylor method is convergent of order three, i.e.*

$$\|u_n - u(t_n)\| \leq Ch^3$$

*with a constant $C$ that is uniform on compact intervals $0 \leq nh \leq T$.*

# Outline

# Accumulation of local errors

Consider a simple one-dimensional partial differential equation

$$\partial_t u = u_{xx} + \gamma u(1-u), \quad x \in [-\frac{5}{2}, \frac{5}{2}]$$

with periodic boundary conditions and the initial value

$$u(x,0) = \exp(-10x^2), \quad x \in [-\frac{5}{2}, \frac{5}{2}].$$

We set $\gamma = 10$.

# Accumulation of local errors

Performing spatial semidiscretization with finite differences gives for the linear part:

$$A := \frac{1}{(\Delta x)^2} \begin{bmatrix} -2 & 1 & & & 1 \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ 1 & & & 1 & -2 \end{bmatrix},$$

where $\Delta x = L/n$.

Eigenvalues of $A$ are on the negative real axis,
the smallest being: $\lambda_{min} = -4/(\Delta x)^2$.

# Accumulation of local errors

The term $w_p$ contains the highest powers of $A$, namely

$$g'(u_n)A^{p-1}u_n.$$

Using the inequality

$$|g'(u)| = \gamma|1-2u| \leq \gamma$$

the stability of the exponential Taylor scheme is governed by the factor

$$\left|\gamma h^p \varphi_p(h\lambda_{\text{min}})\lambda_{\text{min}}^{p-1}\right|$$

which has to be power-bounded, i.e.

$$\gamma h^p \varphi_p(h\lambda_{\text{min}})\left|\lambda_{\text{min}}\right|^{p-1} \leq 1.$$

Similarly for $p$th order linearized scheme:

$$2(p-1)\gamma h^p \varphi(h\lambda_{min})\left|\lambda_{min}\right|^{p-2} \leq 1.$$

# Accumulation of local errors

| $p$ | $d = 500$ | $d = 1000$ |
|---|---|---|
| 3 | 2.3E-3 / 2.4E-3 | 1.1E-3 / 1.2E-3 |
| 4 | 7.3E-4 / 7.8E-4 | 2.9E-4 / 3.0E-4 |
| 5 | 4.5E-4 / 4.8E-4 | 1.5E-4 / 1.6E-4 |

Table: Step sizes determined by the stability condition vs. experimentally observed largest admissible step sizes.

# Accumulation of local errors

The spatial discretization $d = 1000$:

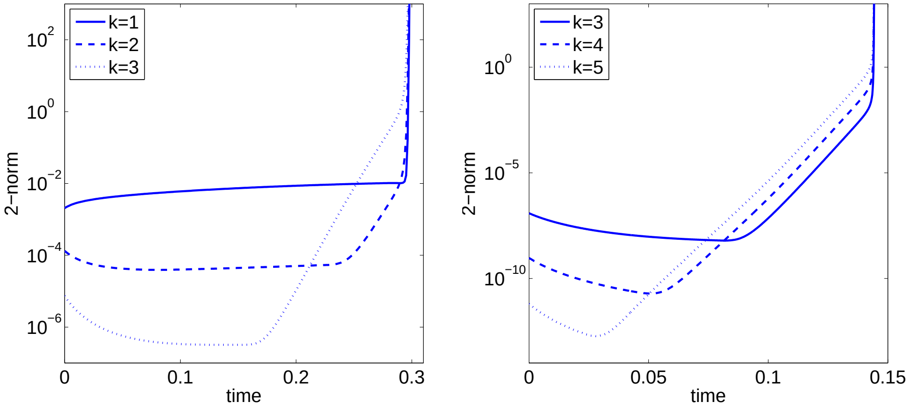


Figure: 2-norms of the highest $h^k \varphi_k(hA) w_k$-terms for $p = 3$ and $p = 5$, when the step size larger than the admissible step size.

# Outline

# A linear example with inhomogeneity

If the nonlinearity is state-independent, no numerical instabilities are expected.

We consider a finite difference spatial discretization (with 500 points) of the equation

$$
\begin{aligned}
\partial_t u &= \partial_{xx} u + 10\,\mathrm{e}^{-10t} x(1-x), \quad x \in [0,1], \quad t \in [0, 0.1] \\
u(x,0) &= 16x^2(1-x)^2, \\
u(0,t) &= u(1,t) = 0.
\end{aligned}
$$

# A linear example with inhomogeneity

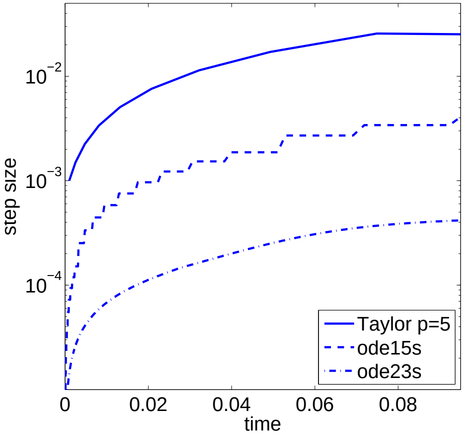


Figure: Step sizes taken by the exponential Taylor method with $p = 5$, ode15s and ode23s. Number of steps taken 11, 148 and 868, respectively.

# Conclusions

- Presented the Exponential Taylor Methods
- Second order convergence for the semilinear equations
- Third order convergence for the linearized semilinear equations
- Methods of arbitrary order for the linear problems