Functionally Fitted Explicit Two-Step Peer Methods

M. Calvo, J.I. Montijano, L. Rández & M. Van Daele

IUMA-Universidad de Zaragoza

Vakgroep Toegepaste Wiskunde en Informatica-Universiteit Gent



Instituto Universitario de Investigación de Matemáticas y Aplicaciones

Universidad Zaragoza



Instituto Universitario de Investigación de Matemáticas y Aplicaciones

Universidad Zaragoza

This talk deals with the numerical solution of IVPs for ODE systems

$$y'(t) = f(t, y(t)), \quad y(t_0) = y_0 \in \mathbb{R}^N,$$

with oscillating or periodic solutions by means of explicit two-stage peer methods.

We present a class of numerical methods called "fitted two-step peer methods" for the numerical integration of periodic problems whose frequency is approximately known in advance.

- These methods combine the advantages of Runge-Kutta and multistep ones to obtain high stage order.
- Introduced by Weiner *et al* (2004, 2005, 2009), ... for parallel computation and extended to sequential computation.

A step of a RK method



A step of a Peer method



Functionally Fitted Peer

- Standard methods for IVPs are fitted to a polynomial approximation to the local solution. The fitting space is $\mathcal{F} = \{1, t, t^2, \ldots\}$.
- Exponential Fitted methods The fitting space is $\mathcal{F} = \{1, e^{\pm iwt}, e^{\pm i2wt}, \ldots\}.$
- Functional Fitted methods The fitting space is $\mathcal{F} = \{1, \varphi_1(t), \varphi_2(t), \ldots\}.$

Ref: Bettis (1979), Paternoster (1998), Simos (1998), Vanden Berghe *et al* (1999), Coleman *et al* (2000), Franco (2002), Ixaru *et al* (2004), ...

Background

In Functionally Fitted s-stages RK methods the solution of the IVP (1) advances to $(t_n, y_n) \rightarrow (t_{n+1} = t_n + h, y_{n+1})$ by means of the formulas

$$y_{n+1} = \gamma_0 y_n + h \sum_{j=1}^{\infty} b_j f(t_n + c_j h, Y_{n,j}),$$
(2)

$$Y_{n,j} = \gamma_j y_n + h \sum_{k=1}^{s} a_{jk} f(t_n + c_k h, Y_{n,k}), \quad j = 1, \dots, s, \quad (3)$$

where

$$\begin{array}{c|c} c = (c_j)_{j=1}^s & \gamma = (\gamma_j)_{j=1}^s & A = (a_{jk}) \in \mathbb{R}^{s \times s} \\ \hline & & \gamma_0 & b^T = (b_j)_{j=1}^s \end{array}$$
(4)

are the real coefficients that define the method.

In standard RK methods all $\gamma_j = 1$ and the remaining coefficients are fixed numbers. In fitted methods they depend in general on the time step h, the starting time t_n and the space \mathcal{F} of fitting functions.

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We will assume (q + 1)-dim. fitting spaces

$$\mathcal{F} = \mathcal{F}_q = \langle \varphi_0(t), \varphi_1(t), \dots, \varphi_q(t) \rangle,$$

of smooth linearly independent real functions in $\left[t_0,t_0+T\right]$ in the sense that the Wronskian matrix

$$W(\varphi_0,\varphi_1,\ldots,\varphi_q)(t) = \begin{pmatrix} \varphi_0(t) & \varphi_1(t) & \ldots & \varphi_q(t) \\ \dot{\varphi}_0(t) & \dot{\varphi}_1(t) & \ldots & \dot{\varphi}_q(t) \\ \vdots & \vdots & & \vdots \\ \varphi_0^{(q)}(t) & \varphi_1^{(q)}(t) & \ldots & \varphi_q^{(q)}(t) \end{pmatrix}$$

is non singular for all $t \in [t_0, t_0 + T]$.

To have a RK method fitted to \mathcal{F}_q , the available coefficients a_{ij} , c_i , γ_i , b_i are selected so that they satisfy the fitting conditions

$$\varphi(t_n + h) = \gamma_0 \varphi(t_n) + h \sum_{j=1}^{s} b_j \dot{\varphi}(t_n + c_j h),$$
(5)
$$\varphi(t_n + c_j h) = \gamma_j \varphi(t_n) + h \sum_{k=1}^{s} a_{jk} \dot{\varphi}(t_n + c_k h), \quad j = 1, \dots, s$$
(6)

for all $\varphi \in \mathcal{F}_q$.

The above conditions imply by linearity that the corresponding RK method integrates exactly any local solution $y(t; t_n, y_n)$ of y' = f(t, y) such that $y(t; t_n, y_n) \in \mathcal{F}_q$.

Drawback

For explicit RK fitted methods $c_1=0, \gamma_1=1$ and then the second one

$$\varphi(t_n + c_2 h) = \gamma_2 \varphi(t_n) + h a_{21} \dot{\varphi}(t_n),$$

for a fixed node c_2 , has only the two free parameters (γ_2 , a_{21}) and $q \leq 1$ and this implies serious restrictions in the dimensionality of the fitting space.

One remedy

We consider the so called explicit two-step peer methods, recently introduced by R. Weiner, B. A. Schmitt *et al* as an alternative to classical Runge–Kutta (RK) and multistep methods attempting to combine the advantages of these two classes of methods.

Two-Step Peer Methods

Given a set of admissible fixed nodes $\{c_j\}_{j=1}^s$ in the sense that

$$c_1, c_2, \ldots, c_s, 1 + c_1, 1 + c_2, \ldots, 1 + c_s$$

is a non confluent set of nodes, and starting from known approximations $Y_{0,j}$ to $y(t_0+c_jh)$, $j=1,\ldots,s$ we obtain the new approximations

$$Y_{1,j}\simeq y(t_1+c_jh) \quad \text{where} \quad t_1=t_0+h,$$

by means of

$$Y_{1,j} = \sum_{k=1}^{s} a_{jk} Y_{0,k} + h \sum_{k=1}^{s} b_{jk} f(t_0 + c_k h, Y_{0,k})$$

$$+ h \sum_{k=1}^{j-1} r_{jk} f(t_1 + c_k h, Y_{1,k}), \quad (j = 1, \dots, s).$$
(7)

 $A, B \in \mathbb{R}^{s \times s}$ full matrices and $R \in \mathbb{R}^{s \times s}$ strictly lower triangular are the free parameters that define the method with $A\mathbf{e} = \mathbf{e}$ to ensure the preconsistency condition.

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Extending the definition of fitted RK methods to PEER methods, we will say that the explicit two-step peer method is fitted to \mathcal{F}_q if

$$\varphi(t_1 + c_j h) = \sum_{k=1}^{s} a_{jk} \varphi(t_0 + c_k h) + h \sum_{k=1}^{s} b_{jk} \dot{\varphi}(t_0 + c_k h) + h \sum_{k=1}^{s} b_{jk} \dot{\varphi}(t_0 + c_k h) + h \sum_{k=1}^{s} c_{jk} \dot{\varphi}(t_1 + c_k h), \quad j = 1, \dots, s$$
(8)

holds for all $\varphi \in \mathcal{F}_q$.

- At each stage we have at least 2s 1 free parameters
- It is possible to obtain explicit methods that attain high stage order
- Are good candidates to obtain explicit methods fitted to spaces *F_q* with *q* large.
- The authors have derived in (2010), s stage methods with q = 2s 1 taking into account some stability and accuracy requirements

In our study of the order of a Fitted Peer Methods it will be sufficient to consider a scalar (non-linear) equation (m = 1), and they can be written in the vector form

$$\mathbf{Y}_{1} = A \ \mathbf{Y}_{0} + h \ B \ \mathbf{F}_{0} + h \ R \ \mathbf{F}_{1}, \qquad (9)$$

$$\mathbf{Y}_{k} = (Y_{k,1}, \dots, Y_{k,s})^{T} \in \mathbb{R}^{s},$$

$$\mathbf{e} = (1, \dots, 1)^{T} \in \mathbb{R}^{s},$$

$$\mathbf{c} = (c_{1}, \dots, c_{s})^{T} \in \mathbb{R}^{s},$$

$$\mathbf{F}_{k} = f(t_{k}\mathbf{e} + h\mathbf{c}, \mathbf{Y}_{k}) = (f(t_{k} + hc_{j}, Y_{k,j}))_{j=1}^{s} \in \mathbb{R}^{s}.$$

where

0-Stability

For the zero stability we only consider Peer Methods with the stronger requirement

$$\lambda_1(A) = 1, \qquad \lambda_j(A) = 0, \quad j = 2, \dots, s,$$
 (10)

and take A with the form

$$A = P^{-1} \hat{A} P, \tag{11}$$

with P and \widehat{A} of type

	(1	0		0 \			/ 1	\widehat{a}_{12}		\widehat{a}_{1s}	\	
	p_{21}	1	• • •	0				0	\widehat{a}_{23}	\widehat{a}_{2s}		
P =	p_{31}	p_{32}	•••	0	,	$\widehat{A} =$			·	:	,	
	:	÷	•••	÷						$\widehat{a}_{s-1.s}$		
	p_{s1}	p_{s2}		1 /						0)	

that satisfy (10). Note that the pre-consistency condition Ae = e implies that $Pe = e_1$.

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We associate to $\mathbf{Y}_1 = A\mathbf{Y}_0 + hB\mathbf{F}_0 + hR\mathbf{F}_1$ the linear *s*-dim vector valued operator $\mathcal{L}[\varphi;h]$ defined by

$$\mathcal{L}[\varphi;h](t) \equiv \varphi((t+h)\mathbf{e} + h\mathbf{c}) - A \varphi(t\mathbf{e} + h\mathbf{c}) - h B \dot{\varphi}(t\mathbf{e} + h\mathbf{c}) - h R \dot{\varphi}((t+h)\mathbf{e} + h\mathbf{c}).$$
(12)

Definition

For a given set of admissible nodes and a fitting space $\mathcal{F}_q = \langle \varphi_0(t), \varphi_1(t), \dots, \varphi_q(t) \rangle$ the Peer Method is fitted to the linear space \mathcal{F}_q with step size h at t_0 if

$$\mathcal{L}[\varphi;h](t_0) = 0, \qquad \forall \varphi \in \mathcal{F}_q.$$
(13)

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Remarks:

- If the starting values $(Y_{0,j})_{j=1}^s$ belong to a solution of the differential equation contained in the fitting space \mathcal{F}_q , then the Peer method gives the exact values of the solution.
- ullet In the polynomial case, $\mathcal{F}_q=\Pi_q,\,q$ is the stage order and

$$\mathcal{L}[y;h](t) = \mathcal{O}(h^{q+1}) \quad \text{for all} \quad y \in \mathcal{C}^{\infty},$$

and this condition turns out to be independent of t.

• If
$$\mathbf{Z}(t) = P \ \varphi(t\mathbf{e} + h\mathbf{c})$$
, we have $\mathcal{L}[\varphi; h](t_0) = P^{-1} \ \widehat{\mathcal{L}}[\varphi; h](t_0)$, with
 $\widehat{\mathcal{L}}[\varphi; h](t_0) = \mathbf{Z}(t+h) - \widehat{A} \ \mathbf{Z}(t) - h\widehat{B} \ \dot{\mathbf{Z}}(t) - h\widehat{R} \ \dot{\mathbf{Z}}(t+h)$

Then, the Peer method is fitted to \mathcal{F}_q iff $\widehat{\mathcal{L}}[\varphi;h](t_0) = 0, \forall \varphi \in \mathcal{F}_q$.

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When the coefficients are independent of t_n ?

We give sufficient conditions on the functions of \mathcal{F}_q that ensure that $\mathcal{L}[\varphi;h](t_0)$ is independent of t_0 and therefore the coefficients of the fitted method can be chosen independent of t_0 .

Theorem

Let \mathcal{F}_q be the (q+1)-dim space of solutions of an homogeneous linear differential equation with constant coefficients with order (q+1). If the linear operator \mathcal{L} with A, B and R independent of t satisfies

$$\mathcal{L}[\varphi;h](t_0) = 0, \quad \forall \varphi \in \mathcal{F}_q$$

then

$$\mathcal{L}[\varphi;h](t) = 0, \quad \forall \varphi \in \mathcal{F}_q, \quad \forall t \in [t_0, t_0 + T].$$

Remarks

- For fitting spaces of solutions of linear homogeneous solutions with constant coefficients if the available coefficients A, B, R (that may depend of the nodes and the step size h) are fitted for some particular t_0 then they are fitted for all t.
- For fitting spaces that satisfy the assumptions of the above Theorem, if we take as basis point $t_0 = -hc_1$ then $\widehat{\mathcal{L}}[\varphi; h](-hc_1)$ depends on the nodes in the form of differences $(c_2 c_1), \ldots, (c_s c_1)$.



We assume that $F_q = \langle \varphi_0(t) = 1, \varphi_1(t), \dots, \varphi_q(t) \rangle$ is a (q+1)-dim basis of solutions of the linear equation with constant coefficients

$$Q(D)u(t) \equiv u^{(q+1)}(t) + a_q u^{(q)}(t) + \ldots + a_1 u^{(1)}(t) = 0,$$

whose characteristic polynomial is

$$Q(z) = z^{q+1} + a_q z^q + \ldots + a_1 z = z^{\beta_0} (z - w_1)^{\beta_1} \ldots (z - w_r)^{\beta_r},$$

with $\beta_0 + \beta_1 + ... + \beta_r = q + 1$.

In the polynomial case it has been shown that:

- i) Given a set of admissible nodes $c_1, \ldots, c_s, 1 + c_1, \ldots, 1 + c_s$.
- ii) Given a lower triangular matrix $P = (p_{ij})$ with $p_{ii} = 1$ and $Pe = e_1$.

The parameters in \widehat{A} , \widehat{B} and \widehat{R} can be obtained, under usual hypothesis, as solutions of s independent sets of linear equations in the unknowns

It has been proved that if the free parameters are selected by attempting its exactness for the polynomials $\varphi(t) = t^k$, $k = 1, \ldots, 2s - 1$ then the corresponding method would have (stage) order p = 2s - 1.

We extend this situation to a more general case of spaces \mathcal{F}_q .

Theorem

Suppose that for a given set of admissible fixed nodes and constant matrix P the polynomially fitted two-step peer method with s stages has a unique solution with stage order 2s - 1, then:

• For any linear space $\mathcal{F}_{2s-1} = \langle 1, \varphi_1(t), \dots, \varphi_{2s-1}(t) \rangle$ there exist a unique s-stage two step peer method fitted to this space for h sufficiently small. This peer method has the same nodes and P-matrix as the polynomially fitted method to Π_{2s-1} and the coefficients

$$\widehat{A}_{\mathcal{F}} = \widehat{A}(t_0, h), \quad \widehat{B}_{\mathcal{F}} = \widehat{B}(t_0, h), \quad \widehat{R}_{\mathcal{F}} = \widehat{R}(t_0, h),$$

may depend (apart of the fitting space) on t_0 and h.

- 2 If \mathcal{F}_{2s-1} is a basis of solutions of a linear equation with constant coefficients, $\widehat{A}_{\mathcal{F}}$, $\widehat{B}_{\mathcal{F}}$, $\widehat{R}_{\mathcal{F}}$, are independent of t_0 and depend only on the roots of Q(D).
- Further when all the roots of the polynomial Q(D) tend to zero the coefficients $\hat{A}_{\mathcal{F}}$, $\hat{B}_{\mathcal{F}}$, $\hat{R}_{\mathcal{F}}$ tend to those of the polynomial case.

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Two-stage Peer Methods

With s = 2 the pre consistency condition $Pe = e_1$ implies that

$$P = \begin{pmatrix} 1 & 0 \\ -1 & 1 \end{pmatrix}. \tag{15}$$

On the other hand, the matrices $\widehat{A}, \widehat{B}, \widehat{R}$ will have the form

$$\widehat{A} = \begin{pmatrix} 1 & \widehat{a}_{12} \\ 0 & 0 \end{pmatrix}, \quad \widehat{B} = \begin{pmatrix} \widehat{b}_{11} & \widehat{b}_{12} \\ \widehat{b}_{21} & \widehat{b}_{22} \end{pmatrix}, \quad \widehat{R} = \begin{pmatrix} 0 & 0 \\ \widehat{r}_{21} & 0 \end{pmatrix}, \quad (16)$$

and

$$\mathbf{Z}(t) = P \varphi(t\mathbf{e} + h\mathbf{c}) = \begin{pmatrix} \varphi(t + c_1h) \\ -\varphi(t + c_1h) + \varphi(t + c_2h) \end{pmatrix}.$$
 (17)

Since the linear operator $\widehat{\mathcal{L}}$ is

$$\widehat{\mathcal{L}}[\varphi;h](t) = \mathbf{Z}(t+h) - \widehat{A} \,\mathbf{Z}(t) - h\widehat{B} \,\dot{\mathbf{Z}}(t) - h\widehat{R} \,\dot{\mathbf{Z}}(t+h)$$

we have two order conditions and in each condition there are three free parameters. The first equation with the parameters $\hat{a}_{12}, \hat{b}_{11}, \hat{b}_{12}$ can be written in the form

$$\begin{split} &[\varphi(t+c_2h) - \varphi(t+c_1h)]\hat{a}_{12} + h\dot{\varphi}(t+c_1h)\hat{b}_{11} \\ &+ h[\dot{\varphi}(t+c_2h) - \dot{\varphi}(t+c_1h)]\hat{b}_{12} = \varphi(t+h+c_1h) - \varphi(t+c_1h), \end{split}$$

and the second one with the parameters $\widehat{b}_{21}, \widehat{b}_{22}, \widehat{r}_{21}$ is

$$\begin{split} h\dot{\varphi}(t+c_{1}h)\widehat{b}_{21} + h[\dot{\varphi}(t+c_{2}h) - \dot{\varphi}(t+c_{1}h)]\widehat{b}_{22} \\ h\dot{\varphi}(t+h+c_{1}h)\widehat{r}_{21} = \varphi(t+h+c_{2}h) - \varphi(t+h+c_{1}h). \end{split}$$

These parameters will be determined by imposing that the above equations hold for the functions $\varphi_j(t), j = 1, 2, 3$ of the fitting space

$$\mathcal{F}_3 = \langle 1, t, \cos \omega t, \sin \omega t \rangle.$$

Solving the equations for
$$\hat{r}_{21}$$
, \hat{a}_{12} , \hat{b}_{11} , \hat{b}_{12} , \hat{b}_{21} , \hat{b}_{22} we obtain
 $\hat{a}_{12} = \frac{-1 + \cos \nu + \cos(d\nu) - \cos \nu \cos(d\nu) + \nu \sin(d\nu) - \sin \nu \sin(d\nu)}{\Delta_1}$,
 $\hat{b}_{11} = \frac{(-2 + d - d \cos \nu)(1 - \cos(d\nu) + d \sin \nu \sin(d\nu)}{\Delta_1}$,
 $\hat{b}_{12} = -\frac{\nu - d\nu + d\nu \cos \nu - \nu \cos(d\nu) - \sin \nu + \sin(d\nu) \sin(\nu - d\nu)}{\nu \Delta_1}$,
with $d = c_2 - c_1$, $\nu = hw$ and $\Delta_1 = -2 + 2\cos(d\nu) + d\nu \sin(d\nu)$.
In a similar way, we get
 $\hat{r}_{21} = \frac{\sin(d\nu/2) (d\nu \cos(d\nu/2) - 2\cos\nu \sin(d\nu/2))}{\Delta_2}$,
 $\hat{b}_{21} = -\frac{\sin(d\nu/2) (d\nu \cos(\nu - d\nu/2) - 2\cos\nu \sin(d\nu/2))}{\Delta_2}$,
 $\hat{b}_{22} = -\frac{\sin(\nu/2) (d\nu \cos(\nu/2) + \sin(\nu/2) - \sin(d\nu + \nu/2))}{\Delta_2}$,
with $\Delta_2 = 2\nu \sin(d\nu/2) \sin(\nu/2) \sin((\nu - d\nu)/2)$.

Three-stages Peer Methods

In the case of three stages Peer Methods, we have several possibilities,

•
$$\mathcal{F}_q = \{1, t, \cos wt, \sin wt, \cos 2wt, \sin 2wt\}$$

•
$$\mathcal{F}_q = \{1, t, t^2, t^3, \cos wt, \sin wt\}$$

•
$$\mathcal{F}_q = \{1, t, \cos w_1 t, \sin w_1 t, \cos w_2 t, \sin w_2 t\}$$

•
$$\mathcal{F}_q = \{1, t, \cos wt, \sin wt, t \cos wt, t \sin wt\}$$

For the sake of simplicity, we derive the fitted method associated to the 3-stage method developed by the authors (2010) and given by the coefficients:

[A B] =	$\begin{bmatrix} 0.0003 \\ 5.040 \\ 2.631 \end{bmatrix}$	855 0.69200 47 6.1955 53 3.5648	$\begin{array}{rrrr} 06 & 0.30 \ 2 & -10 \ 4 & -5. \end{array}$	7138).236 1963	$\begin{array}{c} 0.000172 \\ 1.11675 \\ 0.593029 \end{array}$	$\begin{array}{c} 0.041579 \\ 41.799 \\ 20.477 \end{array}$	-0.01777 21.9221 10.6664	
[c R] =	0 0.904 1.141	$\begin{array}{c} 0.000172 \\ -56.8554 \\ -27.3595 \end{array}$	$\begin{array}{c} 0\\ 0\\ 0.47041\end{array}$	$\begin{array}{c} 0\\ 0\\ 2 \end{array}$				

Test Problems

Duffing's equation

$$\begin{split} y'' + (\lambda^2 + k^2)y &= 2k^2y^3, \quad t \in [0, 20] \\ y(0) &= 0, \quad y'(0) = \lambda, \end{split}$$

with k = 0.035 and $\lambda = 5$. The analytic solution is given by:

$$y(t) = \operatorname{sn}\left(\lambda t, \left(\frac{k}{\lambda}\right)^2\right).$$

where sn represents the elliptic Jacobi function. We choose $\omega = 5i$, and the numerical results have been computed with the integration steps

$$\Delta t = \frac{1}{5 \times 2^m}, \ m = 1, \dots, 6.$$



The Euler equations

$$y' = f(y) = ((\alpha - \beta)y_2y_3, (1 - \alpha)y_3y_1, (\beta - 1)y_1y_2)^T,$$

with the initial values $y(0) = (0, 1, 1)^T$.

- It possesses two quadratic invariants: $G_1=y_1^2+y_2^2+y_3^2$ and $G_2=y_1^2+\beta y_2^2+\alpha y_3^2$
- Parameter values $\alpha = 1 + \frac{1}{\sqrt{1.51}}$ and $\beta = 1 \frac{0.51}{\sqrt{1.51}}$. $\omega = 2\pi/T$, with T = 7.45056320933095. The exact solution of this IVP is given by

$$y(t) = \left(\sqrt{1.51}\operatorname{sn}(t, 0.51), \operatorname{cn}(t, 0.51), \operatorname{dn}(t, 0.51)
ight)^T$$

where sn, cn, dn are the elliptic Jacobi functions.

• The integration is carried out on the interval [0, 40] with step sizes $h = 1/(5 \times 2^{j-2})$, $j = 1, \ldots, 5$ and $w = 2\pi/Ti$.





A perturbed Kepler's problem

The Hamiltonian function is

$$H(p,q) = \frac{1}{2} \left(p_1^2 + p_2^2 \right) - \left(q_1^2 + q_2^2 \right)^{-1/2} - (2\varepsilon + \varepsilon^2) / 3 \left(q_1^2 + q_2^2 \right)^{-3/2},$$

Initial conditions:

 $q_1(0) = 1, \ q_2(0) = 0, \ p_1(0) = 0, \ p_2(0) = 1 + \varepsilon, \quad 0 < \varepsilon << 1$

The exact solution of this IVP is given by

 $q_1(t) = \cos(t + \varepsilon t), \quad q_2(t) = \sin(t + \varepsilon t), \quad p_i(t) = q'_i(t), \ i = 1, 2.$

• The numerical results have been computed with the integration steps $\Delta t = \frac{\pi}{10 \times 2^m}, m = 0, \dots, 3$. We take the parameter values $\varepsilon = 10^{-3}, \lambda = i$ and the problem is integrated up to $t_{end} = 10\pi$.

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Conclusions

- In our numerical experiments, we have considered fitted methods for systems of equations with all components fitted to the same given frequency ω.
- It appear that an accurate estimation of the frequency is essential for the integrators based on fitted methods. This fact was already recognised by Vanden Berghe *et al* (2001)
- The accuracy of the fitted methods is in general superior to the non fitted ones of the same order.

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