# Exponential Integrators - History and Recent Developments

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# Outline

- Introduction and Motivation
- Main classes of exponential integrators
  - Exponential linear multistep methods
  - Exponentila Runge–Kutta methods
  - Exponential general linear methods
- Exponential integrators for parabolic PDEs
- Exponential integrators and Schrödinger equation
- Exponential integrators for oscillatory problems
- Implementation issues
- Conclusions
- Open problems

# Introduction and Motivation

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- Lawson'69 - multistage type

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A new interest in exponential integrators for semilinear problems

$$u' = Lu + N(u,t), \ u(t_0) = u_0, \tag{1}$$

where $u : \mathbb{R} \to \mathbb{R}^d, \ L \in \mathbb{R}^{d\times d}, N : \mathbb{R}^d \to \mathbb{R}^d$ and $d$ is a discretization parameter equal to the number of spatial grid points.

# Exponential multistep methods

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$$v(t) = e^{-tL}u(t).$$

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Solve exactly the linear part and then make a change of variables (also known as Lawson transformation)

$$v(t) = e^{-tL} u(t).$$

The initial value problem written in the new variable is then given by

$$v'(t) = e^{-tL} N(e^{tL} v(t), t) = \mathrm{g}(v,t), \qquad v(t_0) = v_0,$$

where $v_0 = e^{-t_0 L} u_0$.

# Integrating Factor

Consider the Jacobian of the transformed equation

$$\frac{\partial \mathrm{g}}{\partial v} = e^{-tL}\,\frac{\partial N}{\partial u}\,e^{tL},$$

Since $e^{-tL} = (e^{tL})^{-1}$, it follows that the eigenvalues of $\partial \mathrm{g}/\partial v$ are those of $\partial N/\partial u$.

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The idea now is to apply any numerical method on the transformed equation and then to transform back the result into the original variable.

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For example:
IF Euler method is

$$u_n = e^{hL}u_{n-1} + e^{hL}hN_{n-1},$$

where $h$ represents the stepsize of the method and $N_{n-1} = N(u_{n-1}, t_{n-1})$.

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IF implicit Euler method is

$$u_n = e^{hL}u_{n-1} + e^{hL}hN_n.$$

# More IF multistep methods

Similarly $k$-step IF Adams methods are defined as

$$u_n = e^{hL} u_{n-1} + \sum_{i=0}^{k} \beta_i e^{ihL} h N_{n-i},$$

where $\beta_i$ are the coefficients of the Adams method and $N_{n-i} = N(u_{n-i}, t_{n-i})$ for $i = 0, 1, 2, \ldots, k$.

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IF BDF methods are defined as

$$u_n = \sum_{i=1}^{k} \alpha_i e^{ihL} u_{n-i} + \beta_0 h N_n,$$

where $\beta_0$ and $\alpha_i$ are the coefficients of the underlying BDF method.

# ETD multistep methods

Similar approach to the $IF$ methods, but we do not make a complete change of variables. Premultiplying the original problem (1) by the integrating factor $e^{-tL}$ we get

$$\begin{aligned} e^{-tL}u' &= e^{-tL}Lu + e^{-tL}N(u,t), \\ (e^{-tL}u)' &= e^{-tL}N(u,t). \end{aligned}$$

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Integrating the last equation between $t_{n-1}$ and $t_n = t_{n-1} + h$, we obtain

$$\text{(vcf)} \quad u(t_{n-1}+h) = e^{hL}u_{n-1} + \int_0^h e^{(h-\tau)L} N(u(t_{n-1}+\tau), t_{n-1}+\tau)\mathrm{d}\tau.$$

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- When $N(u(t_{n-1}+\tau), t_{n-1}+\tau) \approx N_{n-1}$ we obtain the ETD Euler method

$$u_n = e^{hL}u_{n-1} + \phi^{[1]}(hL)hN_{n-1},$$

where $\phi^{[1]}(z)$ is

$$\phi^{[1]}(z) = \frac{e^z - 1}{z}.$$

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- In general, using higher order approximations to the nonlinear part $N$ we obtain

  ETD Adams–Bashforth (Nørsett'69,..., Cox–Matthews'02).

# An alternative approach

An alternative approach for deriving exponential Adams methods, both explicit and implicit, is to use the following result (Beylkin at al.'98)

**Lemma 1.** *The exact solution of the initial value problem*

$$u' = Lu + N(u,t), \qquad u(t_{n-1}) = u_{n-1},$$

*can be expressed in the form*

$$u(t_{n-1}+h) = e^{hL}u_{n-1} + \sum_{i=0}^{\infty} h^{i+1}\phi^{[i+1]}(hL)N_{n-1}^{(i)},$$

*where* $N_{n-1}^{(i)} = \frac{d^i}{dt^i}\Big|_{t=t_{n-1}} N(u(t),t)$, *and* $\phi^{[i]}(z)$ *are recursively defined as*

$$\phi^{[0]}(z) = e^z, \quad \phi^{[i+1]}(z) = \frac{\phi^{[i]}(z) - \frac{1}{i!}}{z}, \quad \text{for } i = 0,1,2,\ldots.$$

# ETD Adams methods

The exact solution

$$u(t_{n-1}+h) = e^{hL}u_{n-1} + \sum_{i=0}^{\infty} h^{i+1}\phi^{[i+1]}(hL)N_{n-1}^{(i)}.$$

Its numerical approximation

$$u_n = e^{hL}u_{n-1} + h\sum_{l=0}^{k}\beta_l N_{n-l},$$

where $\beta_0, \beta_1, \ldots, \beta_k$ are coefficients which have to be computed by expanding in Taylor series the nonlinear terms.

# ETD Adams methods

$$u_n = e^{hL} u_{n-1} + h \sum_{l=0}^{k} \beta_l N_{n-l},$$

| k | $\beta_1$ | $\beta_2$ | $\beta_3$ | $\beta_4$ |
|---|---|---|---|---|
| 1 | $\phi^{[1]}$ | 0 | 0 | 0 |
| 2 | $\phi^{[1]} + \phi^{[2]}$ | $-\phi^{[2]}$ | 0 | 0 |
| 3 | $\phi^{[1]} + \frac{3}{2}\phi^{[2]} + \phi^{[3]}$ | $-2(\phi^{[2]} + \phi^{[3]})$ | $\frac{1}{2}\phi^{[2]} + \phi^{[3]}$ | 0 |
| 4 | $\phi^{[1]} + \frac{11}{6}\phi^{[2]} + 2\phi^{[3]} + \phi^{[4]}$ | $-3\phi^{[2]} - 5\phi^{[3]} - 3\phi^{[4]}$ | $\frac{3}{2}\phi^{[2]} + 4\phi^{[3]} + 3\phi^{[4]}$ | X |

where X $= -\frac{1}{3}\phi^{[2]} - \phi^{[3]} - \phi^{[4]}$

Coefficients of ETD Adams–Bashforth methods.

# ETD Adams methods

$$u_n = e^{hL} u_{n-1} + h \sum_{l=0}^{k} \beta_l N_{n-l},$$

| k | $\beta_0$ | $\beta_1$ | $\beta_2$ | $\beta_3$ |
|---|---|---|---|---|
| 0 | $\phi^{[1]}$ | 0 | 0 | 0 |
| 1 | $\phi^{[2]}$ | $\phi^{[1]} - \phi^{[2]}$ | 0 | 0 |
| 2 | $\frac{1}{2}\phi^{[2]} + \phi^{[3]}$ | $\phi^{[1]} - 2\phi^{[3]}$ | $-\frac{1}{2}\phi^{[2]} + \phi^{[3]}$ | 0 |
| 3 | $\frac{1}{3}\phi^{[2]} + \phi^{[3]} + \phi^{[4]}$ | $\phi^{[1]} + \frac{1}{2}\phi^{[2]} - 2\phi^{[3]} - 3\phi^{[4]}$ | $-\phi^{[2]} + \phi^{[3]} + 3\phi^{[4]}$ | X |

where X $= \frac{1}{6}\phi^{[2]} - \phi^{[4]}$

Coefficients of ETD Adams–Moulton methods.

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$$u_n = e^{hL} u_{n-1} + h \sum_{l=0}^{k} \beta_l N_{n-l},$$

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where X $= \frac{1}{6}\phi^{[2]} - \phi^{[4]}$

Coefficients of ETD Adams–Moulton methods.

It is not possible to construct ETD BDF methods !

# Exponential Runge–Kuta methods

IF Runge–Kuta methods (Lawson'69)

For simplicity, we represent the initial value problem (1) in autonomous form

$$u' \; = \; Lu + N(u(t)), \quad u(t_0) = u_0.$$

Similarly to the the multistep case, the idea now is to apply an arbitrary $s$-stage Runge–Kutta method to the transformed equation

$$v'(t) = e^{-tL} N(e^{tL} v(t)) = \mathrm{g}(v), \qquad v(t_0) = v_0,$$

and then to transform back the result into the original variable. If $\mathcal{A} = (\alpha_{ij})$, $b = (\beta_i)$ and $c = (c_i)$ are the coefficients of the underlying multistage method then in terms of the original variable the computations performed are

# Exponential Runge–Kuta methods

IF Runge–Kuta methods (Lawson'69)

$$\begin{aligned}
U_1 &= u_0 \\
U_2 &= e^{c_2 hL}(u_0 + \alpha_{21} hN(U_1)) \\
U_3 &= e^{c_3 hL}(u_0 + \alpha_{31} hN(U_1) + \alpha_{32} h e^{-c_2 hL} N(U_2)) \\
U_4 &= e^{c_4 hL}(u_0 + \alpha_{41} hN(U_1) + \alpha_{42} h e^{-c_2 hL} N(U_2) \\
&\quad + \alpha_{43} h e^{-c_3 hL} N(U_3)) \\
u_1 &= e^{hL}(u_0 + \beta_1 hN(U_1) + \beta_2 h e^{-c_2 hL} N(U_2) \\
&\quad + \beta_3 h e^{-c_3 hL} N(U_3) + \beta_4 h e^{-c_4 hL} N(U_4))
\end{aligned}$$

# Exponential Runge–Kuta methods

IF Runge–Kuta methods (Lawson'69)

General form of an order 4 integrating factor method is

$$\left[\begin{array}{cccc|c} 0 & 0 & 0 & 0 & e^{c_1 hL} \\ \alpha_{21} e^{c_2 hL} & 0 & 0 & 0 & e^{c_2 hL} \\ \alpha_{31} e^{c_3 hL} & \alpha_{32} e^{(c_3 - c2) hL} & 0 & 0 & e^{c_3 hL} \\ \alpha_{41} e^{c_4 hL} & \alpha_{42} e^{(c_3 - c2) hL} & \alpha_{43} e^{(c_4 - c3) hL} & 0 & e^{c_4 hL} \\ \hline \beta_1 e^{hL} & \beta_2 e^{(1 - c_2) hL} & \beta_3 e^{(1 - c_3) hL} & \beta_4 e^{(1 - c_4) hL} & e^{hL} \end{array}\right]$$

# Exponential Runge–Kutta methods

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- Uniformly distributed $c$ vector provides cheapest methods.
- This structure requires only classical order conditions.
- IF RK methods perform poorly for stiff problems.

# History of ETD RK methods

ETD Runge–Kuta methods

- Friedli'78
  - Explicit ETD RK methods, nonstiff order 5 conditions
- Steihaug and Wolfbrand'79
  - $W$ methods, order conditions
- Hairer, Bader and Lubich'82
  - Linearly implicit methods
- Strehmel and Weiner'82
  - Adaptive RK methods, order theory, B-stability

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This methods can be seen as exponential integrators which use Padé approximations to the exponential and the related functions

# History of ETD RK methods

Pure exponential Runge–Kuta methods

- Hochbruck and Lubich'97
  - Rosenbrock-like exponential integrators, which use the first ETD function $\phi^{[1]}$
- Munthe-Kaas'99
  - Runge–Kutta Munthe-Kaas (RKMK) methods with affine action
- Celledoni Marthinsen and Owren'03
  - Commutator Free (CF) Lie group methods
- Krogstad'03
  - Generalized IF methods, connection with CF
- Hochbruck and Osterman'04
  - Exponential collocation methods, convergence analyze for parabolic PDEs

# General format of Exp. RK methods

Aims:

- Construct a class of exponential integrators which overcome the stiffness by using a set of precomputed functions $\phi^{[l]}$ along with evaluations of the nonlinear part of the differential equation.
- Include all exponential integrators of Runge–Kutta type in one framework.
- Derive the nonstiff order theory for this class of method

# The $\phi$ functions

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$$\phi^{[i]}(c_j)(hL) = e^{(c_i - c_j)hL} \quad i = 1, 2, \ldots .$$

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$$\begin{aligned} \phi^{[0]}(c_j)(hL) &= e^{c_j hL}, \\ \phi^{[i]}(c_j)(hL) &= \frac{\phi^{[i-1]}(c_j)(hL) - \frac{1}{(i-1)!}}{c_j hL} \end{aligned}$$

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$$\phi^{[i]}(c_j)(hL) = e^{(c_i - c_j)hL} \quad i = 1, 2, \ldots,$$

- The ETD $\phi$ functions are

$$\phi^{[i]}(c_j)(hL) = \frac{1}{i!}I + \frac{c_j}{(i+1)!}hL + \frac{c_j^2}{(i+2)!}(hL)^2 + \cdots \quad i = 1, 2, \ldots.$$

# The $\phi$ functions

In general, for $l \in \mathbb{N}$ and $\lambda \in \mathbb{R}$, the $\phi^{[l]}$ functions could be

$$\phi^{[l]}(\lambda)(hL) = \sum_{j \geq 0} \phi_j^{[l]}(\lambda)(hL)^j,$$

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and must:

- Be computed exactly or to arbitrary high order cheaply
- Map the spectrum of $hL$ to a bounded region

Given the IF and ETD $\phi$ functions as basis elements then
- linear combinations
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- inverses
produce mehods.

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Given the IF and ETD $\phi$ functions as basis elements then
- linear combinations
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produce mehods.
Other choices are also posible (approximations with trigonometric polynomials in vcf).
The exact structure of $\phi^{[l]}$, which leads to methods is still unclear!

# Formulation of the methods

The computations performed are

$$
\begin{aligned}
U_i &= \sum_{j=1}^{s} \sum_{l=1}^{m} \alpha_{ij}^{[l]} \phi^{[l]}(c_i)(hL) h N(U_j) + e^{c_i hL} u_{n-1}, \\
u_n &= \sum_{j=1}^{s} \sum_{l=1}^{m} \beta_{j}^{[l]} \phi^{[l]}(1)(hL) h N(U_j) + e^{hL} u_{n-1},
\end{aligned}
$$

where $m$ puts a limit on the number of $\phi^{[l]}$ functions which can be computed, $h$ represents the stepsize and $U_i$ denotes the internal stage approximation.

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Interpreted in a Runge–Kutta type tableau

$$
\begin{array}{c|c|c|c|c|c}
 & \phi^{[1]} & \phi^{[2]} & & \phi^{[m-1]} & \phi^{[m]} \\
c & \alpha^{[1]} & \alpha^{[2]} & \cdots & \alpha^{[m-1]} & \alpha^{[m]} \\
\hline
 & \beta^{[1]^T} & \beta^{[2]^T} & \cdots & \beta^{[m-1]^T} & \beta^{[m]^T}
\end{array}
$$

# Nonstiff order conditions

Use rooted trees and B-series.

Represent the elementary differentials using trees:

- Associate a closed node with $L$ and an open node with $N$
- 2T$^*$ - Bi-coloured rooted trees with one child closed nodes

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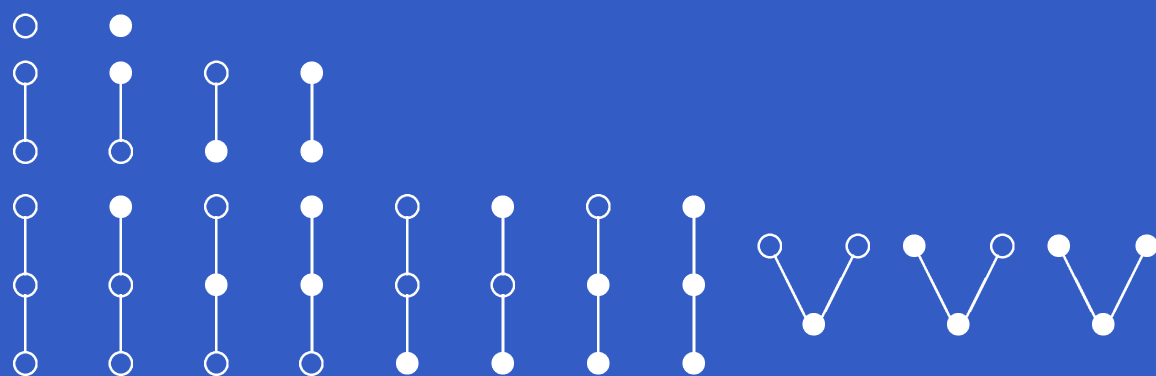
Order 1:
Order 2:
Order 3:



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| $n$ | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---|---|---|---|---|---|---|---|---|---|---|
| $\theta_n$ | 2 | 4 | 11 | 34 | 117 | 421 | 1589 | 6162 | 24507 | 99268 |
| $\Theta = \sum_i^n \theta_n$ | 2 | 6 | 17 | 51 | 168 | 589 | 2178 | 8340 | 32847 | 132115 |

The number of rooted trees in $2$T$^*$ for all orders up to ten.

# Elementary differentials and B-series

The elementary differentials are recursively generated as

$$F(\tau)(u) = \begin{cases} LF(\tau_1)(u) & \text{if } \tau = [\circ; \tau_1] \\ N^{(\ell)}(u)(F(\tau_1)(u), \dots, F(\tau_\ell)(u)) & \text{if } \tau = [\bullet; \tau_1, \dots, \tau_\ell] \end{cases}$$

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For an elementary weight function $a : 2\mathrm{T}^* \to \mathbb{R}$ the B-series is

$$B(a,u) = a(\emptyset)u + \sum_{\tau \in 2\mathrm{T}^*} h^{|\tau|} \frac{a(\tau)}{\sigma(\tau)} F(\tau)(u)$$

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The elementary weight function for the exact solution is

$$a(\tau) = \frac{1}{\gamma(\tau)},$$

where $\gamma$ is the density of single coloured tree

# The lemmas

To obtain B-series expansions of the numerical solution we need three Lemmas.

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**Lemma 2.** *Let* $a : 2\mathrm{T}^* \to \mathbb{R}$, *with* $a(\emptyset) = 1$, *then*

$$hN(B(a,u)) = B(a',u),$$

*where*

$$a'(\tau) = \begin{cases} 0 & \text{if } \tau = [\circ; \tau_1] \\ a(\tau_1)\dots a(\tau_\ell) & \text{if } \tau = [\bullet; \tau_1, \dots, \tau_\ell] \end{cases}$$

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**Lemma 3.** *Let* $a : 2\mathrm{T}^* \to \mathbb{R}$*, with* $a(\emptyset) = 1$*, then*

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**Lemma 4.** *Let* $a : 2\mathrm{T}^* \to \mathbb{R}$*, then*

$$(hL)^l B(a,u) = B(\mathcal{L}^l a, u),$$

*where*

$$(\mathcal{L}^l a)(\tau) = \begin{cases} (\mathcal{L}^{l-1}a)(\tau_1) & \textit{if } \tau = [\circ; \tau_1] \\ 0 & \textit{if } \tau = [\bullet; \tau_1, \dots, \tau_\ell] \end{cases}$$

# The lemmas

**Lemma 5.** *Let $\psi_x(z)$ be a power series*

$$\psi_x(z) = \sum_{l \geq 0} x^{[l]} z^l$$

*and let $a : 2\mathrm{T}^* \to \mathbb{R}$, then*

$$\psi_x(hL)B(a,u) = B(\psi_x(\mathcal{L})a,u),$$

*where the elementary weight function satisfies, $(\psi_x(\mathcal{L})a)(\emptyset) = x^{[0]}a(\emptyset)$, and*

$$(\psi_x(\mathcal{L})a)(\tau) = \sum_{l \geq 0} x^{[l]}(\mathcal{L}^l a)(\tau)$$

# General rule

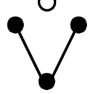
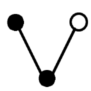
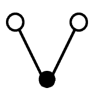
The rule for computing the elementary weight is:

- Attach ${b^{[i]}}^T$ to the root open (black) node
- Attach $A^{[i]}$ to all remaining nonterminal open (black) nodes
- Attach $A^{[i]}e$ to all terminal open (black) nodes
- Attach $C^{[i]}e$ to all terminal closed (white) nodes
- Attach $I$ to all remaining closed (white) nodes

where $i$ is the number of closed (white) nodes below the corresponding node and

$$A^{[i]} = \sum_{k=1}^{m} \phi_l^{[k]}(c)\alpha^{[k]}, \qquad {b^{[i]}}^T = \sum_{k=1}^{m} \phi_l^{[k]}(1){\beta^{[k]}}^T,$$

$$C^{[i]} = \frac{1}{(i+1)!}C^{i+1}.$$

| $\tau$ | $\gamma(\tau)$ | $F(\tau)(u)$ | $\alpha(\tau)$ |
|---|---|---|---|
|  | 1 | $N$ | ${b^{[0]}}^T e$ |
|  | 2 | $N'N$ | ${b^{[0]}}^T A^{[0]} e$ |
|  | 2 | $N'Lu$ | ${b^{[0]}}^T C^{[0]} e$ |
|  | 2 | $LN$ | ${b^{[1]}}^T e$ |
|  | 6 | $N'N'N$ | ${b^{[0]}}^T A^{[0]} A^{[0]} e$ |
|  | 6 | $N'N'Lu$ | ${b^{[0]}}^T A^{[0]} C^{[0]} e$ |
|  | 6 | $N'LN$ | ${b^{[0]}}^T A^{[1]} e$ |
|  | 6 | $LN'N$ | ${b^{[1]}}^T A^{[0]} e$ |
|  | 6 | $N'LLu$ | ${b^{[0]}}^T C_1 e$ |
|  | 6 | $LN'Lu$ | ${b^{[1]}}^T C^{[0]} e$ |
|  | 6 | $LLN$ | ${b^{[2]}}^T e$ |
|  | 3 | $N''(N, N)$ | ${b^{[0]}}^T (A^{[0]} e)(A^{[0]} e)$ |
|  | 3 | $N''(N, Lu)$ | ${b^{[0]}}^T (A^{[0]} e)(C^{[0]} e)$ |
|  | 3 | $N''(Lu, Lu)$ | ${b^{[0]}}^T (C^{[0]} e)(C^{[0]} e)$ |

Relations between elementary differentials and elementary weights

# Exp. RK methods for parabolic PDEs

- Stiff order theory for ETD RK methods for parabolic PDEs (Hochbruck–Ostermann'04)
  - Abstract ODEs on a Banach spaces
  - Sectorial operators
  - Locally Lipschitz continuous functions

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The error bounds depend form the space where the solution evolves!

It is not possible to construct stiff fourth order
explicit exponential Runge–Kutta method with only four stages

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The methods converge at least with their stage order. Higher and even fractional order of convergence is possible if additional temporal and spatial regularity are required Hochbruck–Ostermann'04.

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- No need of new order theory
- Higher stage order
- Solve the nonlinear equations by fixed-point iterations

# General linear methods

Consider $u' = f(u(t)), \quad u(t_0) = u_0, \quad f(u(t)) : \mathbb{R}^d \to \mathbb{R}^d$.
Assume that at the beginning of step number $n$, $r$ quantities

$$u_1^{[n-1]}, u_2^{[n-1]}, \ldots, u_r^{[n-1]},$$

are available from approximations computed in the previous steps. If

$$U_1, U_2, \ldots, U_s$$

are the internal stage approximations to the solution at points near the current time step, then then the quantities imported into and evaluated in step number $n$ are related by the equations

$$U_i = \sum_{j=1}^{s} a_{ij} h f(Uj) + \sum_{j=1}^{r} d_{ij} u_j^{[n-1]}, \quad i = 1, 2, \ldots s,$$

$$u_i^{[n]} = \sum_{j=1}^{s} b_{ij} h f(Uj) + \sum_{j=1}^{r} v_{ij} u_j^{[n-1]}, \quad i = 1, 2, \ldots r,$$

# Vector notations

$$U_i = \sum_{j=1}^{s} a_{ij} h f(Uj) + \sum_{j=1}^{r} d_{ij} u_j^{[n-1]}, \quad i = 1, 2, \ldots s,$$

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Introducing the vector notations

$$U = \begin{bmatrix} U_1 \\ U_2 \\ \vdots \\ U_s \end{bmatrix}, \quad f(U) = \begin{bmatrix} f(U_1) \\ f(U_2) \\ \vdots \\ f(U_s) \end{bmatrix}, \quad u^{[n-1]} = \begin{bmatrix} u_1^{[n-1]} \\ u_2^{[n-1]} \\ \vdots \\ u_r^{[n-1]} \end{bmatrix}, \quad u^{[n]} = \begin{bmatrix} u_1^{[n]} \\ u_2^{[n]} \\ \vdots \\ u_r^{[n]} \end{bmatrix},$$

# Vector notations

$$U_i = \sum_{j=1}^{s} a_{ij} h f(Uj) + \sum_{j=1}^{r} d_{ij} u_j^{[n-1]}, \quad i = 1, 2, \ldots s,$$

$$u_i^{[n]} = \sum_{j=1}^{s} b_{ij} h f(Uj) + \sum_{j=1}^{r} v_{ij} u_j^{[n-1]}, \quad i = 1, 2, \ldots r,$$

allows us to rewrite the above method in the following more compact form

$$\left[\begin{array}{c} U \\ \hline u^{[n]} \end{array}\right] = \left[\begin{array}{c|c} A \otimes I_d & D \otimes I_d \\ \hline B \otimes I_d & V \otimes I_d \end{array}\right] \left[\begin{array}{c} hf(U) \\ \hline u^{[n-1]} \end{array}\right],$$

where $\otimes$ is the Kronecker product and $I_d$ is the $d \times d$ identity matrix.

# Examples of GLMs

Consider $k$-step linear multistep methods of Adams type

$$u_n = u_{n-1} + h \sum_{i=0}^{k} \beta_i f(u_{n-i}).$$

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In general linear form

$$\left[\begin{array}{c} U_1 \\ \hline u_n \\ hf(U_1) \\ hf(u_{n-1}) \\ \vdots \\ hf(u_{n-k-1}) \end{array}\right] = \left[\begin{array}{c|ccccc} \beta_0 & 1 & \beta_1 & \cdots & \beta_{k-1} & \beta_k \\ \hline \beta_0 & 1 & \beta_1 & \cdots & \beta_{k-1} & \beta_k \\ 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & 0 \end{array}\right] \left[\begin{array}{c} hf(U_1) \\ \hline u_{n-1} \\ hf(u_{n-1}) \\ hf(u_{n-2}) \\ \vdots \\ hf(u_{n-k}) \end{array}\right].$$

# Examples of GLMs

The classical fourth order Runge–Kutta method

$$\begin{array}{c|cccc} 0 & & & & \\ \frac{1}{2} & \frac{1}{2} & & & \\ \frac{1}{2} & 0 & \frac{1}{2} & & \\ 1 & 0 & 0 & 1 & \\ \hline & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6} \end{array},$$

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1 & 0 & 0 & 1 & \\
\hline
 & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6}
\end{array},
$$

can be written as

$$
\left[\begin{array}{c}
U_1 \\ U_2 \\ U_3 \\ U_4 \\ \hline u_n
\end{array}\right]
=
\left[\begin{array}{cccc|c}
0 & 0 & 0 & 0 & 1 \\
\frac{1}{2} & 0 & 0 & 0 & 1 \\
0 & \frac{1}{2} & 0 & 0 & 1 \\
0 & 0 & 1 & 0 & 1 \\
\hline
\frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6} & 1
\end{array}\right]
\left[\begin{array}{c}
hf(U_1) \\ hf(U_2) \\ hf(U_3) \\ hf(U_4) \\ \hline u_{n-1}
\end{array}\right].
$$

# Examples of GLMs

It is not always appropriate to represent a Runge–Kutta method like a general liner method with $r = 1$. Example is the Lobatto IIIA method

$$\begin{array}{c|ccc} 0 & & & \\ \frac{1}{2} & \frac{5}{24} & \frac{1}{3} & -\frac{1}{24} \\ \frac{1}{2} & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \\ \hline & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \end{array}.$$

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\hline
 & \frac{1}{6} & \frac{2}{3} & \frac{1}{6}
\end{array}.$$

It has the following general linear form

$$\left[\begin{array}{c} U_1 \\ U_2 \\ \hline u_n \\ hf(U_2) \end{array}\right] = \left[\begin{array}{cc|cc} \frac{1}{3} & -\frac{1}{24} & 1 & \frac{5}{24} \\ \frac{2}{3} & \frac{1}{6} & 1 & \frac{1}{6} \\ \hline \frac{2}{3} & \frac{1}{6} & 1 & \frac{1}{6} \\ 0 & 1 & 0 & 0 \end{array}\right] \left[\begin{array}{c} hf(U_1) \\ hf(U_2) \\ \hline u_{n-1} \\ hf(u_{n-1}) \end{array}\right].$$

# Practical GLMs

Introduce initial assumptions

- Stage order equal to the overall order of the method
- Quantities passed from step to step to be approximations of the Nordsieck vector
- Stability regions identical to those corresponding to RK methods (IRKS)

Wright'02
Butcher, Wright'03
Butcher, Zackiewicz'04

# Exp. general linear methods

Consider the following unified format of Exp. GLMs

$$U_i = \sum_{j=1}^{s}\sum_{l=1}^{m}\alpha_{ij}^{[l]}\,\phi^{[l]}(c_i)(hL)\,hN(U_j) + \sum_{j=1}^{r}\sum_{l=1}^{m}\delta_{ij}^{[l]}\,\phi^{[l]}(c_i)(hL)\,u_j^{[n-1]},$$

$$u_i^{[n]} = \sum_{j=1}^{s}\sum_{l=1}^{m}\beta_{ij}^{[l]}\,\phi^{[l]}(1)(hL)\,hN(U_j) + \sum_{j=1}^{r}\sum_{l=1}^{m}\nu_{ij}^{[l]}\,\phi^{[l]}(1)(hL)\,u_j^{[n-1]}.$$

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$$u_i^{[n]} = \sum_{j=1}^{s} \sum_{l=1}^{m} \beta_{ij}^{[l]} \, \phi^{[l]}(1)(hL) \, hN(U_j) + \sum_{j=1}^{r} \sum_{l=1}^{m} \nu_{ij}^{[l]} \, \phi^{[l]}(1)(hL) \, u_j^{[n-1]}.$$

Similarly, to the traditional GLMs, we can represent the method in the following matrix form

$$\left[\begin{array}{c} U \\ \hline u^{[n]} \end{array}\right] = \left[\begin{array}{c|c} A(\phi) & D(\phi) \\ \hline B(\phi) & V(\phi) \end{array}\right] \left[\begin{array}{c} hN(U) \\ \hline u^{[n-1]} \end{array}\right],$$

where each of the coefficient matrices $A(\phi), B(\phi), D(\phi), V(\phi)$ has entries which are linear combinations of the $\phi^{[l]}$ functions.

# Generalized IF methods

Seek for a solution of the form

$$u(t_n + t) = \phi_{t,\widehat{F}}(v(t)),$$

where $\phi_{t,\widehat{F}}$ is the flow of the differential equation

$$u' = \widehat{F}(u,t), \qquad u(0) = u_n.$$

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The vector field $\widehat{F}(u,t)$ must:

- Approximates the original vector field $f(u, t_n + t)$ around the point $u_n$.
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The corresponding differential equation for the $v$ variable is

$$v'(t) = \left(\frac{\partial u}{\partial v}\right)^{-1} \left(f(u, t_n + t) - \widehat{F}(u,t), \right), \qquad v(0) = u_n.$$

Use numerical method on the transformed equation and then transform back.

# GIF for semilinear problems

For the semilinear problem (1), we can choice $\widehat{F}(u,t) = Lu + \mathsf{L}_k(N,t)$, where $\mathsf{L}_k(N,t)$ is the Lagrange interpolating polynomial of degree $k-1$ for the function $N(u(t_n+t),\, t_n+t)$, which passes through the $k$ points $N_n, N_{n-1}, \ldots, N_{n-k+1}$.

The transformed equation is

$$v'(t) = e^{-tL}\big(N(u(t_n+t),\, t_n+t) - \mathsf{L}_k(N,t)\big) \qquad v(0) = u_n.$$

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The transformed equation is

$$v'(t) = e^{-tL}\big(N(u(t_n+t),\, t_n+t) - \mathsf{L}_k(N,t)\big) \qquad v(0) = u_n.$$

- Applying a multistep method to the transformed equation leads to a class of methods which includes as a special cases all exponential multistep methods considered so far.
- Applying a multistage method to the transformed equation leads to a new class of methods known as GIF/RK methods (Krogstad'03).

# GIF/RK methods

$$\begin{aligned}
\mathsf{L}_0(N,t) &= 0 && - \quad \text{IF RK (Lawson)},\\
\mathsf{L}_1(N,t) &= N_n && - \quad \text{GIF1/RK (Krogstad)},\\
\mathsf{L}_2(N,t) &= N_n + t\left(\frac{N_n - N_{n-1}}{h}\right) && - \quad \text{GIF2/RK (Krogstad)},
\end{aligned}$$

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\end{aligned}
$$

$$
\left[\begin{array}{cccc|cc}
0 & 0 & 0 & 0 & I & 0\\
a_{21}(hL) & 0 & 0 & 0 & e^{c_2 hL} & d_{22}(hL)\\
a_{31}(hL) & \alpha_{32}e^{(c_3-c_2)hL} & 0 & 0 & e^{c_3 hL} & d_{32}(hL)\\
a_{41}(hL) & \alpha_{42}e^{(c_4-c_2)hL} & \alpha_{43}e^{(c_4-c_3)hL} & 0 & e^{c_4 hL} & d_{42}(hL)\\
\hline
b_1(hL) & \beta_2 e^{(1-c_2)hL} & \beta_3 e^{(1-c_3)hL} & \beta_4 e^{(1-c_4)hL} & e^{hL} & v_{12}(hL)\\
I & 0 & 0 & 0 & 0 & 0
\end{array}\right],
$$

Fourth order GIF2/RK method

# GIF/RK methods

$$\begin{aligned} \mathsf{L}_0(N,t) &= 0 &&- \quad \text{IF RK (Lawson)},\\ \mathsf{L}_1(N,t) &= N_n &&- \quad \text{GIF1/RK (Krogstad)},\\ \mathsf{L}_2(N,t) &= N_n + t\left(\frac{N_n - N_{n-1}}{h}\right) &&- \quad \text{GIF2/RK (Krogstad)}, \end{aligned}$$

where

$$a_{21}(hL) = c_2\phi^{[1]} + c_2^2\phi^{[2]},$$

$$a_{31}(hL) = c_3\phi^{[1]} + c_3^2\phi^{[2]} - \alpha_{32}\,(1+c_2)\,e^{(c_3-c_2)hL},$$

$$a_{41}(hL) = c_4\phi^{[1]} + c_4^2\phi^{[2]} - \alpha_{42}\,(1+c_2)\,e^{(c_4-c_2)hL} - \alpha_{43}\,(1+c_3)\,e^{(c_4-c_3)hL},$$

$$b_1(hL) = \phi^{[1]}+\phi^{[2]}-\beta_2(1+c_2)e^{(1-c_2)hL}-\beta_3(1+c_3)e^{(1-c_3)hL}-\beta_4(1+c_4)e^{(1-c_4)hL},$$

$$d_{22}(hL) = -c_2^2\phi^{[2]},$$

$$d_{32}(hL) = -c_3^2\phi^{[2]} + c_2\alpha_{32}e^{(c_3-c_2)hL},$$

$$d_{42}(hL) = -c_4^2\phi^{[2]} + c_2\alpha_{42}e^{(c_4-c_2)hL} + c_3\alpha_{43}e^{(c_4-c_3)hL},$$

$$v_{12}(hL) = -\phi^{[2]} + c_2\beta_2e^{(1-c_2)hL} + c_3\beta_3e^{(1-c_3)hL} + c_4\beta_4e^{(1-c_4)hL}.$$

# GIF/RK methods

Similarly, if $\widehat{F}(u,t) = Lu + \mathsf{T}_k(N,t)$, where

$$\mathsf{T}_k(N,t) = b + \sum_{\alpha=1}^{k} \left(c_\alpha \sin(\alpha t) + d_\alpha \cos(\alpha t)\right); \qquad k \in \mathbb{N},\ c_\alpha, d_\alpha \in,$$

it is possible to construct new GIF methods.

This approach leads to the followig $\phi^{[l]}$ funactions

$$\phi^{[\alpha]}_{\sin}(hL) = \frac{e^{hL}\alpha - L\sin(\alpha h) - \alpha\cos(\alpha h)I}{\alpha^2 I + L^2},$$

$$\phi^{[\alpha]}_{\cos}(hL) = \frac{e^{hL}L - L\cos(\alpha h) + \alpha\sin(\alpha h)I}{\alpha^2 I + L^2}.$$

# Exp. Int. and Schrödinger equation

- Symmetric exponential integrators of firs, second and third order - convergence analysis (Hochbruck, Lubich'99).

- Higher order Exp. RK methods for the nonlinear Schrödinger equation are studied by Berland, Skaflestad, Owren'04.

IF RK methods seems to be the best for this problem.

# Exp. Int. for oscillatory problems

Consider the following oscillatory second-order differential equation

$$u'' = Lu + g(u), \qquad u(0) = u_0,\ y'(0) = y_0',$$

where $-L$ is positive semi-definite and has arbitrarily large norm.

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where $-L$ is positive semi-definite and has arbitrarily large norm.

Again base the methods on (vcf) (Hochbruck, Lubich'99)

$$u(t+\tau) = \cos(\tau\Omega)u(t) + \Omega^{-1}\sin(\tau\Omega)u'(t) + \int_0^\tau \Omega^{-1}\sin\left((\tau - s)\Omega\right) g(u(t+s))ds,$$

where $\Omega = \sqrt{-L}$.

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where $-L$ is positive semi-definite and has arbitrarily large norm.

Again base the methods on (vcf) (Hochbruck, Lubich'99)

$$u(t+\tau) = \cos(\tau\Omega)u(t) + \Omega^{-1}\sin(\tau\Omega)u'(t) + \int_0^\tau \Omega^{-1}\sin\left((\tau - s)\Omega\right) g(u(t+s))ds,$$

where $\Omega = \sqrt{-L}$.

Approximating $g(u(t))$ by a suitable constant $g_n$ we obtain the following numerical scheme

$$u_{n+1} - 2u_n + u_{n-1} = h^2\sigma(-h^2L)(Lu + g_n)$$
$$u_1 = \cos(h\Omega)u_0 + \Omega^{-1}\sin(h\Omega)u_0' + \tfrac{1}{2}h^2\sigma(-h^2L)g_0,$$

where

$$\sigma(z^2) = 2\frac{1-\cos z}{z^2}.$$

# Implementation issues

Consider the ETD $\phi^{[i]}$ functions

$$\phi^{[1]}(z) = \frac{e^z - 1}{z}, \qquad \phi^{[i+1]}(z) = \frac{\phi^{[i]}(z) - \frac{1}{i!}}{z}, \quad \text{for} \quad i = 2, 3, \ldots .$$

A straightforward implementation suffers from cancellation errors (Kassam and Trefethen).

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Numerical techniques

- Decomposition methods
- Cauchy integral approach
- Krylov subspace approximations

# Implementation issues

- At the heart of all decomposition methods is the similarity transformation

$$A = SBS^{-1},$$

where $A = \gamma h L$. Therefore

$$\phi^{[i]}(A) = S\phi^{[i]}(B)S^{-1}.$$

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Two conflicting tasks:

- Make $B$ close to diagonal so that $\phi^{[i]}(B)$ is easy to compute.
- Make $S$ well conditioned so that errors are not magnified.

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  - Based on the Cauchy integral formula

$$\phi^{[i]}(A) = \frac{1}{2\pi i}\int_{\Gamma_A} \phi^{[i]}(\lambda)(\lambda I - A)^{-1} d\lambda,$$

where $\Gamma_A$ is a contour in the complex plane that encloses the eigenvalue of $A$, and it is also well separated from $0$.

# Implementation issues

- At the heart of all decomposition methods is the similarity transformation

$$A = SBS^{-1},$$

where $A = \gamma h L$. Therefore

$$\phi^{[i]}(A) = S\phi^{[i]}(B)S^{-1}.$$

- Using the trapezoid rule, we obtain the following approximation

$$\phi^{[i]}(A) \approx \frac{1}{k}\sum_{j=1}^{k} \lambda_j \phi^{[i]}(\lambda_j)(\lambda_j I - A)^{-1},$$

where $k$ is the number of the equally spaced points $\lambda_j$ along the contour $\Gamma_A$.

# Krylov subspace approximations

Approximately project the action of $\phi^{[i]}(A)$ on a state vector $v \in \mathbb{C}^d$, to a small Krylov subspace

$$K_{\mathsf{m}} \equiv \mathrm{span}\{v, Av, \ldots, A^{\mathsf{m}-1}v\}.$$

Construct a orthogonal basis $V_{\mathsf{m}} = [v_1, v_2, \ldots, v_{\mathsf{m}}]$ of $K_{\mathsf{m}}$ (Arnoldi, Lanczos)
If $H_{\mathsf{m}}$ is the $\mathsf{m} \times \mathsf{m}$ upper Hessenberg matrix generated by the process then

$$V_{\mathsf{m}}^T A V_{\mathsf{m}} = H_{\mathsf{m}}.$$

Therefore, $H_{\mathsf{m}}$ is the orthogonal projection of $A$ to the subspace $K_{\mathsf{m}}$ and

$$\begin{aligned} \phi^{[i]}(A)v = V_{\mathsf{m}} V_{\mathsf{m}}^T \phi^{[i]}(A)v &= \beta V_{\mathsf{m}} V_{\mathsf{m}}^T \phi^{[i]}(A) V_{\mathsf{m}} e_1 \\ &\approx \beta V_{\mathsf{m}} \phi^{[i]}(H_{\mathsf{m}}) e_1, \end{aligned}$$

where $e_1$ is the first unit vector in $\mathbb{R}^{\mathsf{m}}$ and $\beta \equiv ||v||_2$.

# Krylov subspace approximations

- Superlinear convergence (Hochbruck, Lubich'98)
- Preconditioning the Lanczos process (Hochbruck,Van der Eshof'04)
- At every step we need to construct several Krylov bases
- Multiple Arnldi methods (Schmitt, Weiner'95)

# Conclusions

- The exponential integrators have a long history
- A general framework for analyzing the non-stiff order based on GLMs can help
- IF, ETD, GIF, CF, EC are special cases
- Exp. integrators with Krylov approximation techniques are very promising

# Open problems

- Need to understand the role of the $\phi^{[i]}$ functions.
- Effective algorithms for their computation.
- Are these methods competitive with variable stepsize.
- Extensive numerical experiments.
- Stability analysis - generalize the concept of IRKS
- Exponential integrators for oscillatory problems.

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