# Deferred correction based on exponentially-fitted mono-implicit Runge-Kutta methods

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- EFRK methods
- EF as a correction technique

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- The overall order of a DC-scheme

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- Mono-implicit Runge-Kutta methods

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- Analysis of the error
- The scheme-level approach
- The method-level approach
- A priori knowledge

# Exponential fitting

PART ONE

# Exponential fitting

Since about 1990, the research group of Guido Vanden Berghe at Ghent University did a lot of work on EF methods.

- interpolation
- quadrature (Newton-Cotes, Gauss)
- differentiation
- integration (linear multistep methods, Runge-Kutta(-Nystrom) methods for IVP and BVP, eigenvalue problems, ...)
- integral equations (Fredholm, Volterra)
- . . .

Aim : build methods which perform very good when the solution has a known exponential of trigonometric behaviour.

# A model problem

Consider the initial value problem

$$y'' + \omega^2 y = g(y) \qquad y(a) = y_a \qquad y(a) = y'_a\,.$$

If $|g(y)| \ll |\omega^2 y|$ then

$$y(x) \approx \alpha \cos(\omega x + \phi)$$

To mimic this oscillatory behaviour, we construct methods which yield exact results when the solution is of trigonometric (in the complex case : exponential) type.
These methods are called Exponentially-fitted methods.

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# Exponentially fitted methods

- researchers involved at Ghent University:
  Guido Vanden Berghe, Hans De Meyer, Jan Vanthournout, Marnix Van Daele, Philippe Bocher, Hans Vande Vyver, Veerle Ledoux and Davy Hollevoet
- collaboration with Liviu Ixaru (Bucarest)
- work on EF by Vigo-Aguiar, Calvo, Paternoster, Simos, . . . and co-workers.

# Different ways to develop EF methods

- starting from interpolation function

$$p_{n-2}^{(\omega)}(x) = a \cos \omega x + b \sin \omega x + \sum_{i=0}^{n-2} c_i x^i$$

with

$$\lim_{\omega \to 0} p_{n-2}^{(\omega)}(x) = p_n(x) = \sum_{i=0}^{n} c_i x^i$$

- starting from linear functional and imposing that for the set of functions $\{\cos \omega x, \sin \omega x, 1, x, x^2, \ldots, x^{n-2}\}$ the method produces exact results.

$\omega$ which is either real (trigonometric case) or purely imaginary (exponential case), is determined from the expression for the local error.

# Example : Numerov method

$$y'' = f(y) \qquad y(a) = y_a \qquad y(b) = y_b$$

classical Numerov method :

$$y_{n+1} - 2\,y_n + y_{n-1} = \frac{1}{12} h^2 \left( f(y_{n+1}) + 10\,f(y_n) + f(y_{n-1}) \right)$$

$$n = 1, 2, \ldots, N \qquad h = \frac{b-a}{N+1}$$

Construction :

impose $\mathcal{L}[z(x); h] = 0$ for $z(x) \in \mathcal{S} = \{1, x, x^2, x^3, x^4\}$ where

$$\begin{aligned}\mathcal{L}[z(x); h] := {} & z(x+h) + a_0\, z(x) + a_{-1}\, z(x-h) \\ & -h^2 \left( b_1\, z''(x+h) + b_0\, z''(x) + b_{-1}\, z''(x-h) \right)\end{aligned}$$

$$\mathcal{L}[z(x); h] = -\frac{1}{240} h^6\, z^{(6)}(x) + \mathcal{O}(h^8) \qquad \Longrightarrow \text{order } 4$$

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Construction : impose $\mathcal{L}[z(x);h] = 0$ for $z(x) \in \mathcal{S}$ with

$$\mathcal{S} = \{1, x, x^2, \sin(\omega x), \cos(\omega x)\}$$

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$$y_{n+1} - 2\, y_n + y_{n-1} = h^2 \left(\lambda f(y_{n-1}) + (1 - 2\,\lambda) f(y_n) + \lambda f(y_{n+1})\right)$$

$$\lambda \quad = \quad \frac{1}{4\sin^2\frac{\theta}{2}} - \frac{1}{\theta^2} = \frac{1}{12} + \frac{1}{240}\theta^2 + \frac{1}{6048}\theta^4 + \dots \qquad \theta := \omega h$$

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$$\lambda \;=\; \frac{1}{4\,\sin^2\frac{\theta}{2}}-\frac{1}{\theta^2}=\frac{1}{12}+\frac{1}{240}\theta^2+\frac{1}{6048}\theta^4+\dots \qquad \theta:=\omega\,h$$

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# Exponential Fitting

L. Ixaru and G. Vanden Berghe
*Exponential fitting*
Kluwer Academic Publishers, Dordrecht, 2004

$$\xi(Z) = \begin{cases} \cos(|Z|^{1/2}) & \text{if } Z < 0 \\ \cosh(Z^{1/2}) & \text{if } Z \geq 0 \end{cases}$$

$$\eta(Z) = \begin{cases} \sin(|Z|^{1/2})/|Z|^{1/2} & \text{if } Z < 0 \\ 1 & \text{if } Z = 0 \\ \sinh(Z^{1/2})/Z^{1/2} & \text{if } Z > 0 \end{cases} \qquad Z := (\mu h)^2 = -(\omega h)^2$$

Extension to $Z \in \mathbb{C}$ :

$$\xi(Z) = \cos(\mathrm{i}\sqrt{Z}) \quad \text{and} \quad \eta(Z) = \begin{cases} \dfrac{\sin(\mathrm{i}\sqrt{Z})}{\mathrm{i}\sqrt{Z}} & \text{if } Z \neq 0 \\ 1 & \text{if } Z = 0 \end{cases}$$

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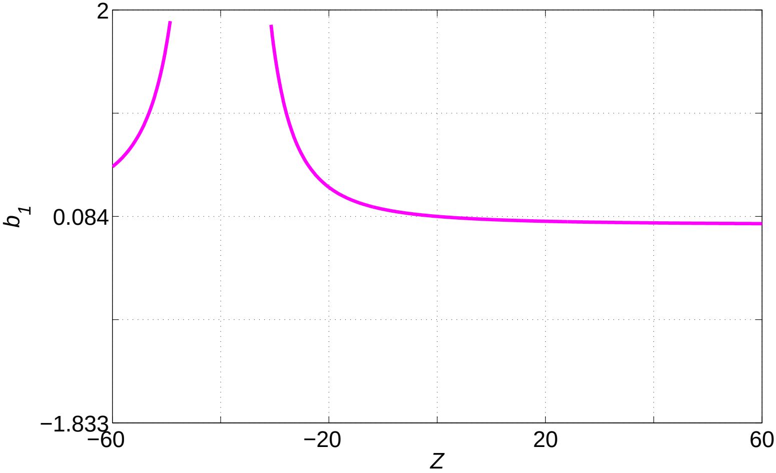
$$\lambda = \frac{1}{4\sin^2\frac{\theta}{2}} - \frac{1}{\theta^2} = \frac{1}{12} + \frac{1}{240}\theta^2 + \frac{1}{6048}\theta^4 + \dots \qquad \theta := \omega\, h$$

$$= -\frac{1}{4\sinh^2\frac{\nu}{2}} + \frac{1}{\nu^2} = \frac{1}{12} - \frac{1}{240}\nu^2 + \frac{1}{6048}\nu^4 + \dots \qquad \nu := \mu\, h$$

$$= \frac{1}{Z}\left(1 - \frac{1}{\eta^2(\frac{Z}{4})}\right) = \frac{1}{12} - \frac{1}{240}Z + \frac{1}{6048}Z^2 + \dots \quad Z := \nu^2 = -\theta^2$$

# $\lambda$ as a function of $Z$



# Choice of $\omega$

- local optimization
  based on local truncation error (lte)
  $\omega$ is step-dependent

- global optimization
  Preservation of geometric properties (periodicity, energy, $\ldots$)
  $\omega$ is constant over the interval of integration

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$$\mathcal{L}[z(x);h] = -\frac{1}{240}h^6\left(z^{(6)}(x) + \omega^2 z^{(4)}(x)\right) + \mathcal{O}(h^8) \qquad \Longrightarrow \text{order } 4$$

A value for the parameter $\omega$ can be obtained from the expression for the lte :

$$y^{(6)}(x_n) + \omega_n^2 y_n^{(4)}(x_n) = 0\,.$$

# Exponentially-fitted Runge-Kutta methods

For methods of collocation type (Gauss, LobattoIIIA, . . . ) linear functionals can be introduced

$$\begin{cases} \mathcal{L}_i[y(x);h] = y(x+c_i\,h) - y(x) - h\displaystyle\sum_{j=1}^{s} a_{ij}\,y'(x+c_j\,h) \\ \qquad\qquad i = 1,\ldots,s \\ \mathcal{L}[y(x);h] = y(x+h) - y(x) - h\displaystyle\sum_{i=1}^{s} b_i\,y'(x+c_i\,h)\,. \end{cases}$$

A fitting space $\mathcal{S}$ is introduced such that $\forall u \in \mathcal{S}$

$$\begin{cases} \mathcal{L}_i[u(x);h] = 0 \qquad i = 1,\ldots,s \\ \mathcal{L}[u(x);h] = 0 \end{cases}$$

# Exponentially-fitted trapezoidal rule

$$\mathcal{S} = \{1, \exp(\omega x), \exp(-\omega x)\}$$

$$\begin{array}{c|cc}
0 & 0 & 0 \\
1 & \frac{s(\omega/2)}{c(\omega/2)\,\omega\,h} & \frac{s(\omega/2)}{c(\omega/2)\,\omega\,h} \\
\hline
 & \frac{s(\omega/2)}{c(\omega/2)\,\omega\,h} & \frac{s(\omega/2)}{c(\omega/2)\,\omega\,h}
\end{array}$$

$$c(t) := \cosh(t\,h) \qquad\qquad s(t) := \sinh(t\,h)$$

$$\mathrm{lte}_{EFTR} = -\frac{h^3}{12}\left(y^{(3)}(x_k) - \omega^2\, y'(x_k)\right) + \mathcal{O}(h^4)$$

# EF as a correction technique

In the past, EF has been successfully applied as a correction technique, see e.g.

- G. Vanden Berghe, H. De Meyer, On a correction of Numerov-like eigenvalue approximations for Sturm-Liouville problems, JCAM **37** (1991) 179-186.
- G. Vanden Berghe, H. De Meyer, A modified Numerov integration method for second order periodic initial-value problems, Intern. J. Comput. Math. **37** (1990) 233-242.
- G. Vanden Berghe, M. Van Daele, Exponentially-fitted Numerov methods, JCAM **200** (2007) 140-153.

# EF as a correction technique . . .

- Sturm-Liouville problem in normal form :
  $-y'' + q(x)\,y = \lambda\,y,\ y(0) = y(\pi) = 0$
- Numerov's method is used to discretize the differential equation, leading to the algebraic eigenvalue problem

  $$A\,v + B\,Q\,v = \Sigma\,B\,v$$

  of size $N$, whereby $(N+1)\,h = \pi$
- The eigenvalues $\lambda_1 < \lambda_2 < \lambda_3 < \cdots$ of the differential equation are approximated by the eigenvalues $\Lambda_1 < \Lambda_2 < \Lambda_3 < \cdots < \Lambda_N$ of the algebraic eigenvalue problem
- $\|\Lambda_k - \lambda_k\| = \mathcal{O}(k^{6}\,h^{4})$
- with EF, the error can be reduced seriously . . .

# ...EF as a correction technique

- suppose you need a better approximation for $\lambda_k$
- first the approximation $y_k$ of the eigenvector $v_k$ is computed
- this approximation is used to annihilate the error-expression of the EF Numerov method $y_k^{(6)}(t_n)+\omega_n^2 y_k^{(4)}(t_n) = 0, n = 1, \ldots, N$
- the $\omega_n^2$ values thus obtained are then used to apply the EF Numerov method
- this leads to a new EF algebraic eigenvalue problem

$$A_{EF}\, v + B_{EF}\, Q\, v_{EF} = \Sigma_{EF}\, B_{EF}\, v_{EF}$$

- the eigenvalues $\lambda_1 < \lambda_2 < \lambda_3 < \cdots$ of the differential equation are approximated by the eigenvalues $\Lambda_{EF,1} < \Lambda_{EF,2} < \Lambda_{EF,3} < \cdots < \Lambda_{EF,N}$ of the algebraic eigenvalue problem
- $\|\Lambda_{EF,k} - \lambda_k\| = \mathcal{O}(k^3\, h^4)$

# Deferred Correction

PART TWO

# Deferred correction

Following idea's of Fox (1947), Lindberg (1980)

Consider the nonlinear two-point boundary value problem

$$\frac{dy}{dx} = f(x, y(x)), \quad g(y(a), y(b)) = 0, \quad a \leq x \leq b$$

- discretise the ODE by Runge-Kutta method $\phi_p$ of order $p$
- this leads to a system of nonlinear algebraic conditions

$$\phi_p(\eta) = 0$$

- In Lindbergs approach, the basic deferred correction algorithm is then to use a second Runge-Kutta formula $\phi_{p+r}$ of order $p + r$ as follows

$$\phi_p(\overline{\eta}) = -\phi_{p+r}(\eta).$$

$-\phi_{p+r}(\eta)$ provides an estimate of the local truncation error of the lower order formula $\phi_p$.

# Iterated deferred correction

- This idea can be extended to allow for more deferred correction iterations.
- In the widely used code `TWPBVP.f` (Cash, Mazzia), the algorithm is

$$\begin{aligned}
\phi_4(\eta) &= 0 \\
\phi_4(\bar{\eta}) &= -\phi_6(\eta) \\
\phi_4(\bar{\bar{\eta}}) &= -\phi_6(\eta) - \phi_8(\bar{\eta})
\end{aligned}$$

where the Runge-Kutta formulae $\phi_4, \phi_6$ and $\phi_8$ are MIRK formulae of order 4, 6 and 8, respectively.

# Iterated deferred correction

- Lindberghs (iterated) approach offers important computational advantages:
  - the solutions $\eta$, $\overline{\eta}$, $\ldots$ are computed on the same grid, and this generally leads to a large saving in the cost of the linear algebra
  - The local error estimates $\overline{\eta} - \eta$, $\overline{\overline{\eta}} - \overline{\eta}$ are immediately available at no extra cost
- If the error is less than a user supplied tolerance, then the most accurate solution is accepted. If the error criterion is not satisfied, then the mesh is refined and the deferred correction scheme is applied on the new mesh.

# The overall order of a DC-scheme

The criteria under which the numerical solution of a deferred correction scheme reaches a certain order, were established by Skeel for the problem

$$\phi(\eta) = 0 \tag{1}$$

$$\phi(\bar{\eta}) = \psi(\eta). \tag{2}$$

$\phi$ : basic discretization scheme $\quad \psi(\eta)$ : estimate of the residual

We assume that the solutions $\eta$ and $\bar{\eta}$ are computed on a grid

$$\pi : a = x_1 < x_2 < \ldots < x_{N+1} = b.$$

$\Delta y$ : restriction of continuous solution $y(x)$ to the finite grid $\pi$

# The overall order of a DC-scheme

SKEEL, R. D.,A THEORETICAL FRAMEWORK FOR PROVING ACCURACY RESULTS FOR DEFERRED CORRECTIONS, SINUM **19** (1982) 171-196

Let $\phi$ be a stable numerical method and assume that the following conditions hold for the deferred correction scheme (1), (2) :

(i) $\|\eta - \Delta y\| = O(h^p)$

(ii) $\|\psi(\Delta y) - \phi(\Delta y)\| = O(h^{r+p})$

(iii) $\psi(\Delta w) = O(h^r)$

for arbitrary functions $w$ having at least $r$ continuous derivatives and $\|.\|$ is a suitable finite norm. If $\phi(\bar{\eta}) = \psi(\eta)$ then

$$\|\bar{\eta} - \Delta y\| = O(h^{r+p}) \,.$$

# The overall order of a DC-scheme

The real difficulty in satisfying the conditions of Skeel's theorem comes from condition (iii).

- For general implicit Runge-Kutta formulae it can be shown that $r = 1$, and so the deferred correction scheme only gives an increase of one order of accuracy.
- To obtain $r = 2$ it was necessary to rewrite the Runge-Kutta formula defining $\psi$ in a symmetrized way, and this is possible by the introduction of parameterized IRK (PIRK) methods

# Mono-implicit Runge-Kutta methods

PART THREE

# Parameterized Runge-Kutta methods

Any Runge-Kutta method

$$\begin{aligned} y_{k+1} &= y_k + h\sum_{i=1}^{s} b_i f(x_k + c_i h, Y_i) \\ Y_i &= y_k + h\sum_{j=1}^{s} a_{ij} f(x_k + c_j h, Y_j), \quad i = 1 \dots s \end{aligned}$$

can be written in a parameterized form

$$\begin{aligned} y_{k+1} &= y_k + h\sum_{i=1}^{s} b_i f(x_k + c_i h, Y_i) \\ Y_i &= (1 - v_i) y_k + v_i y_{k+1} + h\sum_{j=1}^{s} x_{ij} f(x_k + c_j h, Y_j), \quad i = 1 \dots s \end{aligned}$$

# Parameterized Runge-Kutta methods

Any Runge-Kutta method

$$\begin{array}{c|c} c & A \\ \hline & b^T \end{array}$$

can be written in a parameterized form

$$\begin{array}{c|c|c} c & v & X \\ \hline & & b^T \end{array}$$

whereby

$$A = X + v\, b^T$$

# Example 1: the trapezoidal rule

$$y_{k+1} = y_k + \frac{h}{2}\left(f(x_k, y_k) + f(x_{k+1}, y_{k+1})\right)$$

- written as a Runge-Kutta method ($=$ 2-stage Lobatto IIIA)

$$\begin{aligned} y_{k+1} &= y_k + \tfrac{h}{2}\left(f(x_k, Y_1) + f(x_{k+1}, Y_2)\right) \\ Y_1 &= y_k \\ Y_2 &= y_k + \tfrac{h}{2}\left(f(x_k, Y_1) + f(x_{k+1}, Y_2)\right) \end{aligned} \qquad \begin{array}{c|cc} 0 & 0 & 0 \\ 1 & \frac{1}{2} & \frac{1}{2} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

- written as a PIRK method

$$\begin{aligned} y_{k+1} &= y_k + \tfrac{h}{2}\left(f(x_k, Y_1) + f(x_{k+1}, Y_2)\right) \\ Y_1 &= y_k \\ Y_2 &= y_{k+1} \end{aligned} \qquad \begin{array}{c|c|cc} 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ \hline & & \frac{1}{2} & \frac{1}{2} \end{array}$$

# Example 2: the 3-stage Lobatto IIIA method

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

- PIRK version 1: $\begin{array}{c|c|ccc} 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{5}{24} & \frac{1}{3} & \frac{-1}{24} \\ 1 & 1 & 0 & 0 & 0 \\ \hline & & \frac{1}{6} & \frac{4}{6} & \frac{1}{6} \end{array}$

$$y_{k+1} = y_k + \frac{h}{6}\left(f(x_k, y_k) + 4\,f(x_k + \frac{h}{2}, Y_2) + f(x_{k+1}, y_{k+1})\right)$$

$$Y_2 = y_k + \frac{h}{24}\left(5\,f(x_k, y_k) + 8\,f(x_k + \frac{h}{2}, Y_2) - f(x_{k+1}, y_{k+1})\right)$$

# Example 2: the 3-stage Lobatto IIIA method

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

- PIRK version 2: $\begin{array}{c|c|ccc} 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{8} & -\frac{1}{8} & 0 \\ \hline & & \frac{1}{6} & \frac{1}{6} & \frac{4}{6} \end{array}$

$$y_{k+1} = y_k + \frac{h}{6}\left(f(x_k, y_k) + 4\,f(x_k + \tfrac{h}{2}, Y_2) + f(x_{k+1}, y_{k+1})\right)$$

$$Y_2 = \tfrac{1}{2}y_k + \tfrac{1}{2}y_{k+1} + \tfrac{h}{8}\,(\,f(x_k, y_k) - f(x_{k+1}, y_{k+1}))$$

# Example 2: the 3-stage Lobatto IIIA method

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

- PIRK version 2: $\begin{array}{c|c|ccc} 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{8} & -\frac{1}{8} & 0 \\ \hline & & \frac{1}{6} & \frac{1}{6} & \frac{4}{6} \end{array}$

MIRK: mono-implicit RK

$$y_{k+1} = y_k + \frac{h}{6}\left(f(x_k, y_k) + 4\,f(x_k + \tfrac{h}{2}, Y_2) + f(x_{k+1}, y_{k+1})\right)$$

$$Y_2 = \tfrac{1}{2}y_k + \tfrac{1}{2}y_{k+1} + \frac{h}{8}\left(f(x_k, y_k) - f(x_{k+1}, y_{k+1})\right)$$

# Parameterized Runge-Kutta methods

- For a given Rung-Kutta method, there thus exist infinitely many PIRK versions.
- As standalone method, all parameterized versions of a given Runge-Kutta method give (in exact arithmetic) the same result
- But in a deferred correction setting, all PIRK versions are quite different.

## Example : $y' = y \qquad y(0) = 1 \qquad y(x) = \exp(x)$

- $\phi$: trapezoidal rule: $-y_1 + y_0 + \frac{h}{2}(y_0 + y_1) = 0$

$$\Longrightarrow y_1 = \frac{1 + \frac{h}{2}}{1 - \frac{h}{2}} = \exp(h) + \frac{1}{12}h^3 + \mathcal{O}(h^4)$$

- $\psi$: PIRK version 1 of Lobatto IIIA

$$-\bar{y}_1 + \bar{y}_0 + \frac{h}{2}(\bar{y}_0 + \bar{y}_1) = -\mathrm{est}_1$$

$$\mathrm{est}_1 = -y_1 + y_0 + \frac{h}{6}(y_0 + 4\,Y_2 + y_1)$$

$$Y_2 = y_0 + \frac{h}{24}(5\,y_0 + 8\,Y_2 - y_1)$$

$$\Longrightarrow \bar{y}_1 = \exp(h) - \frac{1}{36}h^4 + \mathcal{O}(h^5)$$

## Example : $y' = y \qquad y(0) = 1 \qquad y(x) = \exp(x)$

- $\phi$: trapezoidal rule: $-y_1 + y_0 + \frac{h}{2}(y_0 + y_1) = 0$

$$\Longrightarrow y_1 = \frac{1 + \frac{h}{2}}{1 - \frac{h}{2}} = \exp(h) + \frac{1}{12}h^3 + \mathcal{O}(h^4)$$

- $\psi$: PIRK version 2 of Lobatto IIIA

$$-\bar{y}_1 + \bar{y}_0 + \frac{h}{2}(\bar{y}_0 + \bar{y}_1) = -\mathrm{est}_2$$

$$\mathrm{est}_2 = -y_1 + y_0 + \frac{h}{6}(y_0 + 4\,Y_2 + y_1)$$

$$Y_2 = (y_0 + y_1)/2$$

$$\Longrightarrow \bar{y}_1 = \exp(h) - \frac{1}{120}h^5 + \mathcal{O}(h^6)$$

# Mono-implicit Runge-Kutta methods

Restricting $X$ to lower triangular matrices only reveals the class of mono-implicit Runge-Kutta (MIRK) methods.
A MIRK method is only implicit in the next knot point, which makes such a method very suitable for solving boundary value problems and using deferred correction, while maintaining a good stability:

- if $\phi_p$ is an $s$-stage MIRK method, then the dimension of the system to be solved in each step of the deferred correction process is equal to the number of gridpoints in the integration interval, whereas for a general PIRK method the dimension will be $s$ times larger
- if $\psi$ is a MIRK method, then the error estimator can be computed explicitly, i.e. at a very low cost.

# Deferred correction with EF

PART FOUR

joint work with Davy Hollevoet

# Exponentially-fitted mono-implicit trapezoidal rule

$$\mathcal{S} = \{1, \exp(\omega x), \exp(-\omega x)\}$$

$$\begin{array}{c|c|cc} 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ \hline & & \frac{s(\omega/2)}{c(\omega/2)\,\omega\,h} & \frac{s(\omega/2)}{c(\omega/2)\,\omega\,h} \end{array}$$

$$c(t) := \cosh(t\,h) \qquad s(t) := \sinh(t\,h)$$

$$\text{lte}_{EFTR} = -\frac{h^3}{12}\left(y^{(3)}(x_k) - \omega^2 y'(x_k)\right) + \mathcal{O}(h^4)$$

# Exponentially-fitted mono-implicit Lobatto IIIA method

$$\mathcal{S} = \{1, x, \exp(\mu x), \exp(-\mu x)\}$$

$$\begin{array}{c|c|ccc}
0 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 \\
\frac{1}{2} & \frac{1}{2} & \frac{s(\mu/2)}{2\,\mu\,h(1+c(\mu/2))} & \frac{s(\mu/2)}{-2\,\mu\,h(1+c(\mu/2))} & 0 \\
\hline
 & & \frac{\mu\,h-2\,s(\mu/2)}{2\,\mu\,h(1-c(\mu/2))} & \frac{\mu\,h-2\,s(\mu/2)}{2\,\mu\,h(1-c(\mu/2))} & \frac{2\,s(\mu/2)-c(\mu/2)\,\mu\,h}{\mu\,h(1-c(\mu/2))}
\end{array}$$

$$c(t) := \cosh(t\,h) \qquad\qquad s(t) := \sinh(t\,h)$$

$$\begin{aligned}
\mathrm{lte}_{EFLob} \quad = \quad & -\frac{h^5}{2880}\Big(y^{(5)}(x_k) - \mu^2\,y^{(3)}(x_k) \\
& \qquad -5\,f_y\,\Big(y^{(4)}(x_k) - \mu^2 y^{(2)}(x_k)\Big)\Big) + \mathcal{O}(h^6)
\end{aligned}$$

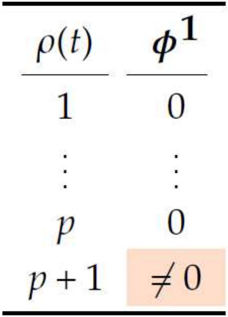
# Analysis of the error

As it is the spirit of EF methods, we want to increase the accuracy of the overall method by the introduction of EF methods

This requires a detailed analysis of the expression for the error of a DC scheme.

Analysis in terms of P-series (details can be found in Ph.D. thesis of Davy Hollevoet)

# Residual of a RK method



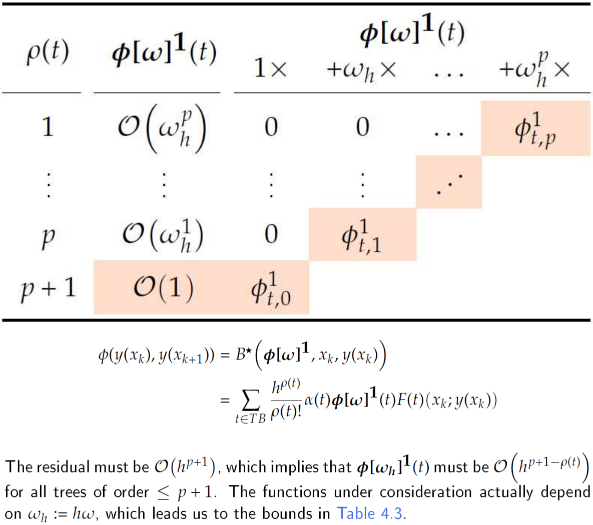
| $\rho(t)$ | $\phi^1$ |
|---|---|
| $1$ | $0$ |
| $\vdots$ | $\vdots$ |
| $p$ | $0$ |
| $p+1$ | $\neq 0$ |

# Example: trapezoidal rule

| $\rho(t)$ | t | $\phi^{\mathbf{1}}(t)$ |
|---|---|---|
| 1 | $\bullet$ | 0 |
| 2 | $\overset{\bullet}{\bullet}, \overset{\star}{\bullet}$ | 0, 0 |
| 3 | $\overset{\bullet\,\bullet}{\vee}, \overset{\star\,\bullet}{\vee}, \overset{\star\,\star}{\vee}, \overset{\bullet}{\underset{\bullet}{\bullet}}, \overset{\star}{\underset{\bullet}{\bullet}}$ | $-\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}$ |

$$
\begin{aligned}
\phi\left(y(x_k), y(x_{k+1})\right) = -\frac{1}{2}\frac{h^3}{6}\Big[ & F(\overset{\bullet\,\bullet}{\vee}) + 2F(\overset{\star\,\bullet}{\vee}) + F(\overset{\star\,\star}{\vee}) \\
& + F(\overset{\bullet}{\underset{\bullet}{\bullet}}) + F(\overset{\star}{\underset{\bullet}{\bullet}})\Big] (x_k; y(x_k)) + \mathcal{O}\left(h^4\right) \\
= -\frac{1}{12} h^3 y^{(3)}(x_k) + \mathcal{O}\left(h^4\right).
\end{aligned}
$$

# Residual of an EF RK method

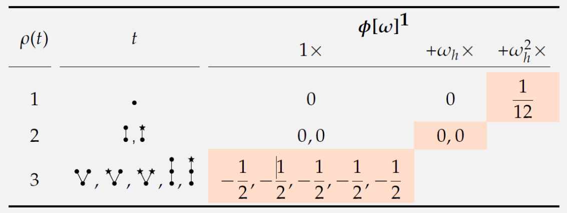


| $\rho(t)$ | $\boldsymbol{\phi}[\omega]^{\mathbf{1}}(t)$ | $\boldsymbol{\phi}[\omega]^{\mathbf{1}}(t)$ | | | |
|---|---|---|---|---|---|
| | | $1\times$ | $+\omega_h\times$ | $\dots$ | $+\omega_h^p\times$ |
| $1$ | $\mathcal{O}\left(\omega_h^p\right)$ | $0$ | $0$ | $\dots$ | $\phi_{t,p}^1$ |
| $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\iddots$ | |
| $p$ | $\mathcal{O}\left(\omega_h^1\right)$ | $0$ | $\phi_{t,1}^1$ | | |
| $p+1$ | $\mathcal{O}(1)$ | $\phi_{t,0}^1$ | | | |

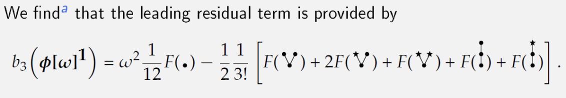
$$\begin{aligned}
\phi(y(x_k), y(x_{k+1})) &= B^\star\left(\boldsymbol{\phi}[\omega]^{\mathbf{1}}, x_k, y(x_k)\right) \\
&= \sum_{t\in TB} \frac{h^{\rho(t)}}{\rho(t)!}\alpha(t)\boldsymbol{\phi}[\omega]^{\mathbf{1}}(t)F(t)(x_k; y(x_k))
\end{aligned}$$

The residual must be $\mathcal{O}\left(h^{p+1}\right)$, which implies that $\boldsymbol{\phi}[\omega_h]^{\mathbf{1}}(t)$ must be $\mathcal{O}\left(h^{p+1-\rho(t)}\right)$ for all trees of order $\leq p+1$. The functions under consideration actually depend on $\omega_h := h\omega$, which leads us to the bounds in Table 4.3.

# Example: The EF trapezoidal rule

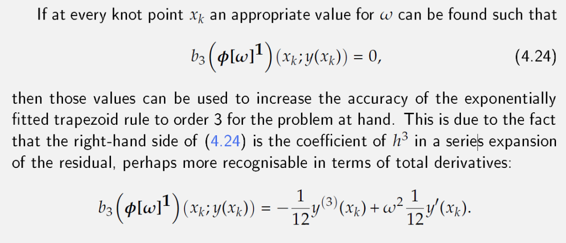


| $\rho(t)$ | $t$ | $\phi[\omega]^{\mathbf{1}}$ | | |
|---|---|---|---|---|
| | | $1\times$ | $+\omega_h\times$ | $+\omega_h^2\times$ |
| 1 | $\bullet$ | $0$ | $0$ | $\frac{1}{12}$ |
| 2 | $[\bullet], [\star]$ | $0, 0$ | $0, 0$ | |
| 3 | $[\bullet,\bullet], [\star,\bullet], [\star,\star], [[\bullet]], [[\star]]$ | $-\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}$ | | |



We find[a] that the leading residual term is provided by

$$b_3\left(\boldsymbol{\phi}[\omega]^{\mathbf{1}}\right) = \omega^2 \frac{1}{12} F(\bullet) - \frac{1}{2}\frac{1}{3!}\left[F([\bullet,\bullet]) + 2F([\star,\bullet]) + F([\star,\star]) + F([[\bullet]]) + F([[\star]])\right].$$



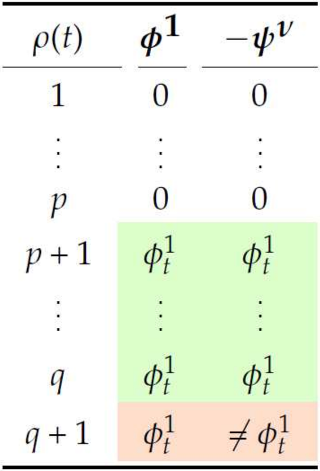
If at every knot point $x_k$ an appropriate value for $\omega$ can be found such that

$$b_3\left(\boldsymbol{\phi}[\omega]^{\mathbf{1}}\right)(x_k; y(x_k)) = 0, \qquad (4.24)$$

then those values can be used to increase the accuracy of the exponentially fitted trapezoid rule to order 3 for the problem at hand. This is due to the fact that the right-hand side of (4.24) is the coefficient of $h^3$ in a series expansion of the residual, perhaps more recognisable in terms of total derivatives:

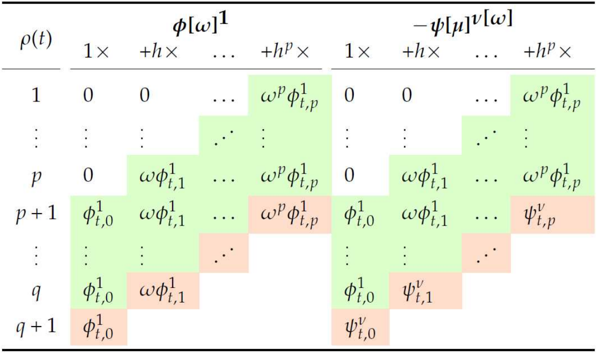
$$b_3\left(\boldsymbol{\phi}[\omega]^{\mathbf{1}}\right)(x_k; y(x_k)) = -\frac{1}{12} y^{(3)}(x_k) + \omega^2 \frac{1}{12} y'(x_k).$$

# Residual of a DC scheme



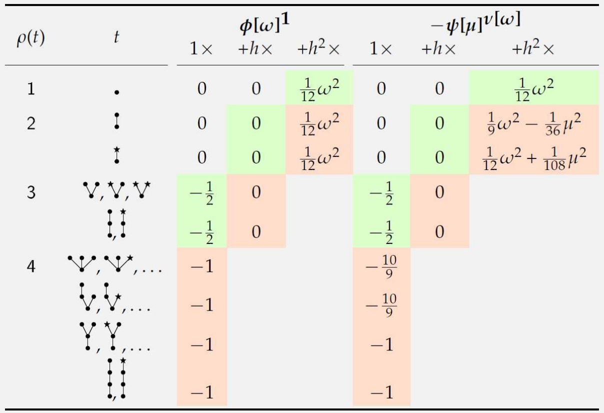
| $\rho(t)$ | $\boldsymbol{\phi}^{\mathbf{1}}$ | $-\psi^{\nu}$ |
|---|---|---|
| $1$ | $0$ | $0$ |
| $\vdots$ | $\vdots$ | $\vdots$ |
| $p$ | $0$ | $0$ |
| $p+1$ | $\phi_t^1$ | $\phi_t^1$ |
| $\vdots$ | $\vdots$ | $\vdots$ |
| $q$ | $\phi_t^1$ | $\phi_t^1$ |
| $q+1$ | $\phi_t^1$ | $\neq \phi_t^1$ |

# Residual of an EF DC scheme



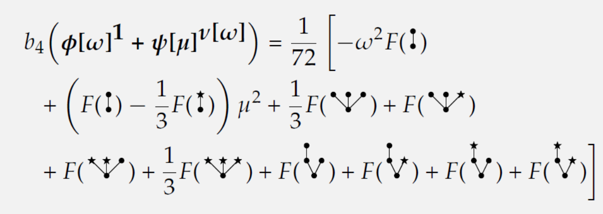
| $\rho(t)$ | $\phi[\omega]^1$ | | | | $-\psi[\mu]^\nu[\omega]$ | | | |
|---|---|---|---|---|---|---|---|---|
| | $1\times$ | $+h\times$ | $\dots$ | $+h^p\times$ | $1\times$ | $+h\times$ | $\dots$ | $+h^p\times$ |
| $1$ | $0$ | $0$ | $\dots$ | $\omega^p\phi^1_{t,p}$ | $0$ | $0$ | $\dots$ | $\omega^p\phi^1_{t,p}$ |
| $\vdots$ | $\vdots$ | $\vdots$ | $\iddots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\iddots$ | $\vdots$ |
| $p$ | $0$ | $\omega\phi^1_{t,1}$ | $\dots$ | $\omega^p\phi^1_{t,p}$ | $0$ | $\omega\phi^1_{t,1}$ | $\dots$ | $\omega^p\phi^1_{t,p}$ |
| $p+1$ | $\phi^1_{t,0}$ | $\omega\phi^1_{t,1}$ | $\dots$ | $\omega^p\phi^1_{t,p}$ | $\phi^1_{t,0}$ | $\omega\phi^1_{t,1}$ | $\dots$ | $\psi^\nu_{t,p}$ |
| $\vdots$ | $\vdots$ | $\vdots$ | $\iddots$ | | $\vdots$ | $\vdots$ | $\iddots$ | |
| $q$ | $\phi^1_{t,0}$ | $\omega\phi^1_{t,1}$ | | | $\phi^1_{t,0}$ | $\psi^\nu_{t,1}$ | | |
| $q+1$ | $\phi^1_{t,0}$ | | | | $\psi^\nu_{t,0}$ | | | |

# The overall error of TR - RadauI



| $\rho(t)$ | $t$ | $\phi[\omega]^1$ | | | $-\psi[\mu]^\nu[\omega]$ | | |
|---|---|---|---|---|---|---|---|
| | | $1\times$ | $+h\times$ | $+h^2\times$ | $1\times$ | $+h\times$ | $+h^2\times$ |
| 1 | | $0$ | $0$ | $\frac{1}{12}\omega^2$ | $0$ | $0$ | $\frac{1}{12}\omega^2$ |
| 2 | | $0$ | $0$ | $\frac{1}{12}\omega^2$ | $0$ | $0$ | $\frac{1}{9}\omega^2 - \frac{1}{36}\mu^2$ |
| | | $0$ | $0$ | $\frac{1}{12}\omega^2$ | $0$ | $0$ | $\frac{1}{12}\omega^2 + \frac{1}{108}\mu^2$ |
| 3 | | $-\frac{1}{2}$ | $0$ | | $-\frac{1}{2}$ | $0$ | |
| | | $-\frac{1}{2}$ | $0$ | | $-\frac{1}{2}$ | $0$ | |
| 4 | … | $-1$ | | | $-\frac{10}{9}$ | | |
| | … | $-1$ | | | $-\frac{10}{9}$ | | |
| | … | $-1$ | | | $-1$ | | |
| | | $-1$ | | | $-1$ | | |

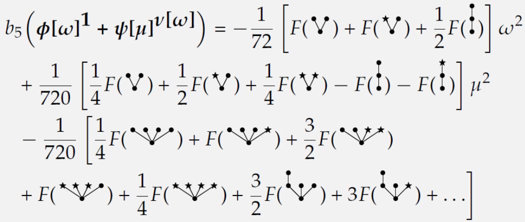
# The overall error of TR - RadauI



$$
b_4\left(\boldsymbol{\phi}[\omega]^{\mathbf{1}} + \boldsymbol{\psi}[\mu]^{\nu[\omega]}\right) = \frac{1}{72}\Bigg[-\omega^2 F(\overset{\bullet}{\bullet})
+ \left(F(\overset{\bullet}{\bullet}) - \frac{1}{3}F(\overset{\star}{\bullet})\right)\mu^2 + \frac{1}{3}F(\overset{\bullet\bullet\bullet}{\bullet}) + F(\overset{\bullet\bullet\star}{\bullet})
+ F(\overset{\star\star\bullet}{\bullet}) + \frac{1}{3}F(\overset{\star\star\star}{\bullet}) + F(\overset{\overset{\bullet}{\bullet}\,\bullet}{\bullet}) + F(\overset{\overset{\bullet}{\bullet}\,\star}{\bullet}) + F(\overset{\overset{\star}{\bullet}\,\bullet}{\bullet}) + F(\overset{\overset{\star}{\bullet}\,\star}{\bullet})\Bigg]
$$

# The overall error of TR - LobattaIIIA

**Leading residual term**



# Analysis of the error

Three approaches

- scheme-level approach
- method-level approach
- a priori knowledge

# 1. The scheme-level approach

Goal : annihilate (or minimize) the leading term of the error of the entire DC scheme.

- one first applies a classical method (such as trapezoidal rule)
- with this numerical solution locally appropriate values for the parameters $\omega$ and $\mu$ are determined.
  - problems with 2 components at most : annihilate the leading error term
  - problems with more than 2 components : minimize the leading error term
- Once these values have been obtained, the entire EFDC scheme is applied, giving rise to a method of order
  - $p + r + 1$ for problems with 2 components at most
  - $p + r$ for problems with more than 2 components

# 1. The scheme-level approach

This algorithm has following properties:

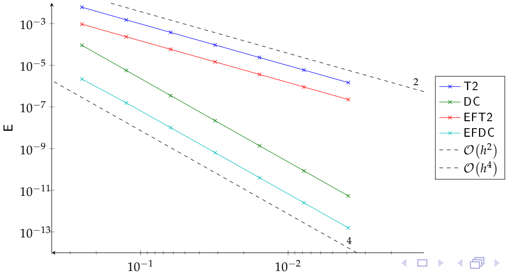
- extra work involved to obtain an initial solution (with a classical method) to estimate values for the parameters $\omega_k$ and $\mu_k$.
- computation of the error expression is rather expensive (the higher the order, the higher the number of elementary differentials involved)
- The values for $\omega_k$ and $\mu_k$ that are obtained in this way, depend upon the specific methods used and they do not necessarily reflect the nature of the problem.
- The raise of order is only possible iff $r < p$. For $r = p$, it can be shown that there is an uncontrollable error accumulation (such that the order remains $p + r$).

# 1. The scheme-level approach

$$\epsilon y'' = y \qquad y(0) = 1 \quad y(1) = 0 \qquad \epsilon = 0.3$$

$$y(x) = \frac{e^{\frac{x}{\sqrt{\epsilon}}} - e^{\frac{2-x}{\sqrt{\epsilon}}}}{1 - e^{\frac{2}{\sqrt{\epsilon}}}} \qquad \text{(test set of J. Cash, Problem 1)}$$

This problem can be solved exactly by any EF method if the parameter is chosen as $1/\sqrt{\epsilon} \approx 1.8$, but in the scheme-level approach $(\omega_k, \mu_k) \approx (1, -0.7\,i)$



# 2. The method-level approach

Goal : annihilate (or minimize) the leading term of the error of the base method and of the error estimator seperately

- one first applies a classical method (such as trapezoidal rule)
- with this numerical solution locally appropriate values for the parameter $\omega$ (of the base method) are determined and the EF base method is applied
- with this numerical solution locally appropriate values for the parameter $\mu$ (of the error estimator) are determined
- the second step of the DC scheme is applied with the EF base method and the EF error estimator

This gives rise to a method of order

- $p + r + 1$ for scalar problems
- $p + r$ for non-scalar problems

# 2. The method level approach

This algorithm has following properties:

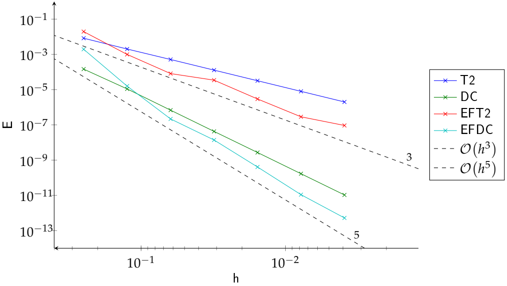
- still some extra work involved to obtain estimate values for the parameters $\omega_k$ and $\mu_k$.
- the values for $\omega_k$ and $\mu_k$ that are obtained in this way, do reflect the nature of the problem.
- The raise of order is also possible if $r = p$.

# 2. Method level approach

A Bernoulli-problem

$$y' = \frac{2y + xy^4}{6} \qquad\qquad y(0) = -2$$

$$y(x) = \frac{-2}{(4x - 4 + 5e^{-x})^{\frac{1}{3}}}$$

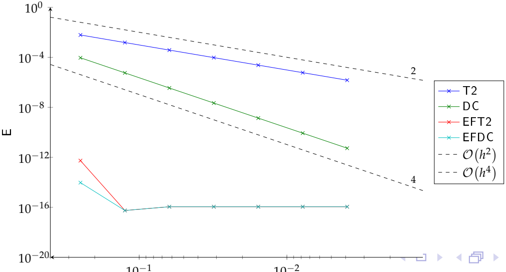


# 2. Method level approach

$$\epsilon y'' = y \qquad y(0) = 1 \quad y(1) = 0 \qquad \epsilon = 0.3$$

$$y(x) = \frac{e^{\frac{x}{\sqrt{\epsilon}}} - e^{\frac{2-x}{\sqrt{\epsilon}}}}{1 - e^{\frac{2}{\sqrt{\epsilon}}}} \qquad \text{(test set of J. Cash, Problem 1)}$$

This problem can be solved exactly by any EF method if the parameter is chosen as $1/\sqrt{\epsilon} \approx 1.8$. In the method-level approach $(\omega_k, \mu_k) \approx (1.8, 1.8)$



## 2. The method level approach

$$y'' = -y - y^3 + 0.002\cos(1.01x) \qquad \text{(Duffing problem)}$$

$$y(0) = 0.200426728067 \quad y(2) = -0.08668702310$$

Approximate solution:

$$\begin{aligned} y(x) = {} & 0.200179477536\cos(1.01x) + 0.000246946143\cos(3.03x) \\ & + 0.000000304014\cos(5.05x) + 0.000000000374\cos(7.07x) \\ & + \ldots \end{aligned}$$

EF methods can produce very accurate results for this problem if the parameter is approximately equal to 1.01

# 2. The method level approach

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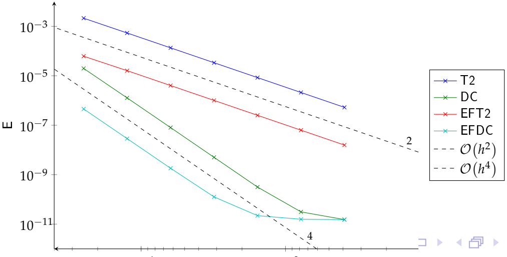
EF methods can produce very accurate results for this problem if the parameter is approximately equal to 1.01.

The computed values for $\omega_k$ and $\mu_k$ vary in the integration interval from 1.5 to 1

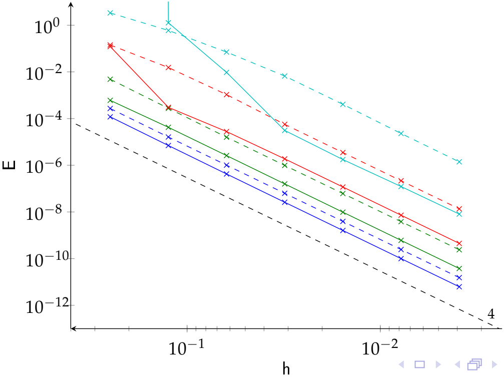


# 2. The method level approach

$$\epsilon y'' + y' = (1+\epsilon)y \qquad y(-1) = 1 + e^{-2}, \quad y(1) = 1 + e^{-2(1+\epsilon)}\epsilon$$

$$y(x) = e^{x-1} + e^{-\frac{(1+\epsilon)(1+x)}{\epsilon}}$$

$\epsilon$ : 1, 0.29240177382129, 0.085498797333835 and 0.025.



# 3. A priori knowledge

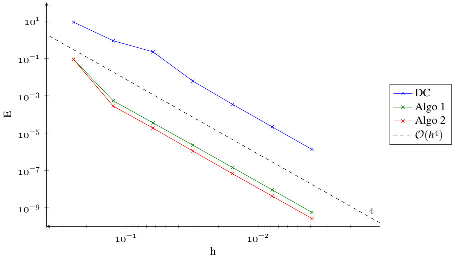
Suppose we already have a good estimate for the EF parameter $\omega$.

- One then immediately applies an EF method (such as EF trapezoidal rule) with that estimate
- with this numerical solution locally appropriate values for the parameter $\mu$ (of the error estimator) are determined
- the second step of the DC scheme is applied with the original EF base method and the EF error estimator

# 3. A priori knowledge

$$y'' = -\left(100 + \frac{1}{4x^2}\right) y \qquad y(1) = J_0(10), \quad y(2) = \sqrt{2} J_0(20)$$

$$y(x) = \sqrt{x} J_0(10x)$$ (Bessel problem)



DC : classical DC scheme

Algorithm 1 : a priori fixed $\omega$-values : $\omega_k = 10\,i$

Algorithm 2 : the method-level approach

# The end

Thank you for your attention