Dissipative high phase-lag order methods.

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September 16, 1998

ABSTRACT. New explicit hybrid Numerov type methods are presented in this paper. They share eighth algebraic order while their phase lag order varies between 18 and 22. Their main characteristic is that they are dissipative so they posses an empty interval of periodicity, Numerical illustrations indicate that this choice was successful since the new methods outperforms the older ones which were scheduled to integrate effectively periodic problems.

Keywords : explicit methods for periodic ODEs, phase lag, dissipation, eighth algebraic order.

1. INTRODUCTION.

The initial value problem of second order

$$y'' = f(x, y), \quad y(x_0) = y_0, \quad y'(x_0) = y_0', \tag{1}$$

especially when the solution is periodic, is of continued interest in many fields of celestial mechanics, quantum mechanics, scattering theory, theoretical physics and chemistry, and electronics (see [7, 8]).

When solving (1) numerically we have to pay attention in the algebraic order of the method used, since this is the main factor of achieving higher accuracy with lower computational cost, i.e. this is the main factor of increasing the efficiency of our effort. If we also feel that the solution of (1) is of periodic nature then it is essential to consider *phase-lag* (or dispersion) and *amplification* (or dissipation). These are actually two types of truncation errors. The first is the angle between the true and the approximated solution, while the second is the distance from a standard cyclic solution.

One of the most widely used method for solving (1) is the Numerov method which is fourth algebraic and fourth phase-lag order. This method is implicit and its implementation involve computations of Jacobians and solutions of non-linear systems of equations, [1]. So many authors proposed explicit modifications of Numerov method trying simultaneously to increase the phase-lag order. The algebraic orders achieved were at most only six, [2, 3, 10]. Recently Tsitouras and Simos [14], presented an explicit method of eighth algebraic order and of phase-lag order 14, which is the

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best method of this type appeared in the literature until then. That method was of zero dissipation, something common when implementing two step hybrid methods for problems with periodic solutions.

At the same time Papakostas and Tsitouras [9], presented high phase-lag order Runge-Kutta and Runge-Kutta-Nyström methods with non zero amplification error. Even in [12], it was notified that the zero amplification error is not so promising. The former results was the motivation for this paper which deals with the derivation of dissipative two-step eighth order methods of very high phase-lag order. This will became possible since degrees of freedom during the construction of the new scheme can be used for increasing phase-lag order instead of trying to keep amplification to zero.

2. Basic theory.

To study the stability properties of methods posed for solving (1), it is constructive to consider the scalar test problem

$$y' = -\omega^2 y. \tag{2}$$

When applying an explicit two step hybrid method to the problem (2) we obtain a difference equation of the form

$$y_{n+1} + S\left(v^2\right) y_n + C\left(v^2\right) y_{n-1} = 0, \tag{3}$$

where $y_n \approx y(nh)$ the computed approximations at $n = 1, 2, \ldots, v = \omega h$, h the step size used, and $S(v^2), C(v^2)$ polynomials in v^2. All the methods until now, make the assumption $C(v^2) \equiv 1$. This was not obligatory but mostly a pleasant (as believed) outcome of oversimplifications due to the symmetries of the methods proposed. The characteristic equation associated with (3) is

$$\lambda^2 + S\left(v^2\right)\lambda + C\left(v^2\right) = 0. \tag{4}$$

Following Lambert and Watson [6], we say that the numerical method (3) has interval of periodicity $(0, v_0^2)$ if $C(v^2) \equiv 1$ and $\mid S(v^2) \mid < 2$ for all $v^2 \in (0, v_0^2)$. Consequently the method is called P-stable if $v_0 = \infty$. In our new proposal here $C(v^2) \neq 1$ so it is of interest to consider the *amplification* (or dissipation) order q as the number satisfying

$$1 - C\left(v^2\right) = O\left(v^q\right).$$

The phase-lag order of the method is p if

$$e^{2v} + S\left(v^2\right) \cdot e^v + C\left(v^2\right) = O\left(v^p\right).$$

We intend to use the 10-stage family of methods introduced in [14], in order to produce two methods. The first has $p = 22$ and $q = 10$, while the other one $p = 18$ and $q = 14$.

3. THE NEW METHODS

In [14] a 10 stage family of eighth algebraic order was introduced. It uses the smallest number of stages per step but also leaves many parameters free in order to manipulate some improvements. These family has the following general form.

$$
\begin{aligned}
&f_n = f(x_n, y_n)\\
&\overline{y}_{n+1} = 2y_n - y_{n-1} + h^2 f_n\\
&\overline{\overline{y}}_{n+1} = 2y_n - y_{n-1} + \tfrac{h^2}{12}\left(\overline{f}_{n+1} + 10 f_n + f_{n-1}\right)\\
&\overline{y}_{n-1/2} = \tfrac{1}{2}y_n + \tfrac{1}{2}y_{n-1} + \tfrac{h^2}{384}\left(5\overline{\overline{f}}_{n+1} - 34 f_n + -19 f_{n-1}\right)\\
&\overline{y}_{n+1/2} = \tfrac{3}{2}y_n - \tfrac{1}{2}y_{n-1} + h^2\left(g_1\overline{\overline{f}}_{n+1} + g_2 f_n + g_3 f_{n-1} + g_4\overline{f}_{n-1/2}\right)\\
&\overline{y}_{n-3/4} = \tfrac{1}{4}y_n + \tfrac{3}{4}y_{n-1} + h^2\left(d_1\overline{\overline{f}}_{n+1} + d_2 f_n + d_3 f_{n-1} + d_4\overline{f}_{n+1/2} + d_5\overline{f}_{n-1/2}\right)\\
&\overline{y}_{n+3/4} = \tfrac{7}{4}y_n - \tfrac{3}{4}y_{n-1}\\
&\qquad +h^2\left(c_1\overline{\overline{f}}_{n+1} + c_2 f_n + c_3 f_{n-1} + c_4\overline{f}_{n+1/2} + c_5\overline{f}_{n-1/2} + c_6\overline{f}_{n-3/4}\right)\\
&\overline{y}_{n-2/5} = \tfrac{3}{5}y_n + \tfrac{2}{5}y_{n-1}\\
&\qquad +h^2\left(\begin{array}{c} k_1 f_{n+1} + k_2 f_n + k_3 f_{n-1} + k_4\overline{f}_{n+\frac{1}{2}}\\ +k_5\overline{f}_{n-\frac{1}{2}} + k_6\overline{f}_{n+\frac{3}{4}} + k_7\overline{f}_{n-\frac{3}{4}}\end{array}\right)\\
&\overline{y}_{n+2/5} = \tfrac{7}{5}y_n - \tfrac{2}{5}y_{n-1}\\
&\qquad +h^2\left(\begin{array}{c} r_1\overline{\overline{f}}_{n+1} + r_2 f_n + r_3 f_{n-1} + r_4\overline{f}_{n+\frac{1}{2}}\\ +r_5\overline{f}_{n-\frac{1}{2}} + r_6\overline{f}_{n+\frac{3}{4}} + r_7\overline{f}_{n-\frac{3}{4}} + r_8\overline{f}_{n-\frac{2}{5}}\end{array}\right)\\
&\tilde{y}_n = 2y_n - y_{n-1}\\
&\qquad +h^2\left(s_1\overline{\overline{f}}_{n+1} + s_2 f_n + s_3 f_{n-1} + s_4\left(\overline{f}_{n+\frac{3}{4}} + \overline{f}_{n-\frac{3}{4}}\right) + s_6\left(\overline{f}_{n+\frac{2}{5}} + \overline{f}_{n-\frac{2}{5}}\right)\right)\\
&y_{n+1} - 2y_n + y_{n-1} = h^2\cdot\left(\begin{array}{c} \frac{107}{30870}\left(\tilde{f}_{n+1} + f_{n-1}\right) + \frac{2831}{7560} f_n +\\ \frac{80384}{1065015}(\overline{f}_{n+\frac{3}{4}} + \overline{f}_{n-\frac{3}{4}}) + \frac{265625}{1136016}(\overline{f}_{n+\frac{2}{5}} + \overline{f}_{n-\frac{2}{5}})\end{array}\right)
\end{aligned}
$$

Actually we added g_4, c_6 and r_8 in the family of [14]. They were useless then, but now we need any available degree of freedom in order to increase either phase-lag or dissipation order. Only six parameters remain free at last, because most of the parameters of the family are fixed due to algebraic order restrictions of each layer, forming the final method. We observe that 1-$C\left(v^2\right) = a_{10}v^{10} + a_{12}v^{12} + a_{14}v^{14} + a_{16}v^{16}$, with a depending on the sufficient parameters of the family. On the other hand phase lag is an infinite series of the form $l_{10}v^{10} + l_{12}v^{12} + O\left(v^{14}\right)$. In [14], following tradition we asked for 1-$C\left(v^2\right) \equiv 0$ and we were lucky enough to achieve a special solution at a cost of one parameter but then we could satisfy only $l_{10} = l_{12} = 0$, getting a forced $l_{14} \neq 0$. Unfortunately this holds even now with the extra freedoms, so we can not get zero dissipation and a higher phase-lag order together.

The choices mentioned earlier are two.

Table 1: Parameters for the 1st choice.

$g_1 = -0.32786618933175$	$g_2 = 2.2484471359905$
$g_3 = 1.01484856799525$	$g_4 = -2.560429514654$
$d_1 = 0.001285807291666666$	$d_2 = 0.01064453125$
$d_3 = -0.01466471354166666$	$d_4 = -0.006770833333333334$
$d_5 = -0.08424479166666666$	$c_1 = 0.01569149760700887$
$c_2 = 0.5856314873314576$	$c_3 = -0.1112076707490621$
$c_4 = 0.01576042590075025$	$c_5 = -0.3067447454962486$
$c_6 = 0.457119005406094$	$k_1 = -0.0004766854383154811$
$k_2 = -0.02431196195189366$	$k_3 = -0.003494149915634853$
$k_4 = 0.003684031277186183$	$k_5 = -0.08164166925930805$
$k_6 = 7.81360527358 \cdot 10^{-9}$	$k_7 = -0.01375957252563939$
$r_1 = 0.008179617736005171$	$r_2 = 0.2358016708666944$
$r_3 = 0.1195199889374067$	$r_4 = 0.05955674442839562$
$r_5 = 1.899787462877609$	$r_6 = -0.04240495495488127$
$r_7 = -0.5916663848162211$	$r_8 = -1.408774145075008$
$s_1 = -1.377668289974674$	$s_2 = 11.65373547923761$
$s_3 = -1.377668289974674$	$s_4 = 5.199685801866009$
$s_6 = -9.148885251510144$	

3.1. 1st choice.

$p = 22$, $q = 10$, achieved for $l_{10} = \cdots = l_{20} = 0$ and $a_{10} \neq 0$.

The parameters are given in Table 1.

The local truncation error is evaluated for the scalar case according to the guidelines in [11, 14].

So taking in account that $y'' = f$, $y''' = \frac{\partial f}{\partial x} = \frac{\partial f}{\partial y}\frac{\partial y}{\partial x} = f'y'$ etc., we arrive at a Local Truncation Error (LTE) of the form $h^{10}\left(t_1F_1 + t_2F_2 + \cdots + t_{72}F_{72}\right) + O\left(h^{11}\right)$ where t are numbers and F are elementary differentials involving only y', f and partial derivatives of f with respect to y. There are 72 elementary differentials of 10th order, according to the theory of one step methods [4]. Only 27 of the t_i are independent since the internal stages are at least of second order. We must also notice that assuming a scalar case, compression of different F_is may occur. For example $f^{(6)}f'y'^{\,6} = f'f^{(6)}y'^{\,6}$ in the scalar case since f', $f^{(6)}$ and y' are numbers, but this is not true for a system of ODEs since these differentials are matrices.

Finally we get for this case

$$
\begin{aligned}
LTE \;=\; & h^{10}(0.0000105 \cdot f^2 f'^2 f'' + 0.0025468 \cdot f'^3 y'^2 f'' - 2.7 \cdot 10^{-7} \cdot f^3 f''^2 \\
& +0.0074077 \cdot f f' y'^2 f''^2 - 0.0000385 \cdot y'^4 f''^3 \\
& -0.0000251 \cdot f^3 f' f''' - 0.0000542 \cdot f f'^2 y'^2 f''' \\
& -0.0001185 \cdot f^2 y'^2 f'' f''' + 0.0024133 \cdot f' y'^4 f'' f'''
\end{aligned}
$$

Table 2: Parameters for the 2nd choice.

$g_1 = -0.3275064808539252$	$g_2 = 2.246288885123552$
$g_3 = 1.013769442561776$	$g_4 = -2.557551846831402$
$d_1 = 0.001285807291666666$	$d_2 = 0.01064453125$
$d_3 = -0.01466471354166666$	$d_4 = -0.006770833333333334$
$d_5 = -0.08424479166666666$	$c_1 = 0.01569686332120066$
$c_2 = 0.5857066073301425$	$c_3 = -0.1112452307484046$
$c_4 = 0.01573037790127627$	$c_5 = -0.3068949854936185$
$c_6 = 0.4572563676894037$	$k_1 = -0.0004776893915544161$
$k_2 = -0.02431531295954992$	$k_3 = -0.003491709816257519$
$k_4 = 0.003683230812710925$	$k_5 = -0.08163282637645776$
$k_6 = 2.454519362719256 \cdot 10^{-6}$	$k_7 = -0.01376814678825401$
$r_1 = 0.00820226463177012$	$r_2 = 0.2357706404459578$
$r_3 = 0.1195813195859239$	$r_4 = 0.0596717574254971$
$r_5 = 1.900670459112769$	$r_6 = -0.04249926804562959$
$r_7 = -0.5919828216271334$	$r_8 = -1.409414351529155$
$s_1 = -1.378402397366143$	$s_2 = 11.65973068960128$
$s_3 = -1.378402397366143$	$s_4 = 5.202409446680736$
$s_6 = -9.153872394115232$	

$$
\begin{aligned}
& -1.07 \cdot 10^{-6} \cdot f y'^4 f'''^2 - 3.36 \cdot 10^{-7} \cdot f^4 f^{(4)} \\
& -0.0000774 \cdot f^2 f' y'^2 f^{(4)} - 0.0000219 \cdot f'^2 y'^4 f^{(4)} \\
& -0.0000789 \cdot f y'^4 f'' f^{(4)} - 2.68 \cdot 10^{-7} \cdot y'^6 f''' f^{(4)} \\
& -1.34 \cdot 10^{-6} \cdot f^3 y'^2 f^{(5)} - 0.0000264 \cdot f f' y'^4 f^{(5)} \\
& -7.92 \cdot 10^{-6} \cdot y'^6 f'' f^{(5)} - 6.72 \cdot 10^{-7} \cdot f^2 y'^4 f^{(6)} - 1.81 \cdot 10^{-6} \cdot f' y'^6 f^{(6)} \\
& -8.95 \cdot 10^{-8} \cdot f y'^6 f^{(7)} - 3.19 \cdot 10^{-9} \cdot y'^8 f^{(8)}).
\end{aligned}
$$

3.2. 2nd choice.

$p = 18$, $q = 14$, achieved for $l_{10} = \cdots = l_{16} = 0$ and $a_{10} = a_{12} = 0$.
The parameters are given in Table 2.
The local truncation error is

$$
\begin{aligned}
LTE \;=\; & h^{10}(0.0000104 \cdot f^2 f'^2 f'' + 0.0025478 \cdot f'^3 y'^2 f'' - 2.7 \cdot 10^{-7} \cdot f^3 f''^2 \\
& +0.0074109 \cdot f f' y'^2 f''^2 - 0.0000386 \cdot y'^4 f''^3 - 0.0000252 \cdot f^3 f' f''' \\
& -0.0000546 \cdot f f'^2 y'^2 f''' - 0.0001185 \cdot f^2 y'^2 f'' f''' \\
& +0.0024143 \cdot f' y'^4 f'' f''' - 1.07 \cdot 10^{-6} \cdot f y'^4 f'''^2 - 3.36 \cdot 10^{-7} \cdot f^4 f^{(4)} \\
& -0.0000776 \cdot f^2 f' y'^2 f^{(4)} - 0.0000220 \cdot f'^2 y'^4 f^{(4)} \\
& -0.0000789 \cdot f y'^4 f'' f^{(4)} - 2.68 \cdot 10^{-7} \cdot y'^6 f''' f^{(4)}
\end{aligned}
$$

$$-1.34 \cdot 10^{-6} \cdot f^3 y'^2 f^{(5)} - 0.0000265 \cdot f f' y'^4 f^{(5)}$$
$$-7.92 \cdot 10^{-6} \cdot y'^6 f'' f^{(5)} - 6.72 \cdot 10^{-7} \cdot f^2 y'^4 f^{(6)} - 1.81 \cdot 10^{-6} \cdot f' y'^6 f^{(6)}$$
$$-8.95 \cdot 10^{-8} \cdot f y'^6 f^{(7)} - 3.19 \cdot 10^{-9} \cdot y'^8 f^{(8)}).$$

The truncation errors of the two methods presented in this article differ slightly.

4. Numerical results

Four methods of eighth algebraic order with reduced phase errors are tested numerically. These methods are:

i) PL14, $p = 14$, $q = \infty$, [14].
ii) PL22, $p = 22$, $q = 10$, 1st choice above.
iii) PL18, $p = 18$, $q = 14$, 2nd choice above.
iv) RKN, $p = 16$, $q = 10$, [9].

The problems chosen are well known in the relevant literature.

4.1. Bessel equation.

equation $y'' = \left(-100 + \frac{1}{4x^2}\right) y,\ x \in [1, 32.59406213134967]$,
initial values $y(1) = J_0(10x),\ y'(1) = -0.5576953439142885$
exact solution $y(x) = \sqrt{x} J_0(10x),\ y(32.59406213134967) = 0.$

4.2. Inhomogeneous equation.

equation $y'' = -100y + 99 \sin x,\ x \in [0, 10\pi]$
initial values $y(0) = 1,\ y'(1) = 11$
exact solution $y(x) = \cos 10x + \sin 10x + \sin x,\ y(10\pi) = 1.$

4.3. Wave equation, [5].

equation $\frac{\partial^2 u}{\partial t^2} = gd(x) \frac{\partial^2 u}{\partial x^2} + \frac{1}{4}\lambda^2(x, u)\, u,\ x \in [0, b],\ t \geq 0$
initial (and boundary) values
$\frac{\partial u}{\partial x}(t, 0) = \frac{\partial u}{\partial x}(t, b) = 0,$
$u(0, x) = \sin \frac{\pi x}{b},\ \frac{\partial u}{\partial t}(0, x) = -\frac{\pi}{b}\sqrt{gd} \cos \frac{\pi x}{b}.$

We implemented the case $b = 100,\ g = 9.81,\ d = 10\left(2 + \cos \frac{2\pi x}{b}\right),\ \lambda = \frac{g|u|}{2500d}$ as in [5]. By using the method of lines with $\Delta x = 10$, this problem was converted into a system of ODEs with eleven equations. The ninth component u_9 of the system approximates $u(t, x)$ at $x = 8\Delta x = 80$. A very accurate integration calculated the 10th zero of u_9 to be 63.35062926689779. So we integrated the methods to this point and recorded the values of the 9th component there.

In all cases tested we recorded the end-point errors observed for a variety of function evaluations used. The two step methods used fixed step size during the integration. The Runge-Kutta-Nyström pair of algebraic orders 8(6) [9], was implemented in variable step mode using the technique introduced in [13]. Since it was

Table 3: Results for Bessel equation

	stages					
	2000	3000	4000	5000	6000	7000
PL14	$3.2 \cdot 10^{-4}$	$1.9 \cdot 10^{-6}$	$5.7 \cdot 10^{-8}$	$3.9 \cdot 10^{-9}$	$4.4 \cdot 10^{-10}$	$7.1 \cdot 10^{-11}$
PL22	$4.5 \cdot 10^{-6}$	$4.7 \cdot 10^{-8}$	$4.9 \cdot 10^{-10}$	$3.0 \cdot 10^{-10}$	$1.3 \cdot 10^{-10}$	$4.9 \cdot 10^{-11}$
PL18	$5.3 \cdot 10^{-6}$	$6.0 \cdot 10^{-8}$	$1.2 \cdot 10^{-9}$	$2.3 \cdot 10^{-10}$	$1.2 \cdot 10^{-10}$	$4.6 \cdot 10^{-11}$
RKN	$2.5 \cdot 10^{-5}$	$2.0 \cdot 10^{-7}$	$2.4 \cdot 10^{-8}$	$4.4 \cdot 10^{-9}$	$1.2 \cdot 10^{-9}$	$5.4 \cdot 10^{-10}$

Table 4: Results for the inhomogeneous equation

	stages					
	1600	2000	2400	2800	3200	3600
PL14	$2.3 \cdot 10^{-2}$	$1.2 \cdot 10^{-3}$	$1.1 \cdot 10^{-4}$	$1.7 \cdot 10^{-5}$	$3.2 \cdot 10^{-6}$	$7.4 \cdot 10^{-7}$
PL22	$3.1 \cdot 10^{-5}$	$2.6 \cdot 10^{-6}$	$3.1 \cdot 10^{-7}$	$4.8 \cdot 10^{-8}$	$8.2 \cdot 10^{-9}$	$1.2 \cdot 10^{-9}$
PL18	$1.8 \cdot 10^{-4}$	$6.4 \cdot 10^{-6}$	$4.3 \cdot 10^{-7}$	$4.3 \cdot 10^{-8}$	$5.8 \cdot 10^{-9}$	$9.8 \cdot 10^{-10}$
RKN	$3.4 \cdot 10^{-4}$	$1.8 \cdot 10^{-4}$	$3.2 \cdot 10^{-5}$	$4.3 \cdot 10^{-6}$	$6.9 \cdot 10^{-7}$	$4.8 \cdot 10^{-7}$

difficult to integrate it at exactly the stages used by the hybrid methods, we simply integrated RKN86 for various tolerances. Then we estimated the errors that might be generated for the requested stages by interpolating the respective values.

The results are given in Tables 3, 4 and 5.

Interpreting the results it is obvious that the new methods outperform the older ones. It worth mentioning that the advantage is clear even in the non-linear realistic model of wave equation.

REFERENCES

[1] M. M. Chawla and P. S. Rao, Numerov type method with minimal phase lag for the integration of second order periodic initial value problems, *J. Comput. Appl. Math.* 11 (1984) 277-281.

[2] M. M. Chawla and P. S. Rao, Numerov type method with minimal phase lag for the integration of second order periodic initial value problems II. Explicit method, *J. Comput. Appl. Math.* 15 (1986) 329-337.

Table 5: Results for the wave equation

	stages					
	1000	1500	2250	3000	3750	4500
PL14	$3.4 \cdot 10^{-3}$	$1.2 \cdot 10^{-5}$	$6.9 \cdot 10^{-8}$	$2.0 \cdot 10^{-9}$	$1.3 \cdot 10^{-10}$	$1.5 \cdot 10^{-11}$
PL22	$6.9 \cdot 10^{-7}$	$2.4 \cdot 10^{-8}$	$5.0 \cdot 10^{-10}$	$3.1 \cdot 10^{-11}$	$3.6 \cdot 10^{-12}$	$6.5 \cdot 10^{-13}$
PL18	$1.0 \cdot 10^{-5}$	$2.0 \cdot 10^{-8}$	$3.5 \cdot 10^{-11}$	$4.9 \cdot 10^{-13}$	$8.1 \cdot 10^{-14}$	$5.9 \cdot 10^{-14}$
RKN	$1.3 \cdot 10^{-5}$	$8.0 \cdot 10^{-7}$	$1.1 \cdot 10^{-8}$	$3.7 \cdot 10^{-10}$	$4.0 \cdot 10^{-11}$	$1.5 \cdot 10^{-11}$

[3] M. M. Chawla and P. S. Rao, An explicit sixth-order method with phase-lag of order eight for $y'' = f(t, y)$, *J. Comput. Appl. Math.* 17 (1987) 365-368.

[4] E. Fehlberg, Classical eighth and lower order Runge-Kutta-Nyström formulas with stepsize control for special second order differential equations, NASA Tech. Rep. TR R-381, March 1972, G. C. Marsal Space Flight Center, Ala. 35812.

[5] P. J. Van Der Houwen and B. P. Sommeijer, Explicit Runge-Kutta (-Nystrom) methods with reduced phase errors for computing oscilating solutions, *SIAM J. Numer. Anal.* 24 (1987) 595-617.

[6] J. D. Lambert and I. A. Watson, Symmetric multistep methods for periodic initial value problems, *J. Inst. Math. Appl.* 18 (1976) 189-202.

[7] L. D. Landau and F. M. Lifshitz, Quantum Mechanics, *Pergamon Press*, New York, 1965.

[8] R. L. Liboff, Introductory Quantum Mechanics, *Addison-Wesley*, Reading MA, 1980.

[9] S. N. Papakostas and Ch. Tsitouras, High algebraic order, high phase-lag order Runge-Kutta and Nystrom pairs, *SIAM J. Sci. Comput.* **20** (1999) to appear.

[10] T. E. Simos, Explicit two-step methods with minimal phase-lag for the numerical integration of special second order initial value problems and their application to the one dimensional Schrodinger equation, *J. Comput. Appl. Math.* 39 (1992) 89-94.

[11] T. E. Simos and Ch. Tsitouras, A P-stable eighth order method for the numerical integration of periodic initial value problems, *J. Comput. Phys.* 130 (1997) 123-128.

[12] Ch. Tsitouras, A parameter study of a Runge-Kutta pair of orders 6(5), *Appl. Math. Letters* 11 (1998) 65-69.

[13] Ch. Tsitouras and S. N. Papakostas, Cheap error estimation for Runge-Kutta methods, *SIAM J. Sci. Comput.* **20** (1999) to appear.

[14] Ch. Tsitouras and T. E. Simos, Explicit high order methods for the numerical integration of periodic initial value problems, *Appl. Math.& Comput.* 95 (1998) 15-26.