Higher-order exponential Rosenbrock-type methods

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joint work with Alexander Ostermann

Innovative Time Integration

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Outline

- 1. **Problem class**
- 2. **Exponential Rosenbrock-type methods (EXPRB)**
- 3. **A new approach to construct stiff order conditions**
- 4. **Error analysis**
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Problem class

Consider the time integration of large systems of stiff DEs:

$$u'(t) = F(t, u(t)), \quad u(t_0) = u_0$$

characterized by a Jacobian that possesses eigenvalues with large negative real parts.

Stiffness: the implicit Euler method works better than the explicit Euler method (Explicit methods lack stability and are forced to use tiny time steps).

$\Longrightarrow$ Exponential Integrators: very good approach!
Hochbruck, Ostermann (Acta Numerica, Vol. **19**, 2010).

Method: Linearised exponential integrators

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

Idea: Linearising the problem in each step at u_n to get

$$u' = J_n u + g_n(u),$$

$$J_n = DF(u_n) = A + \frac{\partial g}{\partial u}(u_n), \quad g_n(u) = g(u) - \frac{\partial g}{\partial u}(u_n)u.$$

By the variation of constants formula:

$$u(t_{n+1}) = \mathrm{e}^{hJ_n}u(t_n) + \int_0^h \mathrm{e}^{(h-\tau)J_n} g_n(u(t_n+\tau))d\tau$$

Hochbruck, Ostermann, Schweitzer (SINUM, Vol. **47**, 2009), Tokman (JCP, Vol. **213**, 2006)

Exponential Rosenbrock-Euler method

Approximating $g_n(u(t_n+\tau)) \approx g_n(u_n)$ yields the exponential Rosenbrock-Euler method:

$$u_{n+1} = \mathrm{e}^{hJ_n} u_n + \int_0^h \mathrm{e}^{(h-\tau)J_n} g_n(u_n) d\tau = \mathrm{e}^{hJ_n} u_n + h\,\varphi_1(hJ_n)\, g_n(u_n)$$

where $\quad \varphi_1(hJ_n) = \frac{1}{h}\int_0^h \mathrm{e}^{(h-\tau)J_n} d\tau = \int_0^1 \mathrm{e}^{(1-\theta)hJ_n} d\theta.$

The method can be reformulated as

$$\begin{aligned} u_{n+1} &= \mathrm{e}^{hJ_n} u_n + h\,\varphi_1(hJ_n)\big(F(u_n) - J_n u_n\big) \\ &= u_n + h\,\varphi_1(hJ_n) F(u_n). \end{aligned}$$

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

The method has order two.

Exponential Rosenbrock-type methods (EXPRB)

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

$$u_{n+1} = u_n + h_n \varphi_1(h_n J_n) F(u_n) + h_n \sum_{i=2}^{s} b_i(h_n J_n) D_{ni}$$

- $D_{ni} = g_n(U_{ni}) - g_n(u_n)$ are expected to be small in norm
- $a_{ij}(z)$ and $b_i(z)$ are linear combinations of

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

▶ Advantage for efficient implementation.

See: Hochbruck, Ostermann, Schweitzer (SINUM, Vol. **47**, 2009).

Analytic framework

Let

$$J = J(u) = \frac{\partial F}{\partial u}(u)$$

be the Fréchet derivative of F in a neighborhood of u.

Assumption 1. The linear operator J is the generator of a C_0 semigroup e^{tJ} on a Banach space X. This implies

$$\|\mathrm{e}^{tJ}\|_{X\leftarrow X} \leq C\mathrm{e}^{\omega t}, \quad t \geq 0.$$

Assumption 2. The problem possesses a sufficiently smooth solution u with derivative in X;
g is sufficiently often Fréchet differentiable in a strip along the exact solution.

Typical examples: advection-diffusion-reaction equations, the Chafee-Infante problem, Allen-Cahn equations (D. Henry, 1981).

New approach to construct stiff order conditions

- **Previous approaches:** Insert the exact solution into the numerical scheme $\Longrightarrow$ defects $\overset{\text{estimate}}{\Longrightarrow}$ order conditions.
- **New approach:**
  - exponential Rosenbrock-type methods

$$u_{n+1} = u_n + h_n \varphi_1(h_n J_n) F(u_n) + h_n \sum_{i=2}^{s} b_i(h_n J_n) D_{ni}$$

can be seen as small perturbations of exponential Rosenbrock-Euler method which has order two

$$u_{n+1} = u_n + h_n \varphi_1(hJ_n) F(u_n).$$

To get higher order methods $\Longrightarrow$ investigate D_{ni}

EXPRB: local error analysis

We also consider:

$$u'(t) = F\big(u(t)\big) = \tilde{J}_n u(t) + \tilde{g}_n\big(u(t)\big), \quad u(t_n) =: \tilde{u}_n$$

here

$$\tilde{J}_n = A + \frac{\partial g}{\partial u}(\tilde{u}_n)$$

$$\tilde{g}_n = F(u) - \tilde{J}_n u = g(u) - \frac{\partial g}{\partial u}(\tilde{u}_n)u.$$

$$\widehat{U}_{ni} = \tilde{u}_n + c_i h_n \varphi_1(c_i h_n \tilde{J}_n)F(\tilde{u}_n) + h_n \sum_{j=2}^{i-1} a_{ij}(h_n \tilde{J}_n)\widehat{D}_{nj},$$

$$\hat{u}_{n+1} = \tilde{u}_n + h_n \varphi_1(h_n \tilde{J}_n)F(\tilde{u}_n) + h_n \sum_{i=2}^{s} b_i(h_n \tilde{J}_n)\widehat{D}_{ni},$$

$$\widehat{D}_{ni} = \tilde{g}_n(\widehat{U}_{ni}) - \tilde{g}_n(\tilde{u}_n).$$

A new approach to construct stiff order conditions

Expanding $\widehat{D}_{ni}$ into a Taylor series at $\tilde{u}_n$, we get:

$$\widehat{D}_{ni} = \sum_{q=2}^{k} \frac{h_n^q}{q!} \tilde{g}_n^{(q)}(\tilde{u}_n)(\underbrace{V_i, ..., V_i}_{q-times}) + \mathcal{O}(h_n^{k+1}),$$

where

$$V_i = \frac{1}{h_n}(\widehat{U}_{ni} - \tilde{u}_n) = c_i \varphi_1(c_i h_n \tilde{J}_n) F(\tilde{u}_n) + \sum_{j=2}^{i-1} a_{ij}(h_n \tilde{J}_n) \widehat{D}_{nj}.$$

Remark. *As $u(t)$ is smooth, we have*

a) $\tilde{g}_n'(\tilde{u}_n) = 0.$

b) $\tilde{J}_n u^{(k)}(t)$ *are bounded for all* $k = 0, 1, 2, \ldots$ *In particular,*
$\tilde{J}_n \tilde{u}_n' = \tilde{u}_n''$; $\quad \tilde{J}_n \tilde{u}_n'' = \tilde{u}_n^{(3)} - \tilde{g}_n''(\tilde{u}_n)(\tilde{u}_n', \tilde{u}_n').$

A new approach to construct stiff order conditions

Lemma

For $k = 4$, by employing the above remark, we obtain:

$$\varphi_1(c_i h_n \tilde{J}_n) F(\tilde{u}_n) = \tilde{u}'_n + \frac{1}{2!} c_i h_n \tilde{u}''_n + \frac{1}{3!} c_i^2 h_n^2 \Big(\tilde{u}_n^{(3)} - 3! \varphi_3(c_i h_n \tilde{J}_n) \tilde{g}''_n(\tilde{u}_n)(\tilde{u}'_n, \tilde{u}'_n) \Big) + \mathcal{O}(h_n^3).$$

Corollary

$$V_i = c_i \tilde{u}'_n + \frac{1}{2!} c_i^2 h_n \tilde{u}''_n + \frac{1}{3!} c_i^3 h_n^2 \tilde{u}_n^{(3)} + h_n^2 \psi_{3,i} \tilde{g}''_n(\tilde{u}_n)(\tilde{u}'_n, \tilde{u}'_n) + \mathcal{O}(h_n^3),$$

where

$$\psi_{3,i} = \sum_{j=2}^{i-1} a_{ij}(h_n \tilde{J}_n) \frac{c_j^2}{2!} - c_i^3 \varphi_3(c_i h_n \tilde{J}_n).$$

Numerical and exact solution at time t_{n+1}

Using the above Lemma, we obtain:

- $\hat{u}_{n+1} =$

$$\tilde{u}_n + h_n\varphi_1(h_n\tilde{J}_n)F(\tilde{u}_n) + h_n^3\Big(\sum_{i=2}^{s} b_i(h_n\tilde{J}_n)\frac{c_i^2}{2!}\Big)\tilde{g}_n''(\tilde{u}_n)(\tilde{u}_n',\tilde{u}_n') + h_n^4\Big(\sum_{i=2}^{s} b_i(h_n\tilde{J}_n)\frac{c_i^3}{3!}\Big)\mathbf{M} + h_n^5\Big(\sum_{i=2}^{s} b_i(h_n\tilde{J}_n)\frac{c_i^4}{4!}\Big)\mathbf{N} + h_n^5\sum_{i=3}^{s} b_i(h_n\tilde{J}_n)c_i\tilde{g}_n''(\tilde{u}_n)(\tilde{u}_n',\psi_{3,i}\tilde{g}_n''(\tilde{u}_n)(\tilde{u}_n',\tilde{u}_n')) + \mathcal{O}(h_n^6).$$

Exact solution t_{n+1} by the variation-of-constants formula:

$$\tilde{u}_{n+1} = u(t_{n+1}) = \mathrm{e}^{h_n\tilde{J}_n}\tilde{u}_n + h_n\int_0^1 \mathrm{e}^{(1-\theta)h_n\tilde{J}_n}\tilde{g}_n(u(t_n+\theta h_n))d\theta.$$

Expanding $\tilde{g}_n(u(t_n+\theta h_n))$ in a Taylor series at $u(t_n) = \tilde{u}_n$:

- $$\tilde{u}_{n+1} = u(t_{n+1}) = \tilde{u}_n + h_n\varphi_1(h_n\tilde{J}_n)F(\tilde{u}_n) + h_n^3\varphi_3(h_n\tilde{J}_n)\tilde{g}_n''(\tilde{u}_n)(\tilde{u}_n',\tilde{u}_n') + h_n^4\varphi_4(h_n\tilde{J}_n)\mathbf{M} + h_n^5\varphi_5(h_n\tilde{J}_n)\mathbf{N} + \mathcal{O}(h_n^6).$$

New stiff order conditions (up to order 5)

- Comparing $\hat{u}_{n+1}$ and $u(t_{n+1}) = \tilde{u}_{n+1}$ we obtain the stiff order conditions:

No.	order condition	order
1	$\sum_{i=1}^{s} b_i(Z) = \varphi_1(Z)$	1
2	$\sum_{j=1}^{i-1} a_{ij}(Z) = c_i\varphi_1(c_i Z)$	2
3	$\sum_{i=2}^{s} b_i(Z)c_i^2 = 2\varphi_3(Z)$	3
4	$\sum_{i=2}^{s} b_i(Z)c_i^3 = 6\varphi_4(Z)$	4
5 6	$\sum_{i=2}^{s} b_i(Z)c_i^4 = 24\varphi_5(Z)$ $\sum_{i=3}^{s} b_i(Z)c_i K\Psi_{3,i}(Z) = 0$	5

- Again, we see the result up to order 4 which resulted in **exprb43** by Hochbruck, Ostermann, Schweitzer (SINUM, Vol. **47**, 2009).

Luan, Ostermann (submitted, 2012a)

Error analysis: Stability bounds

Solving the error recursion yields

$$e_n = \sum_{i=0}^{n-1} h_i \Big(\prod_{j=1}^{n-i-1} \mathrm{e}^{h_{n-j} J_{n-j}} \Big) \big(T_i + \frac{1}{h_i} \tilde{e}_{i+1} \big).$$

$\Longrightarrow$ stability bounds for the discrete evolution operators are crucial.

Theorem (M.Hochbruck, A. Ostermann, J. Schweitzer, 2009)

Under Assumptions 1 and 2, there exist constants C, C_E and Ω such that

$$\| \prod_{j=0}^{n} \mathrm{e}^{h_{n-j} J_{n-j}} \|_{X \leftarrow X} \leq C \mathrm{e}^{\Omega(h_0 + \ldots + h_n) + C_E \sum_{j=1}^{n} \|e_j\|}.$$

as long as the numerical solution remains in a neighborhood of the exact solution.

Convergence results: main result

Theorem (Th. 3.7 (V.T. Luan, A. Ostermann, 2012))

Under the previous assumptions, consider an EXPRB method that fulfills the order conditions up to order p for some $2 \leq p \leq 5$. *Further, let the step size sequence* h_i *satisfy* $\sum_{k=1}^{n-1} \sum_{i=0}^{k-1} h_i^{p+1} \leq C_H$ *(uniformly in* $t_0 \leq t_n \leq T$*). Then, for* C_H *sufficiently small, the method converges with order p. In particular, the numerical solution satisfies the error bound*

$$\|u_n - u(t_n)\| \leq C \sum_{i=0}^{n-1} h_i^{p+1}$$

uniformly on $t_0 \leq t_n \leq T$. *The constant C is independent of the chosen step size sequence satisfying the above condition.*

Convergence results: refined result

Assumption 3. We assume that the operators A and $g(u)$:

$$\tilde{J}_n \mathbf{N} \quad \text{and } \tilde{J}_n \tilde{g}''_n(\tilde{u}_n)\big(\tilde{u}'_n, \psi_{3,i} \tilde{g}''_n(\tilde{u}_n)(\tilde{u}'_n, \tilde{u}'_n)\big)$$

are uniformly bounded on X for all $2 \le i \le s$.

Theorem (Th. 3.8 (V.T. Luan, A. Ostermann, 2012))

In extension of the above theorem, assume the above reasonable assumption holds and that the order conditions are satisfied up to order $p-1$ and $\psi_p(0) = 0$. The conditions for order p are satisfied with $b_i(0)$ instead of $b_i(z)$ for $2 \le i \le s$. Then, the method converges with order p.

No.	order condition	order
1	$\sum_{i=1}^{s} b_i(Z) = \varphi_1(Z)$	1
2	$\sum_{j=1}^{i-1} a_{ij}(Z) = c_i \varphi_1(c_i Z)$	2
3	$\sum_{i=2}^{s} b_i(Z) c_i^2 = 2\varphi_3(Z)$	3
4	$\sum_{i=2}^{s} b_i(Z) c_i^3 = 6\varphi_4(Z)$	4
5 6	$\sum_{i=2}^{s} b_i(0) c_i^4 = 24\varphi_5(0)$ $\sum_{i=3}^{s} b_i(0) c_i K \Psi_{3,i}(Z) = 0$	5

The 5-stage methods of order 5

$$b_i = b_i(h_n J_n),\ a_{ij} = a_{ij}(h_n J_n),\ \text{and } \varphi_{i,j} = \varphi_i(c_j h_n J_n).$$

exprb54s5:

$$\begin{array}{c|ccccc}
0 & & & & & \\
\frac{1}{2} & \frac{1}{2}\varphi_{1,2} & & & & \\
\frac{1}{2} & \frac{1}{2}\varphi_{1,3} - \varphi_{3,3} & \varphi_{3,3} & & & \\
\frac{1}{3} & \frac{1}{3}\varphi_{1,4} - \frac{8}{27}\varphi_{3,4} & a_{42} & \frac{8}{27}\varphi_{3,4} - a_{42} & & \\
1 & \varphi_{1,5} - 8\varphi_{3,5} - \frac{5}{9}a_{54} & a_{52} & a_{53} & a_{54} & \\
\hline
 & \varphi_1 - 50\varphi_3 + 360\varphi_4 - 864\varphi_5 & 0 & b_3 & b_4 & b_5 \\
 & \varphi_1 - 50\varphi_3 + 360\varphi_4 & 0 & \breve{b}_3 & 81\varphi_3 - 729\varphi_4 & \varphi_3 - 15\varphi_4
\end{array}$$

with $b_3 = -32\varphi_3 + 384\varphi_4 - 1152\varphi_5$,
$b_4 = 81\varphi_3 - 729\varphi_4 + 1944\varphi_5$, $b_5 = \varphi_3 - 15\varphi_4 + 72\varphi_5$,
$a_{52} = 8\varphi_{3,5} - \frac{4}{9}a_{54} - a_{53}$, $\breve{b}_3 = -32\varphi_3 + 384\varphi_4$.
Coefficients a_{42}, a_{53}, and a_{54}: free parameters.

The 3-stage and 4-stage methods of order 5

exprb53s3:

$$
\begin{array}{c|ccc}
0 & & & \\
\frac{1}{2} & \frac{1}{2}\varphi_{1,2} & & \\
\frac{9}{10} & \frac{9}{10}\varphi_{1,3} - \frac{27}{25}\varphi_{3,2} - \frac{729}{125}\varphi_{3,3} & \frac{27}{25}\varphi_{3,2} + \frac{729}{125}\varphi_{3,3} & \\
\hline
 & \varphi_1 - \frac{1208}{81}\varphi_3 + \frac{1120}{27}\varphi_4 & 18\varphi_3 - 60\varphi_4 & -\frac{250}{81}\varphi_3 + \frac{500}{27}\varphi_4 \\
 & \varphi_1 - 8\varphi_3 & 8\varphi_3 & 0
\end{array}
$$

exprb54s4:

$$
\begin{array}{c|cccc}
0 & & & & \\
\frac{1}{4} & \frac{1}{4}\varphi_{1,2} & & & \\
\frac{1}{2} & \frac{1}{2}\varphi_{1,3} - 4\varphi_{3,3} & 4\varphi_{3,3} & & \\
\frac{9}{10} & 0 & \frac{6}{5}\varphi_{1,4} - \frac{972}{125}\varphi_{3,4} & \frac{972}{125}\varphi_{3,4} - \frac{3}{10}\varphi_{1,4} & \\
\hline
 & \varphi_1 - \frac{1208}{81}\varphi_3 + \frac{1120}{27}\varphi_4 & 0 & 18\varphi_3 - 60\varphi_4 & -\frac{250}{81}\varphi_3 + \frac{500}{27}\varphi_4 \\
 & \varphi_1 - 56\varphi_3 + 288\varphi_4 & 64\varphi_3 - 384\varphi_4 & -8\varphi_3 + 96\varphi_4 & 0
\end{array}
$$

Non-autonomous case

$$u'(t) = F(t, u(t)), \quad u(t_0) = u_0.$$

By rewriting the problem in autonomous form:

$$
\begin{aligned}
U_{ni} &= u_n + c_i h_n \varphi_1(c_i h_n J_n) F(t_n, u_n) \\
&\qquad + h_n^2 c_i^2 \varphi_2(c_i h_n J_n) v_n + h_n \sum_{j=2}^{i-1} a_{ij}(h_n J_n) D_{nj}, \\
u_{n+1} &= u_n + h_n \varphi_1(h_n J_n) F(t_n, u_n) + h_n^2 \varphi_2(h_n J_n) v_n \\
&\qquad + h_n \sum_{i=2}^{s} b_i(h_n J_n) D_{ni},
\end{aligned}
$$

with $J_n = \frac{\partial F}{\partial u}(t_n, u_n)$, $v_n = \frac{\partial F}{\partial t}(t_n, u_n)$

$D_{nj} = g_n(t_n + c_j h_n, U_{nj}) - g_n(t_n, u_n)$,

$g_n(t, u) = F(t, u) - J_n u - v_n v$.

Example 1: 1D semilinear parabolic problem

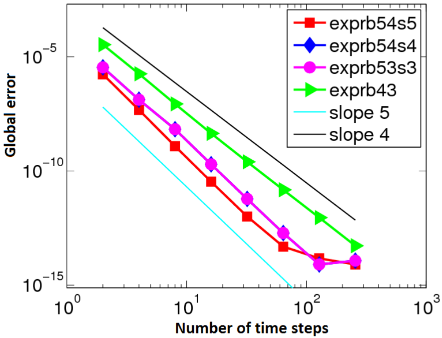
Hochbruck-Ostermann's example: for $u = u(x,t)$

$$\frac{\partial u}{\partial t} - \partial_{xx} u = \frac{1}{1+u^2} + \Phi(x,t), \qquad (x,t) \in [0,1]^2$$

BC: homogeneous Dirichlet.

Φ is chosen in such a way $u(x,t) = x(1-x)\mathrm{e}^t$.

Standard FDM, $\Delta x = 1/200 \Longrightarrow$ **stiff problem!**$(\lambda_{max} \approx -10^5)$



Example 2: 2D advection-diffusion-reaction eq.

For $u = u(x, y, t)$: $(x, y) \in [0, 1]^2, t \in [0, 0.08]$, we consider

$$\frac{\partial u}{\partial t} = \epsilon(\partial_{xx} u + \partial_{yy} u) - \alpha(u_x + u_y) + \gamma u\big(u - \frac{1}{2}\big)(1 - u)$$

IC: $u(x, y, 0) = 256((1 - x)x(1 - y)y)^2 + 0.3$

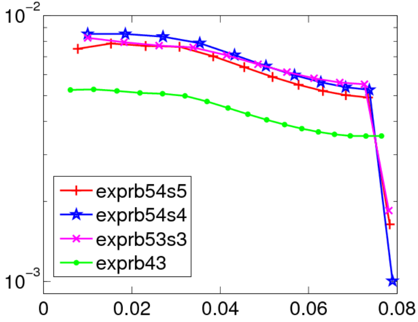
BC: Homogeneous Neumann

Parameters: $\epsilon = 1/100, \alpha = -10$, and $\gamma = 100$
Using standard FDM with $\Delta x = \Delta y = 1/100$

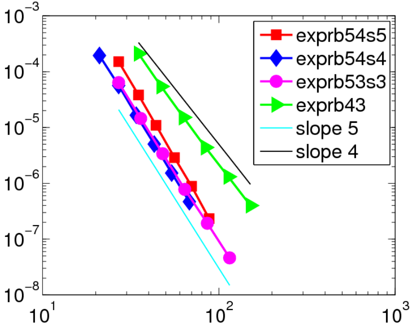
$\Longrightarrow$ **mildly stiff problem!**

This example was considered in Hochbruck, Ostermann, Schweitzer (SINUM, Vol. **47**, 2009) in which used **exprb43**.

Example 2: 2D advection-diffusion-reaction eq.



(a) Time versus step sizes
TOL : accuracy $\approx 4.10^{-3}$



(b) Number of time steps versus accuracy
$ATOL = RTOL = 10^{-4}, 10^{-4.5}, ..., 10^{-6.5}$

Conclusions

- A new and simpler approach has been proposed to derive high-order EXPRB methods (even extend to methods of arbitrary order)
- EXPRB methods of order 5 were constructed with five, four and three stages only!
- Convergence results were proved for variable step size methods.

Reference: V. T. Luan, A. Ostermann, Exponential Rosenbrock methods of order five - derivation, analysis and numerical comparisons (submitted, 2012a).

Thank you very much for your attention!