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Phase-fitted Runge–Kutta pairs of orders 8(7)

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ABSTRACT

A new phase fitted Runge–Kutta pair of orders 8(7) which is a modification of a well known explicit Runge–Kutta pair for the integration of periodic initial value problems is presented. Numerical experiments show the efficiency of the new pair in a wide range of oscillatory problems.

1. Introduction

For the numerical solution of the initial value problem

$$y' = f(x, y), \qquad y(x_0) = y_0 \in \Re^m, \quad x \in [x_0, x_e] \tag{1}$$

where $f : \Re \times \Re^m \mapsto \Re^m$, the Explicit Runge–Kutta (RK) pairs are widely used. Such pairs can be presented by the extended Butcher tableau [1,2]:

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

with $b^T, \hat{b}^T, c \in \Re^s$ and $A \in \Re^{s\times s}$ is strictly lower triangular. Such methods advance the solution from x_n to $x_{n+1} = x_n + h_n$ using the following two approximations at each step, $y_{n+1}, \hat{y}_{n+1}$ to $y(x_{n+1})$ of orders p and $p - 1$ respectively,

$$y_{n+1} = y_n + h_n \sum_{i=1}^{s} b_i f_{ni}$$

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and

$$\hat{y}_{n+1} = y_n + h_n \sum_{i=1}^{s} \hat{b}_i f_{ni},$$

where

$$f_{ni} = f\left(x_n + c_i h_n, y_n + h_n \sum_{j=1}^{i-1} a_{ij} f_{nj}\right)$$

for $i = 1, 2, \ldots, s$. Using this embedded form we can obtain an estimate $E_{n+1} = \left\|y_{n+1} - \hat{y}_{n+1}\right\|$ of the local truncation error of the $p-1$ order formula. Then the next step of the numerical solution can be computed using a step-size control algorithm

$$h_{n+1} = 0.9 \cdot h_n \cdot \left(\frac{\mathrm{TOL}}{E_{n+1}}\right)^{1/p}, \tag{2}$$

where TOL being the requested tolerance. If $E_{n+1} > \mathrm{TOL}$ the step h_n computed to advance the approximation of the solution from x_n to x_{n+1} is rejected and the same formula (2) is assumed to recompute the new smaller current step. In (2) the 0.9 is a safety factor that is used so that the error will be acceptable the next time with high probability. For more details on the implementation of these types of step size policies see [2,3].

2. Basic theory

When a RK method is applied to solve the test problem

$$y' = i\omega y, \quad \omega \in \Re,\ i = \sqrt{-1}, \tag{3}$$

we are led to the numerical scheme

$$y_{n+1} = P\left(i\omega h_n\right) y_n,$$

$h_n = x_{n+1} - x_n$, where the function $P\left(iv\right) = P\left(i\omega h\right)$ satisfies the relation

$$P\left(iv\right) = 1 + ivb\left(I - ivA\right)^{-1} e = \sum_{j=0}^{\infty} t_j \left(iv\right)^j, \tag{4}$$

and for $j \geq 1$, $t_j = bA^{j-1}e$, $t_0 = 1$ and $e = [1, 1, \ldots, 1] \in \Re^s$ [4]. The quantities t_j depend only on the coefficients of the method. For explicit methods (e.g. A strictly lower triangular), the above sum in the determination of $P\left(iv\right)$ is finite and j runs from 0 to s.

Following [5], we define the phase-lag (or dispersion) order of a RK method as the order of approximation of the argument of the exponential function by the argument of P along the imaginary axis. Equivalently, the phase-lag order of a method is q, whenever $\delta\left(v\right) = O\left(v^{q+1}\right)$, for $\delta\left(v\right) = v - \arg\left(P\left(iv\right)\right)$. We define also, the imaginary stability interval of a RK method $I_I = \left(0, v_0\right)$ by the relations $\left|P\left(iv\right)\right| < 1$ and $\left|P\left(i\left(v_0 + \theta\right)\right)\right| > 1$, for every $v \in I_I$ and every suitably small positive θ. When a method has a non-vanishing imaginary stability interval then it is called dissipative.

Even though in the definition for a RK method the phase-lag property is based on the solution of a special problem (3), the numerical tests presented in [6,4] strongly indicated that the RK pairs of high phase-lag order exhibit a remarkable numerical performance on a much wider class of test problems. Especially for a certain class of initial value problems (as those whose solutions are described by free oscillations or free oscillations of low frequency with forced oscillations of high frequency superimposed, over long integration intervals), one should use pairs of methods of high phase-lag order with minimized leading truncation error coefficients instead of pairs of the same algebraic order which attain the minimal algebraic order and phase-lag order allowed by the number of method's stages.

3. Methods with known frequency

Gautschi [7] has been the first who tried to fit a method to a set of linearly independent trigonometric functions. Since then a lot of methods trying to do something similar have been constructed. Here we will exploit the knowledge of $v = \omega h$ in the direction of the ideas presented in the previous section.

We observe that

$$\begin{aligned} P\left(iv\right) &= Q\left(v\right) + iR\left(v\right) \\ &= \left(1 - t_2 v^2 + t_4 v^4 - t_6 v^6 \pm \cdots\right) + i\left(v - t_3 v^3 + t_5 v^5 - t_7 v^7 \pm \cdots\right) \end{aligned}$$

which is a finite series for explicit methods, as we have mentioned.

Requiring $\delta(v) = v - \arg(P(iv)) = 0$ and $\tan v = \frac{R(v)}{Q(v)}$ then

$$Q(v)\tan v = R(v)$$

holds, restricting just one t_{ji} to some expression of v. A new method can be derived by solving all the order conditions and the equation for the restricted t_j. As the number of stages of a method is greater than its order (e.g. $s > p$) when $p > 4$, there is always some free t_j, $j > p$ to solve for. Such a method is characterized as a *phase-fitted* method and these ideas where first introduced by Raptis and Simos [8].

In the next section we construct explicit phase-fitted RK formulas of orders 8(7) with 13 stages and we derive coefficients for a phase fitted pair based on a classical similar pair of Prince and Dormand [9].

4. Phase-fitted Runge–Kutta pairs of orders 8(7)

For the popular family that PD8(7) [9] belongs to we set $c_{12} = 1$, $a_{13,12} = 0$ and when solving the set of order conditions we have the following free parameters $c_2, c_5, c_6, c_7, c_8, c_{10}, c_{11}, a_{8,7}, b_{13}, \hat{b}_{12}, \hat{b}_{13}$ to use for the minimization of the principal local truncation error term. For the classical DP8(7) the choice of the parameters set is $c_2 = \frac{1}{18}$, $c_5 = \frac{5}{16}$, $c_6 = \frac{3}{8}$, $c_7 = \frac{59}{400}$, $c_8 = \frac{93}{200}$, $c_{10} = \frac{13}{20}$, $c_{11} = \frac{1201146811}{1299019798}$, $a_{8,7} = -\frac{180193667}{1043307555}$, $b_{13} = \frac{1}{4}$, $\hat{b}_{12} = \frac{2}{45}$, $\hat{b}_{13} = 0$.

For such methods (4) takes the form

$$\begin{aligned} P &= Q(v) + \sqrt{-1}R(v) \\ &= \left(1 - \frac{1}{2}v^2 + \frac{1}{24}v^4 - \frac{1}{720}v^6 + \frac{1}{40320}v^8 - t_{10}v^10 + t_{12}v^{12}\right) \\ &\quad + \sqrt{-1}\left(v - \frac{1}{6}v^3 + \frac{1}{120}v^5 - \frac{1}{5040}v^7 + t_9v^9 - t_{11}v^{11}\right) \end{aligned}$$

and for phase-fitted methods we require $v = \arg(P(iv))$. So we solve

$$Q(v)\tan v = R(v)$$

for $a_{8,7}$ to get its expression with respect to v and $\tan(v)$. Asking a high precision least squares approximation of the solution over a dense uniform grid of the interval [0, 1.5] we finally get

$$a_{8,7} = \frac{C(v)}{D(v)}$$

where

$$\begin{aligned} C(v) = &-0.19781108078634084 - 0.164050909125528499v^2 \\ &+ 0.042578310088756321v^4 - 0.002300513610963998v^6 \\ &+ 0.000033467244551879287v^8 - 7.8661142036921924 \cdot 10^{-8}v^{10} \end{aligned}$$

and

$$\begin{aligned} D(v) = &\ 1 - 0.296457092123567400v^2 + 0.015793885907465726v^4 \\ &- 0.00018913011771688527v^6 + 0.0000017089234650765179v^8 - 1.2705211682518626 \cdot 10^{-7}v^{10}. \end{aligned}$$

The behavior of $a_{8,7}$ for $v \in [0, 1.5]$ is presented in Fig. 1. Now, only the following coefficients of the method depend on $a_{8,7}$:

$$\begin{aligned} a_{8,1} &= 0.026876256 + 0.0576576a_{8,7}, \\ a_{8,4} &= 0.22464336 - 0.944944a_{8,7}, \\ a_{8,5} &= 0.000369024 - 0.2061696a_{8,7}, \\ a_{8,6} &= 0.21311136 + 0.093456a_{8,7}, \\ a_{9,1} &= 0.07239997637512857 + 0.01913119863380767a_{8,7}, \\ a_{9,4} &= -0.688400520601143 - 0.3135390887207368a_{8,7}, \\ a_{9,5} &= -0.688400520601143 - 0.3135390887207368a_{8,7}, \\ a_{9,6} &= -0.17301267570583073 - 0.06840852844816077a_{8,7}, \\ a_{9,7} &= 0.1440060555560846 + 0.031009360422930017a_{8,7}, \\ a_{9,8} &= 0.9982362892760762 + 0.33180705811215994a_{8,7}, \\ a_{10,1} &= 0.16261514523236525 - 0.12125171966747463a_{8,7}, \\ a_{10,4} &= -2.1255544052061124 + 1.9871809612169453a_{8,7}, \\ a_{10,5} &= -0.216403903283323 + 0.43356675517460624a_{8,7}, \end{aligned}$$

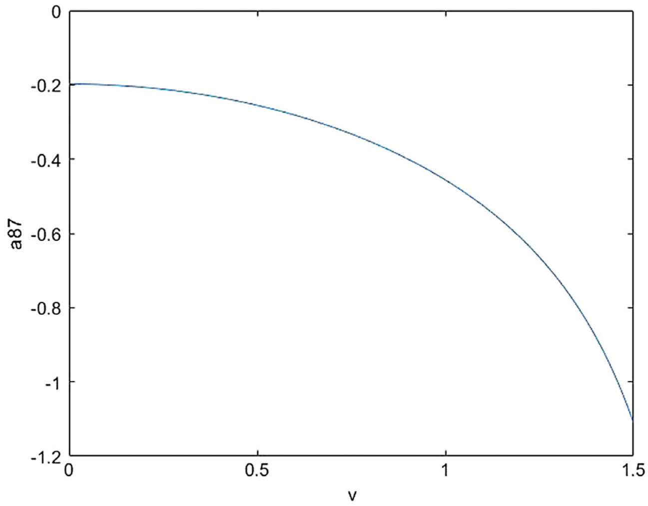

Fig. 1. The $a_{8,7}(v)$ for $v \in [0, 1.5]$.

$$a_{10,6} = -0.060417230254934076 - 0.1965343807796979 a_{8,7},$$
$$a_{10,7} = -0.060417230254934076 - 0.1965343807796979 a_{8,7},$$
$$a_{10,8} = 2.4846281621788395 - 2.102961615944379 a_{8,7},$$
$$a_{11,1} = -1.0320124180911034 + 1.061943768952537 a_{8,7},$$
$$a_{11,4} = 13.666683232895137 - 17.40407843561103 a_{8,7},$$
$$a_{11,5} = 0.25990355211486116 - 3.797253476860588 a_{8,7},$$
$$a_{11,6} = -5.759316475814002 + 1.7212824826428488 a_{8,7},$$
$$a_{11,7} = -12.822511612651839 + 18.41810566087623 a_{8,7},$$
$$a_{12,1} = 0.2478349764611783 - 0.06383934946543009 a_{8,7},$$
$$a_{12,4} = -4.593782880309185 + 1.046256005127882 a_{8,7},$$
$$a_{12,5} = -0.39566692537411896 + 0.22827403748244698 a_{8,7},$$
$$a_{12,6} = -3.0673550479691665 - 0.10347586863902129 a_{8,7},$$
$$a_{12,7} = 5.386688702227177 - 1.1072148245058775 a_{8,7},$$
$$a_{13,1} = 0.7332242174431163 - 0.5164807626867616 a_{8,7},$$
$$a_{13,4} = -10.196728938160977 + 8.464545832921925 a_{8,7},$$
$$a_{13,5} = -0.43865244706547707 + 1.846809999910238 a_{8,7},$$
$$a_{13,6} = 0.5693856884667226 - 0.8371528845746959 a_{8,7},$$
$$a_{13,7} = 10.52865228002416 - 8.957722185570706 a_{8,7},$$

whereas, the other coefficients are the same ones of classical PD8(7) pair. It is obvious that the computational overhead for evaluating these coefficients is negligible.

5. Numerical experiments

The new phase fitted pair of order 8(7), which we call NEW8(7)v, was based on the classical Runge–Kutta pair of orders 8(7) due to Prince and Dormand [9], in this work called PD8(7), and so we chose this method for the comparison of the new method. The pairs were run for tolerances $10^{-3}, 10^{-4}, \ldots, 10^{-9}$ in variable step-size and measure the $-\log_{10}$(end-point error) at y and the total number of function evaluations needed for the following well known problems from the literature problems.

The model equation

$$y'' = -25y,$$

with $y(0) = 1, y'(0) = 0$ for $x \in [0, 20\pi]$. Its exact solution is $y(x) = \cos 5x$. For this problem $\omega = 5$.

Bessel equation

$$y'' = -\left(100 + \frac{1}{4x^2}\right) y,$$

Table 1
The model equation results.

Tolerance	10^{-3}	10^{-4}	10^{-5}	10^{-6}	10^{-7}	10^{-8}	10^{-9}
Correct digits							
PD8(7)	2.08	3.00	4.08	5.22	6.38	7.54	8.69
NEW8(7)v	12.45	13.11	12.40	13.70	12.49	13.06	13.07
Fun. Ev.							
PD8(7)	1781	2418	3211	4264	5668	7540	10 036
NEW8(7)v	3112	2924	3640	4654	6032	7891	10 387

Table 2
The Bessel equation results.

Tolerance	10^{-3}	10^{-4}	10^{-5}	10^{-6}	10^{-7}	10^{-8}	10^{-9}
Correct digits							
PD8(7)	2.86	3.87	4.48	5.51	6.73	7.94	9.12
NEW8(7)v	7.49	8.03	9.83	10.43	11.48	12.75	13.05
Fun. Ev.							
PD8(7)	2429	3754	3282	4186	5577	7436	9932
NEW8(7)v	3185	3264	3627	4628	5993	7865	10 309

Table 3
The hyperbolic PDE results.

Tolerance	10^{-3}	10^{-4}	10^{-5}	10^{-6}	10^{-7}	10^{-8}	10^{-9}
Correct digits							
PD8(7)	2.20	2.96	3.93	5.18	5.67	6.63	7.73
NEW8(7)v	2.55	3.73	4.99	6.38	8.03	9.00	10.07
Fun. Ev.							
PD8(7)	5382	5486	5850	7384	10 335	13 897	18 512
NEW8(7)v	6187	6801	7051	9229	14 921	16 406	20 709

with initial conditions $y\,(1) = -0.2459357644513483$,

$$y'\,(1) = -0.5576953439142885, \quad \text{for } x \in [1, 32.59406213134967].$$

The theoretical solution of this problem is $y(x) = \sqrt{x}J_0\,(10x)$. The 100th zero of this problem was observed for $x = 32.59406213134967$, [10]. We used $\omega = 10$ for derivation of the coefficients of phase-fitted methods.

Hyperbolic problem

The hyperbolic PDE,

$$\frac{\vartheta u}{\vartheta x} = \frac{\vartheta u}{\vartheta r}, \qquad u\,(x, 0) = 0, \qquad u\,(0, r) = \sin \pi^2 r^2,$$
$$0 \le r \le 1, \; x \ge 0$$

is semi-discretized by symmetric differences (with $\Delta r = 1/50$) to the system of ODEs

$$\begin{bmatrix} y_1' \\ y_2' \\ \\ y_{50}' \end{bmatrix} = \frac{1}{2} \cdot \frac{1}{(1/50)} \begin{bmatrix} 0 & -1 & & & \\ 1 & 0 & -1 & & \\ & & & & \\ & & 1 & 0 & -1 \\ & & -1 & 4 & -3 \end{bmatrix} \cdot \begin{bmatrix} y_1 \\ y_2 \\ \\ y_{50} \end{bmatrix}.$$

In [5] it was found that the 500th zero of the 20th component in the above equation was reached for $x = 33.509996948$. So we integrated the methods to that point. As, there is not some dominant frequency for this problem, we use a rough estimation of $\omega = 50$ which is not far from the largest eigenvalue of the problem.

Nonlinear problem

$$y'' = -100y + \sin y,$$

with $y\,(0) = 0,\; y\,(0) = 1$ for $x \in [0, 20\pi]$. The analytic solution is not known but with a quadruple precision integration at high tolerance it can be found that $y\,(20\pi) = 3.92823991 \cdot 10^{-4}$, [11]. We used $\omega = 10$ for this problem.

Most of the problems we choose have oscillatory solutions that are not described by trivial trigonometric solutions. The results over the problems are presented in Tables 1–4 and reveal the superiority of the proposed phase fitted method in a competitive computational cost.

Table 4
The nonlinear problem results.

Tolerance	10^{-3}	10^{-4}	10^{-5}	10^{-6}	10^{-7}	10^{-8}	10^{-9}
Correct digits							
PD8(7)	2.75	3.45	4.58	5.40	6.53	7.71	8.89
NEW8(7)v	4.83	6.02	7.02	8.09	9.12	10.02	11.32
Fun. Ev.							
PD8(7)	3706	4670	7050	7799	10 374	13 884	18 551
NEW8(7)v	5534	7013	8448	10 187	12 649	14 689	19 318

6. Conclusion

A new phase-fitted pair of orders 8(7) is presented in this article. The numerical experiments on problems with oscillatory solutions indicate that the new phase fitted pair is appropriate for initial value problems with oscillatory solutions.

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