

Multiparameter symplectic, symmetric exponentially-fitted modified Runge-Kutta methods of Gauss type

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ICNAAM, Rhodes, September 2010

Outline

Exponential fitting

Multiparameter EF methods

The case $s = 2$

The case $s = 3$

Numerical results

Conclusions

Exponential fitting

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

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

$$\lim_{\omega \rightarrow 0} p_{n-2}^{(\omega)}(x) = p_n(x) = \text{a polynomial of degree } \leq n$$

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

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

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Example : Numerov method

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

classical Numerov method :

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

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

Construction :

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

$$\begin{aligned} \mathcal{L}[z(t); h] := & z(t+h) + a_0 z(t) + a_{-1} z(t-h) \\ & - h^2 (b_1 z''(t+h) + b_0 z''(t) + b_{-1} z''(t-h)) \end{aligned}$$

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

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

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Exponential Fitting



L. Ixaru and G. Vanden Berghe

Exponential fitting

Kluwer Academic Publishers, Dordrecht, 2004

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

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

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

A value for the parameter ω can be obtained from the expression for the lte :

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Generalisations

To determine the coefficients of a method, we impose conditions on a linear functional. These conditions are related to the fitting space \mathcal{S} which contains $\{1, t, t^2, \dots, t^K\}$ and

- possibility 1 (Calvo et al.) : trigonometric polynomials $\{\exp(\pm\mu t), \exp(\pm 2\mu t), \dots, \exp(\pm(P+1)\mu t)\}$
- possibility 2 (Ixaru, Vanden Berghe, V.D., ...) : exponential-fitting $\{\exp(\pm\mu t), t \exp(\pm\mu t), \dots, t^P \exp(\pm\mu t)\}$

A method can be characterized by the couple (K, P)

Here, we consider a generalisation of both classes :

- possibility 3 : $\{\exp(\pm\mu_0 t), \exp(\pm\mu_1 t), \dots, \exp(\pm\mu_P t)\}$

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work by Hollevoet, V.D. and Vanden Berghe

- “On the leading error term of exponentially fitted Numerov methods”, ICNAAM 2008
- “The optimal exponentially-fitted Numerov method for solving two-point boundary value methods”, J. CAM 2009

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μ is determined from the Ité :

$$h^6 \phi_P(Z) D^{K+1} (D^2 - \mu^2)^{P+1} y(t_j) + \mathcal{O}(h^8) \quad \phi_P(Z) = -\frac{1}{240} + \mathcal{O}(Z)$$

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To solve this problem, we propose the new type of EF methods : EF multiparameter methods

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To solve this problem, we propose the new type of EF methods : EF multiparameter methods

Motivation

μ is determined from the Ité :

$$h^6 \phi_P(Z) D^{K+1} (D^2 - \mu^2)^{P+1} y(t_j) + \mathcal{O}(h^8) \quad \phi_P(Z) = -\frac{1}{240} + \mathcal{O}(Z)$$

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The construction of symmetric, symplectic EF multiparameter Runge-Kutta methods Gauss-type methods

Previous work on

- EF symplectic RK-like methods by Van de Vyver (2006)
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General approach

Associate linear functionals to the **internal stages**

$$\mathcal{L}_i[y(x); h; \mathbf{a}] = y(x + c_i h) - y(x) - h \sum_{j=1}^s a_{ij} y'(x + c_j h)$$

where $i = 1, \dots, s$ and the **final stage**

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and impose $\begin{cases} \mathcal{L}_i[y(x); h; \mathbf{a}] = 0 & \text{for } y(x) \in S_{int} \\ \mathcal{L}[y(x); h; \mathbf{b}] = 0 & \text{for } y(x) \in S_{fin} \end{cases}$

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Van de Vyver's approach

In order to construct a symplectic EF version of the Gauss $s = 2$ method with fixed knots $c_1 = \frac{3-\sqrt{3}}{6}$ and $c_2 = \frac{3+\sqrt{3}}{6}$ and

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Van de Vyver considers **modified** RK-methods

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Extra conditions

A **modified** Runge-Kutta method is called **symplectic** iff

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The case $s = 2$

We consider a 2-stage modified Runge-Kutta method

c_1	γ_1	a_{11}	a_{12}
c_2	γ_2	a_{21}	a_{22}
		b_1	b_2

$$\text{Symmetry : } c_1 = \frac{1}{2} - \theta \quad c_2 = \frac{1}{2} + \theta \quad b_1 = b_2$$

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Special cases :

- $\mu_2 = 2\mu$ (Calvo)
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leads to formula's also obtained by Vanden Berghe et al.

$$b_1 = \frac{1}{2} \frac{\sinh(z/2)}{\cosh(z\theta) (z/2)} = b_2$$

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This leads to a formula for θ : $F(z) = F(z_2)$ where

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In general, an iterative procedure is needed to determine θ .

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For this value of θ : $\gamma_1 = \gamma_2 = 1$

This is the EFRK method of Calvo et al.

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$$S_{fin} = \{\exp(\mu x), \exp(-\mu x)\} \cup \{x \exp(\mu x), x \exp(-\mu x)\}$$

- $z_2 = 0 : F(z) = 1 \Rightarrow \theta = \frac{1}{z} \operatorname{acosh} \left(\frac{\sinh(z/2)}{(z/2)} \right)$

This is the method of Vanden Berghe et al. with

$$S_{fin} = \{\exp(\mu x), \exp(-\mu x)\} \cup \{1, x\}$$

...the case $s = 2$...

$$F(z) = F(z_2) \text{ where } F(u) = \frac{\sinh(u/2)}{\cosh(u\theta)(u/2)}$$

Special cases :

- $z_2 = z : F'(z) = 0$

$$\Rightarrow \theta = \frac{1}{z} \frac{\cosh(z\theta)}{\sinh(z\theta)} \left(\frac{\cosh(z/2)}{\sinh(z/2)/(z/2)} - 1 \right)$$

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...the case $s = 2$...

What if

- $z \approx 0$
- $z_2 \approx 0$
- $z \approx 0$ and $z_2 \approx 0$
- $z_2 \approx z$

...the case $s = 2$...

If $z \rightarrow 0$ and $z_2 \rightarrow 0$:

$$\begin{aligned}\theta = & \frac{\sqrt{3}}{6} + \frac{\sqrt{3}}{2160} \left(z^2 + z_2^2 \right) \\ & - \frac{\sqrt{3}}{10886400} \left(27 z^4 - 106 z^2 z_2^2 + 27 z_2^4 \right) \\ & + \frac{\sqrt{3}}{435456000} \left(3 z_2^4 - 34 z^2 z_2^2 + 3 z^4 \right) \left(z^2 + z_2^2 \right) \\ & + \dots\end{aligned}$$

...the case $s = 2$...

$$F(z_2) = F(z)$$

If $z_2 - z$ is very small :

$$F(z_2) = F(z) + (z_2 - z) F'(z) + \frac{1}{2} (z_2 - z)^2 F''(z) + \dots$$

$$F'(z) + (z_2 - z) F''(z) = 0$$

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The case $s = 3$

A symmetric, symplectic modified EF Runge-Kutta method has the form

$\frac{1}{2} - \theta$	γ_1	$\frac{\gamma_1 b_1}{2}$	$\frac{\gamma_1 b_2}{2} - \alpha_2$	$\frac{\gamma_1 b_1}{2} - \alpha_3$	
$\frac{1}{2}$	γ_2	$\frac{\gamma_2 b_1}{2} - \alpha_4$	$\frac{\gamma_2 b_2}{2}$	$\frac{\gamma_2 b_1}{2} + \alpha_4$	
$\frac{1}{2} + \theta$	γ_1	$\frac{\gamma_1 b_1}{2} + \alpha_3$	$\frac{\gamma_1 b_2}{2} + \alpha_2$	$\frac{\gamma_1 b_1}{2}$	$\frac{b_1}{\gamma_1} \alpha_2 + \frac{b_2}{\gamma_2} \alpha_4 = 0$
		b_1	b_2	b_1	

Parameters : $b_1, b_2, \gamma_1, \gamma_2, \alpha_2, \alpha_3, \theta$

The case $s = 3$

We consider the construction of a method for which

$$S_{int} = \{1, \exp(\mu x), \exp(-\mu x)\}$$

and

$$S_{fin} = \{1, \exp(\mu x), \exp(-\mu x), \exp(\mu_2 x), \exp(-\mu_2 x)\}$$

Special cases :

- $\mu_2 = 2\mu$ (Calvo)
- $\mu_2 \rightarrow \mu$ (Vanden Berghe)

First we impose

$$S_{int} = \{1, \exp(\mu x), \exp(-\mu x)\}$$

$$S_{fin} = \{1, \exp(\mu x), \exp(-\mu x)\}$$

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Imposing

$$S_{int} = \{1, \exp(\mu x), \exp(-\mu x)\} \quad S_{fin} = \{1, \exp(\mu x), \exp(-\mu x)\}$$

leads to formula's also obtained by **Calvo et al.** since

$$\gamma_1 = 1 = \gamma_2$$

$$b_1 = \frac{1}{2} \frac{\frac{\sinh(z)}{z} - \frac{\sinh(z/2)}{z/2}}{\cosh(2z\theta) - \cosh(z\theta)}$$

$$b_2 = \dots \quad \alpha_2 = \dots \quad \alpha_3 = \dots$$

Following Ixaru :

$$b_1 = \frac{1}{2} \frac{\eta(Z) - \eta(Z/4)}{\xi(4Z\theta^2) - \xi(Z\theta^2)}$$

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We then obtain

$$b_1 = \frac{1}{2 \cosh(z_2 \theta) - \cosh(z \theta)} \frac{\frac{\sinh(z_2/2)}{z_2/2} - \frac{\sinh(z/2)}{z/2}}{b_2 = \dots}$$

which has exactly the same form as the expression we already had :

$$b_1 = \frac{1}{2 \cosh(2z \theta) - \cosh(z \theta)} \frac{\frac{\sinh(z)}{z} - \frac{\sinh(z/2)}{z/2}}$$

The first expression makes clear that the final stage **by accident** also integrates $\{\exp(2\mu x), \exp(-2\mu x)\}$ exactly :

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...the case $s = 3$...

Combining both results, we obtain the relation from which θ can be determined :

$$\frac{1}{2} \frac{\frac{\sinh(z_2/2)}{z_2/2} - \frac{\sinh(z/2)}{z/2}}{\cosh(z_2\theta) - \cosh(z\theta)} = \frac{1}{2} \frac{\frac{\sinh(z)}{z} - \frac{\sinh(z/2)}{z/2}}{\cosh(2z\theta) - \cosh(z\theta)}$$

$$G(z, z_2) = G(z, 2z)$$

$$\text{with } G(a, b) := \frac{\frac{\sinh(a/2)}{a/2} - \frac{\sinh(b/2)}{b/2}}{\cosh(a\theta) - \cosh(b\theta)}$$

In general, an iterative procedure is needed to determine θ .

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In general, an iterative procedure is needed to determine θ .

...the case $s = 3$...

Special case : $z_2 = 3z$: the method of Calvo et al.

$$\theta = \frac{2}{z} \operatorname{acosh}(\beta_1)$$

$$\beta_1 = \frac{1}{6} \sqrt{15 + 6 \cosh(z/2) + 3 \sqrt{15 + 8 \cosh(z/2) + 2 \cosh(z)}}$$

$$\theta = \frac{\sqrt{15}}{10} \left(1 + \frac{z^2}{150} - \frac{31 z^4}{240000} + \frac{89 z^6}{144000000} + \dots \right)$$

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...the case $s = 3$...

Special case : $z_2 = z/2$:

$$\theta = \frac{4}{z} \operatorname{acosh}(\beta_3)$$

$$\beta_3 = \frac{1}{4} \sqrt{6 + 2 \sqrt{9 + 8 (\cosh(z/4))^2 + 8 \cosh(z/4)}}$$

$$\theta = \frac{\sqrt{15}}{10} \left(1 + \frac{z^2}{400} - \frac{253 z^4}{11520000} + \frac{1241 z^6}{9216000000} - \dots \right)$$

...the case $s = 3$...

Special case : $z_2 = z$:

$$G(z, z) = G(z, 2z)$$

$$G(a, b) := \frac{\frac{\sinh(a/2)}{a/2} - \frac{\sinh(b/2)}{b/2}}{\cosh(a\theta) - \cosh(b\theta)} = \frac{G_N(a, b)}{G_D(a, b)}$$

$$\begin{aligned} G(z, z) &= \lim_{z_2 \rightarrow z} G(z, z_2) &= \left(\frac{0}{0} \right) = \frac{\frac{\partial}{\partial z_2} G_N(z, z_2) \Big|_{z_2=z}}{\frac{\partial}{\partial z_2} G_D(z, z_2) \Big|_{z_2=z}} \\ &= \frac{\cosh(z/2) - \frac{\sinh(z/2)}{z/2}}{z\theta \sinh(z\theta)} \end{aligned}$$

$$S_{fin} = \{1, \exp(\pm\mu x), \exp(\pm 2\mu x), x \exp(\pm\mu x)\}$$

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...the case $s = 3$...

If $z \rightarrow 0$ and $z_2 \rightarrow 0$:

$$\begin{aligned}\theta = & \frac{\sqrt{15}}{10} + \frac{\sqrt{15}}{21000} \left(5z^2 + z_2^2 \right) \\ & - \frac{\sqrt{15}}{1058400000} \left(2295z^4 + 85z^2z_2^2 + 131z_2^4 \right) \\ & + \frac{\sqrt{15}}{97796160000000} \times \\ & \left(1730250z^6 - 1653665z^4z_2^2 - 5765z^2z_2^4 + 26974z_2^6 \right) \\ & + \dots\end{aligned}$$

Some tests for the $s = 3$ case

We have considered three problems

- Kepler's problem
- a perturbed Kepler problem
- Euler's problem

and four methods

- Classical Gauss method of order 6
- Calvo method with variable c_i -values
- Calvo method with fixed c_i -values
- my 2 parameter method

Problem 1 : Kepler's problem

$$H(p, q) = \frac{1}{2} \left(p_1^2 + p_2^2 \right) - \frac{1}{\sqrt{q_1^2 + q_2^2}}$$

$$\text{at } t = 0 : (q_1, q_2, p_1, p_2) = \left(1 - e, 0, 0, \sqrt{\frac{1+e}{1-e}} \right)$$

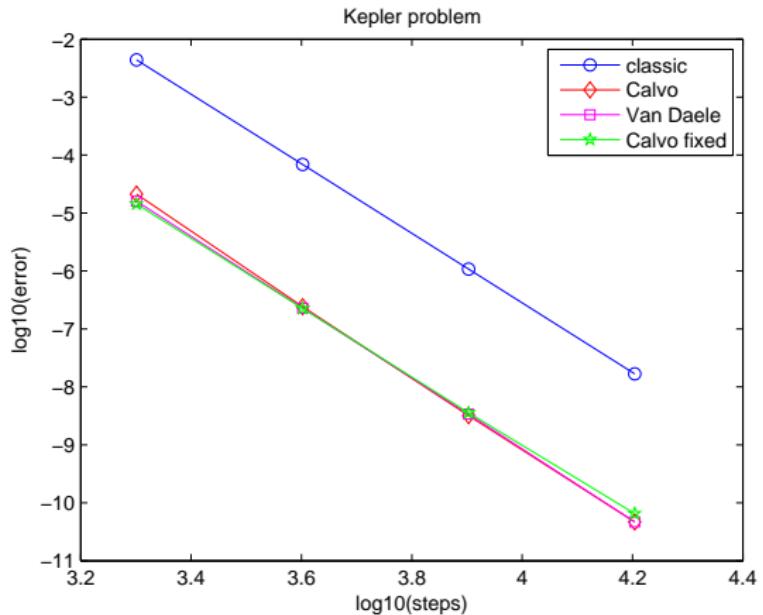
whereby $e = 0.001$

Integrated in $[0, 1000]$ with $h = 2^{-m}$, $m = 1, \dots, 4$.

$$(q_1(t), q_2(t), p_1(t), p_2(t)) = (\cos(E) - e, \sqrt{1 - e^2} \sin(E), q'_1(t), q'_2(t))$$

whereby $t = E - e \sin(E)$

Problem 1 : Kepler's problem



$$z = \frac{i}{(q_1^2 + q_2^2)^{3/2}} h \quad z_2 = z/2$$

Problem 2 : a Perturbed Kepler problem

$$H(p, q) = \frac{1}{2} (p_1^2 + p_2^2) - \frac{1}{\sqrt{q_1^2 + q_2^2}} - \frac{2\epsilon + \epsilon^2}{3\sqrt{(q_1^2 + q_2^2)^3}}$$

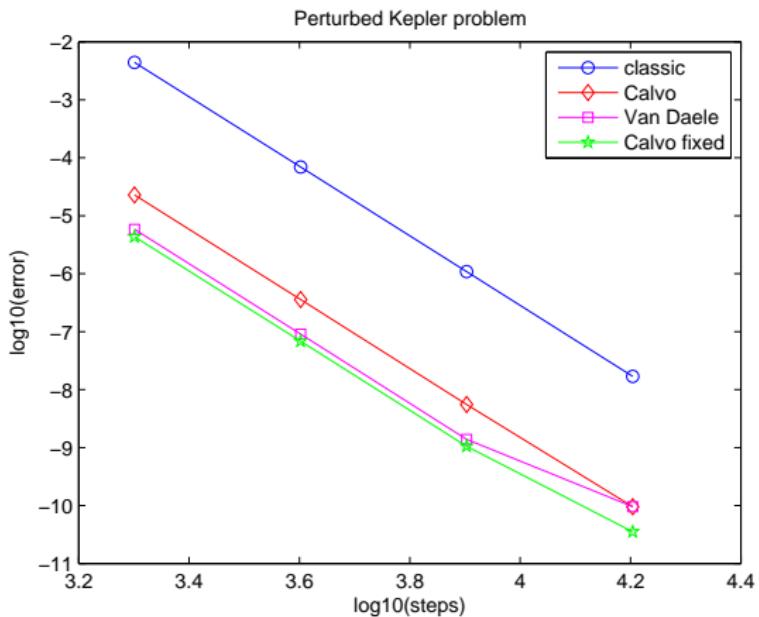
at $t = 0$: $(q_1, q_2, p_1, p_2) = (1, 0, 0, 1 + \epsilon)$

whereby $\epsilon = 0.001$

Integrated in $[0, 1000]$ with $h = 2^{-m}$, $m = 1, \dots, 4$.

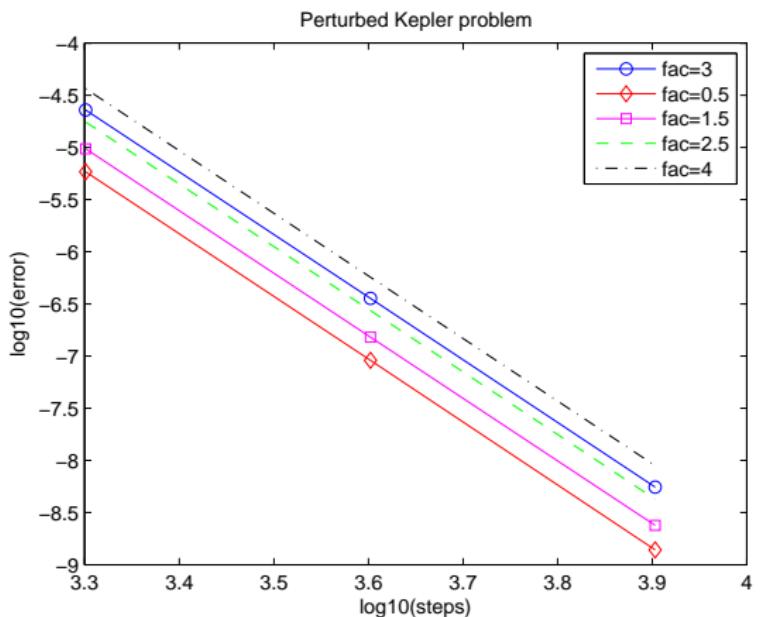
$$(q_1(t), q_2(t), p_1(t), p_2(t)) = (\cos((1+\epsilon)t), \sin((1+\epsilon)t), q'_1(t), q'_2(t))$$

Problem 2 : a Perturbed Kepler problem



$$z = i h \quad z_2 = z/2$$

Problem 2 : a Perturbed Kepler problem



$$z = i h \quad z_2 = \text{fac } z$$

Problem 3 : Euler's problem

$$\dot{q} = ((\alpha - \beta) q_2 q_3, (1 - \alpha) q_1 q_3, (\beta - 1) q_1 q_2)^T$$

at $t = 0$: $(q_1, q_2, q_3) = (0, 1, 1)$

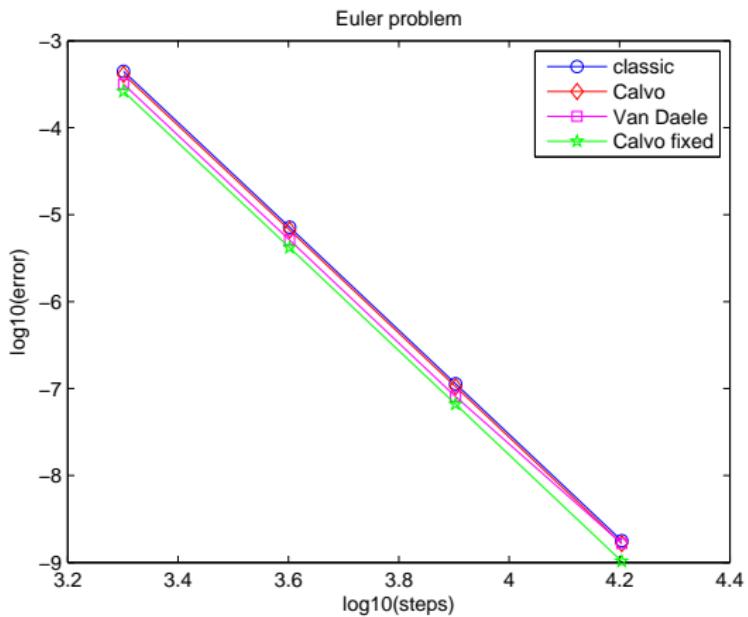
whereby $\alpha = 1 + \frac{1}{\sqrt{1.51}}$ and $\beta = 1 - \frac{0.51}{\sqrt{1.51}}$

Integrated in $[0, 1000]$ with $h = 2^{-m}$, $m = 1, \dots, 4$.

$$(q_1(t), q_2(t), q_3(t)) = (\sqrt{1.51} \operatorname{sn}(t, 0.51), \operatorname{cn}(t, 0.51), \operatorname{dn}(t, 0.51))$$

Problem is periodic with $T = 7.45056320933095$.

Problem 3 : Euler's problem



$$z = i \frac{2\pi}{T} h \quad z_2 = z/2$$

Conclusions

- we constructed a new family of exponentially-fitted variants of the Runge-Kutta methods of Gauss type
- these methods contain parameters μ_0, μ_1, \dots
- special case $\mu_0 = \mu_1 = \mu_2 \dots$ and $\mu_0 = \mu_1/2 = \mu_2/3 \dots$ gives known families of EF methods
- open problem (needs more testing) : how to choose the parameters