

EXPLORING EFFICIENT
NUMERICAL METHODS FOR
DIFFERENTIAL EQUATIONS

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Professor Dr. Fudziah
Ismail



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ABSTRACT

Numerical analysis is a way to do higher mathematical problems on a computer, a technique widely used by scientists and engineers to solve their problems. A major advantage of numerical analysis is that a numerical answer can be obtained even when a problem has no “analytical” solution. Results from numerical analysis are an approximation, which can be made as accurate as desired. The analysis of errors in numerical methods is a critically important part of the study of numerical analysis. Hence, we will see in this research that computation of the error is a must as it is a way to measure the efficiency of the numerical methods developed

Numerical methods require highly tedious and repetitive computations that can only be done using the computer. Hence in this research, it is shown that computer programs must be written for the implementation of numerical methods. In the early part of related research the computer language used was Fortran. Subsequently more and more computer programs used the C programming language. Additionally, now computations can also be carried out using softwares like MATLAB, MATHEMATICA and MAPLE.

Many physical problems that arise from ordinary differential equations (ODEs) have magnitudes of eigenvalues which vary greatly, and such systems are commonly known as stiff systems. Stiff systems usually consist of a transient solution, that is, a solution which varies rapidly at the beginning of the integration. This phase is referred to as the transient phase and during this phase, accuracy rather than stability restricts the stepsize of the numerical methods used. Thus the generally the structure of the solutions suggests application of specific methods for non-stiff equations in the transient phase and specific methods for stiff equations during

the steady-state phase in a manner whereby computational costs can be reduced.

Consequently, in this research we developed embedded Runge-Kutta methods for solving stiff differential equations so that variable stepsize codes can be used in its implementation. We have also included intervalwise partitioning, whereby the system is considered as non-stiff first, and solved using the method with simple iterations, and once stiffness is detected, the system is solved using the same method, but with Newton iterations. By using variable stepsize code and intervalwise partitioning, we have been able to reduce the computational costs.

With the aim of increasing the computational efficiency of the Runge-Kutta methods, we have also developed methods of higher order with less number of stages or function evaluations. The method used is an extension of the classical Runge-Kutta method and the approximation at the current point is based on the information at the current internal stage as well as the previous internal stage. This is the idea underlying the construction of Improved Runge-Kutta methods, so that the resulting method will give better accuracy.

Usually higher order ordinary differential equations are solved by converting them into a system of first order ODEs and using numerical methods suitable for first order ODEs. However it is more efficient, in terms of accuracy, number of function evaluations as well as computational time, if the higher order ODEs can be solved directly (without being converted to a system of first order ODEs), using numerical methods. In this research we developed numerical methods, particularly Runge-Kutta type methods, which can directly solve special third order and fourth order ODEs.

Special second order ODE is an ODE which does not depend on the first derivative. The solution from this type of ODE often exhibits a pronounced oscillatory character. It is well known that it is difficult

to obtain accurate numerical results if the ODEs are oscillatory in nature. In order to address this problem a lot of research has been focused on developing methods which have high algebraic order, reduced phase-lag or dispersion and reduced dissipation. Phase-lag is the angle between the true and approximate solution, while dissipation is the difference between the approximate solution and the standard cyclic solution. If a method has high algebraic order, high order of dispersion and dissipation, then the numerical solutions obtained will be very accurate. Hence in this research we have developed numerical methods, specifically hybrid methods which have all the abovementioned properties.

If the solutions are oscillatory in nature, it means that the solutions will have components which are trigonometric functions, that is, sine and cosine functions. In order to get accurate numerical solutions we thus phase-fitted the methods using trigonometric functions. In this research, it is proven that trigonometrically-fitting the hybrid methods and applying them to solve oscillatory delay differential equations result in better numerical results.

These are the highlights of my research journey, though a lot of work has also been done in developing numerical methods which are multistep in nature, for solving higher order ODEs, as well as implementation of methods developed for solving fuzzy differential equations and partial differential equations, which are not covered here.

INTRODUCTION

This research is basically to find numerical solutions to differential equations. Hence, here we give a brief introduction to differential equations and the numerical methods used to solve them.

Introduction to Differential Equations

A differential equation is a mathematical equation that relates some function with its derivatives. In applications, the functions usually represent physical quantities while the derivatives represent their rates of change, and the equation defines the relationship between the two. Since such relations are extremely common, differential equations play a prominent role in many disciplines, including engineering, physics, economics and biology. In mathematics, differential equations are studied from several different perspectives, but mostly concerned with their solutions.

Ordinary Differential Equations

The Ordinary Differential Equation (ODE) is a differential equation that contains only ordinary derivatives of one or more unknown functions with respect to a single independent variable. We have listed some of the applications of ODEs below.

Population Models

One of the most basic examples of differential equations is the Malthusian Law of population growth $\frac{dN}{dt} = rN$, which shows how the population (N) changes with respect to time. The constant r will change depending on the species. This law is used to predict how a species would grow over time.

Logistic Growth

In many situations where there is growth of a population, the growth is bound by some maximum. This kind of growth is called logistic growth, where the growth of a population is proportional to both the size of the population and the difference between the size of the population and the maximum.

Let $N(t)$ represent the size of the population at time t , and suppose $0 < N(t) < L$. That is N is always bound between zero and L , then the resulting differential equation can be written as $\frac{dN}{dt} = rN(L - N)$.

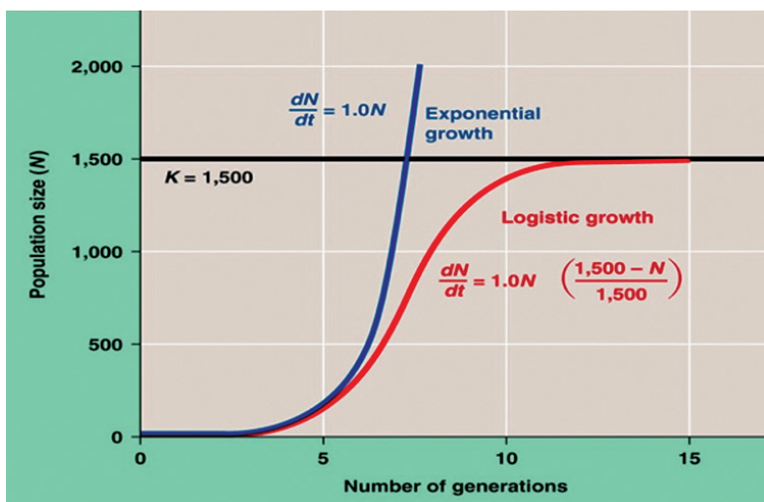


Figure 1 The graphs of Exponential Growth and Logistic Growth

Predator-prey Models

More complicated differential equations can be used to model the relationship between predators and prey. For example, as predators increase the prey will decrease as more get eaten. However then the

predators will have less to eat and start to die out, which allows more prey to survive. The interactions between these two populations are connected by differential equations.

Consider two populations whose sizes at a reference time t are denoted by $x(t)$ and $y(t)$, respectively. The functions x and y might denote population numbers or concentrations (number per area) or some other scaled measure of the population sizes, but are taken to be continuous functions. Changes in population size with time are then described by the system of two autonomous differential equations:

$$\frac{dx}{dt} = xf(x, y)$$

$$\frac{dy}{dt} = yg(x, y)$$

The functions f and g denote the respective per capita growth rates of the two species.

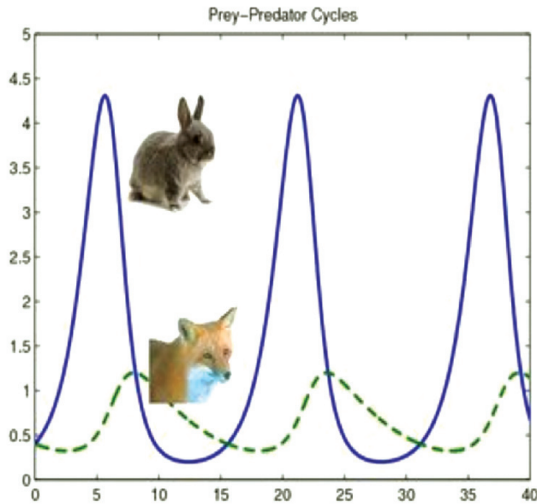


Figure 2 Periodic activity generated by the Predator-Prey model

The graph above shows the predator and prey population and it is very dependent on the prey. This particular relationship generates a population boom and crash – the predator rapidly eats the prey population and grows rapidly before it runs out of prey to eat and then it has no other food and thus starts to die off again.

Some other uses of differential equations include:-

1. In medicine, for modelling cancer growth or the spread of disease.
2. In engineering, for describing the movement of electricity.
3. In chemistry, for modelling chemical reactions.
4. In economics, to find optimum investment strategies.
5. In physics, to describe the motion of waves, pendulums or chaotic systems.

Delay Differential Equations

Delay differential equations (DDEs) are a type of differential equation in which the derivative of the unknown function at a certain time is given in terms of the values of the function at previous times. DDE is a model which incorporates past history. A more realistic model must include some of the past history of the system to determine future behavior.

It can include for example, population dynamics, epidemiology and reforestation. In the latter the replanting process will take at least 20 years before reaching maturity. Hence, time delay must be applied in the mathematical model for forest harvesting and regeneration.

The Nicholas Blowfly Equation: $\frac{dN}{dt} = \beta N(t - \tau) \exp\left(\frac{-N(t - \tau)}{\kappa}\right) - \delta N(t)$ where β is the birth rate, δ is the death rate, τ

is the age at which adult flies emerge from their pupal cases and K the population's carrying capacity (See Brillinger, 2011).

A vector disease model: $\frac{dy}{dt} = by(t - \tau)[1 - y(t)] - cy(t)$ where $y(t)$ is the infected host population. The disease is transmitted to the host by an insect vector, assumed to have a large and constant population. Within the vector there is an incubation period τ , before a disease agent can infect the host while c is the recovery rate and b is the contact rate (See Cooke, 1978).

Stiff Differential Equations

Stiffness is a subtle, difficult and important concept in the numerical solution of ordinary differential equations. It depends on the differential equation, the initial conditions and the numerical method. An ordinary differential equation problem is stiff if the solution being sought is varying slowly, but there are nearby solutions that vary rapidly, so the numerical method used must take small steps to obtain satisfactory results. A stiff differential equation is numerically unstable unless the step size is extremely small.

Numerical Methods for Ordinary Differential Equations

Many differential equations cannot be solved analytically. For practical purposes however, such as in engineering, a numeric approximation to the solution is often sufficient. Numerical methods for ODEs are methods used to find numerical approximations to the solutions of ODEs.

Computer Software

The most popular programming language for implementing numerical methods is Fortran, a language developed in the 1950s that continues to be updated to meet changing needs. Other languages, such as, C and C++, are also used for the implementation of numerical methods. MATLAB, is a commercial package that is arguably the most popular to do numerical computing. Two other popular computer programs for handling algebraic-analytic mathematics (manipulating and displaying formulas) are MAPLE and MATHEMATICA.

Methods

Conceptually, a numerical method starts from an initial point and then takes a short step forward in time to find the next solution point. First let us introduce the following equation

$$y' = f(x, y), y(x_0) = y_0, x_0 < x < X \quad (1.1)$$

ODE together with the initial condition is called the initial value problem (IVP). Numerical methods for solving first-order IVPs often fall into one of two large categories:

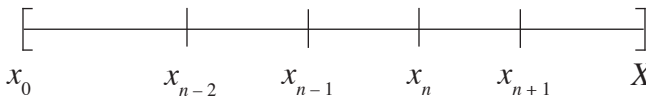
i. Single-step methods (such as Euler's method) which refer to only one previous point and its derivative to determine the current value. Methods such as Runge-Kutta (RK) take some intermediate steps (for example, a half-step) to obtain a higher order method, but then discard all previous information before taking a second step.



Single step method

A further division can be realized by dividing methods into those that are explicit and those that are implicit. Implicit RK methods include the diagonally implicit RK (DIRK), singly diagonally implicit RK (SDIRK) and the Gauss-Radau method, and any RK method with a lower diagonal Butcher tableau is explicit.

ii. Multistep methods which attempt to gain efficiency by keeping and using the information from previous steps rather than discarding it. Consequently, multistep methods refer to several previous points and derivative values. In the case of *linear* multistep methods, a linear combination of the previous points and derivative values are used.



Multistep Method

For example, implicit linear multistep methods include Adams-Moulton methods and backward differentiation methods (BDF). Explicit methods include the Adams-Bashforth methods, and the so-called general linear methods (GLMs) which are a generalization of the earlier mentioned two large classes of methods.

Analysis

Numerical analysis involves not only the design of numerical methods but also their analysis. Three central concepts in this analysis are: *convergence*: whether the method approximates the solution; *order*: how well it approximates the solution; and *stability*: whether errors are damped out.

Convergence

A numerical method is said to be *convergent* if the numerical solution approaches the exact solution as the step size h goes to 0. In fact, a numerical scheme has to be convergent to be of any use.

Consistency and Order

Suppose the numerical method is: $y_{n+k} = \Phi(t_{n+k}; y_n, y_{n+1}, \dots, y_{n+k-1}; h)$. The local (truncation) error of the method is the error committed by one step of the method. That is, it is the difference between the result given by the method, assuming that no error was made in earlier steps, and the exact solution:

$$\delta_{n+k}^h = \Phi(t_{n+k}; y(t_n), y(t_{n+1}), \dots, y(t_{n+k-1}); h) - y(t_{n+k})$$

The method is said to be *consistent* if: $\lim_{h \rightarrow 0} \frac{\delta_{n+k}^h}{h} = 0$

The method has *order* p if: $\delta_{n+k}^h = O(h^{p+1})$ as $h \rightarrow 0$

Hence a method is consistent if it has an order greater than 0. Most methods being used in practice attain a higher order. Consistency is a necessary condition for convergence, but not sufficient. For a method to be convergent, it must be both consistent and zero-stable.

DIAGONALLY IMPLICIT RUNGE-KUTTA METHODS FOR STIFF DIFFERENTIAL EQUATIONS

The initial value problems with stiff ordinary differential equations arise in fluid mechanics, elasticity, electrical networks, chemical reactions and many other areas of physical importance. The stiffness

arises due to the large difference in time scales exhibited in the physical models. These time scales are usually responsible for the decaying rates of the model.

$$y'(x) = f(x, y), y(x_0) = y_0, y \in \Re \quad (2.1)$$

Several schemes have been developed for the numerical solution of stiff initial value problems for ordinary differential equations, and among them we note Gear's method (1969) and the method of Bulirsch and Stoer (1996). While these schemes work well for moderately stiff systems, however, as the stiffness increases they all require the use of very small mesh spacing over portions of the domain of integration. Thus, computational cost increases and accuracy decreases as the stiffness increases.

In line with this, there has been recent interest in integrating stiff systems of first order ODEs numerically, using the diagonally implicit RK method. The method was introduced to overcome some of the limitations of the fully implicit and explicit RK method. This is due to the fact that computational effort involved in using the DIRK method is generally less compared to that for the fully implicit RK methods. Such methods can be written as

$$k_i = f\left(x_n + c_i h, y_n + h \sum_{j=1}^i a_{ij} k_j\right), \quad i = 1, \dots, q \quad (2.2a)$$

$$\bar{y}_{n+1} = y_n + h \sum_{i=1}^q b_i k_i \quad (2.2b)$$

If we assume that all the diagonal elements of the method are equal, $a_{ii} = \gamma$, thus all the eigenvalues of the method will be equal, hence the method is called a singly diagonally implicit Runge-Kutta

(SDIRK) method. Next, suppose (2.2a) is solved successively using Newton-type iterations, where the linear system with a coefficient matrix of the form

$$I - ha_{ii} \frac{\partial f}{\partial y}.$$

is solved at each stage, then the stored LU-factorization of the matrix may be used repeatedly, thereby making the method computationally more efficient. Such formulae were first suggested by Norsett (1974) and studied further by Alexander (1977) and Cash (1979). The embedded SDIRK formulae have a built-in local truncation error estimate, and as a result, the stepsize can be controlled at virtually no extra cost. Norsett and Thompson (1984) continued the work using the semi-implicit RK method, where they developed a SDIRK method of order two embedded in the method of order three. Further, Al-Rabeh (1987) derived a SDIRK method of third order embedded in the fourth order. Preliminary experiments have shown that these methods are suitable for solving stiff ODEs.

Here, we derive a SDIRK method of fourth-order five-stage embedded in method of fifth-order six- stage, where we define the embedding method to equation (2.2) as

$$k_i = f \left(x_n + c_i h, y_n + h \sum_{j=1}^i a_{ij} k_j \right), \quad i = 1, \dots, q + 1 \quad (2.3a)$$






$$y_{n+1} = y_n + h \sum_{i=1}^{q+1} b_i k_i \quad (2.3b)$$

Then the local truncation error could be estimated using the higher order method and the lower order method. The derivation can be also seen in Ismail *et al.* (1998) and work related to stiff ODEs can be referred to in Suleiman *et. al.* (1996).

Derivation of Embedded Singly Diagonally Implicit Runge-Kutta Method

For the RK method, $c_i = \sum_{j=1}^i a_{ij}$, \bar{b}_i is for the lower order method and b_i is for the higher order method, and $a_{ii} = \gamma$ are the diagonal elements of the method. Butcher (1987) has listed the expressions for the elementary differentials for up to order 8. Table 1 contains the required equations up to order 5.

Table 1 Equations of Conditions for order 1 to 5

Graph of t	$\phi(t) = \frac{1}{\gamma(t)}$	
	$\sum_i b_i = 1$	(2.2.1)
	$\sum_i b_i c_i = \frac{1}{2}$	(2.2.2)
	$\sum_i b_i c_i^2 = \frac{1}{3}$	(2.2.3)
	$\sum_{ij} b_i a_{ij} c_j = \frac{1}{6}$	(2.2.4)
	$\sum_i b_i c_i^3 = \frac{1}{4}$	(2.2.5)



$$\sum_{ij} b_i c_i a_{ij} c_j = \frac{1}{8} \quad (2.2.6)$$



$$\sum_{ij} b_i a_{ij} c_j^2 = \frac{1}{12} \quad (2.2.7)$$



$$\sum_{ijk} b_i a_{ij} a_{jk} c_k = \frac{1}{24} \quad (2.2.8)$$



$$\sum_i b_i c_i^4 = \frac{1}{5} \quad (2.2.9)$$



$$\sum_{ij} b_i c_i^2 a_{ij} c_j = \frac{1}{10} \quad (2.2.10)$$



$$\sum_{ij} b_i c_i a_{ij} c_j^2 = \frac{1}{15} \quad (2.2.11)$$



$$\sum_{ijk} b_i c_i a_{ij} a_{jk} c_k = \frac{1}{30} \quad (2.2.12)$$



$$\sum_{ij} b_i a_{ij} c_j^3 = \frac{1}{20} \quad (2.2.13)$$



$$\sum_{ijk} b_i a_{ij} c_j a_{ik} c_k = \frac{1}{20} \quad (2.2.14)$$



$$\sum_{ijk} b_i a_{ij} c_j a_{jk} c_k = \frac{1}{40} \quad (2.2.15)$$



$$\sum_{ijk} b_i a_{ij} a_{jk} c_k^2 = \frac{1}{60} \quad (2.2.16)$$



$$\sum_{ijkl} b_i a_{ij} a_{jk} a_{kl} c_l = \frac{1}{120} \quad (2.2.17)$$

Using the Simplifying Assumption $\sum_{ij} a_{ij}c_j = \frac{1}{2}c_i^2$, which holds for all $i = 1, \dots, 6$.

Butcher (1987) referred to the equation as the row-simplifying assumption. Meanwhile, equation

$$\sum_i a_{ij} c_j = b_j(1 - c_j), j = 1, \dots, 6$$

is referred to as a column simplifying assumption.

Using the order conditions and the simplifying assumptions we derived two embedded SDIRK methods (4,5) in (5,6).

Table 2 SDIRK Method (4, 5) Embedded in (5, 6) with $\gamma = 0.27805384$

γ	γ				
$2\gamma + \gamma\sqrt{2}$	a_{21}	γ			
-0.7	a_{31}	1.06004330	γ		
0.25653741	a_{41}	-0.03682839	0.00789379	γ	
0.82839417	a_{51}	-0.03380531	0.00608165	0.53925854	γ
$1-\gamma$	a_{61}	-0.63238912	-0.04238439	0.55765932	0.75299105 γ
	0	-0.06318768	0.00318654	0.56747397	0.57361772 -0.810905
	0	-0.02185092	0.00356539	0.56010910	0.45817642

Table 3 SDIRK Method (4,5) Embedded in (5,6) with $r = \frac{4}{15}$

γ	γ				
$2\gamma + \gamma\sqrt{2}$	a_{21}	γ			
-0.7	a_{31}	1.07091464	γ		
0.25109432	a_{41}	-0.03707993	0.00766549	γ	
0.56536452	a_{51}	-0.07272339	0.00883329	0.97869993	γ
$1 - \gamma$	a_{61}	-0.02745363	0.00216163	0.91306419	-0.05734425 γ
	0	-0.11018458	0.00277906	0.57280038	-0.16289019 0.4771267
	0	0.26135316	0.006320993	0.46956348	0.26277236

Stability of the Method

When the SDIRK method is applied to the test equation $y' = \lambda y$, the following equations are obtained: $y_{n+1} = y_n + h\lambda b^T (I - h\lambda A)^{-1} y_n u$ or $y_{n+1} = R(h\lambda) y_n$ with $R(\bar{h}) = 1 + \bar{h} b^T (I - \bar{h} A)^{-1} u$, $\bar{h} = h\lambda$ and $b^T = (b_1, \dots, b_q)$. $R(\bar{h})$ is called the stability polynomial of the method. The stability region is the region enclosed by the set of points for which $R(\bar{h}) = 1$. By replacing 1 with $\cos \theta + i \sin \theta$, we can determine this boundary by solving the equation for values of $\theta \in [0, 2\pi]$.

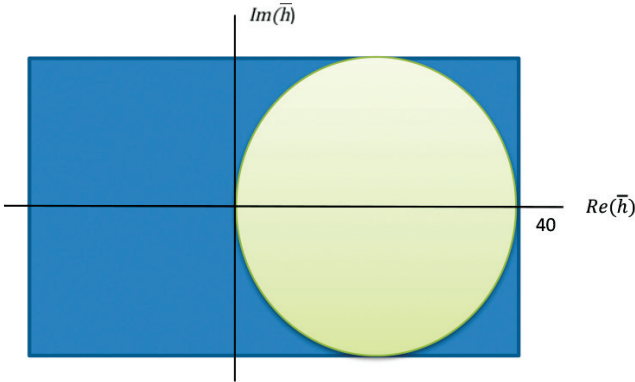


Figure 3 Stability region of F1(A) method lies outside the circle

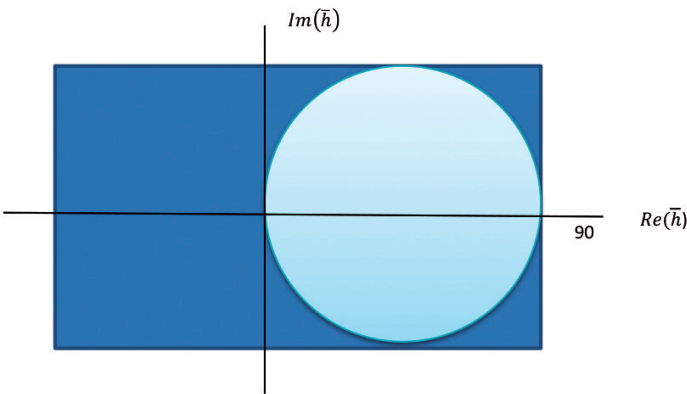


Figure 4 Stability region of F1(B) method lies outside the circle

Problems Tested

In this section, we present some problems which will be tested using the new method. Initially the system is considered as non-stiff, hence we do simple iteration. Once there is an indication of stiffness through step failure and trace of the Jacobian is negative, the whole system is considered stiff and solved using Newton iterations.

Problem 1. $y_1' - (55 + y_3)y_1 + 65y_2, \quad y_1(0) = 1$
 $y_2' = -0.0785(y_1 - y_2), \quad y_2(0) = 1$
 $y_3' = 0.1y_1, \quad y_3(0) = 0, \quad 0 \leq x \leq 20$

Problem 2: $y_1' = -10y_1 + 3y_2, \quad y_2' = -3y_1 - 10y_2$
 $y_3' = -4y_3, \quad y_4' = -y_4 \quad y_i(0) = 1, (i = 1(1)6)$
 $y_5' = -0.5y_5, \quad y_6' = -0.1y_6 \quad 0 \leq x \leq 20.$

Problem 3: $y_1' = -y_1 + y_2^2 + y_3^2 + y_4^2$
 $y_2' = -10y_2 + 10(y_3^2 + y_4^2)$
 $y_3' = -40y_3 + 40y_4^2 \quad y_i(0) = 1, (i = 1(1)4)$
 $y_4' = -100y_4 + 2 \quad 0 \leq x \leq 20.$

Problem 4: $y_1' = -1800y_1 + 900y_2$
 $y_i' = y_{i-1} - 2y_i + y_{i+1}, (i=2(1)8) \quad y_i(0) = 1, (i = 1(1)9)$
 $y_9' = 1000y_8 - 2000y_9 + 1000 \quad 0 \leq x \leq 20.$

Numerical Results and Discussions

The results obtained from the new method are compared with the results obtained when the same problems are solved using the SDIRK method (3,3) embedded in (4,4), which was derived by Rabeh (1987). The numerical results are given in Tables 4 – 7. The notations used are as follows:

TOL \sim the chosen tolerance; FCN \sim the number of function evaluations;

STEP \sim the number of successful steps; FSTEP \sim the number of failure steps; and

JACO \sim the number of Jacobian evaluations.

The methods used are:

F1(A): SDIRK method (4, 5) in (5, 6) with $\gamma = 0.27895384$, in this section.

F1(B): SDIRK method (4, 5) in (5, 6) with $\gamma = \frac{4}{15}$, in this section.

R1: SDIRK method (3, 3) in (4, 4) with $\gamma = 0.43586652$, in Rabeh (1987).

Table 4 Numerical Results for Problem 1, Using Tolerances 10^{-2} , 10^{-4} , 10^{-6} , 10^{-8}

Tol 10^{-2}					Tol 10^{-4}			
Method	FCN	STEP	JACO	FSTEP	FCN	STEP	JACO	FSTEP
F1(A)	221	16	1	2	689	52	1	2
F1(B)	221	16	1	2	637	48	1	2
R1	153	16	1	1	557	61	1	2

Tol 10^{-6}					Tol 10^{-8}			
Method	FCN	STEP	JACO	FSTEP	FCN	STEP	JACO	FSTEP
F1(A)	3288	251	1	3	10630	815	1	3
F1(B)	3106	237	1	3	10032	769	1	3
R1	3347	370	1	3	17413	911	1	3

Table 5 Numerical Results for Problem 2, Using Tolerances 10^{-2} , 10^{-4} , 10^{-6} , 10^{-8}

Tol 10^{-2}					Tol 10^{-4}			
Method	FCN	STEP	JACO	FSTEP	FCN	STEP	JACO	FSTEP
F1(A)	261	19	1	1	598	44	1	2
F1(B)	261	19	1	1	572	42	1	2
R1	291	31	1	1	875	95	1	2

Tol 10^{-6}					Tol 10^{-8}			
Method	FCN	STEP	JACO	FSTEP	FCN	STEP	JACO	FSTEP
F1(A)	1391	105	1	2	3406	260	1	2
F1(B)	1352	102	1	2	3302	252	1	2
R1	2667	295	1	2	14618	1622	1	2

Table 6 Numerical Results for Problem 3, Using Tolerances 10^{-2} , 10^{-4} , 10^{-6} , 10^{-8}

Tol 10^{-2}					Tol 10^{-4}			
Method	FCN	STEP	JACO	FSTEP	FCN	STEP	JACO	FSTEP
F1(A)	337	25	1	1	750	56	1	2
F1(B)	337	25	1	1	731	55	1	2
R1	370	40	1	1	1063	117	1	1

Tol 10^{-6}					Tol 10^{-8}			
Method	FCN	STEP	JACO	FSTEP	FCN	STEP	JACO	FSTEP
F1(A)	1770	134	1	3	4375	333	1	5
F1(B)	1710	130	1	3	4235	323	1	5
R1	1312	336	1	2	17319	1917	2	9

Table 7 Numerical Results for Problem 4, Using Tolerances 10^{-2} , 10^{-4} , 10^{-6} , 10^{-8}

Tol 10^{-2}					Tol 10^{-4}			
Method	FCN	STEP	JACO	FSTEP	FCN	STEP	JACO	FSTEP
F1(A)	305	22	1	2	578	43	1	2
F1(B)	292	21	1	2	603	44	1	3
R1	294	31	1	1	806	87	1	2

Tol 10^{-6}					Tol 10^{-8}			
Method	FCN	STEP	JACO	FSTEP	FCN	STEP	JACO	FSTEP
F1(A)	1370	103	1	4	3306	251	1	4
F1(B)	1331	100	1	3	3202	343	1	4
R1	2399	264	1	2	9288	1022	2	4

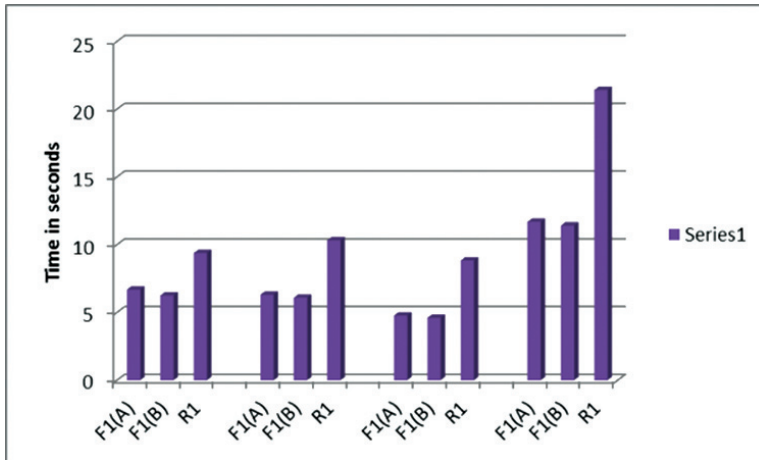


Figure 5 Total Time Taken to solve the problems over all the tolerances (in seconds)

We derived embedded SDIRK methods of order (4,5) in (5,6), denoted as F1(A) and F1(B). The methods have large regions of stability and are hence suitable for solving stiff differential equations. These methods performed better compared to Rabeh's method in terms of Jacobian evaluations, number of steps and also the total time taken to solve each system of equations over tolerances 10^{-2} , 10^{-4} , 10^{-6} and 10^{-8} . Even though methods F1(A) and F1(B) have more function evaluations to be evaluated at each step, they are more economical compared to the existing method.

IMPROVED RUNGE-KUTTA METHODS FOR SOLVING ORDINARY DIFFERENTIAL EQUATIONS

Most efforts to increase the order of the RK method have been accomplished by increasing the number of Taylor series terms used and thus the number of function evaluations. The RK method of order p has a local error over the step size h of (h^{p+1}) . Many authors have attempted to increase the efficiency of RK methods by trying to lower the number of function evaluations required. Goeken and Johnson (2000) proposed a class of RK methods with higher derivatives approximations for the third and fourth-order methods; Xinyuan (2003) presented a class of RK formulae of order three and four with reduced evaluations of functions; Phohomsiri and Udwadia (2004) constructed the accelerated RK integration schemes for the third-order method using two function evaluations per step; and Udwadia and Farahani (2008) developed the higher order accelerated Runge-Kutta methods. However these methods are for the autonomous system. Improved Runge-Kutta methods (IRK) can be used for autonomous as well as non-autonomous systems. Rabiei and Ismail (2011) extended the work and constructed the third-order Improved Runge-Kutta method for non-autonomous systems, solving ordinary differential equations

without minimization of the error norm. The IRK methods that arise from the classical RK methods can also be considered as a special class of two-step methods. That is, the approximate solution y_{n+1} is calculated using the values of y_n and y_{n-1} . The IRK method introduces the new terms of k_{-i} , which are calculated using k_i , ($i > 2$), from the previous step. The scheme proposed here has a lower number of function evaluations than the RK methods.

Derivation of the IRK Method

The proposed IRK method can be presented as follows:

$$y_{n+1} = y_n + h \left(b_1 k_1 - b_{-1} k_{-1} + \sum_{i=2}^s b_i (k_i - k_{-i}) \right), \quad (3.1)$$

$$k_1 = f(x_n, y_n), \quad k_{-1} = f(x_{n-1}, y_{n-1}),$$

$$k_i = f \left(x_n + c_i h, y_n + h \sum_{j=1}^{i-1} a_{ij} k_j \right), \quad k_{-i} = f \left(x_{n-1} + c_i h, y_{n-1} + h \sum_{j=1}^{i-1} a_{ij} k_{-j} \right),$$

$$2 \leq i \leq s.$$

Taylor Series expansion for y_{n+1} around y_n is given by

$$y_{n+1} = y_n + hf + \frac{h^2}{2!} (f_x + f f_y) + \frac{h^3}{3!} (f_{xx} + 2f_{xy}f + f_{yy}f^2 + f_y f_x + f_y^2 f) + O(h^4),$$

where $y' = f(x, y)$ and by expanding (3.1) in the Taylor series expansion and comparing both the series in terms of h , we have the order conditions of the method:

Table 8 Order Conditions of the Method

<i>First order</i>	$b_1 - b_{-1} = 1$	<i>Fifth order :</i>	$\sum_i^s b_i c_i^3 = \frac{31}{120}$
<i>Second order</i>	$b_{-1} + \sum_{i=2}^s b_i = \frac{1}{2}$		$\sum_i^s b_i c_i a_{ij} c_j^2 = \frac{31}{240}$
<i>Third order</i>	$\sum_i^s b_i c_i = \frac{5}{12}$		$\sum_i^s b_i a_{ij} c_j^2 = \frac{31}{360}$
<i>Fourth order</i>	$\sum_i^s b_i c_i^2 = \frac{5}{12}$		$\sum_i^s b_i a_{ij} a_{jk} c_k = \frac{31}{720}$
	$\sum_i^s b_i a_{ij} c_j^2 = \frac{1}{6}$		

Using the order conditions in Table 8, we derived the IRK methods of orders $p = 3$ and $p = 4$. To determine the free parameters of the third and fourth order methods we minimized the error norm for the methods of order 4 and 5, respectively. Hence, the third order method (IRK3) with two stages ($p = 3, s = 2$), IRK3-3, ($p = 3, s = 3$) and the fourth order method with three stages ($p = 4, s = 3$) are obtained. Then, by satisfying as many equations as possible, for the fifth order method, we obtained the optimized fourth order method with 4-stages ($p = 4, s = 4$), which is denoted as the IRK4-4 method. The coefficients of the IRK3, IRK4 and IRK4-4 methods are presented in Table 9. The derivation can also be seen in Rabiei *et al.* (2013).

Table 9 Coefficients of IRK3, IRK4 and IRK4-4 methods

						0				
						$\frac{1}{5}$	$\frac{1}{5}$			
0			$\frac{31}{60}$	$\frac{31}{60}$	$\frac{31}{60}$	$\frac{3}{5}$	0	$\frac{3}{5}$		
$\frac{1}{2}$	$\frac{1}{2}$		$\frac{31}{60}$	$\frac{31}{60}$	$\frac{31}{60}$	$\frac{4}{5}$	$\frac{2}{15}$	$\frac{4}{25}$	$\frac{38}{75}$	
$-\frac{1}{3}$	$\frac{2}{3}$	$\frac{5}{6}$	$-\frac{157}{23064}$	$\frac{23221}{23064}$	$-\frac{1800}{161448}$	$\frac{19}{288}$	$\frac{307}{288}$	$-\frac{25}{144}$	$\frac{25}{144}$	$\frac{125}{288}$
IRK3			IRK4			IRK4-4				

Numerical Results and Discussions

In this section, we tested a set of initial value problems to show the efficiency and accuracy of the proposed methods. The following problems are solved for $x \in [0,10]$.

Problem 1: $y' = -xy/(1 + x^2)$, $y(0) = 1$;

Exact solution: $y(x) = -1/\sqrt{(1 + x^2)}$

(Source: Udwadia and Farahani (2008))

Problem 2: (an oscillatory problem)

$y' = y\cos(x)$, $y(0) = 1$;

Exact solution: $y(x) = e^{\sin(x)}$

(Source: Hull *et al.* (1972))

Problem 3: (1-body gravitational problem with eccentricity $e = 0$)

$y_1'' = -y_1(y_1^2 + y_2^2)^{-3/2}$, $y_1(0) = 1, y_1'(0) = 0$

$$y_2'' = -y_2(y_1^2 + y_2^2)^{-3/2}, \quad y_2(0) = 0, y_2'(0) = 1$$

Exact solution: $y_1(x) = \cos(x)$, $y_2(x) = \sin(x)$

(Source: Hull *et al.* (1972))

Notations used are as follows:

IRK3 ~ Improved Runge-Kutta Method ($p = 3, s = 2$)

IRK3-3 ~ Improved Runge-Kutta Method ($p = 3, s = 3$)

IRK4 ~ Improved Runge-Kutta Method ($p = 4, s = 3$)

IRK4-4 ~ Improved Runge-Kutta Method ($p = 4, s = 4$)

RK2 ~ Existing RK Method ($p = 2, s = 2$)

RK3 ~ Existing Runge-Kutta Method ($p = 3, s = 3$)

RK4 ~ Existing Runge-Kutta Method ($p = 4, s = 4$)

(Existing RK method in Dormand J.R.(1996)).

The number of function evaluations versus the $\log(\text{maximum global error})$ for the tested problems are shown in Figures 6 – 8.

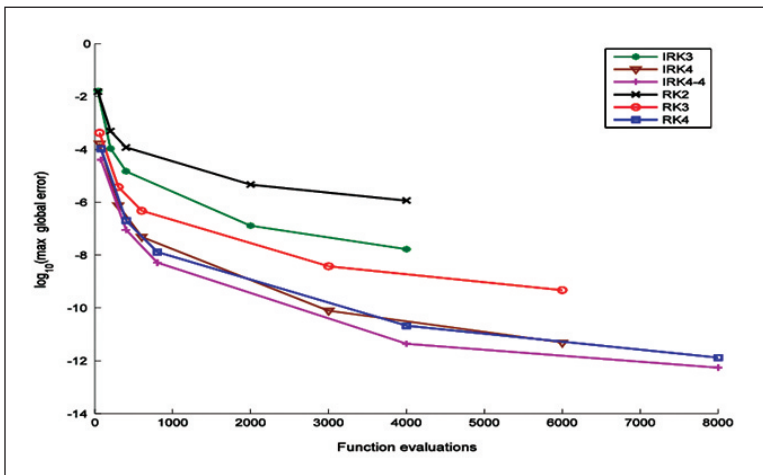


Figure 6 Maximum global error versus number of function evaluations for problem 1

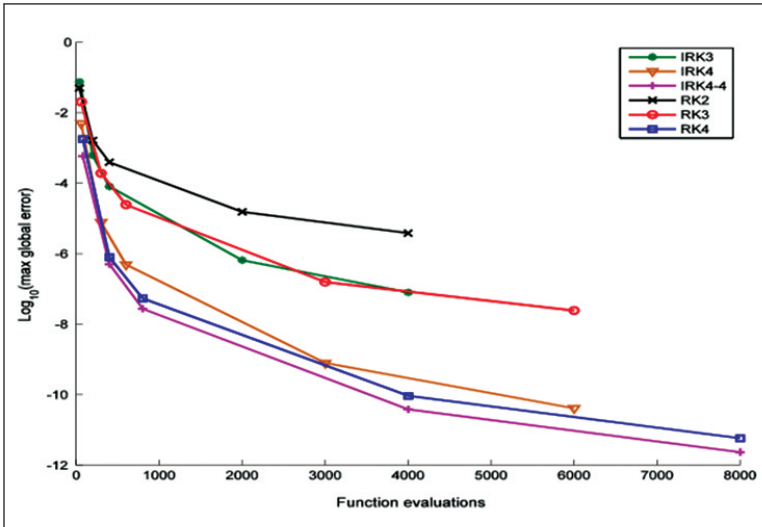


Figure 7 Maximum global error versus number of function evaluations for problem 2

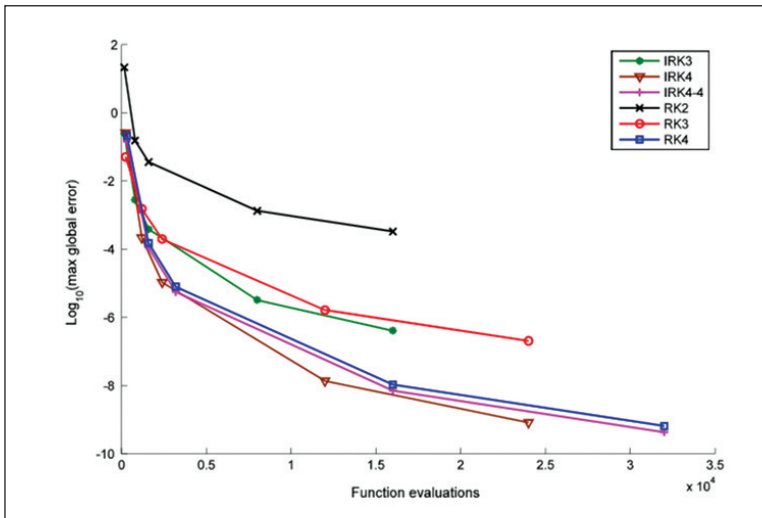


Figure 8 Maximum global error versus number of function evaluations for problem 3

In this research, the order conditions of the IRK method up to order five are derived. Based on these order conditions, we obtained IRK methods of order three and four with different stages. From the numerical results, we observed that for the same order, IRK methods with less number of stages require less number of function evaluations, which leads to less computational time needed for approximating numerical solutions of the problems as compared with the existing RK methods. Thus, we can conclude that IRK methods are computationally more efficient compared to the existing RK methods.

RUNGE-KUTTA TYPE METHODS FOR DIRECTLY SOLVING SPECIAL THIRD ORDER ORDINARY DIFFERENTIAL EQUATIONS

A special third order ODE can be written in the following form:

$$y'''(t) = f(t, y(t)), t \geq t_0, y(t_0) = \alpha, y'(t_0) = \beta, y''(t_0) = \gamma, \quad (4.1)$$

where $f: \mathfrak{R} \times \mathfrak{R} \rightarrow \mathfrak{R}$, which is not explicitly dependent on the first derivative $y'(t)$ and the second derivative $y''(t)$ of the solution. The ODE (4.1) is frequently found in many physical problems such as thin film flow, gravity and electromagnetic waves. Most researchers, scientists and engineers used to solve (4.1) by converting the third order differential equations to a system of first order equations three times the dimension. However, it is more efficient if the problem can be solved directly using numerical methods. Such work can be seen in Awoyemi, 2005; Waeleh, 2011; Noraini, 2011; Jator, 2011 and Yap *et al.* 2014. All the methods previously discussed are multistep methods, hence they need the starting values when used to solve the equation. Here we are going to derive a RK method for

solving the third order ODEs directly, and the method is denoted as the RKD method

Derivation of the RKD Method

The general form of an s -stage RK method for directly solving the initial value problem (4.1), denoted as the RKD method, can be written as

$$y_{n+1} = y_n + hy'_n + \frac{h^2}{2} y''_n + h^3 \sum_{i=1}^s b_i k_i \quad (4.2)$$

$$y'_{n+1} = y'_n + hy''_n + h^2 \sum_{i=1}^s b'_i k_i \quad (4.3)$$

$$y''_{n+1} = y''_n + h \sum_{i=1}^s b''_i k_i \quad (4.4)$$

$$\text{where } k_1 = f(t_n, y_n) \quad (4.5)$$

$$k_i = f \left(t_n + c_i h, y_n + hc_i y'_n + \frac{(c_i h)^2}{2} y''_n + h^3 \sum_{j=1}^{i-1} a_{ij} k_j \right) \quad (4.6)$$

for $i = 2, 3, \dots, s$. The parameters of the RKD method are $c_i, a_{ij}, b_i, b'_i, b''_i$ for $i = 1, 2, 3, \dots, s$ and $j = 1, 2, 3, \dots, s$ are assumed to be real.

To determine the coefficients of the RKD method, the expressions given in (4.3) - (4.7) are expanded using Taylor's series expansion. After some algebraic manipulations these expansions are equated to the Taylor's series expansion of the true solution. Comparison of the Taylor series expansion between the true solution

and the RKD method gives the order conditions, which can be seen in Mechee *et al.* (2014a).

To obtain the higher order RKD method, the following simplifying assumptions are used in order to reduce the number of equations to be solved:

$$b'_i = b''_i(1 - c_i), i = 1, \dots, s, \quad b_i = b'_i \frac{(1 - c_i)^2}{2}, i = 1, \dots, s$$

The following strategies are used for developing the efficient pairs.

The quantities $\|\tau^{(p+1)}\|_2$ and $\|\bar{\tau}^{(p+1)}\|_2$ should be as small as possible for higher and lower order RKD formulas. Further, a local truncation error (*LTE*) estimation at the point x_n is determined by the formula

$$LTE = \max\{\|\delta_n\|_\infty, \|\delta'_n\|_\infty, \|\delta''_n\|_\infty\},$$

where $\delta_n = \bar{y}_n - y_n$, $\delta'_n = \bar{y}'_n - y'_n$, $\delta_n = \bar{y}_n'' - y_n''$.

\bar{y}_n , \bar{y}'_n , \bar{y}_n'' and y_n , y'_n , y_n'' are the solutions for the lower and higher order formulas, respectively and the *LTE* can be used to control the stepsize h .

Derivation of RKD 5(4) Pair

For the three-stage fifth order formula, the algebraic order conditions up to the fifth order, together with the simplifying assumptions, are solved simultaneously. Based on the values of a_{ij} and c_i , for the fifth order method, we derived the three-stage fourth order method, where the free parameters are obtained using the minimized error norm. This gives us the following formula:

Table 10 Embedded RKD 5(4) method

0	0		
$\frac{3}{5} + \frac{\sqrt{6}}{10}$	$\frac{27}{500} + \frac{19\sqrt{6}}{1000}$	0	
$\frac{3}{5} - \frac{\sqrt{6}}{10}$	$\frac{33}{2500} - \frac{51\sqrt{6}}{5000}$	$\frac{51}{1250} - \frac{11\sqrt{6}}{1250}$	0
	$\frac{1}{18}$	$\frac{1}{18} - \frac{\sqrt{6}}{48}$	$\frac{1}{18} + \frac{\sqrt{6}}{48}$
	$\frac{1}{9}$	$\frac{7}{36} - \frac{\sqrt{6}}{18}$	$\frac{7}{36} + \frac{\sqrt{6}}{36}$
	$\frac{1}{9}$	$\frac{4}{9} - \frac{\sqrt{6}}{36}$	$\frac{4}{9} + \frac{\sqrt{6}}{36}$
	$\frac{1}{15}$	$\frac{1}{20} - \frac{11\sqrt{6}}{720}$	$\frac{1}{20} + \frac{11\sqrt{6}}{720}$
	$\frac{1}{9}$	$\frac{7}{36} - \frac{\sqrt{6}}{18}$	$\frac{7}{36} + \frac{\sqrt{6}}{18}$
	$\frac{1}{9}$	$\frac{4}{9} - \frac{\sqrt{6}}{36}$	$\frac{4}{9} + \frac{\sqrt{6}}{36}$

Derivation of RKD 6(5) Pair

Here, we are going to derive the RKD6(5) pair with four stages. For the 6th order formula the order conditions of up to order six for y, y', y'' need to be solved. Imposing the simplifying assumptions the number of equations are reduced to 12 with 13 unknowns, which leaves us with one degree of freedom. The free parameter is chosen to be c_3 where it is in the interval $[0,1]$ and choosing $c_3 = \frac{1}{2}$ gives the smallest error norm. Now based on the values of A and c, we derived the fifth order embedded formula by solving the order conditions up to order five.

Table 11 Embedded RKD 6(5) Method

0	0					
$\frac{1}{2} + \frac{\sqrt{15}}{10}$	$\frac{7}{120}$	$-\frac{3\sqrt{15}}{200}$	0			
$\frac{1}{2}$	$\frac{-1}{90}$	$+\frac{\sqrt{15}}{480}$	$\frac{1}{32}$	$-\frac{\sqrt{15}}{480}$	0	
$\frac{1}{2} + \frac{\sqrt{15}}{10}$	$\frac{-1}{600}$	$+\frac{\sqrt{15}}{600}$	$\frac{\sqrt{15}}{50}$	$\frac{3}{50}$	$-\frac{\sqrt{15}}{150}$	0
	0	$\frac{1}{18}$	$+\frac{\sqrt{15}}{72}$	$\frac{1}{18}$	$\frac{1}{18}$	$-\frac{\sqrt{15}}{72}$
	0	$\frac{5}{36}$	$+\frac{\sqrt{15}}{36}$	$\frac{2}{9}$	$\frac{5}{36}$	$-\frac{\sqrt{15}}{36}$
	0	$\frac{5}{18}$		$\frac{4}{9}$	$\frac{5}{18}$	
	$\frac{7}{600}$	$-\frac{43\sqrt{15}}{3000}$	$\frac{49}{600} + \frac{43\sqrt{15}}{1800}$	$\frac{19}{300} - \frac{43\sqrt{15}}{4500}$	$\frac{1}{100}$	
	0	$\frac{5}{36}$	$+\frac{\sqrt{15}}{36}$	$\frac{2}{9}$	$\frac{5}{36}$	$-\frac{\sqrt{15}}{36}$
	0	$\frac{5}{18}$		$\frac{4}{9}$	$\frac{5}{18}$	

Numerical Results

Below are some of the third order problems to be tested and the numerical results will be compared with that using the existing numerical methods.

Problem 1: (Inhomogeneous linear problem)

$$y''' = (y(t))^2 + \cos(t) (\cos(t) - 1) - 1, \quad 0 < t \leq 5,$$

$$y(0) = 0, \quad y'(0) = 1, \quad y''(0) = 0.$$

The exact solution is given by $y(t) = \sin(t)$.

Problem 2:

$$y''' = y(t) + \cos(t), \quad 0 < x \leq 10,$$

$$y(0) = 0, \quad y'(0) = 0, \quad y''(0) = 1.$$

The exact solution is given by $y(x) = \frac{1}{2}e^t - \frac{1}{2}(\cos(t) + \sin(t))$

Problem 3:

$$y''' = 2e^t \cos(t) - 2y(t), \quad 0 < x \leq 3,$$

$$y(0) = 0, \quad y'(0) = 1, \quad y''(0) = 2.$$

The exact solution is given by $y(x) = e^t \sin(t)$.

Problem 4:

$$y_1''' = -e^{2t} y_3(t), \quad y_1(0) = 1, y_1'(0) = -1, y_1''(0) = 1,$$

$$y_2''' = -8e^{2t} y_1(t), \quad y_2(0) = 1, y_2'(0) = -2, y_2''(0) = 4,$$

$$y_3''' = -27e^{-t} y_2(t), \quad y_3(0) = 1, y_3'(0) = -3, y_3''(0) = 9.$$

The system is integrated in the interval $[0,2]$.

The exact solution is: $y_1(t) = e^{-t}$, $y_2(t) = e^{-2t}$, $y_3(t) = e^{-3t}$.

The following notations are used in Figures 4.1 - 4.4:

RKD 5(4): Runge-Kutta type method, 5(4) pair derived here.

RKD 6(5): Runge-Kutta type method, 6(5) pair derived here.

DOPRI 5(4): Runge-Kutta method, 5(4) pair derived by Dormand and Prince (1980).

RK5(4) B: Runge-Kutta method, 5(4) pair derived by Butcher (2008).

RK5(4) F: Runge-Kutta method, 5(4) pair derived by Fehlberg (1968).

RK6(5) D:): Runge-Kutta method, 6(5) pair derived by Dormand and Prince (1981).

RK6(5) B: Runge-Kutta method, 5(4) pair derived by Butcher (2008).

RK6(5) F: Runge-Kutta method, 5(4) pair derived by Fehlberg (1968).

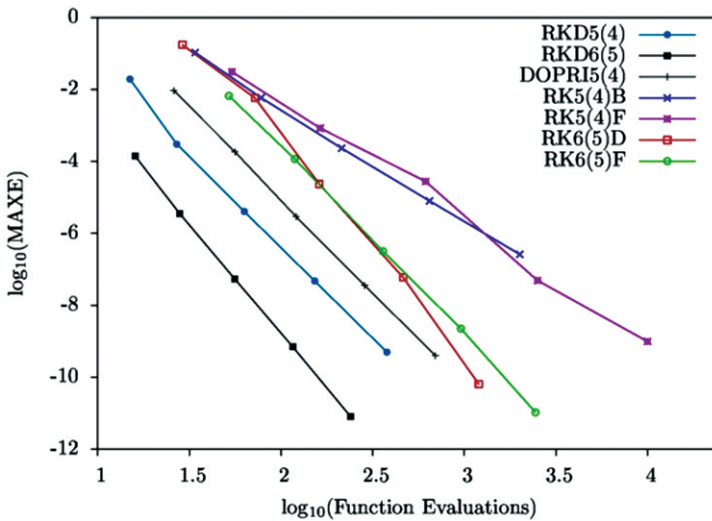


Figure 9 The efficiency curves of the methods and their comparisons for problem 1

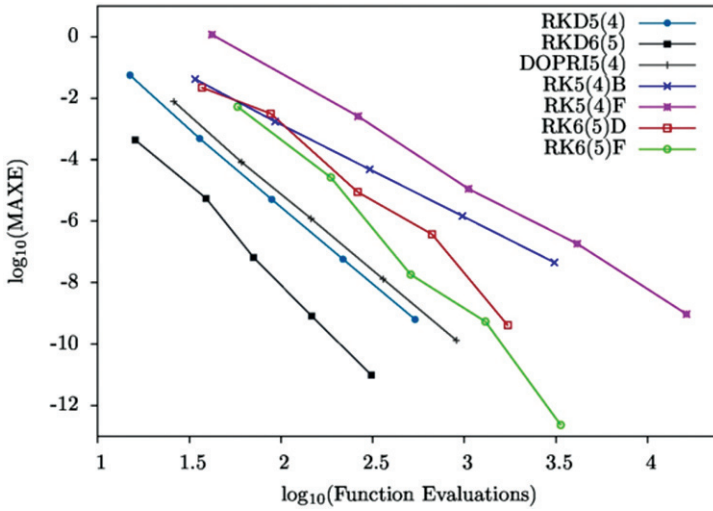


Figure 10 The efficiency curves of the methods and their comparisons for problem 2

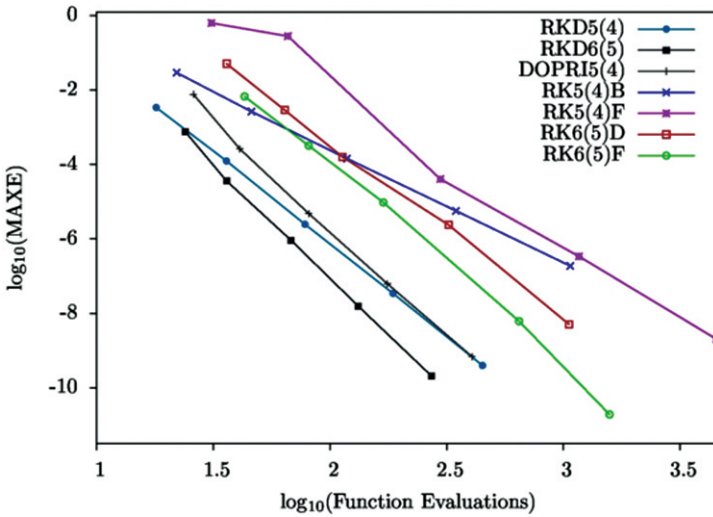


Figure 11 The efficiency curves of the methods and their comparisons for problem 3

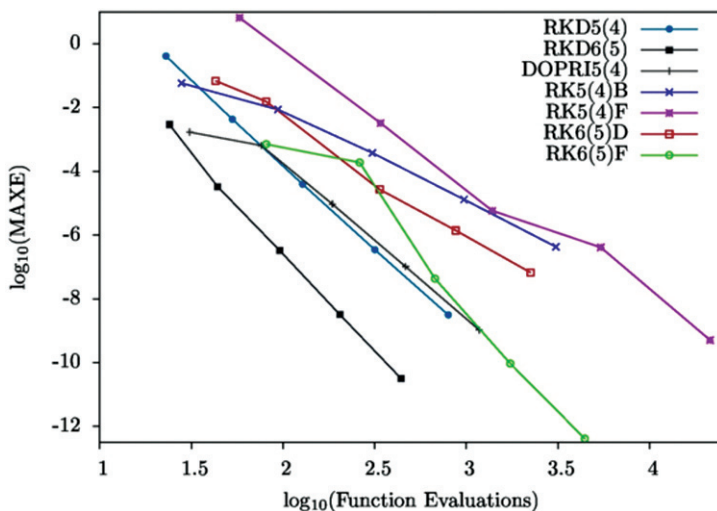


Figure 12 The efficiency curves of the methods and their comparisons for problem 4

Here, we derived the order conditions of the RKD method and constructed two pairs of embedded methods. Variable stepsize codes based on the methods are developed and used to solve the special third order ODEs directly. From the numerical results, it is observed that the new methods are more efficient compared to the existing embedded RK pairs in scientific literature. In fact the RKD5(4) is more efficient compared to the existing RK6(5) methods.

RUNGE-KUTTA TYPE METHODS FOR DIRECTLY SOLVING SPECIAL FOURTH ORDER ORDINARY DIFFERENTIAL EQUATIONS

In this section we are concerned with the efficient numerical integration of the special fourth-order ODEs of the form

$$y^{(iv)}(x) = f(x, y), \quad (5.1)$$

with initial conditions

$$y(x_0) = y_0, \quad y'(x_0) = y'_0, \quad y''(x_0) = y''_0, \quad y'''(x_0) = y'''_0$$

where $f: \mathbb{R} \times \mathbb{R}^m \rightarrow \mathbb{R}^m$ is a continuous valued function which does not contain the first, second and third derivatives. Normally, researchers and engineers solve the fourth-order ODEs by converting them into a first-order system of ODEs and then applying a suitable numerical method to solve the resulting system. However, the application of such technique takes a lot of computational time. Direct integration method is proposed to avoid this computational burden and to increase the efficiency of the method. Many authors have proposed several numerical methods for directly approximating the solutions for the higher order ODEs. For example, Kayode (2008) proposed a zero stable predictor-corrector method for solving fourth-order ordinary differential equations and Yap *et al.* (2015) derived a one point block method to solve a system of higher order ODEs. All these methods are multistep and are not self-starting. These methods require the starting values to obtain the initial values for solving equation (5.1).

This research primarily aims to construct a one-step method of order six to solve special fourth-order ODEs directly. Further, this new method will be self-starting in nature. Mechee *et al.* (2014a) and Senu *et al.* (2014) derived RKD methods for direct integration of special third order ODEs and Mechee *et al.* (2014b) also applied the RKD method for solving third order PDEs. Here we will further extend their work to fourth order ODEs.

The General Form of the RKFD Method

In this section we present the general form of the Runge-Kutta method for directly solving special fourth order ODEs, denoted as the RKFD method with s -stage, as follows

$$y_{n+1} = y_n + h y'_n + \frac{h^2}{2} y''_n + \frac{h^3}{6} y'''_n + h^4 \sum_{i=1}^s b_i k_i, \quad (5.2)$$

$$y'_{n+1} = y'_n + h y''_n + \frac{h^2}{2} y'''_n + h^3 \sum_{i=1}^s b'_i k_i, \quad (5.3)$$

$$y''_{n+1} = y''_n + h y'''_n + h^2 \sum_{i=1}^s b''_i k_i, \quad (5.4)$$

$$y'''_{n+1} = y'''_n + h \sum_{i=1}^s b'''_i k_i, \quad (5.5)$$

where

$$k_1 = f(x_n, y_n),$$

$$k_i = f \left(x_n + c_i h, y_n + h c_i y'_n + \frac{h^2}{2} c_i^2 y''_n + \frac{h^3}{6} c_i^3 y'''_n + h^4 \sum_{j=1}^{i-1} a_{ij} k_j \right), \quad i = 2, 3, \dots, s. \quad (5.6)$$

All parameters $b_i, b'_i, b''_i, b'''_i, a_{ij}$ and c_i of the RKFD method are used for $i = 1, 2, \dots, s$; $j = 1, 2, \dots, s$ and is supposed to be real.

To determine the parameters of the RKFD method, expressions (5.2) to (5.6) are expanded using the Taylor series expansion. This expansion is equated to the Taylor series expansion of the true solution. The direct expansion of the truncation error is used to derive the order conditions for the RKFD method. A good deal of

the algebraic and numerical calculations required were carried out using the algebra package MAPLE.

Order Conditions of the RKFD Method

Hussain *et al.* (2015a) and Hussain *et al.* (2016) derived the algebraic order conditions for the RKFD method using the Taylor Series expansion and the theory of B-series. Using the order conditions, embedded pairs of RKFD methods were derived by Hussain *et al.* (2015b). The order conditions for the RKFD method obtained by Hussain *et al.* (2015a), up to order six, are as follows:

The order conditions for y :

$$\text{order 4: } \sum_{i=1}^s b_i = \frac{1}{24}, \quad (5.7) \quad \text{order 5: } \sum_{i=1}^s b_i'' c_i^3 = \frac{1}{20}, \quad (5.18)$$

$$\text{order 5: } \sum_{i=1}^s b_i c_i = \frac{1}{120}, \quad (5.8) \quad \text{order 6: } \sum_{i=1}^s b_i'' c_i^4 = \frac{1}{30}, \quad (5.19)$$

$$\text{order 6: } \sum_{i=1}^s b_i c_i^2 = \frac{1}{360}, \quad (5.9) \quad \sum_{i,j=1}^s b_i'' a_{ij} = \frac{1}{720}, \quad (5.20)$$

$$\text{order 7: } \sum_{i=1}^s b_i c_i^3 = \frac{1}{840}, \quad (5.10) \quad \text{order conditions for } y''':$$

$$\text{The order conditions for } y': \quad \text{order 1: } \sum_{i=1}^s b_i''' = 1 \quad (5.21)$$

$$\text{order 3: } \sum_{i=1}^s b_i' = \frac{1}{6}, \quad (5.11) \quad \text{order 2: } \sum_{i=1}^s b_i''' c_i = \frac{1}{2}, \quad (5.22)$$

$$\text{order 4: } \sum_{i=1}^s b'_i c_i = \frac{1}{24}, \quad (5.12) \quad \text{order 3: } \sum_{i=1}^s b_i''' c_i^2 = \frac{1}{3}, \quad (5.23)$$

$$\text{order 5: } \sum_{i=1}^s b'_i c_i^2 = \frac{1}{60}, \quad (5.13) \quad \text{order 4: } \sum_{i=1}^s b_i''' c_i^3 = \frac{1}{4}, \quad (5.24)$$

$$\text{order 6: } \sum_{i=1}^s b'_i c_i^3 = \frac{1}{120}, \quad (5.14) \quad \text{order 5: } \sum_{i=1}^s b_i''' c_i^4 = \frac{1}{5}, \quad (5.25)$$

$$\text{The order conditions for } y'': \quad \sum_{i,j=1}^s b_i''' a_{ij} = \frac{1}{120}, \quad (5.26)$$

$$\text{order 2: } \sum_{i=1}^s b_i'' = \frac{1}{2}, \quad (5.15) \quad \text{order 6: } \sum_{i=1}^s b_i''' c_i^5 = \frac{1}{6}, \quad (5.27)$$

$$\text{order 3: } \sum_{i=1}^s b_i'' c_i = \frac{1}{6}, \quad (5.16) \quad \sum_{i,j=1}^s b_i''' a_{ij} c_j = \frac{1}{720}, \quad (5.28)$$

$$\text{order 4: } \sum_{i=1}^s b_i'' c_i^2 = \frac{1}{12}, \quad (5.17) \quad \sum_{i,j=1}^s b_i''' c_i a_{ij} = \frac{1}{144}. \quad (5.29)$$

Sixth Order RKFD Method with Four-Stages

In order to construct the four-stage sixth-order RKFD6 method, the algebraic conditions of the RKFD method up to order six for y, y', y'' and y''' need to be solved first. We choose equations (5.11) -to (5.14) from the order conditions for y' , equations (5.15) - (5.19) from order conditions for y'' and equations (5.21) - (5.25) and (5.27) from order conditions for y''' . Here we have one free parameter b_1 , which can be chosen by minimizing the error norm of the seventh order conditions for y , as in Dormand (1987).

By minimizing the error norm of the seventh order condition, $\|\tau^{(7)}\|_2$ with respect to the free parameter b_1 , we obtain $b_1 = \frac{17}{1260}$ as the optimal value. Finally, all the parameters of the four-stage sixth-order RKFD method, denoted as RKFD6, are written in Butcher tableau as follows:

Table 12 Butcher tableau for RKFD6 method

$\frac{1}{2} + \frac{\sqrt{5}}{10}$	$\frac{1}{168} + \frac{11\sqrt{5}}{4200}$			
$\frac{1}{2} - \frac{\sqrt{5}}{10}$	$\frac{1}{420} - \frac{\sqrt{5}}{700}$	$\frac{1}{280} - \frac{\sqrt{5}}{840}$		
1	$\frac{-1}{840} - \frac{\sqrt{5}}{168}$	$\frac{1}{84} - \frac{\sqrt{5}}{140}$	$\frac{5}{168} + \frac{11\sqrt{5}}{840}$	
	$\frac{17}{1260}$	$\frac{1}{72} - \frac{\sqrt{5}}{168}$	$\frac{1}{72} + \frac{\sqrt{15}}{168}$	$\frac{1}{2520}$
	$\frac{1}{24}$	$\frac{1}{16} - \frac{\sqrt{5}}{48}$	$\frac{1}{16} + \frac{\sqrt{5}}{48}$	0
	$\frac{1}{12}$	$\frac{5}{24} - \frac{\sqrt{5}}{24}$	$\frac{5}{24} + \frac{\sqrt{5}}{24}$	0
	$\frac{1}{12}$	$\frac{5}{12}$	$\frac{5}{12}$	$\frac{1}{12}$

Numerical Results

In order to evaluate the performance of the new RKFD6 method, it is used to solve a set of special fourth-order ODEs, chosen from the scientific literature, and then results compared with some existing RK methods of the same order.

Problem 1:

$$y^{(iv)} = \frac{3 \sin(y) (3 + 2 \sin^2(y))}{\cos^7(y)},$$

$$y(0) = 0, \quad y'(0) = 1, \quad y''(0) = 0, \quad y'''(0) = 1.$$

The exact solution is given by $y(x) = \arcsin(x)$. Interval of integration is $\left[0, \frac{\pi}{4}\right]$.

Problem 2:

$$y^{(iv)} = e^{3x} u, \quad y(0) = 1, \quad y'(0) = -1, \quad y''(0) = 1, \quad y'''(0) = -1.$$

$$z^{(iv)} = 16 e^{-x} y, \quad z(0) = 1, \quad z'(0) = -2, \quad z''(0) = 4, \quad z'''(0) = -8.$$

$$w^{(iv)} = 81 e^{-x} z, \quad w(0) = 1, \quad w'(0) = -3, \quad w''(0) = 9, \quad w'''(0) = -27.$$

$$u^{(iv)} = 256 e^{-x} w, \quad u(0) = 1, \quad u'(0) = -4, \quad u''(0) = 16, \quad u'''(0) = -64.$$

The problem is integrated in the interval $[0, 2]$. The exact solution is given by

$$y = e^{-x}, \quad z = e^{-2x}, \quad w = e^{-3x}, \quad u = e^{-4x}.$$

Problem 3:

$$y^{(iv)} = y + \frac{1}{\sqrt{y^2 + z^2}} - \frac{1}{\sqrt{w^2 + u^2}}, \quad y(0) = 1, \quad y'(0) = 0, \quad y''(0) = -1, \quad y'''(0) = 0.$$

$$z^{(iv)} = z - \frac{1}{\sqrt{y^2 + z^2}} + \frac{1}{\sqrt{w^2 + u^2}}, \quad z(0) = 0, \quad z'(0) = 1, \quad z''(0) = 0, \quad z'''(0) = -1.$$

$$w^{(iv)} = 16w + \frac{1}{\sqrt{y^2 + z^2}} - \frac{1}{\sqrt{w^2 + u^2}},$$

$$w(0) = 1, \quad w'(0) = 0, \quad w''(0) = -4, \quad w'''(0) = 0.$$

$$u^{(iv)} = 16u - \frac{1}{\sqrt{y^2 + z^2}} + \frac{1}{\sqrt{w^2 + u^2}}, \quad u(0) = 0, \quad u'(0) = 2, \quad u''(0) = 0, \\ u'''(0) = -8.$$

The problem is integrated in the interval $[0, 2]$. The exact solution is given by

$$y = \cos(x), \quad z = \sin(x), \quad w = \cos(2x), \quad u = \sin(2x).$$

In the numerical comparisons we use the criteria based on the maximum error in the solution $Max\ Error = \max(|y(x_n) - y_n|)$, which is equal to the maximum of absolute errors of the true solutions and the computed solutions.. The following methods are used in the comparison.

- RKFD6: The four-stage sixth-order RKFD method derived here.
- RK6N: The seven-stage sixth-order RK method given in Butcher (1964).
- RK6B: The seven-stage sixth-order RK method derived by Butcher (2008).

Figures 13 – 15 show the efficiency curves of $Log_{10}(Max\ Error)$ against the computational effort, measured by $Log_{10}(Function\ Evaluations)$, which are required by each method.

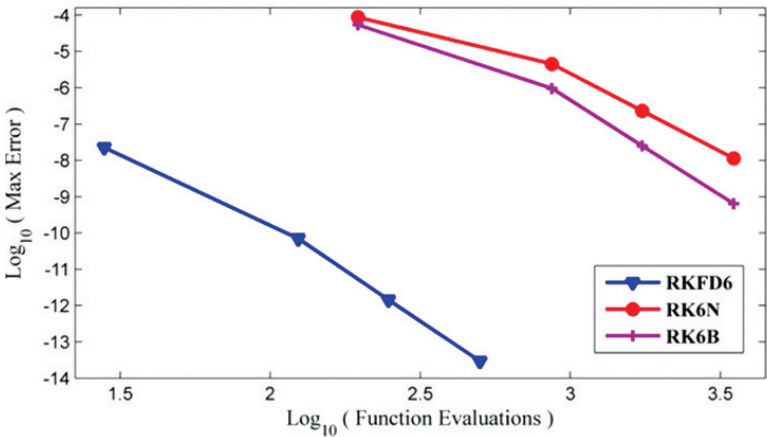


Figure 13 The efficiency curves for Problem 1 with $h = 0.1/2^i, i = 0, 2, 3, 4$

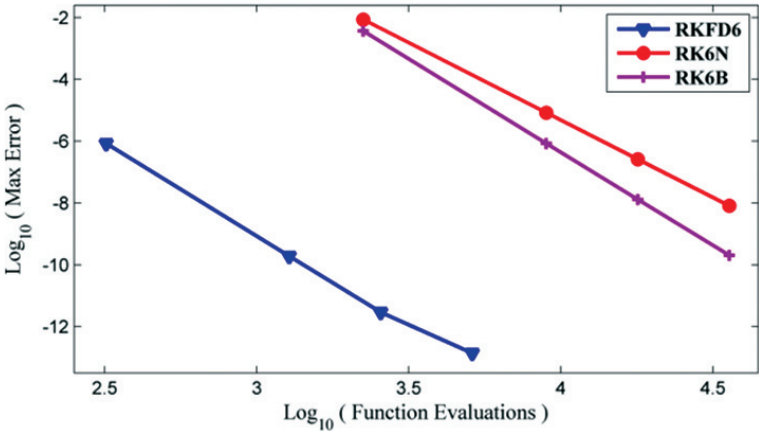


Figure 14 The efficiency curves for Problem 2 with $h = 0.1/2^i, i = 0, 2, 3, 4$

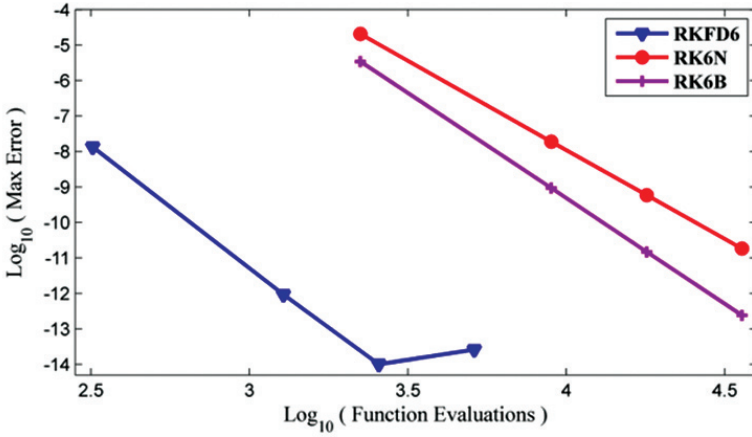


Figure 15 The efficiency curves for Problem 3
with $h = 0.1/2^i, i = 0, 2, 3, 4$

We derived the order conditions of the RKFD methods up to order seven. Based on the order conditions we constructed the four-stage sixth-order RKFD method for directly solving special fourth-order ODEs, and this method is denoted as the RKFD6 method. The numerical results illustrate that the RKFD6 method is more efficient compared to the well known Runge-Kutta methods in literature. In conclusion it can be said that, the new RKFD6 method can directly solve the special fourth-order ODEs efficiently.

SEMI-IMPLICIT HYBRID METHOD FOR SOLVING OSCILLATORY PROBLEMS

Initial value problems (IVPs) for second order ODEs, where the first derivative does not appear explicitly, which can be written as

$$y'' = f(x, y), \quad y(x_0) = y_0, \quad y'(x_0) = y'_0 \quad (6.1)$$

often arise in many scientific areas of engineering and applied science, such as, celestial mechanics, molecular dynamics and quantum mechanics.

The solution for (6.1) also often exhibits a pronounced oscillatory character. It is well known that it is rather difficult to get the accurate numerical results if the initial value problems are oscillatory in nature. In trying to address the problem a lot of research has been focused on developing methods with reduced phase-lag. Phase-lag or dispersion error is the angle between the true and the approximated solution. The performance of numerical methods for solving oscillatory problems can be enhanced by phase-fitting the method.

The idea of Phase-lag of a numerical method was first introduced by Bursa and Nigro (1980). Based on this work, Van der Houwen and Sommeijer (1987) proposed explicit Runge-Kutta Nystrom methods of order 4, 5 and 6, with reduced phase-lag of order $q = 6, 8$ and 10 , respectively. Work on oscillatory problems has also been done by Samat *et al.* (2012).

Derivation of the Method

A Semi-implicit hybrid method for the numerical integration of the IVPs is given as

$$Y_i = (1 + c_i)y_n - c_i y_{n-1} + h^2 \sum_{j=1}^s a_{ij} f(x_n + c_j h, Y_j) \quad (6.2)$$

$$y_{n+1} = 2y_n - y_{n-1} + h^2 \sum_{i=1}^s b_i f(x_n + c_i h, Y_i) \quad (6.3)$$

where $i = 1, \dots, s$ and $i = j$ and the coefficient b_i , c_i , and a_{ij} can be represented as seen in Table 13 and $Y_1 = y_{n-1}$, $Y_2 = y_n$.

Table 13 The s -stage semi-implicit hybrid methods

	-1	0				
	0	0	0			
	c_3	$a_{3,1}$	$a_{3,2}$	γ		
	\vdots	\vdots	\vdots	\ddots	\ddots	
	c_s	$a_{s,1}$	$a_{s,2}$	\dots	$a_{s,s-1}$	γ
		b_1	b_2	\dots	b_{s-1}	b_s

The phase-lag analysis is investigated using the second order equation

$$y''(x) = -\lambda^2 y(x) \text{ for } \lambda > 0, \text{ for } \lambda \in \Re \quad (6.4)$$

By replacing $f(x, y) = -\lambda^2 y$ into equations (6.2) and (6.3), and defining $z = \lambda h$, the equations can be written as

$$y_{n+1} - S(z^2)y_n + P(z^2)y_{n-1} = 0 \quad (6.5)$$

and the stability polynomial is

$$\pi(\xi, z) = \xi^2 - S(z^2)\xi + P(z^2) = 0. \quad (6.6)$$

where $S(z^2) = 2 - z^2 \mathbf{b}^T (\mathbf{I} + z^2 \mathbf{A})^{-1} (\mathbf{e} + \mathbf{c})$ and

$$P(z^2) = 1 - z^2 \mathbf{b}^T (\mathbf{I} + z^2 \mathbf{A})^{-1} \mathbf{c}. \quad (6.7)$$

Solving the difference equation (6.5), gives the solution

$$y_n = 2|c||\rho|^n \cos(\omega + n\phi) \quad (6.8)$$

where ρ is the amplification factor, ϕ is the phase and ω and c are real constants determined by the initial values y_0 and y_0' . The exact solution of $y''(x) = -\lambda^2 y(x)$ is given by

$$y(t_n) = 2|\sigma|\cos(\chi + nz) \quad (6.9)$$

where n is the number of terms and, σ and χ are real constants determined by the initial conditions. Equations (6.8) and (6.9) led to the following definition which was given in Van der Houwen and Sommeijer (1987).

Definition 6.1: The quantity $\varphi(z) = z - \phi$ is called the phase-lag or dissipation error and the quantity $d(z) = 1 - |\rho|$, is called the amplification error. From definition 6.1, it follows that

$$\varphi(z) = z - \cos^{-1}\left(\frac{S(z^2)}{2\sqrt{P(z^2)}}\right) \text{ and } d(z) = 1 - \sqrt{P(z^2)}. \quad (6.10)$$

If $\varphi(z) = O(z^{q+1})$, then the hybrid method is said to be dispersive of order q , while, the quantity $d(z) = 1 - |\rho|$, called the amplification error, and if $d(z) = O(z^{r+1})$, then the hybrid method is said to have dissipation order r .

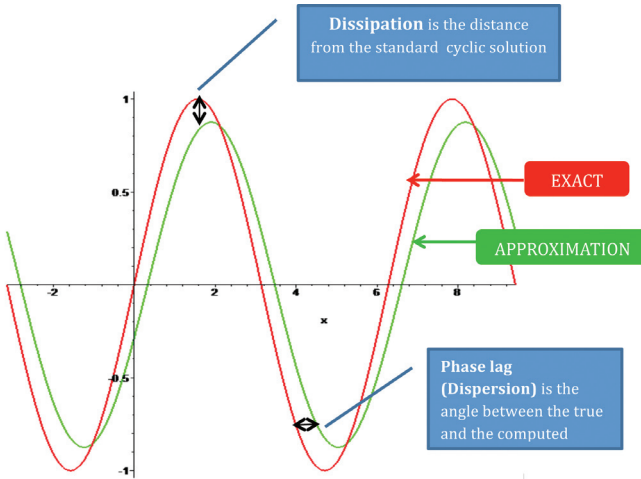


Figure 17 Dissipation and Dispersion or Phase-lag Error

Development of Dispersion and Dissipation Relations

In this section we will develop the dispersion and dissipation relations of the method of stage three and four where $S(z^2)$ and $P(z^2)$ can be written in the following forms

$$S(z^2) = \frac{2 + \alpha_1 z^2 + \cdots + \alpha_{m-1} z^{2(m-1)}}{(1 + \gamma z^2)^{m-2}} \quad (6.11)$$

$$P(z^2) = \frac{1 + \beta_1 z^2 + \cdots + \beta_m z^{2(m-1)}}{(1 + \gamma z^2)^{m-2}} \quad (6.12)$$

and where γ is the diagonal element.

For a zero dissipative method with three stages ($s = 3$), the dispersion relations of order six ($q = 6$) is given as

$$\text{Order 6: } \alpha_2 = \frac{1}{\gamma} \left(\frac{1}{360} - \gamma^2 \right)$$

and the dispersion relations up to order eight for $s = 4$, are given as

$$\text{Order 6: } \beta_3 - 2\beta_2\gamma - \alpha_3 + \gamma\alpha_2 - \frac{1}{2}\beta_2 = -\frac{3}{2}\gamma^2 + \frac{1}{360} - 2\gamma^3$$

$$\begin{aligned} \text{Order 8: } & \frac{1}{4}\beta_2^2 - \left(\frac{7}{2}\gamma^2 + \gamma + \frac{1}{24} \right) \beta_2 - \gamma\alpha_3 + \gamma^2\alpha_2 + \left(2\gamma + \frac{1}{2} \right) \beta_3 \\ & = \frac{1}{20160} - \frac{1}{24}\gamma^2 - 2\gamma^3 - \frac{13}{4}\gamma^4 \end{aligned}$$

The following quantities are used to determine the dissipation of the formula for $s = 3, 4$.

For ($s = 3$) it is

$$\begin{aligned}
 1 - \sqrt{P(z^2)} &= \left(-\frac{1}{2}\beta_1 + \frac{1}{2}\gamma\right)z^2 + \left(-\frac{1}{2}\beta_2 + \frac{1}{4}\gamma\beta_1 - \frac{3}{8}\gamma^2 + \frac{1}{8}\beta_1^2\right)z^4 \\
 &+ \left(\frac{1}{4}\gamma\beta_2 - \frac{3}{16}\gamma^2\beta_1 + \frac{5}{16}\gamma^3 + \frac{1}{4}\beta_1\beta_2 - \frac{1}{16}\gamma\beta_1^2 - \frac{1}{16}\beta_1^3\right)z^6 \\
 &+ \left\{\left(\frac{5}{28}\beta_1^4 - \frac{3}{16}\gamma^2\beta_2 + \frac{5}{32}\gamma^3\beta_1 + \frac{3}{64}\gamma^2\beta_1^2 + \frac{1}{16}\beta_2^2 - \frac{3}{16}\beta_1^2\beta_2\right)\right. \\
 &\left. + \left(\frac{1}{32}\beta_1^3\gamma - \frac{1}{8}\gamma\beta_1\beta_2 - \frac{35}{128}\gamma^4\right)\right\}z^8 + O(z^{10})
 \end{aligned}$$

and for $s = 4$, it is

$$\begin{aligned}
 1 - \sqrt{P(z^2)} &= \left(\gamma - \frac{1}{2}\beta_1\right)z^2 + \left(\frac{1}{2}\beta_1\gamma - \gamma^2 - \frac{1}{2}\beta_2 + \frac{1}{8}\beta_1^2\right)z^4 \\
 &+ \left(-\frac{1}{2}\beta_1\gamma^2 + \frac{1}{2}\beta_2\gamma + \gamma^3 - \frac{1}{2}\beta_3 - \frac{1}{8}\gamma\beta_1^2 + \frac{1}{4}\beta_1\beta_2 - \frac{1}{16}\beta_1^3\right)z^6 \\
 &+ \left\{\left(-\gamma^4 + \frac{1}{2}\beta_1\gamma^3 - \frac{1}{2}\beta_2\gamma^2 + \gamma^3 + \frac{1}{2}\beta_3\gamma - \frac{1}{4}\beta_1\beta_2\gamma + \frac{1}{8}\beta_1^2\gamma^2\right)\right. \\
 &\left. + \left(\frac{1}{4}\beta_1\beta_3 + \frac{1}{8}\beta_2^2 + \frac{1}{16}\beta_1^3\gamma - \frac{3}{16}\beta_1^2\beta_2 + \frac{5}{128}\beta_1^4\right)\right\}z^8 + O(z^{10})
 \end{aligned}$$

while the stability polynomial is

$$\pi(\xi, z) = \xi^2 - S(z^2)\xi + P(z^2) = 0.$$

The integration process is stable if : $P(z^2) < 1$ and $|S(z^2)| < 1 + P(z^2)$, $\forall z^2 \in (0, z_s^2)$. The interval of $(0, z_s^2)$ is called the stability interval.

Derivation of Semi-implicit Hybrid Methods (SIHMs)

The derivation of the methods is based on the order conditions, dispersive and dissipative error and minimization of the error norm of the method. The order conditions of hybrid methods given in Coleman (2003) are:

$$\text{Order 2: } \sum_{i=1}^s b_i = 1, \quad \text{Order 3: } \sum_{i=1}^s b_i c_i = 0,$$

$$\text{Order 4: } \sum_{i=1}^s b_i c_i^2 = \frac{1}{6}, \quad \sum_{i=1}^s b_i a_{ij} = \frac{1}{12},$$

$$\text{Order 5: } \sum_{i=1}^s b_i c_i^3 = 0, \quad \sum_{i=1}^s b_i c_i a_{ij} = \frac{1}{12}, \quad \sum_{i=1}^s b_i a_{ij} c_j = 0,$$

$$\text{Order 6: } \sum_{i=1}^s b_i c_i^4 = 0, \quad \sum_{i=1}^s b_i c_i^2 a_{ij} = \frac{1}{30}, \quad \sum_{i=1}^s b_i c_i a_{ij} c_j = -\frac{1}{60},$$

$$\sum_{i=1}^s b_i a_{ij} a_{ik} = \frac{7}{120}, \quad \sum_{i=1}^s b_i a_{ij} c_j^2 = \frac{1}{180}, \quad \sum_{i=1}^s b_i a_{ij} a_{jk} = \frac{1}{360}.$$

and c_i needs to satisfy

$$\sum_{i=1}^s a_{ij} = \frac{(c_i^2 + c_i)}{2}, j = 1, \dots, i-1, \text{ which is called the simplifying}$$

condition.

We use the notations SIHM $p(q, r)$ which indicate:

SIHM - Semi-implicit hybrid method; p - the algebraic order of the method;

q - the dispersion order of the method; and r - the dissipation order of the method.

Derivation of Three - Stage Fourth - Order SIHM

To derive the fourth order SIHM method, we use the algebraic order conditions up to order four, simplifying conditions, zero dissipation conditions ($\beta_1 = \gamma, \beta_2 = 0$) and dispersion relations of order six ($q = 6$). The resulting system of equations consists of five nonlinear equations and seven unknowns, thus we have two degrees of freedom. The coefficients of the methods are determined in terms of the arbitrary parameters, c_3 and a_{33} . By minimizing the error norm we have $c_3 = \frac{9}{10}$ and $a_{33} = \frac{1}{30}$. This method is denoted as SIHM4(6, ∞), which is given in the table of coefficients (Table 14):

Table 14 The SIHM4(6, ∞) method

-1	0		
0	0	0	
9	3	19	1
$\frac{9}{10}$	$\frac{3}{100}$	$\frac{19}{24}$	$\frac{1}{30}$
	$\frac{5}{57}$	$\frac{22}{27}$	$\frac{50}{513}$

This formula has dispersive order six and is zero-dissipative with a dispersion constant $\frac{13}{302400}z^7 + O(z^9)$. The stability polynomial for SIHM4(6, ∞) is $\pi(\xi, z) = \xi^2 - \frac{120 - 56z^2 + 3z^4}{2(30 + z^2)}\xi + 1$ and the interval of stability of the method is $(0, 2.96)$.

Derivation of Three - Stage Fifth Order SIHM

To develop a three-stage fifth order SIHM, the algebraic conditions up to order five with dispersive of order six ($q = 6$) are first solved. This involved seven equations and seven unknowns, hence it has a unique solution.

Table 15 The SIHM5(6, ∞) method

	-1	0		
	0	0	0	
	1	$\frac{1}{30}$	$\frac{14}{15}$	$\frac{1}{30}$
		$\frac{1}{12}$	$\frac{5}{6}$	$\frac{1}{12}$

Stability polynomial for the method is $\pi(\xi, z) = \xi^2 - \frac{120 - 56z^2 + 3z^4}{2(30 + z^2)}\xi + 1 + 1$ and the stability interval is (0, 2.96).

For the fifth-order SIHM method, eight nonlinear equations from the algebraic conditions, up to order five, with one equation from order condition of dispersive order eight ($q = 8$) are solved using the Maple package, resulting in nine nonlinear equations with eleven free parameters to be solved simultaneously. The coefficients are obtained in terms of two free parameters, b_3 and a_{41} .

Minimizing the error norm we derive $a_{41} = \frac{150617}{771120}$ and $b_3 = \frac{23}{324}$. This method is denoted as SIHM5(8, 5) and is given in Table 16.

Table 16 The SIHM5(8, 5) method

	-1	0			
	0	0	0		
	1	$\frac{199}{38556}$	$\frac{1403}{1428}$	$\frac{1}{81}$	
	1	$\frac{150617}{771120}$	$\frac{18583}{28560}$	$\frac{17}{120}$	$\frac{1}{81}$
		$\frac{1}{12}$	$\frac{5}{6}$	$\frac{23}{324}$	$\frac{1}{81}$

The dispersive order is eight and dissipative order is five with a dispersion and dispersion constant $\frac{241}{881798400}z^9 + o(z^{11})$ and $\frac{277}{44089920}z^6 + o(z^8)$, respectively. The interval of stability of the method is $(0, 5.75)$.

Table 17 Summary of properties of the methods

Methods	Stage	q	r	Err norms	S. I
SIHM4 (6, ∞)	3	6	∞	1.863×10^{-2}	(0, 2.96)
SIHM5 (6, ∞)	3	6	∞	1.147×10^{-1}	(0, 2.96)
SIHM5 (8, 5)	4	8	5	9.772×10^{-2}	(0, 5.75)

Notation: q is dispersive order, r is dissipative order and S.I is the stability interval.

Problems Tested

In order to evaluate the effectiveness of the SIHMs, we solved several problems from scientific literature, which have oscillatory solutions. The test problems are listed below:

Problem 1 (*Homogenous*)

$$y''(x) = -100y(x), \quad y(0) = 1, \quad y'(0) = -2,$$

Exact solution is $y = -\frac{1}{5} \sin(10x) + \cos(10x)$.

Problem 2 (*Inhomogeneous system*)

$$\frac{d^2 y_1(x)}{dt^2} = -v^2 y_1(x) + v^2 f(x) + f''(x), \quad y_1(0) = a + f(0), \quad y_1'(0) = f'(0),$$

$$\frac{d^2 y_2(x)}{dt^2} = -v^2 y_2(x) + v^2 f(x) + f''(x) y_2(0) = f(0), \quad y_2'(0) = va + f'(0)$$

The exact solution is $y_1(x) = a\cos(vx) + f(x) = y_2(x) = a\sin(vx) + f(x)$, $f(x)$ is chosen to be $e^{-0.05x}$ and parameters v and a are 20 and 0.1 respectively.

Problem 3 (*An almost Periodic Orbit problem*)

$$y_1''(x) + y_1(x) = 0.001\cos(x), \quad y_1(0) = 1, \quad y_1'(0) = 0,$$

$$y_2''(x) + y_2(x) = 0.001\sin(x), \quad y_2(0) = 0, \quad y_2'(0) = 0.9995,$$

The exact solution is $y_1 = \cos(x) + 0.0005x\sin(x)$, $y_2 = \sin(x) - 0.0005x\cos(x)$.

Problem 4 (*Oscillatory linear system*)

$$y''(x) + \begin{pmatrix} 13 & -12 \\ -12 & 13 \end{pmatrix} y(x) = \begin{pmatrix} g_1(x) \\ g_2(x) \end{pmatrix}, \quad y(0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad y'(0) = \begin{pmatrix} -4 \\ 8 \end{pmatrix}$$

$g_1(x) = 9\cos(2x) - 12\sin(2x)$, $g_2(x) = -12\cos(2x) + 9\sin(2x)$ and whose analytic

solution is given by $y = \begin{pmatrix} \sin(x) - \sin(5x) + \cos(2x) \\ \sin(x) + \sin(5x) + \sin(2x) \end{pmatrix}$.

Numerical Results and Discussions for the Fourth Order Method

In this section, we test and compare our methods with five other methods in the literature. Following are the notations used:

- **SIHM4(6, ∞)**: A semi - implicit hybrid method of order four with dispersive order six and zero dissipation, developed in the previous section.
- **DIRKN3(4)** --DIRKN method in Senu *et al.* (2010).
- **DIRKN(HS)**: DIRKN method by Sommeijer (1987).

- **RKN3(4)**: RKN method in Hairer *et al.* (2010).
- **RK4**: A classical RK method of order four in Butcher (2008).
- **E-HYBRID3(4)**: hybrid method by Franco (2006).

The methods are compared in terms of absolute error for interval of $T_{end} = 100, 1000, \text{ and } 10000$. The results are given in the form of efficiency curves for $T_{end} = 10,000$. The efficiency curves of the methods are plotted for the largest interval, $T_{end} = 10^4$.

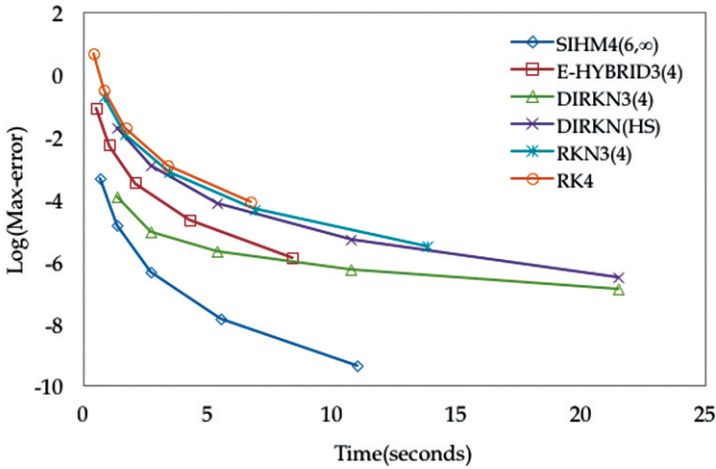


Figure 18 The efficiency curve for SIHM4(6, ∞) for Problem 1 with $T_{end} = 10^4$ and $h = \frac{0.125}{2^i}$ for $i = 3, 4, 5, 6, 7$

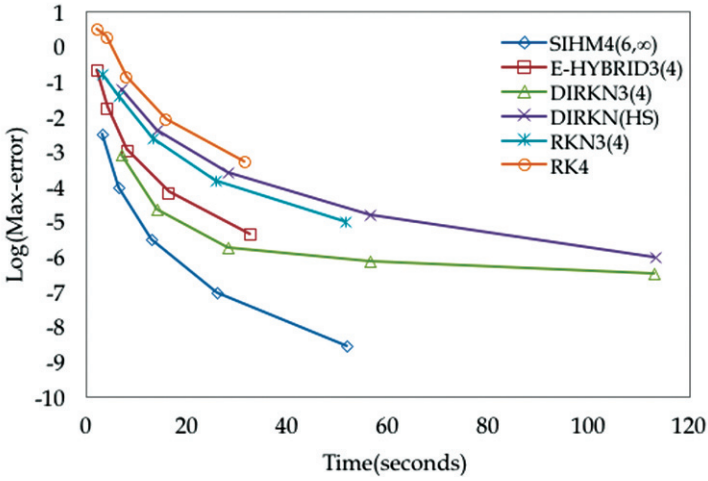


Figure 19 The efficiency curve for SIHM4(6, ∞) for Problem 2 with $T_{end} = 10^4$ and $h = \frac{0.125}{2^i}$ for $i = 3, 4, 5, 6, 7$

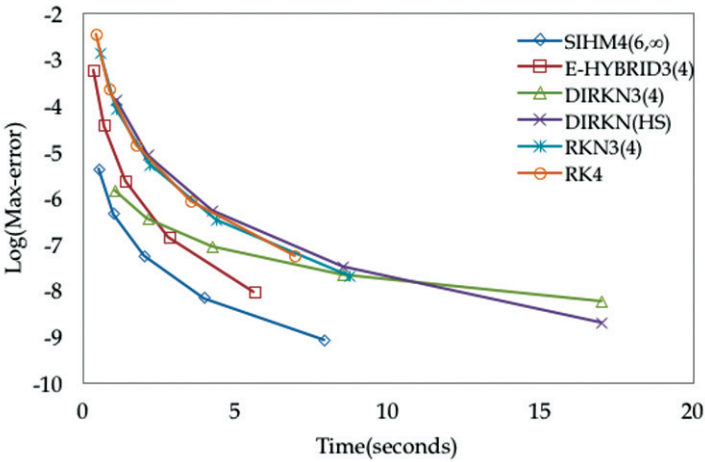


Figure 20 The efficiency curve for SIHM4(6, ∞) for Problem 3 with $T_{end} = 10^4$ and $h = \frac{0.125}{2^i}$ for $i = 1, 2, 3, 4, 5$

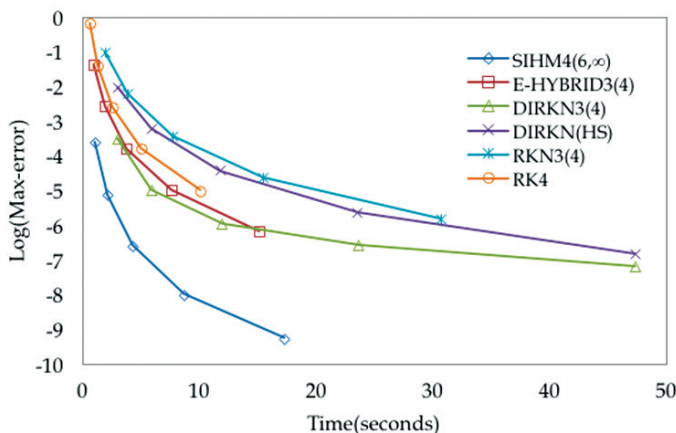


Figure 21 The efficiency curve for SIHM4(6, ∞) for Problem 4 with $T_{end} = 10^4$ and $h = \frac{0.125}{2^i}$ for $i = 2, 3, 4, 5, 6$

Here we present efficiency curves where the common logarithm of the maximum global error along the integration versus the CPU time taken. From the results, we observed that the SIHM4(6, ∞) performs better when integrating second ODEs possessing the oscillatory solution compared to the other implicit and explicit methods.

Numerical Results and Discussions for the Fifth Order Methods

The fifth order methods, SIHM5(6, ∞) and SIHM5(8, 5), are compared with four existing methods that consist of explicit and implicit methods in the literature. We compare the methods using the same problems. The following are the notations used for Figures 22 – 25:

- **SIHM5(6, ∞):** A semi-implicit hybrid method of order five with dispersive order six and zero-dissipation developed in the previous section.

- **SIHM5(8,5)**: A semi-implicit hybrid method of order five with dispersive order eight and dissipation order five developed in the previous section.
- **DIRKN4(4)**: DIRKN method derived by Senu *et al.* (2011)
- **RKN4(5)**: A four-stage fifth-order classical RKN method in Hairer *et al.* (2010).
- **RK7(6)**: A seven-stage sixth-order RK method in Butcher (2008).
- **E-HYBRID4(5)**: A four-stage fifth order hybrid method by Franco (2006).

The efficiency is measured using the absolute error and time taken for solving the problems over a large interval. The graphs of Log (Max-error) versus Time (second) for the largest interval $T_{end}=10000$ are given below.

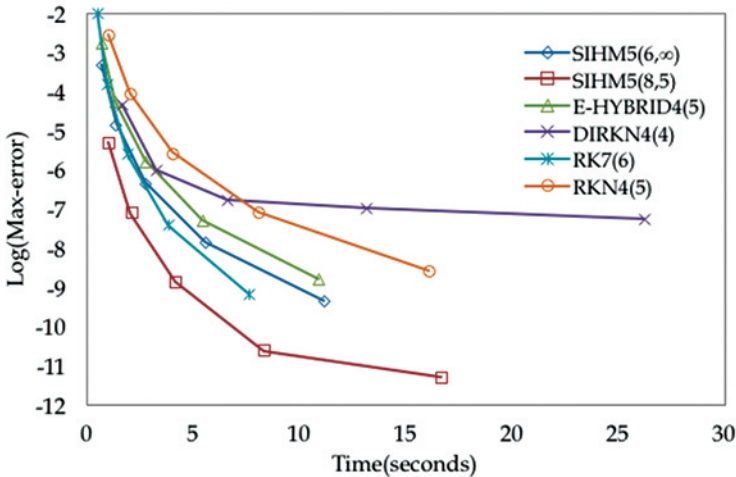


Figure 22 The efficiency curve for SIHM5(6, ∞) and SIHM5(8,5) for Problem 1 with $T_{end} = 10^4$ and $h = \frac{0.125}{2^i}$ for $i = 3, 4, 5, 6, 7$

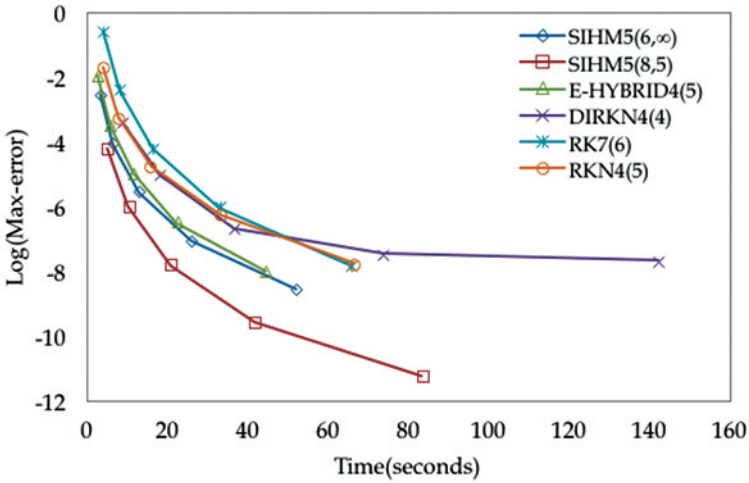


Figure 23 The efficiency curve for SIHM5(6, ∞) and SIHM5(8,5) for Problem 2 with $T_{end} = 10^4$ and $h = \frac{0.125}{2^i}$ for $i = 3, 4, 5, 6, 7$

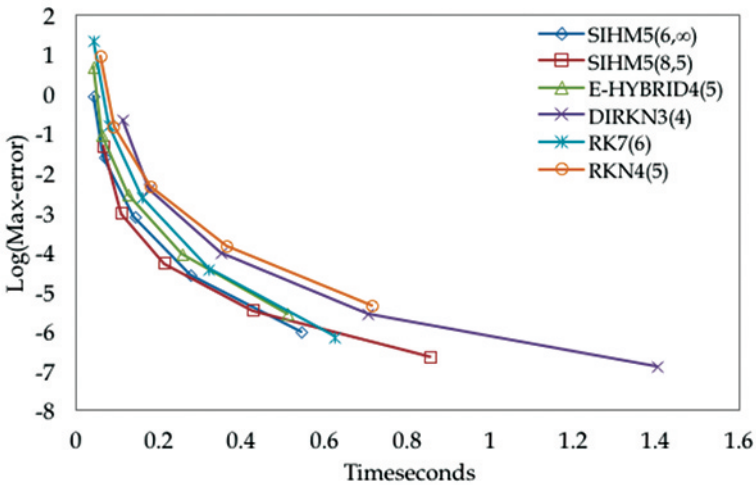


Figure 24 The efficiency curve for SIHM5(6, ∞) and SIHM5(8,5) for Problem 3 with $T_{end} = 10^4$ and $h = \frac{0.9}{2^i}$ for $i = 0, 1, 2, 3, 4$

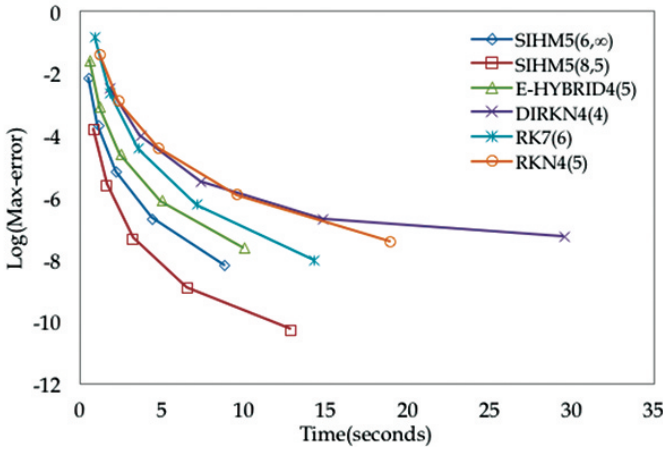


Figure 25 The efficiency curve for SIHM5(6, ∞) and SIHM5(8,5) for Problem 4 with $T_{end} = 10^4$ and $h = \frac{0.125}{2^i}$ for $i = 0, 1, 2, 3, 4, 5$

From the numerical results shown, we observed that SIHM5(8,5) is more efficient than the other existing methods, followed by SIHM5(6, ∞). This is expected because SIHM5(8,5) has dispersion of order eight, hence it is more efficient in integrating oscillatory problems in comparison to methods without the dispersion properties.

PHASE-FITTED HYBRID METHODS FOR SOLVING OSCILLATORY PROBLEMS

Introduction

Ahmad *et al.* (2013a) derived phase-fitted hybrid methods with higher order of dispersion for solving oscillatory problems. As an extension of their work, phase-fitted hybrid methods (PFHMs) based on hybrid methods derived in Franco (2006) will be developed for solving problems which are oscillatory in nature. The purpose of

phase-fitting is to develop a method which has a variable coefficient which depends on the product of the frequency ν of the problems and the step-length of the method. This method will nullify the phase-lag error for a specific product of $z = \nu h$.

Derivation of Phase-fitted Hybrid Methods

In this section three new phase-fitted hybrid methods are developed. The notations used for the phase-fitted hybrid methods PFHM $m(p)$ are as follows:

PFHM-phase-fitted hybrid method; m -the number of stages of the method; and p -the algebraic order of the method.

Given

$$S(z^2) = 2 - \alpha_1 z^2 + \alpha_2 z^4 - \alpha_3 z^6 + \dots + \alpha_i z^{2i} \quad (7.1)$$

$$P(z^2) = 1 - \beta_1 z^2 + \beta_2 z^4 - \beta_3 z^6 + \dots + \beta_i z^{2i} \quad (7.2)$$

and rewriting (7.1) and (7.2) in terms of the coefficients of the hybrid method, we obtained the expressions $S(z^2)$ and $P(z^2)$.

i. **for $m = 3$**

$$S(z^2) = 2 - (1 + c_1)(z^2 b_1 - z^4 b_3 a_{31}) - (1 + c_2)(z^2 b_2 - z^4 b_3 a_{32}) - (1 + c_3)z^2 b_3 \quad (7.3)$$

$$P(z^2) = 1 - c_1(z^2 b_1 - z^4 b_3 a_{31}) - c_2(z^2 b_2 - z^4 b_3 a_{32}) - c_3 z^2 b_3 \quad (7.4)$$

where $z = \nu h$. Recall from the previous section that, in order to have phase-lag of order infinity and zero dissipation the following equations must hold:

$$\phi(z) = z - \cos^{-1} \left(\frac{S(z^2)}{2\sqrt{P(z^2)}} \right) = 0 \quad (7.5)$$

$$d(z) = 1 - \sqrt{P(z^2)} = 0 \quad (7.6)$$

Substituting (7.3) and (7.4) into (7.5), we get

$$\begin{aligned} S(z^2) - 2\sqrt{P(z^2)}\cos(z) \\ &= 2 - (1 + c_1)(b_1z^2 - b_3a_{31}z^4) \\ &\quad - (1 + c_2)(b_2z^2 - b_3a_{32}z^4) - (1 + c_3)b_3z^2 \\ &\quad - 2(1 - c_1(b_1z^2 - b_3a_{31}z^4) - c_2(b_2z^2 - b_3a_{32}z^4) \\ &\quad - c_3b_3z^2)^{1/2}\cos(z) \\ &= 0. \end{aligned} \quad (7.7)$$

Choosing a_{32} as the free parameter and substituting the coefficients of the explicit fourth order hybrid method in Franco (2006) into equation (7.7), we obtained a_{32} where $a_{32} = \frac{12(-2 + z^2 + 2\cos(z))}{z^4}$.

This method is denoted as PFHM3(4) and can be written in Butcher tableau as follows:

Table 18 Table of coefficients for PFHM3(4)

	-1	0		
	0	0	0	
	1	0	a_{32}	0
		$\frac{1}{12}$	$\frac{5}{6}$	$\frac{1}{12}$

and the Taylor expansion of a_{32} is

$$a_{32} = 1 - \frac{1}{30}z^2 + \frac{1}{1680}z^4 - \frac{1}{151200}z^6 + \frac{1}{19958400}z^8 + O(z^{10}).$$

Thus the coefficient a_{32} depends on $z = \nu h$, where ν is the eigenvalue of the problem and h is the stepsize used.

ii. for $m = 4$

$$\begin{aligned} S(z^2) = & 2 - (1 + c_1)(z^2 b_1 - z^4 b_3 a_{31} + h^2 b_4 (h^4 a_{31} a_{43} - h^2 a_{41})) \\ & - (1 + c_2)(z^2 b_2 - z^4 b_3 a_{32} + h^2 b_4 (h^4 a_{32} a_{43} - h^2 a_{42})) \\ & - (1 + c_3)(z^2 b_3 - z^4 b_4 a_{43}) - (1 + c_4)z^2 b_4 \end{aligned} \quad (7.8)$$

$$\begin{aligned} P(z^2) = & 1 - c_1(z^2 b_1 - z^4 b_3 a_{31} + z^2 b_4 (z^4 a_{31} a_{43} - z^2 a_{41})) \\ & - c_2(z^2 b_2 - z^4 b_3 a_{32} + z^2 b_4 (z^4 a_{32} a_{43} - z^2 a_{42})) \\ & - c_3(z^2 b_3 - z^4 b_4 a_{43}) \\ & - c_4 z^2 b_4. \end{aligned} \quad (7.9)$$

Substituting equation (7.8) and (7.9) into (7.5), we obtained the dispersion error as

$$\begin{aligned} S(z^2) - 2\sqrt{P(z^2)}\cos(z) = & 2 - (1 + c_1)(b_1 z^2 - b_3 a_{31} z^4 + z^2 b_4 (z^4 a_{31} a_{43} - z^2 a_{41})) \\ & - (1 + c_2)(b_2 z^2 - b_3 a_{32} z^4 + z^2 b_4 (z^4 a_{32} a_{43} - z^2 a_{42})) - (1 + c_3)(b_3 z^2 \\ & - z^4 b_4 a_{43}) - (1 + c_4)b_4 z^2 \\ & - 2(1 - c_1)(b_1 z^2 - b_3 a_{31} z^4 + z^2 b_4 (z^4 a_{31} a_{43} - z^2 a_{41})) \\ & - c_2(b_2 z^2 - b_3 a_{32} z^4 + z^2 b_4 (z^4 a_{32} a_{43} - z^2 a_{42})) - c_3(b_3 z^2 - z^4 b_4 a_{43}) \\ & - c_4 b_4 z^2)^{\frac{1}{2}}\cos(z) = 0. \end{aligned} \quad (7.10)$$

We substitute all the coefficients of the four-stage fourth-order hybrid method from Franco (2006) and leave a_{32} as the free parameter because we found that by choosing a_{32} as the free parameter the zero-dissipation condition ($d(z) = 0$) is satisfied.

The coefficients of the new method, PFHM4(4) can be written in Butcher tableau as below:

Table 19 Table of coefficients for PFHM4(4)

-1	0			
0	0	0		
33				
50	0	a_{32}	0	
13	314860	1058746	15743000	
-17	20796729	-8268579	686292057	0
	-89	545	625000	83521
	1992	858	3316929	377832

The Taylor expansion of a_{32} is given as

$$a_{32} = \frac{2739}{5000} + \frac{157949}{600000000}z^4 + \frac{12477971}{3000000000000}z^6 + \frac{54306843643}{40500000000000000}z^8 + \frac{5782745038802243}{16584750000000000000000}z^{10} + O(z^{12}).$$

Problems Tested

In order to evaluate the accuracy of the new methods, several problems which have oscillatory solutions are solved using these methods. The test problems used are:

Problem 1 (*Homogenous*)

$y''(x) = -64y(x)$, $y(0) = 1/4$, $y'(0) = -1/2$ The fitted frequency, $\nu = 8$.

The exact solution is $y = \sqrt{17}/16 \sin(8x + \theta)$, $\theta = \pi - \tan^{-1}(4)$.

Problems 2 to 4 are the same as that in the Chapter 6.

Numerical Results and Discussions

In this section, we will test and compare PFHM3(4) and PFHM4(4) with other methods of order four in the literature, using the measure of accuracy, that is absolute error and time taken in seconds. The following are the notations used in Figures 24 – 29:

- **PFHM3(4)**: A phase-fitted hybrid method of three-stage fourth-order and zero dissipation developed in the previous section..
- **E-HYBRID3(4)**: An explicit three-stage fourth-order hybrid method derived by Franco (2006).
- **PFHM4(4)**: A phase-fitted hybrid method of four-stage fourth-order and zero dissipation developed in the previous section.
- **E-HYBRID4(4)**: An explicit four-stage fourth order hybrid method derived by Franco (2006).
- **PFRKN4(4)**: A phase-fitted hybrid method of four-stage fourth-order Runge-Kutta Nyström (RKN) method by Papadopoulos *et al.* (2009).
- **RKN3(4)**: A three-stage fourth-order classical RKN method in Hairer *et al.* (2010).

We compared the methods in terms of accuracy and time taken in seconds for the interval $T_{end}=10000$.

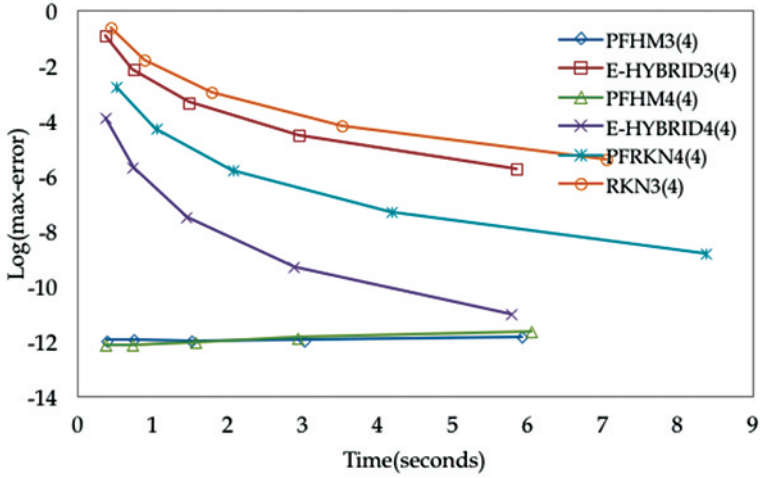


Figure 26 The efficiency curve for PFHM3(4) and PFHM4(4) for Problem 1 with $T_{end} = 10^4$ and $h = \frac{0.125}{2^i}$ for $i = 1, 2, 3, 4, 5$

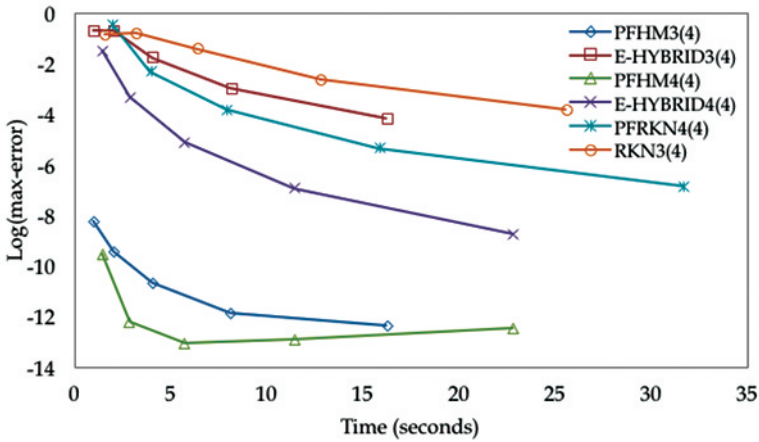


Figure 27 The efficiency curve for PFHM3(4) and PFHM4(4) for Problem 2 with $T_{end} = 10^4$ and $h = \frac{0.125}{2^i}$ for $i = 2, 3, 4, 5, 6$

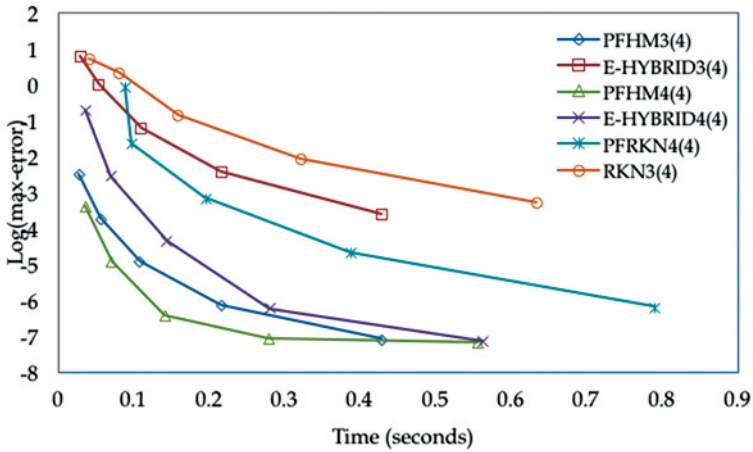


Figure 28 The efficiency curve for PFHM3(4) and PFHM4(4) for Problem 3 with $T_{end} = 10^4$ and $h = \frac{0.8}{2^i}$ for $i = 0, 1, 2, 3, 4$

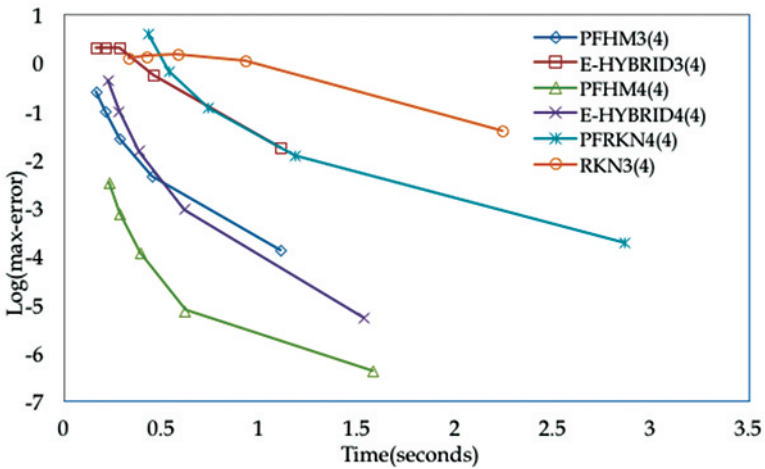


Figure 29 The efficiency curve for PFHM3(4) and PFHM4(4) for Problem 4 with $T_{end} = 10^4$ and $h = 0.2 - i \cdot 0.035$ for $i = 1, 2, 3, 4, 5$

From Figures 26 to 29, we observed that the new fourth order methods, PFHM3(4) and PFHM4(4), are more efficient for integrating second ODEs possessing oscillatory solutions compared to the original hybrid methods E-HYBRID3(4), E-HYBRID4(4), PFRKN4(4) and RKN3(4). Therefore, it is thus shown that phase – fitting the method improved the efficiency of the existing zero - dissipative hybrid methods.

OPTIMIZED HYBRID METHODS FOR SOLVING OSCILLATORY PROBLEMS

In their previous work, Ahmad *et al.* (2013b) have derived zero-dissipative explicit hybrid methods for solving oscillatory problems. Work along the same lines was also done by Jikantoro *et. al.* (2015a, 2015b), who derived zero- dissipative semi-implicit hybrid methods which are also suitable for solving oscillatory problems. To extend the work, we constructed optimized explicit hybrid methods of four-stage fifth-order and five-stage sixth-order. The methods are constructed by nullifying the phase-lag, dissipation and the first derivative of the phase-lag, resulting in methods where the coefficients depend on the problems themselves, provided the frequency values of the problems are known in advance. Work related to this research can also be seen in Ramos and Aguiar (2010) and Papadopoulos and Simos (2011). The new optimized hybrid methods are based on the non-zero-dissipative hybrid method developed by Franco (2006).

Derivation of the New Hybrid Methods

In this section, we construct optimized hybrid methods of four-stage fifth order and five-stage sixth order methods. $S(z^2)$ and $P(z^2)$ for hybrid methods, that satisfied algebraic order conditions up to order six, can be written in these expressions

(i) for $s = 5$:

$$\begin{aligned}
 S(z^2) = & 2 - (1 + c_1)(z^2 b_1 - z^4 b_3 a_{31} + h^2 b_4 (h^4 a_{31} a_{43} - h^2 a_{41})) \\
 & - (1 + c_2)(z^2 b_2 - z^4 b_3 a_{32} + h^2 b_4 (h^4 a_{32} a_{43} - h^2 a_{42})) \\
 & - (1 + c_3)(z^2 b_3 - z^4 b_4 a_{43}) - (1 + c_4)z^2 b_4
 \end{aligned} \tag{8.1}$$

$$\begin{aligned}
 P(z^2) = & 1 - c_1(z^2 b_1 - z^4 b_3 a_{31} + z^2 b_4 (z^4 a_{31} a_{43} - z^2 a_{41})) \\
 & - c_2(z^2 b_2 - z^4 b_3 a_{32} + z^2 b_4 (z^4 a_{32} a_{43} - z^2 a_{42})) \\
 & - c_3(z^2 b_3 - z^4 b_4 a_{43}) - c_4 z^2 b_4
 \end{aligned} \tag{8.2}$$

(ii) for $s = 6$:

$$\begin{aligned}
 S(z^2) = & 2 - z^2 b_2 + z^4 b_3 a_{32} - z^4 b_4 (z^2 a_{43} a_{32} - a_{42}) \\
 & + z^4 b_5 (a_{54} a_{32} z^4 a_{43} - z^2 a_{53} a_{32} - z^2 a_{54} a_{42} + a_{52}) \\
 & - (1 + c_3)(z^2 b_3 - z^4 b_4 a_{43} + z^4 b_5 (z^2 a_{54} a_{43} - a_{53})) \\
 & - (1 + c_4)(z^2 b_4 - z^4 b_5 a_{54}) - (1 + c_5)z^2 b_5
 \end{aligned} \tag{8.3}$$

$$\begin{aligned}
 P(z^2) = & 1 + z^2 b_1 - z^4 b_3 a_{31} + z^4 b_4 (z^2 a_{43} a_{31} - a_{41}) \\
 & - z^4 b_5 (a_{54} a_{31} z^4 a_{43} - z^2 a_{53} a_{31} - z^2 a_{54} a_{41} + a_{51}) \\
 & - c_3(z^2 b_3 - z^4 b_4 a_{43} + z^4 b_5 (z^2 a_{54} a_{43} - a_{53})) \\
 & - c_4(z^2 b_4 - z^4 b_5 a_{54}) - c_5 z^2 b_5
 \end{aligned} \tag{8.4}$$

In order to develop an optimized hybrid method the following relations must hold:

$$\text{The phase-lag condition: } \varphi(z) = z - \cos^{-1}\left(\frac{S(z^2)}{2\sqrt{P(z^2)}}\right) = 0 \quad (8.5)$$

$$\text{Dissipation conditions: } d(z) = 1 - \sqrt{P(z^2)} = 0, \quad (8.6)$$

$$\text{and the first derivative of (8.5), } \varphi'(z) = 0 \quad (8.7)$$

The method developed is based on the non-zero-dissipative hybrid methods developed by Franco (2006). The process involved substituting the coefficients of the hybrid methods in Franco (2006) into equations (8.1) and (8.2), then substituting into equations (8.5) – (8.7) and solving the equations numerically. The coefficients of the fifth order method with a_{41} , a_{42} and a_{43} are taken as free parameters that can be written in Butcher tableau as follows:

Table 20 An Optimized four-stage fifth-order hybrid method

-1	0	0	0	
0	0	0	0	
$25/28$	$1325/43904$	$35775/43904$	0	
$-23/5$	a_{41}	a_{41}	a_{43}	0
<hr/>				
	$173/1908$	$2791/3450$	$307328/3056775$	$-125/636732$

The optimized hybrid method with dissipation order 9 ($r = 9$) is thus obtained and the free parameters in Taylor expansion are given by:

$$a_{41} = 16744/33125 - 17687/74200 z^2 + 14096539/519400000 z^4 + O(z^6)$$

$$a_{42} = 383111/15625 - 53061/875000 z^2 - 11620359/245000000 z^4 + O(z^6)$$

$$\text{and } a_{43} = 13866608/828125 + 247618/828125 z^2 + 336053/16562500 z^4 + O(z^6)$$

For the construction of five-stage sixth-order optimized hybrid methods, we substitute equations (8.3) and (8.4) into (8.5) to (8.7), and using the coefficients of the five-stage sixth order method given in Franco (2006) and choosing a_{52} , a_{53} , and a_{54} as the free parameters, the optimized sixth order hybrid method with $r = 9$ is obtained and given as follows:

Table 21 An Optimized five-stage sixth-order hybrid method

-1	0				
0	0	0			
-1/5	-4/125	-6/125	0		
-2/5	-133/3000	-13/750	-7/120	0	
2/3	-1115/52488	a_{52}	a_{53}	a_{54}	0
	1/60	23/24	-125/156	125/192	729/4160

The Taylor expansion of the parameters are given as

$$a_{52} = 4175/4374 + 23530/137781 z^2 + 95173/4133430 z^4 + O(z^6)$$

$$a_{53} = -2275/1944 - 47060/137781 z^2 - 15977/413343 z^4 + O(z^6)$$

$$a_{54} = 5200/6561 + 23530/137781 z^2 + 2249/118098 z^4 + O(z^6)$$

Phase-fitted Hybrid Methods

To develop phase-fitted of a method, only equation (8.5) must hold. We first substitute equations (8.1) and (8.2) into (8.5). Then, choosing a_{31} as the free parameter and using the same coefficients as in Table 20, together with

$$a_{41} = 16744/33125, a_{42} = 383111/15625, a_{43} = -13866608/828125,$$

we obtained a phase-fitted hybrid method of four-stage fifth-order with $q = 12$ and $r = 5$ and the Taylor expansion of the free parameter is

$$a_{31} = 1325/43904 + 529841/14869757952 z^6 + O(z^8).$$

For the construction of five-stage sixth-order phase-fitted hybrid methods, we substitute equations (8.3) and (8.4) into (8.5) and set a_{52} as the free parameter. We then use the coefficients given in Table 21 together with

$$a_{53} = -2275/1944 \text{ and } a_{54} = 5200/6561.$$

Choosing a_{52} as the free parameter, we thus get a phase-fitted hybrid method of five-stage sixth-order with $q = 12$ and $r = 7$ and the Taylor expansion of a_{52} is

$$a_{52} = 4175/4374 - 2353/688905 z^4 + 15223/20667150 z^6 + O(z^8).$$

Problems Tested and Numerical Results

The methods were used to solve test problems and the results are tabulated and compared and the efficiency curves plotted. The test problems are listed below and most of them are the same problems used in previous chapters. The problems are:

Problem 1

$$\frac{d^2 y_1(t)}{dt^2} = -z^2 y_1(t) + z^2 f(t) + f''(t)$$

$$\frac{d^2 y_2(t)}{dt^2} = -z^2 y_2(t) + z^2 f(t) + f''(t)$$

$$y_1(0) = a + f(0), \quad y_1'(0) = f'(0), \quad y_2(0) = f(0), \quad y_2'(0) = za + f'(0)$$

The exact solution is $y_1(t) = a \cos(zt) + f(t)$, $y_2(t) = a \sin(zt) + f(t)$, $f(t)$ is chosen to be $e^{-0.05t}$ and parameters z and a are 20 and 0.1, respectively.

Problems 2 to 4 are the same as in the previous sections. The following are notations used in the Figures.

- **OPHM(ETSHM5(8,5))**: new optimized hybrid method four-stage fifth order with dissipation of order 9 derived in this section.
- **OPHM(ETSHM6)**: new optimized hybrid method five-stage sixth order with dissipation of order 9 derived in this section.
- **PFHM(ETSHM5(8,5))**: new phase-fitted hybrid method four-stage fifth order with dispersion of order 12 and dissipation of order 5 derived in this section.
- **PFHM(ETSHM6)**: new phase-fitted hybrid method five-stage sixth order with dispersion of order 12 and dissipation of order 7 derived in this section.
- **ETSHM5(8,5)**: explicit hybrid method of four-stage fifth-order with dispersion of order eight and dissipation of order five developed by Franco (2006).
- **ETSHM6**: explicit hybrid method of five-stage sixth-order developed by Franco (2006).
- **OPRKN4(5)**: Optimized Runge-Kutta Nyström method of four-stage fifth-order developed by Kosti *et al.* (2012).

- **PFRKN4(4)**: Phase-fitted Runge-Kutta Nyström method of four-stage fourth-order method by Papadopoulos *et al.* (2009).
- **RKN4(5)**: A classical Runge-Kutta Nyström method of order five in Hairer *et al.* (1987).
- **RK7(6)**: A Runge-Kutta method of order six with seven stages derived by Butcher (2008).
- **PAFRKN4(4)**: A four-stage fourth-order phase-fitted and amplification-fitted Runge-Kutta Nyström method developed by Papadopoulos *et al.* (2010).

A measure of the accuracy is examined using absolute errors which is defined by

$$\text{Absolute error} = \max \{|y(x_n) - y_n|\},$$

where $y(x_n)$ is the exact solution and y_n is the computed solution.

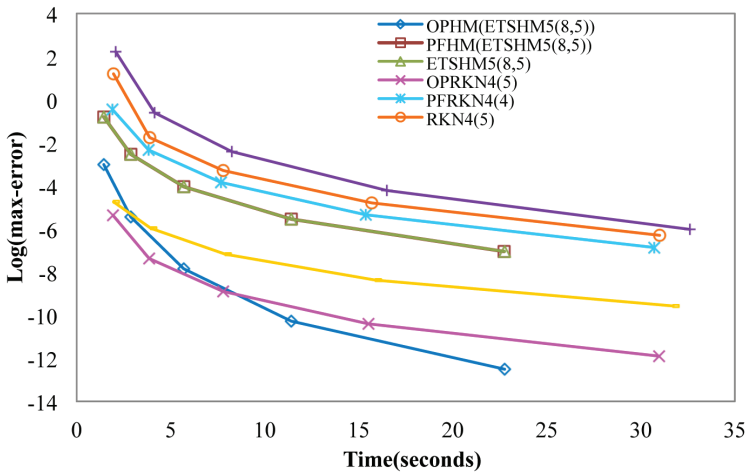


Figure 30 The efficiency curve for OPHMs and PFHMs of order five

for Problem 1 with $t_{end} = 10^4$ and $h = \frac{0.125}{2^i}$ for $i = 1, \dots, 5$

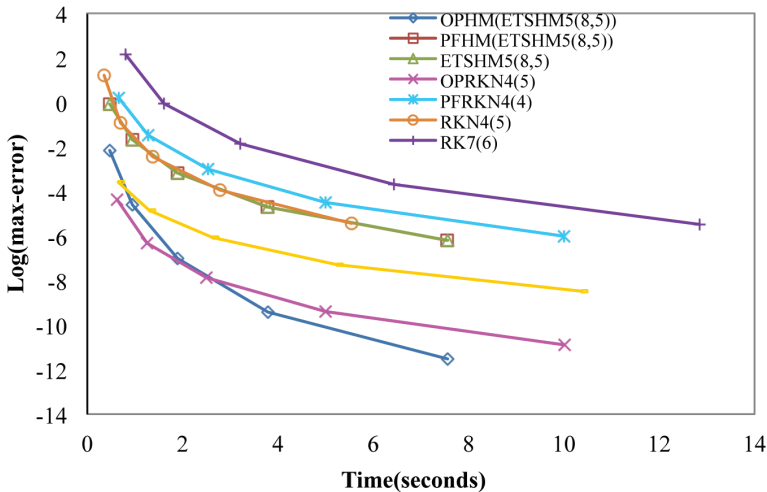


Figure 31 The efficiency curve for OPHMs and PFHMs of order five for Problem 2 with $t_{end} = 10^4$ and $h = \frac{0.125}{2^i}$ for $i = 2, \dots, 6$

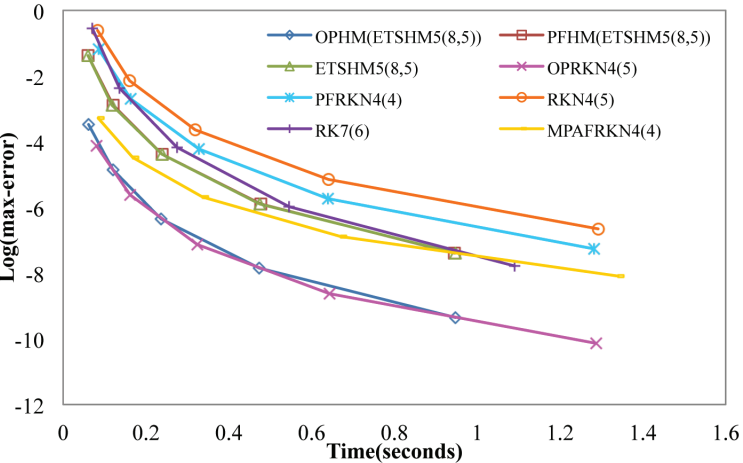


Figure 32 The efficiency curve for OPHMs and PFHMs of order five for Problem 3 with $t_{end} = 10^4$ and $h = \frac{0.5}{2^i}$ for $i = 0, \dots, 4$

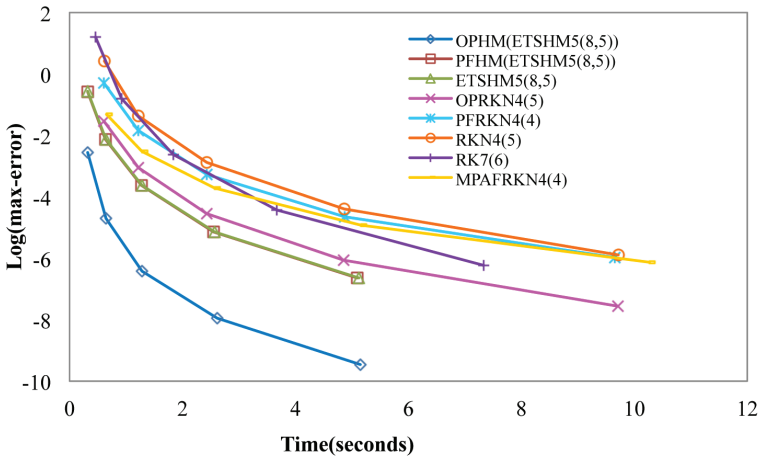


Figure 33 The efficiency curve for OPHMs and PFHMs of order five
for Problem 4 with $t_{end} = 10^4$ and $h = \frac{0.125}{2^i}$ for $i = 0, \dots, 4$

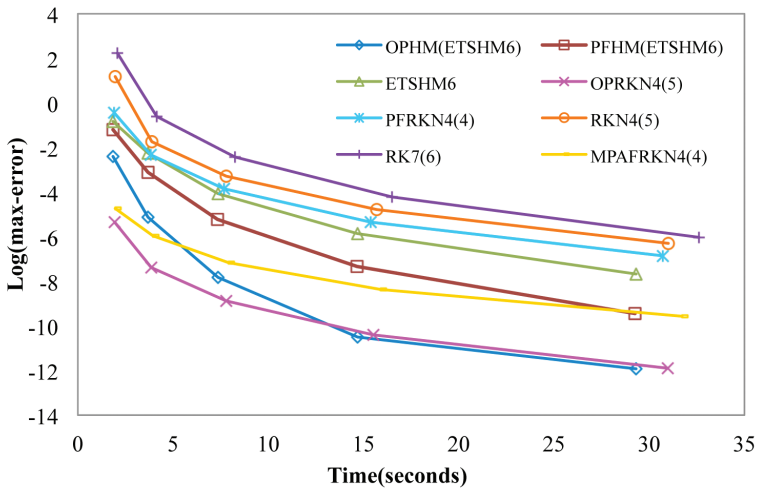


Figure 34 The efficiency curve for OPHMs and PFHMs of order six
for Problem 1 with $t_{end} = 10^4$ and $h = \frac{0.125}{2^i}$ for $i = 2, \dots, 6$

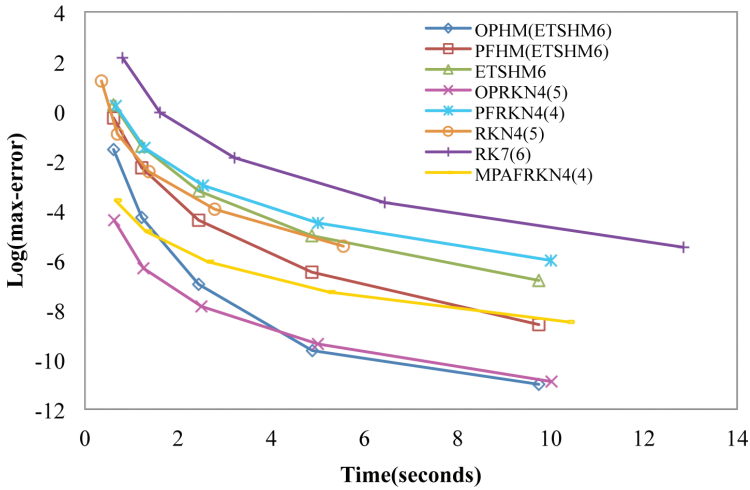


Figure 35 The efficiency curve for OPHMs and PFHMs of order six for Problem 2 with $t_{end} = 10^4$ and $h = \frac{0.125}{2^i}$ for $i = 1, \dots, 5$

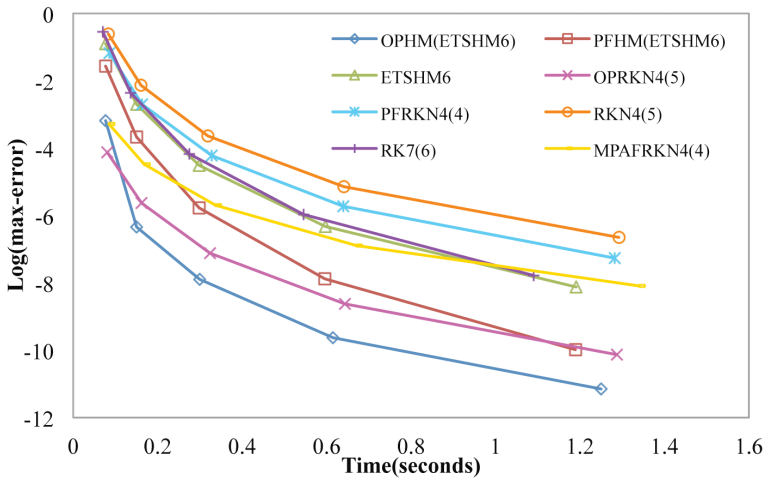


Figure 36 The efficiency curve for OPHMs and PFHMs of order six for Problem 3 with $t_{end} = 10^4$ and $h = \frac{0.5}{2^i}$ for $i = 0, \dots, 4$

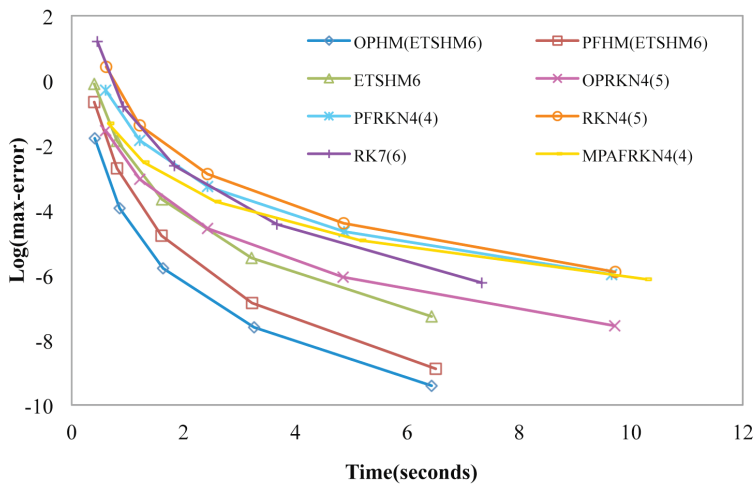


Figure 37 The efficiency curve for OPHMs and PFHMs of order six for Problem 4 with $t_{end} = 10^4$ and $h = \frac{0.125}{2^i}$ for $i = 0, \dots, 4$

Table 22 Summary of the properties of the methods

Methods	Stage	Algebraic order	Phase-lag (dispersive) order	Dissipative efficiency order	
OPHM5	4	5	∞	9	✓
PHFM5	4	5	12	5	
OPHM6	5	6	∞	9	✓
PHFM6	5	6	12	7	
E-HM5	4	5	8	5	

Based on the existing non zero-dissipative hybrid methods of order five and six originally derived by Franco (2006), we constructed the optimized hybrid methods using the phase-lag,

dissipative and derivative of the phase-lag conditions. Then we derived the phase-fitted method using the phase-lag and dissipative conditions only. From the efficiency curves shown, we can conclude that the new optimized methods are more efficient for integrating oscillatory initial value problems of second order ODEs compared to the phase-fitted methods and other well-known existing methods in scientific literature.

TRIGONOMETRICALLY FITTED HYBRID METHOD FOR SOLVING DELAY DIFFERENTIAL EQUATIONS

Research reveals that things do not only depend on the current state of a system but also on past states, resulting in differential equations with a time delay. This kind of equations is called delay differential equations (DDEs) where the derivative at any time depends on the solution from previous times, and is best known as a model that incorporates past history. It is a more realistic model which includes some of the past history of the system to determine future behavior. Here, we are concerned with a numerical method for solving second-order DDEs with constant delay, which can be written in the form of

$$y''(t) = f(t, y(t), y(t - \tau)), a \leq t \leq b, \quad (9.1)$$

$$y(t_0) = y_0, \quad y'(t_0) = y'_0, \quad t \in [-\tau, a]$$

where τ is the delay term and the first derivative does not appear explicitly.

There has been growing interest in the field of DDEs. Kuang (1993) in his book discussed delay differential equations with applications in population dynamics in his book while Ismail and

Suleiman (2000) studied the P-Stability and Q-Stability of Singly diagonally implicit Runge-Kutta Method for delay differential Equations. Ismail and Suleiman (2001) and Suleiman and Ismail (2001) also looked at the intervalwise partitioning and componentwise partitioning, respectively, for stiff DDEs. Ismail *et al.* (2003) have also used the Runge-Kutta method with a few types of interpolations for solving delay differential equations. Work on solving second order DDEs using the Runge-Kutta Nystrom method has also been done by Mechee *et al.* (2012). In their previous work Ahmad *et al.* (2013a) derived the semi implicit hybrid method, where they incorporated the phase-lag and amplification conditions so that a method which has higher order of dissipation and dispersion could be obtained. In this research, we are going to construct a new semi-implicit hybrid method (NSIHM) of four-stage fifth-order using the algebraic order conditions given in Coleman (2003). The derivation will also incorporate the simplifying conditions as well as the technique of minimization of the error constant. The method is then trigonometrically fitted so that it is suitable for solving oscillatory problems. This approach, which is similar to that of Jikantoro *et al.* (2015c), is simpler than incorporating the phase-lag and amplification conditions into the derivation. In all previous work related to phase-fitted methods, the methods have been used to solve oscillatory second order ODEs. Here the method is used for solving retarded second order delay differential equations which are oscillatory in nature.

Derivation of Four-stage Fifth-order Semi-Implicit Hybrid Methods

We derived the four-stage fifth-order NSIHM based on the order conditions and simplifying the conditions given in Coleman (2003).

Minimization of the error constant C_{p+1} of the method is used to find the value of the free parameter. We obtained the coefficients of the four-stage fifth-order semi-implicit hybrid method, denoted as NSIHM4(5), which can be written in Butcher tableau as below and can also be seen in Ahmad *et al.* (2016).

Table 23 The 4-stage fifth order Semi-Implicit Hybrid method

-1	0			
0	0	0		
1	$\frac{1}{81}$	$\frac{79}{81}$	$\frac{1}{81}$	
1	$\frac{150617}{771120}$	$\frac{234943}{385560}$	$\frac{141097}{771120}$	$\frac{1}{81}$
	$\frac{1}{12}$	$\frac{5}{6}$	$\frac{23}{324}$	$\frac{1}{81}$

Trigonometrically Fitting the Semi-Implicit Hybrid Method

To trigonometrically fit the new method, NSIHM4(5), we consider stage three and stage four of the NSIHM4(5) as shown in Table 23. The new method which will be derived is denoted as the four-stage fifth-order trigonometrically-fitted semi-implicit hybrid method or TF-NSIHM4(5), which has fifth algebraic order which is the same as the algebraic order of NSIHM4(5). Note that trigonometrically fitting the method will not change the algebraic order of the method. The method can be written in Butcher tableau as shown below.

Table 24 The 4-stage Fifth Order Trigonometrically Fitted Semi-Implicit Hybrid Method

-1	0			
0	0	0		
1	$\frac{1}{81}$	a_{32}	$\frac{1}{81}$	
1	$\frac{150617}{771120}$	a_{42}	$\frac{141097}{771120}$	$\frac{1}{81}$
	b_1	b_2	b_3	$\frac{1}{81}$

The values of a_{32} , a_{42} , b_1 , b_2 and b_3 are modified using the trigonometrically fitting technique so that it will improve the accuracy of the method and be suitable for solving oscillatory problems.

We require the internal stage (stage- 3 and 4) and the updating stage to integrate exactly the linear combination of the functions $\{\sin(vt), \cos(vt)\}$ for $v \in \mathcal{R}$, subject to the fifth-order formulae. Hence, we obtain the following equations:

$$\cos(c_3 H) = 1 + c_3 - c_3 \cos(H) - H^2 \{a_{31} \cos(H) + a_{32} + a_{33} \cos(c_3 H)\} \quad (9.2)$$

$$\sin(c_3 H) = c_3 \sin(H) + H^2 \{a_{31} \sin(H) - a_{33} \sin(c_3 H)\}, \quad (9.3)$$

$$\cos(c_4 H) = 1 + c_4 - c_4 \cos(H) - H^2 \{a_{41} \cos(H) + a_{42} + a_{43} \cos(c_3 H) + a_{44} \cos(c_4 H)\} \quad (9.4)$$

$$\sin(c_4 H) = c_4 \sin(H) + H^2 \{a_{41} \sin(H) - a_{43} \sin(c_3 H) - a_{44} \sin(c_4 H)\}, \quad (9.5)$$

$$2 \cos(H) = 2 - H^2 \{b_1 \cos(H) + b_2 + b_3 \cos(c_3 H) + b_4 \cos(c_4 H)\} \text{ and} \quad (9.6)$$

$$b_1 \sin(H) = b_3 \sin(c_3 H) + b_4 \sin(c_4 H) \quad (9.7)$$

Solving equations (9.2) to (9.5) with the choice of coefficients

$$c_3 = 1, c_4 = 1, a_{33} = \frac{1}{81},$$

$a_{41} = \frac{150617}{771120}$, $a_{43} = \frac{141097}{771120}$ and, $a_{44} = \frac{1}{81}$ simultaneously, we obtained

$$a_{32} = -\frac{2}{81} \frac{81 \cos(H) - 81 + H^2 \cos(H)}{H^2},$$

and $a_{42} = -\frac{1}{385560} \frac{771120 \cos(H) - 771120 + 150617H^2 \cos(H)}{H^2},$

where $H = vh$; h is step size and v is the fitted frequency. Next, using equations (9.6) and (9.7) and another two additional order conditions for the fifth-order method which are:

$$b_1 + b_2 + b_3 + b_4 = 1 \text{ and } -b_1 + b_3c_3 + b_4c_4 = 0,$$

we solve the equations simultaneously to get b_1 , b_2 , and b_3 , which are given as below:

$$b_1 = -\frac{1}{2} \frac{\cos(H) - 2 + H^2}{Q}, \quad b_2 = \frac{2\cos(H) - 2 + H^2 \cos(H)}{Q}, \text{ and}$$

$$b_3 = -\frac{1}{162} \frac{162 \cos(H) - 162 + 2H^2 \cos(H) + 79H^2}{Q},$$

where $Q = H^2(\cos(H) - 1)$

The parameters can be expressed in Taylor series expansions:

$$a_{32} = \frac{79}{81} - \frac{23}{324}H^2 + \frac{17}{9720}H^4 - \frac{5}{326592}H^6 - \frac{1}{16329600}H^8 + O(H^{10}),$$

$$a_{42} = \frac{234943}{385560} + \frac{86357}{771120}H^2 - \frac{124913}{9253440}H^4 + \frac{136847}{277603200}H^6 - \frac{142049}{15545779200}H^8 + O(H^{10}),$$

$$b_1 = \frac{1}{12} + \frac{1}{240}H^2 + \frac{1}{6048}H^4 + \frac{1}{172800}H^6 + O(H^8),$$

$$b_2 = \frac{5}{6} - \frac{1}{120}H^2 - \frac{1}{3024}H^4 - \frac{1}{86400}H^6 + O(H^{10}), \text{ and}$$

and $b_3 = \frac{23}{324} + \frac{1}{240}H^2 + \frac{1}{6048}H^4 + \frac{1}{172800}H^6 + O(H^8).$

The values of a_{32} , a_{42} , b_1 , b_2 , and b_3 depend on the values of ν and h while the other coefficients remain the same.

Problems Tested and Numerical Results

In this section, the new method NSIHM4(5) and the trigonometrically fitted method, TF-NSIHM4(5) are used to solve a set of oscillatory delay differential equation problems. The delay terms are evaluated using the Newton divided different interpolation. The numerical results are tabulated and compared with the existing explicit and implicit methods in scientific literature. The test problems are as listed below:

Problem 1: $y''(t) = -\frac{1}{2}y(t) + \frac{1}{2}y(t - \pi), 0 \leq t \leq 8\pi, y_0 = 0.$

$\nu = 1$. The exact solution is $y(t) = \sin(t)$.

(Source: Schmidt (1971)).

Problem 2: $y''(t) - y(t) + \eta(t)y\left(\frac{t}{2}\right) = 0, 0 \leq t \leq 2\pi,$

where $\eta(t) = \frac{4\sin(t)}{(2 - 2\cos(t))^{1/2}}, \eta(0) = 4.$

$\nu = 2$. The exact solution is $y(t) = \sin(t)$.

(Source: Schmidt (1971)).

Problem 3: $y''(t) = y(t - \pi), 0 \leq t \leq 8\pi, y_0 = 0.$

$\nu = 1$. The exact solution is $y(t) = \sin(t)$.

(Source: Ladas and Stavroulakis (1982)).

Problem 4: $y''(t) = -\frac{\sin(t)}{2 - \sin(t)}y(t - \pi), 0 \leq t \leq 8\pi, y_0 = 2.$

$\nu = 1$. The exact solution is $y(t) = \sin(t)$.

(Source: Bhagat Singh (1975)).

The following notations are used in Figures 38 to 41:

- SIHM4(5) : SIHM derived in Ahmad *et al.* (2013a).
- NSIHM4(5) : The new semi-implicit hybrid method.
- TF-NSIHM4(5) : The new trigonometrically-fitted semi-implicit hybrid method.
- DIRKN4(4) : A four - stage fourth - order dispersive order six of DIRKN method by Senu (2011).
- MPAFRKN4(4) : Modified Phase - fitted and Amplification fitted RKN method of four stage fourth-order by Papadopoulos *et al.* (2010).
- EHM4(5) : Explicit hybrid method of order five derived in Franco (2006).
- DIRKN3(4) : A three - stage fourth - order dispersive order six of DIRKN method by Senu *et al.* (2011).
- PFRKN4(4) : A phase - fitted RKN method of four-stage fourth-order by Papadopoulos *et al.* (2009).

A measure of the accuracy is examined using the absolute error which is defined by

$$\text{Absolute error} = \max\{|y(t_n) - y_n|\}$$

where $y(t_n)$ is the exact solution and y_n is the computed solution. The efficiency curves with the logarithm of the maximum global error versus the CPU time taken in seconds are analyzed.

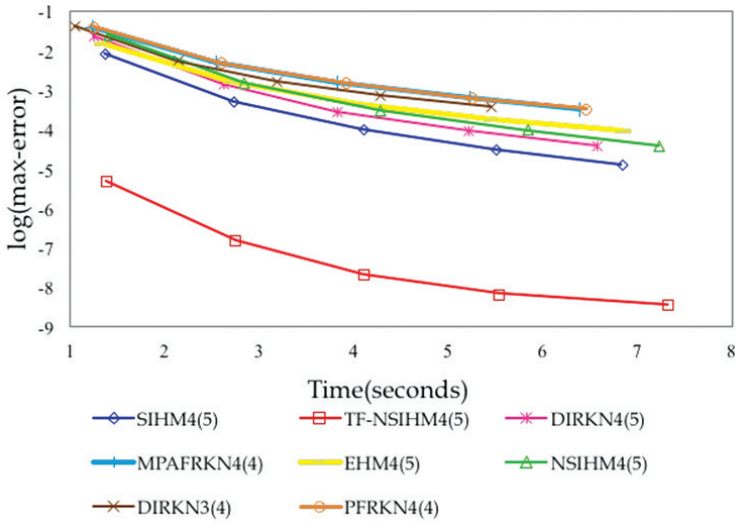


Figure 38 The efficiency curves for problem 1 with $h = \frac{\pi}{4t}$, for $i = 1, \dots, 4$

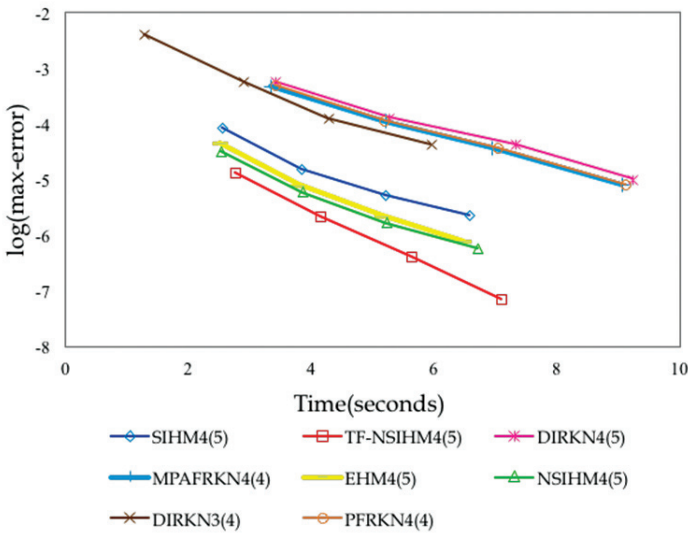


Figure 39 The efficiency curves for problem 2 with $h = \frac{\pi}{16t}$, for $i = 1, \dots, 4$

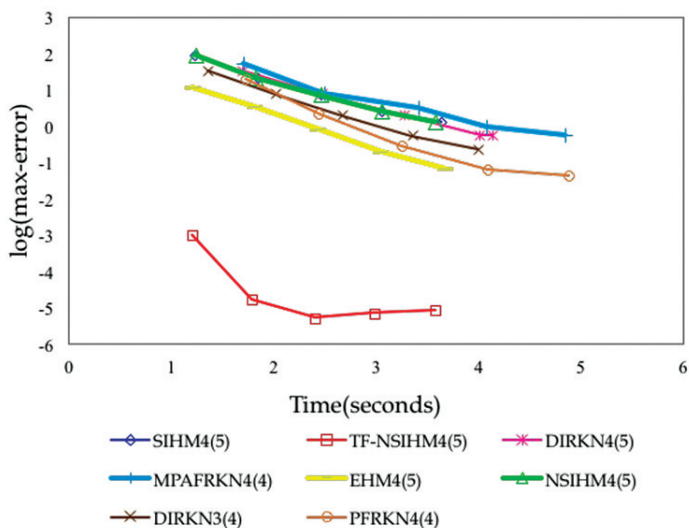


Figure 40 The efficiency curves for problem 3 with $h = \frac{\pi}{2^i}$, for $i = 2, \dots, 6$

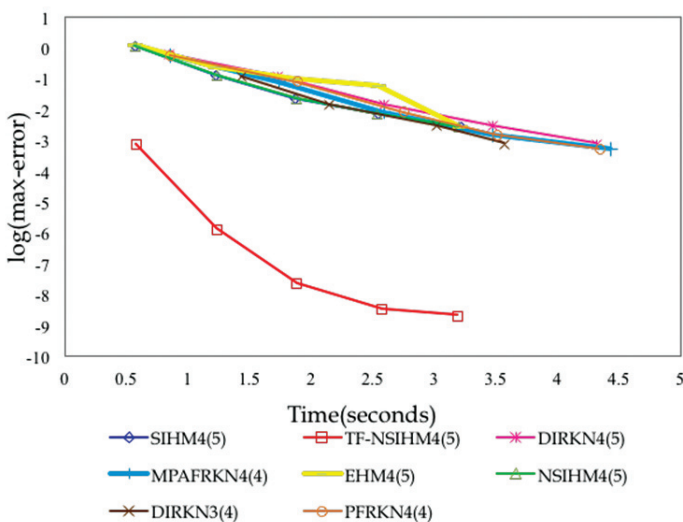


Figure 41 The efficiency curves for problem 4 with $h = \frac{\pi}{2^i}$, for $i = 1, \dots, 5$

In this research we derived a four-stage fifth order semi-implicit hybrid method, which is suitable for solving special second order ODEs directly. The new method, called NSIHM4(5), is then trigonometrically fitted so that it becomes suitable for solving oscillatory problems and is denoted as TF-NSIHM4(5). Both methods are then used for solving oscillatory second order DDEs. The numerical results clearly showed that the TF-NSIHM4(5) is the most efficient in comparison to the original NSIHM4(5) method and other existing methods in the scientific literature. Trigonometrically fitting the method improved the efficiency of the NSIHM4(5) hybrid method and it is much easier to derive compared to the approach where we have to include the dispersion and dissipation equations in the derivation of the method.

CONCLUDING REMARKS

Mathematics plays an important role in society. It shapes and influences many areas of our daily life, from education and culture through technology and industry to physics and information science and more. Mathematics has been important for the development of technology and industry for many centuries and will continue to be so forever. Further, real-world problems inspire and accelerate mathematical research in many ways. While the contribution of mathematics to the development of a new technology is vital it is usually not evident in the end product itself. Indeed these phenomena seem to be the characteristics of research in mathematics.

Many problems in science and engineering are reduced to quantifiable forms through the process of mathematical modelling. The equations arising are often expressed in terms of unknown quantities and their derivatives, and these equations

are called differential equations. The solution of these equations has exercised the ingenuity of great mathematicians since earlier times. However, prior to the development of sophisticated computing machinery, only a small fraction of the differential equations resulting from mathematical modelling were accurately solved. Although a model equation based on established physical laws may be constructed, analytical tools are frequently inadequate for its solution. Such examples concern the gravitational n -body system $n > 3$), whose differential equations are easily constructed but cannot be solved completely. Today these problems can be solved with the aid of a good numerical method.

The advancement in computer technology also has enabled researchers in many fields to perform computations that would have been unthinkable in earlier times. Indeed, computation has become one of the most important modes of scientific discovery, other than theoretical work and laboratory work.

Remarkable as these developments are, there is no indication that research in numerical analysis is slowing down. In fact research in numerical analysis, especially numerical methods for differential equations, will continue to be developed and enhanced as new and improved numerical algorithms are constructed, together with improved computer technology.

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BIOGRAPHY

Fudziah Ismail was born in Rembau, Negeri Sembilan. She received her lower secondary education at the Undang Rembau English Secondary School. After obtaining her Lower Certificate of Education, she furthered her studies for her upper secondary education at Sekolah Menengah Sains Negeri Sembilan in Kuala Pilah. She received a scholarship from Majlis Amanah Rakyat (MARA) after obtaining her Malaysian Certificate of Education in 1977 and went on to pursue her bachelor's degree in Mathematics at Macalester College, a private liberal Arts College in St. Paul, Minnesota, USA. Upon graduation in 1981, she continued to further her studies at Washington State University, in Pullman, Washington, where she obtained her Master of Science in Mathematics in 1983, again under MARA sponsorship. She subsequently came back to Malaysia and joined the Department of Mathematics in Universiti Putra Malaysia in July 1983. In 1995 she enrolled as a PhD student at Universiti Putra Malaysia and obtained her PhD in mathematics in 1999.

Fudziah Ismail is now a Professor in the field of Numerical Analysis at the Department of Mathematics, Faculty of Science, UPM. Her research interest is in numerical methods, particularly Runge-Kutta type methods for solving first order and higher order ordinary differential equations (ODEs). She is also into developing methods which are specifically used for solving second order ODEs which are oscillatory in nature. She also used the numerical methods developed for solving Delay Differential Equations, Stiff differential equations, Partial Differential Equations and Fuzzy Differential Equations.

She was the coordinator of the Department's Long Distance Learning Program from 2002 - 2006 and was the Head of Department for three consecutive terms, from 2007 - 2014. Seven

PhD students and seven Masters students have graduated under her supervision. Currently she is supervising eight postgraduate students (PhD-6, M.S-2).

Fudziah Ismail has published more than 100 research papers in refereed and citation-indexed journals and written two books on her research area. She is a life-member of the Malaysian Mathematical Science Society (PERSAMA), and a member of the American Mathematical Society and International Association of Engineers. She is a member of the Editorial Board for the Malaysian Journal of Mathematical Sciences and the Science Putra Research Bulletin. She has been appointed as a referee for many scientific papers by local and international journals, including the Journal of Applied Mathematics and Computation, a Q1 journal. She was also involved with curriculum development as well as examination questions setting for the Ministry of Education's Matriculation Program. She is also on the curriculum advisory panel for the Master in Mathematics program and the Bachelor of Science in Mathematics program for Universiti Kebangsaan Malaysia and Universiti Teknologi Malaysia, respectively. Her expert opinion has also been sought on a number of occasions by the UKM promotion panel.

During her tenure as an academician, she has received numerous awards for teaching and research. She received the "*Anugerah Adi Pengajar*" in 2007 and "*Anugerah Adi Saintis*" in 2015, from the Faculty of Science, UPM. She also won the bronze medal at the Malaysian Technology Expo 2016 and bronze, silver and gold medals at the UPM PRPI (Pameran Reka cipta Penyelidikan dan Inovasi). She also received the "Excellent Service award" for the years 2002, 2006, 2010 and 2014.

Throughout her thirty-three year stint at UPM, she continuously demonstrated commitment to her work and has been ever willing to impart, share and spread knowledge to her students and the Mathematics community.

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In the name of Allah the most Gracious and the Most Merciful

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My sincere appreciation goes to my supervisor, Prof. Dato' Mohamed Suleiman for believing in me and giving me the chance to work under his supervision. Despite his busy schedule then, Prof. Mad (as he preferred to be called) made time for his students, to provide guidance, support and research direction. I have benefited a lot from his guidance and he was a true mentor. May Allah reward all his good deeds.

Throughout my career at the Department of Mathematics, I was blessed with undivided support, encouragement and advice from the seniors. Now I am doing my best to do the same for the junior staff at the Department. To all my friends, colleagues, management and support staff at the Department and Faculty, thank you for your support and assistance.

I would like to record my appreciation towards my post graduate students for sharing the passion for numerical methods for ODEs, and for their perseverance when things appeared to be heading to a dead end. Their contributions are sincerely appreciated and gratefully acknowledged.

My utmost appreciation goes to my mother Hajjah Ramlah Adam for single handedly bringing us up (my brother - Amir Ismail and me) since we were four and five, respectively. She

is my pillar of strength. May Allah grant her good health and happiness always.

My heartfelt thanks and gratitude goes to my husband Abd. Hamid b. Abd. Samat for his love, support, understanding and prayers. Thank you for being there for me all these years. To the children *Kakak, Afiq, Alif, Hakim* and *Adik*, *mak* loves you all, and to my daughters-in-law, Daila and Amina, welcome to the family and thank you for being part of the family. To the latest addition to the family, eight months old Sara Adriana, you bring so much joy to all of us.

May Allah Bless Us All. Aameen.

LIST OF INAUGURAL LECTURES

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Sejarah Keagungan Bahasa Melayu
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