UNIVERSITI PUTRA MALAYSIA

# *EXPLICIT RUNGE-KUTTA-NYSTRÖM METHODS WITH HIGH ORDER DISPERSION AND DISSIPATION FOR SOLVING OSCILLATORY SECOND ORDER ORDINARY DIFFERENTIAL EQUATION*

MUNIRAH BT MOHAMAD

FS 2013 70

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**MASTER OF SCIENCE**
**UNIVERSITI PUTRA MALAYSIA**

**2013**

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By

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**Thesis Submitted to the School of Graduate Studies, Universiti Putra Malaysia, in Fulfillment of the Requirements for the Degree of Master of Science**

**July 2013**

Abstract of thesis presented to the Senate of Universiti Putra Malaysia
in fulfillment of the requirement for the Master of Science

**EXPLICIT RUNGE-KUTTA-NYSTROM METHODS WITH HIGH ORDER DISPERSION AND DISSIPATION FOR SOLVING OSCILLATORY SECOND ORDER ORDINARY DIFFERENTIAL EQUATION**

By

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**July 2013**

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An explicit Runge-Kutta-Nyström (RKN) method with high order dispersion (phase-lag) and dissipation (amplification error) properties is studied for the integration of initial-value problems (IVP) of second-order ordinary differential equations (ODEs) possessing oscillating solutions. The constructions of RKN methods for constant step size and embedded RKN pair for variable step size have been derived. The effects of dispersion and dissipation relations are tested on homogeneous and non-homogenous test problems which have oscillatory solutions.

Derivation of symplectic explicit Runge-Kutta-Nyström method is studied for Hamiltonian system with oscillating solutions. Symplectic methods can be more efficient than non-symplectic methods for long interval of integration. Numerical results show that the symplectic methods with high order of dispersion are more efficient for solving second order ordinary differential equations.

The new fourth and fifth order explicit RKN methods with dispersion (phase-fitted) and dissipation (amplification-fitted) of order infinity have been derived. The fifth order explicit RKN methods is divided into two parts; methods with phase-fitted and methods with both phase-fitted and amplification-fitted. In this thesis, the phase-fitted methods are derived based on symplectic method by Sharp and method derived in this thesis. For fifth order phase-fitted and amplification-fitted consists of four- and five-stage RKN methods with First Same As Last (FSAL) technique. Numerical results show that our methods are much more efficient than existing method with the same algebraic order.

In conclusion, we have derived explicit RKN methods with dispersion and dissipation for solving second-order ODEs that possessing oscillatory solutions. The dispersion constant, dissipation constant and local truncation error (LTE) terms are also calculated. The homogeneous and non-homogenous test problems with oscillatory solutions are used to prove the efficiency of our methods.

Abstrak tesis yang dikemukakan kepada Senat Universiti Putra Malaysia sebagai memenuhi keperluan untuk Ijazah Master Sains.

**KAEDAH TAK TERSIRAT RUNGE-KUTTA-NYSTRÖM DENGAN CIRI-CIRI SERAKAN DAN LESAPAN PERINGKAT TINGGI UNTUK MENYELESAIKAN PERSAMAAN PEMBEZAAN BIASA PERINGKAT KEDUA BERAYUN**

Oleh

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Kaedah tak tersirat Runge-Kutta-Nyström (RKN) dengan ciri-ciri serakan dan lesapan peringkat tinggi dikaji untuk menyelesaikan kamiran nilai awal berayun bagi persamaan pembezaan biasa peringkat kedua dengan penyelesaian bentuk ayunan. Pembinaan kaedah RKN untuk saiz langkah tetap dan kaedah pasangan benaman RKN untuk saiz langkah berubah telah diterbitkan. Kesan hubungan serakan dan lesapan diuji pada masalah homogen dan tak homogen yang mempunyai penyelesaian bentuk ayunan.

Penerbitan kaedah tak tersirat simplektik RKN dikaji untuk sistem Hamiltonian dengan penyelesaian bentuk berayun. Kaedah simplektik adalah lebih cekap berbanding kaedah tanpa simplektik untuk penyelesaian kamiran dengan selang yang panjang. Keputusan berangka menunjukkan kaedah simplektik dengan serakan peringkat tinggi adalah lebih cekap untuk menyelesaikan persamaan pembezaan biasa peringkat kedua.

Kaedah RKN tak tersirat peringkat keempat dan kelima yang baharu dengan serakan peringkat tak terhingga (suai secara fasa) dan lesapan peringkat tak terhingga (suai secara amplifikasi) telah diterbitkan. Bagi kaedah RKN tak tersirat peringkat kelima, ia dibahagikan kepada dua bahagian iaitu kaedah dengan suai secara fasa dan kaedah dengan suai secara fasa beserta suai secara amplifikasi. Kaedah suai secara fasa adalah berdasarkan kaedah yang telah diterbitkan oleh Sharp dan juga kaedah yang diterbitkan di dalam tesis ini. Untuk kaedah peringkat ke-lima suai secara fasa beserta suai secara amplifikasi merangkumi kaedah RKN tahap empat dan lima dengan teknik Pertama Sama Seperti Akhir (PSSA). Penyelesaian berangka yang diperoleh menunjukkan kaedah yang telah diterbitkan adalah lebih cekap berbanding kaedah sedia ada yang mempunyai peringkat aljabar yang sama.

Kesimpulannya, kami telah menerbitkan kaedah RKN tak tersirat dengan serakan dan lesapan untuk persamaan pembezaan biasa peringkat kedua dengan penyelesaian bentuk berayun. Pemalar serakan, pemalar lesapan dan ralat pemangkasan setempat utama (RPSU) turut dikira. Masalah homogen dan tak homogen yang mempunyai penyelesaian bentuk ayunan digunakan untuk membuktikan kecekapan kaedah-kaedah yang telah diterbitkan.

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Thank you very much.

I certify that a Thesis Examination Committee has met on 4th July 2013 to conduct the final examination of Munirah Bt Mohamad on her thesis entitled "Explicit Runge-Kutta-Nyström Methods with High Order Dispersion and Dissipation for Solving Oscillatory Second Order Ordinary Differential Equations" in accordance with the Universities and University Colleges Act 1971 and the Constitution of the Universiti Putra Malaysia [P.U.(A) 106] 15 March 1998. The Committee recommends that the student be awarded the degree of Master of Science.

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## DECLARATION

I declare that the thesis is my original work except for quotations and citations which have been duly acknowledged. I also declare that it has not been previously, and is not concurrently, submitted for any other degree at Universiti Putra Malaysia or at any other institution.

**MUNIRAH BT MOHAMAD**

Date: 4 July 2013

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# LIST OF ABBREVIATIONS

| | |
|---|---|
| ERKN5(4)-7 | The new embedded 5(4) explicit RKN method with dispersion order eight and dissipation order seven. |
| ERKN5(4)-9 | The new embedded 5(4) explicit RKN method with dispersion order eight and dissipation order nine. |
| ERKN5(4)B | The embedded 5(4) explicit RKN method derived by Bettis(1973). |
| ERKN5(4)D | The embedded 5(4) explicit RKN method by Dormand(1996). |
| ERKN5(4)F | The new embedded 5(4) explicit RKN method with dispersion order eight, dissipation order seven and FSAL technique. |
| ERKN5(4)N | The embedded 5(4) explicit RKN method derived by Senu et al. (2009b). |
| FSAL | First Same As Last technique |
| LTE | Local Truncation Error |
| MAXE | Maximum error |
| PFAFRKN4(4)F | The new fourth order phase-fitted and amplification-fitted RKN method with FSAL technique. |
| PFAFRKN4(5) | The new fourth stage fifth order phase-fitted and amplification-fitted RKN method. |
| PFAFRKN5(5)F | The new fifth stage fifth order phase-fitted and amplification-fitted RKN method with FSAL technique. |
| PFRKN4(4)S | The fourth order phase-fitted RKN method with FSAL techniqu derived by Papadopoulos (2009). |
| PFRKN4(5) | The new fourth stage fifth order phase-fitted RKN method. |
| PFRKN7(5) | The new seventh stage fifth order phase-fitted RKN method based on method derived by Sharp (2000). |
| LTE | Local Truncation Error |
| RKN | Runge-Kutta-Nystrom method |

| | |
|---|---|
| RKN3(3,4,5)G | The third order explicit RKN method with phase-lag order four and amplification error order five derived by Gracia (2002). |
| RKN3(3,6,∞)HS | The third order explicit RKN method with phase-lag order six and zero dissipative derived by Houwen and Sommeijer (1987). |
| RKN3(3,6,∞)N | The third order explicit RKN method with phase-lag order six and zero dissipative derived by Senu et al. (2009c). |
| RKN4(4)F | The fourth order explicit RKN method with FSAL technique. |
| RKN4(4,8,5)P | The fourth order explicit RKN method with dispersion order eight and dissipation order five derived by Papakostas and Tsitouras(1999). |
| RKN4(4,8,7)N | The fourth order explicit RKN method with dispersion order eight and dissipation order seven derived by Senu et al. (2008). |
| RKN4(5,6,5)D | The fifth order explicit RKN method with dispersion order six and dissipation order five derived by Dormand(1996). |
| RKN4(5,8,7)N | The fifth order explicit RKN method with dispersion order eight and dissipation order seven derived by Senu et al. (2009b). |
| RKN5(5,8,7) | The new fifth order explicit RKN method with dispersion order eight and dissipation order seven. |
| RKN5(5,8,9) | The new fifth order explicit RKN method with dispersion order eight and dissipation order nine. |
| RKN5(5,8,7)F | The new fifth order explicit RKN method with dispersion order eight, dissipation order seven and FSAL technique. |
| RKN6(5,6,5)B | The fifth order explicit RKN method with dispersion order six and dissipation order five derived by Bettis (1973). |
| SRKN3(3,6) | The new third order stage three symplectic explicit RKN method with phase-lag of order six. |
| SRKN3(3,4) | The new third order stage three symplectic explicit RKN method with phase-lag of order four. |
| SRKN4(3,6) | The new third order stage four symplectic explicit RKN method with phase-lag of order six. |
| SRKN5(4)C | The fourth order symplectic explicit RKN method derived by Calvo and Serna (1993). |

## CHAPTER 1

## INTRODUCTION

The initial value problems (IVPs) as follow

$$y'' = f(x, y), \quad y(x_0) = y_0, \qquad y'(x_0) = y'_0 \tag{1.1}$$

where $f : \mathbb{R} \times \mathbb{R}^N \to \mathbb{R}^N$, and $y_0, y'_0 \in \mathbb{R}^N$. The solution of (1.1) exhibits a pronounced oscillatory character. One way to solve oscillatory problem is by Runge-Kutta-Nyström (RKN) method. RKN method can be divided into two groups which are explicit and implicit methods. In this study, we are focusing on solving problem (1.1) by using explicit Runge-Kutta-Nyström methods for oscillating problems.

### 1.1 Literature Review

Many RKN methods have been developed for example Bettis (1973) and Dormand et al.(1987) who developed explicit RKN methods. However, their methods do not relate with dispersion or dissipation properties. As we are dealing with oscillating problems, we must consider high order algebraic condition, dispersion (phase-lag) and dissipation (amplification error) properties in order to have accurate methods. The first dispersion and dissipation properties were introduced by Brusa and Nigro (1980). Then, Thomas (1984) uses dispersion and dissipation properties for linear multistep methods. For explicit RKN methods, Van der Houwen and Sommeijer (1987) were the first to introduce these properties for explicit RKN methods.

Another alternative way to develop an efficient method is by using the symplectic condition in RKN methods. A numerical method called symplectic if it preserves the symplectic structure in phase space, thus reproducing the main qualitative property of Hamiltonian systems. A symplectic method is more efficient than non-symplectic methods for large interval of integration. Okunbor and Skeel (1992b) derived symplectic explicit RKN methods up to three stages. Calvo and Sanz Serna (1993) introduced fourth order five-stage method with minimal error coefficients. Our attempt is to derive symplectic explicit RKN methods with highest possible dispersion order and minimum Local Truncation Error (LTE).

The derivation of dispersion of order infinity (phase-fitted) and dissipation of order infinity (amplification-fitted) has been considered widely such as Simos and Aguiar (2000) and (2001) have derived modified phase-fitted RKN method for Schrodinger equation and modified phase-fitted for RK method. Papadopoulos et al.(2010) has developed a modified phase-fitted and amplification-fitted RKN method. In this thesis we will derive phase-fitted and amplification-fitted explicit RKN method with First Same As Last (FSAL) technique and minimum LTE for constant step size.

Therefore, the attempt that will be made here is to derive explicit RKN methods with highest possible dispersion and dissipation order for constant and variable step size, symplectic methods with dispersion and explicit RKN methods with phase-fitted and amplification-fitted. Essentially, our methods should have small error norm of the LTE as define by Dormand (1996) and suitable for solving oscillatory problem.

## 1.2 Runge-Kutta-Nyström (RKN) methods.

Nyström (1925) introduced RK methods for second order differential equations which has been called Runge-Kutta-Nyström (RKN) methods. The construction of RKN methods for integrating system of ordinary differential equations (ODEs) of the form

$$y'' = f(x, y), y(x_0) = y_0, y'(x_0) = y'_0 . \tag{1.2}$$

The form of $s$-stage RKN method of order $p$ is

$$\begin{aligned} y_n &= y_{n-1} + hy'_{n-1} + h^2 \sum_{i=1}^{s} b_i k_i \\ y'_n &= y'_{n-1} + h \sum_{i=1}^{s} b'_i \, k_i \end{aligned} \tag{1.3}$$

where

$$k_i = f(x_{n-1} + c_i h, y_{n-1} + c_i h y'_{n-1} + h^2 \sum_{j=1}^{s-1} a_{ij} k_j) \; i = 1, 2, .., s \tag{1.4}$$

The parameters $a_{ij}, b_i, b'_i$ and $c_i$ are assumed to be real and if $j \geq i$ then $a_{ij} = 0$. $s$ is the number of stages of the method. All the parameter can be tabulated in Butcher Tableau in the following form

$$\begin{array}{c|c} C & A \\ \hline & b^T \\ & b'^T \end{array}$$

where

$C = [c_1, c_2, \dots, c_s]^T,\ A = [a_{ij}],\ b^T = [b_1, b_2, \dots, b_s]^T$ and $b'^T = [b'_1, b'_2, \dots, b'_s]^T$.

RKN methods can be divided into two classes which are the explicit and implicit methods. In this study, we focus on explicit RKN methods where $a_{ij} = 0$ whenever $j \geq i$.

## 1.3 Algebraic condition for RKN method

General order condition for RKN method can be attained from direct expansion of the Local Truncation Error (LTE). The *s*-stage up to order six RKN process are given as follows:

for $y$ :

order 2: $$\sum b_i = \frac{1}{2}, \tag{1.5}$$

order 3: $$\sum b_i c_i = \frac{1}{6}, \tag{1.6}$$

order 4 : $$\frac{1}{2}\sum b_i c_i^2 = \frac{1}{24}, \tag{1.7}$$

order 5: $$\frac{1}{6}\sum b_i c_i^3 = \frac{1}{120}, \tag{1.8}$$

$$\sum b_i a_{ij} c_j = \frac{1}{120}, \tag{1.9}$$

order 6: $$\frac{1}{24}\sum b_i c_i^4 = \frac{1}{720}, \tag{1.10}$$

$$\frac{1}{4}\sum b_i c_i a_{ij} c_j = \frac{1}{720}, \tag{1.11}$$

$$\frac{1}{2}\sum b_i a_{ij} c_j^2 = \frac{1}{720} \tag{1.12}$$

and for $y'$:

order 1: $$\sum b'_i = \frac{1}{2}, \tag{1.13}$$

order 2: $$\sum b'_i c_i^2 = \frac{1}{2}, \tag{1.14}$$

order 3: $$\frac{1}{2}\sum b'_i c_i^2 = \frac{1}{6}, \tag{1.15}$$

order 4: $$\frac{1}{6}\sum b'_i c_i^3 = \frac{1}{24}, \tag{1.16}$$

$$\sum b'_i a_{ij} c_j = \frac{1}{24}, \tag{1.17}$$

order 5: $$\frac{1}{24}\sum b'_i c_i^4 = \frac{1}{120}, \tag{1.18}$$

$$\frac{1}{4}\sum b'_i c_i a_{ij} c_j = \frac{1}{120}, \tag{1.19}$$

$$\frac{1}{2}\sum b'_i a_{ij} c_j^2 = \frac{1}{120}, \tag{1.20}$$

order 6: $$\frac{1}{120}\sum b'_i c_i^5 = \frac{1}{720}, \tag{1.21}$$

$$\frac{1}{20}\sum b'_i c_i^2 a_{ij} c_j = \frac{1}{720}, \tag{1.22}$$

$$\frac{1}{10}\sum b'_i c_i a_{ij} c_i^2 = \frac{1}{720}, \tag{1.23}$$

$$\frac{1}{6}\sum b'_i a_{ij} c_i^3 = \frac{1}{720}, \tag{1.24}$$

$$\sum b'_i a_{ij} a_{jk} c_k = \frac{1}{720}. \tag{1.25}$$

The Nyström row sum conditions that need to be satisfied are

$$\frac{1}{2}c_i^2 = \sum_{i=1}^{s} a_{ij} \ \ (i = 1, \ldots, s). \tag{1.26}$$

The simplifying assumption given by Butcher (2003) which is used in order to reduce the number of equations

$$b_i = b'_i(1 - c_i) \qquad (i = 1, \ldots, s). \tag{1.27}$$

The First Same as Last (FSAL) property where the last stage is evaluated at the same point as the first stage of the next step is used to reduce function evaluation. For method to be FSAL, it must satisfy

$$c_1 = 0,\ \ c_s = 1 \text{ and } \ a_{sj} = b_j,\ \ j = 1, \ldots, s-1 \tag{1.28}$$

## 1.4 Local Truncation Error

Dormand (1996) proposed that having achieved a particular order of accuracy, the best strategy for practical purposes would be minimizing the error norms. The quantities of the norms of (LTE) coefficients are

$$\left\|\tau^{(p+1)}\right\|_2 = \sqrt{\left(\sum_{j=}^{n_{p+1}} \tau_j^{(p+1)}\right)^2} \text{ for } y_n \text{ and } \left\|\tau'^{(p+1)}\right\|_2 = \sqrt{\left(\sum_{j=1}^{n_{p+1}} \tau'^{(p+1)}_j\right)^2} \text{ for } y'_n. \tag{1.29}$$

The error coefficients up to order six for RKN processes are as follows:

for $y$ :

order 2: $$\tau_1^{(2)} = \sum b_i - \frac{1}{2}, \tag{1.30}$$

order 3: $$\tau_1^{(3)} = \sum b_i c_i - \frac{1}{6}, \tag{1.31}$$

order 4 : $$\tau_1^{(4)} = \frac{1}{2}\sum b_i c_i^2 - \frac{1}{24}, \tag{1.32}$$

order 5: $$\tau_1^{(5)} = \frac{1}{6}\sum b_i c_i^3 - \frac{1}{120}, \tag{1.33}$$

$$\tau_2^{(5)} = \sum b_i a_{ij} c_j - \frac{1}{120}, \tag{1.34}$$

order 6: $$\tau_1^{(6)} = \frac{1}{24}\sum b_i c_i^4 - \frac{1}{720}, \tag{1.35}$$

$$\tau_2^{(6)} = \frac{1}{4}\sum b_i c_i a_{ij} c_j - \frac{1}{720}, \tag{1.36}$$

$$\tau_3^{(6)} = \frac{1}{2}\sum b_i a_{ij} c_j^2 - \frac{1}{720} \tag{1.37}$$

and for $y'$:

order 1: $$\tau'^{(1)}_1 = \sum b'_i - \frac{1}{2}, \tag{1.38}$$

order 2: $$\tau'^{(2)}_1 = \sum b'_i c_i^2 - \frac{1}{2}, \tag{1.39}$$

order 3: $$\tau'^{(3)}_1 = \frac{1}{2}\sum b'_i c_i^2 - \frac{1}{6}, \tag{1.40}$$

order 4: $$\tau'^{(4)}_1 = \frac{1}{6}\sum b'_i c_i^3 - \frac{1}{24}, \tag{1.41}$$

$$\tau'^{(4)}_2 = \sum b'_i a_{ij} c_j - \frac{1}{24}, \tag{1.42}$$

order 5: $$\tau'^{(5)}_1 = \frac{1}{24}\sum b'_i c_i^4 - \frac{1}{120}, \tag{1.43}$$

$$\tau'^{(5)}_2 = \frac{1}{4}\sum b'_i c_i a_{ij} c_j - \frac{1}{120}, \tag{1.44}$$

$$\tau'^{(5)}_3 = \frac{1}{2}\sum b'_i a_{ij} c_j^2 - \frac{1}{120}, \tag{1.45}$$

order 6: $$\tau'^{(6)}_1 = \frac{1}{120}\sum b'_i c_i^5 - \frac{1}{720}, \tag{1.46}$$

$$\tau'^{(6)}_2 = \frac{1}{20}\sum b'_i c_i^2 a_{ij} c_j - \frac{1}{720}, \tag{1.47}$$

$$\tau'^{(6)}_3 = \frac{1}{10}\sum b'_i c_i a_{ij} c_i^2 - \frac{1}{720}, \tag{1.48}$$

$$\tau'^{(6)}_4 = \frac{1}{6}\sum b'_i a_{ij} c_i^3 - \frac{1}{720}, \tag{1.49}$$

$$\tau'^{(6)}_5 = \sum b'_i a_{ij} a_{jk} c_k - \frac{1}{720} \tag{1.50}$$

## 1.5 Analysis of Absolute Stability

The phase-lag analysis of the method (1.3) is investigated using the homogeneous test equation

$$y'' = (i\lambda)^2 y(t), \lambda \in \mathbb{R} . \tag{1.51}$$

The general method (1.3) are applied to the test equation (1.51) and we obtain the following recursive relation

$$\begin{bmatrix} y_n \\ hy_n \end{bmatrix} = D^n \begin{bmatrix} y_0 \\ hy'_0 \end{bmatrix}, D = \begin{bmatrix} A(v^2) & B(v^2) \\ A'(v^2) & B'(v^2) \end{bmatrix}, v = \lambda h \tag{1.52}$$

where $A, A', B$ and $B'$ are polynomials in $v^2$. $D$ is the stability matrix and its characteristic equation can be written as

$$\Phi(\xi, v^2) = P_0(v^2)\xi^2 + P_1(v^2)\xi + P_2(v^2) \tag{1.53}$$

which is called the stability equation of RKN method. For explicit RKN method, $P_0(v^2) = 1$ is set and (1.53) is in form of

$$\Phi(\xi, v^2) = \xi^2 + P_1(v^2)\xi + P_2(v^2) \tag{1.54}$$

or

$$\xi^2 - R(v^2)\xi + S(v^2) = 0 . \tag{1.55}$$

Denote

$$R(v^2) = trace(D) = A(v^2) + B'(v^2),$$

$$S(v^2) = \det(D) = A(v^2)B'(v^2) - A'(v^2)B(v^2), v = \lambda h. \tag{1.56}$$

The exact solution of equation (1.51) is given by

$$y(x_n) = \sigma_1[\exp(i\lambda)]^n + \sigma_2[\exp(-i\lambda)]^n, \tag{1.57}$$

where $\sigma_{1,2} = \frac{1}{2}(y_0 \pm \frac{(iy'_0)}{\lambda})$ or $|\sigma|\exp(\pm i\chi)$ where $|\sigma| = \sqrt{\left(\mathrm{Re}\left(\sigma_{1,2}\right)\right)^2 + \left(\mathrm{Im}\left(\sigma_{1,2}\right)\right)^2}$ is the length of the vector $\sigma_{1,2}$. Substituting $\sigma_{1,2}$ into (1.57), we have

$$y_n = 2|\sigma|\cos(\chi + nz). \tag{1.58}$$

Next, we assume that the eigenvalues of $D$ are $\rho_1, \rho_2$ and the corresponding eigenvectors are $[1, v_1]^T, [1, v_2]^T$, $v_i = \dfrac{A'}{\rho_i - B'}$, $i = 1, 2$. The numerical solution of (1.52) is

$$y_n = c_1\rho_1^n + c_2\rho_2^n, \tag{1.59}$$

where

$$c_1 = -\frac{v_2 y_0 - hy'_0}{v_1 - v_2}, \qquad c_2 = -\frac{v_1 y_0 - hy'_0}{v_1 - v_2}. \tag{1.60}$$

If $\rho_1$ and $\rho_2$ are complex conjugates, then $c_{1,2} = |c|\exp(\pm i\omega)$ and $\rho_{1,2} = |\rho|\exp(\pm i\varphi)$ where $|c|$ and $|\rho|$ is the length of the vector $c_{1,2}$ and $\rho_{1,2}$, respectively. By substituting $c_{1,2}$ and $\rho_{1,2}$ into (1.59), we have

$$y_n = 2|c||\rho|^n \cos(\omega + n\varphi). \tag{1.61}$$

From equation(1.3), Van der Houwen and Sommeijer (1987) introduced the following definitions.

**Definition 1.1**

An interval $(-H_a, 0)$ is called the interval of absolute stability of the method if, for all $H \in (-H_a, 0)$, $|\xi_{1,2}| < 1$, where $\xi_{1,2}$ are the roots of polynomial (1.55).

Van der Houwen and Sommeijer (1987) introduced the following absolute stability definition from characteristic polynomial (1.55).

**Definition 1.2**

The interval $(-H_a, 0), H_a > 0,$ where for all $H \in (-H_a, 0)$ such that the conditions

$$|R(v^2)| < S(v^2) + 1 \text{ and } S(v^2) < 1$$

are satisfied, is called the interval of absolute stability for RKN method.

## 1.6 Analysis of Dispersion (Phase-lag) and Dissipation (Amplification error)

The analysis of dispersion and dissipation was first introduced by Brusa and Nigro (1980). Then, Thomas (1984) applied for linear multistep methods and followed by Van der Houwen and Sommeijer (1987) for explicit Runge-Kutta-Nyström methods.

The equation (1.58) and (1.61) led us to the following definition as shown by Van der Houwen and Sommeijer (1987).

**Definition 1.3**

For the RKN method corresponding to the characteristic equation (1.55), the quantities

$$\phi(z) = z - \varphi, \quad \alpha(z) = 1 - |\rho| \tag{1.62}$$

are the dispersion (phase-lag) and dissipation (amplification error) respectively. If $\phi(v) = O(v^{t+1})$, then the method is said to have dispersion order *t* and if $\alpha(v) = O(v^{u+1})$ then the method is said to have dissipation order *u*.

From Definition 1.3, it follows that

$$\phi(v) = v - \cos^{-1}\left(\frac{R(v^2)}{2\sqrt{S(v^2)}}\right), \tag{1.63}$$

$$\alpha(v) = 1 - \sqrt{S(v^2)}. \tag{1.64}$$

where

$$R(v^2) = 2 - \sigma_1 v^2 + \sigma_2 v^4 - \sigma_3 v^6 + \ldots + \sigma_i v^{2i},\ \sigma_i = 0 \text{ for } i > s, \tag{1.65}$$

$$S(v^2) = 1 - \pi_1 v^2 + \pi_2 v^4 - \pi_3 v^6 + \ldots + \pi_i v^{2i},\ \pi_i = 0 \text{ for } i > s. \tag{1.66}$$

If at a point $v$, $\alpha(v) = 0$, then the method is said to have zero dissipative and otherwise it is called dissipative. The error $\phi(v)$ and $\alpha(v)$ are accumulated in numerical process which causes inaccuracy and it leads the need to perform many integration step. Thus, we will focus on high order of dispersion and dissipation.

The dispersion relations which are derived by Van der Houwen and Sommeijer (1987) for algebraic order three, four and five explicit RKN method with dispersion up to order twelve are as shown in Table 1.1 and the dispersion constant are as shown in Table 1.2. Note that *p* is algebraic order of the method and *q* is dispersion order.

**Table 1.1: Dispersion relation in term of $\sigma_i$ and $\pi_j$ .**

| Order | $q \geq$ | |
|---|---|---|
| *p=2,3* | 2 | $\sigma_1 = 1, \pi_1 = 0$ |
| | 4 | $\sigma_2 - \pi_2 = 1/12$ |
| | 6 | $\sigma_2 + 2\sigma_3 - 2\pi_2 - 2\pi_3 = 4/45$ |
| | 8 | $3\sigma_2^2 + 6\sigma_3 + 12\sigma_4 - 4\pi_2 - 12\pi_3 - 12\pi_4 = 4/105$ |
| | 10 | $45\sigma_2\sigma_3 + 45\sigma_4 + 90\sigma_5 - 4\pi_2 - 30\pi_3 - 90\pi_4 - 90\pi_5 = 4/315$ |
| | 12 | $315\sigma_3^2 + 1260\sigma_6 + 630\sigma_5 + 630\sigma_2\sigma_4 - 4\pi_2 - 56\pi_3$ $-420\pi_4 - 1260\pi_5 - 1260\pi_6 = 8/1485$ |
| *p=4,5* | 4 | $\sigma_1 = 1, \sigma_2 = 1/12, \pi_1 = \pi_2 = 0$ |
| | 6 | $\sigma_3 - \pi_3 = 1/360$ |
| | 8 | $\sigma_3 + 2\sigma_4 - 2\pi_3 - 2\pi_4 = 29/10080$ |
| | 10 | $5\sigma_3 + 60\sigma_4 + 120\sigma_5 - 40\pi_3 - 120\pi_4 - 120\pi_5 = 16/945$ |
| | 12 | $630\sigma_3^2 + 2520\sigma_6 + 1260\sigma_5 + 105\sigma_4 - 112\pi_3 - 840\pi_4$ $-2520\pi_5 - 2520\pi_6 = 16/1485$ |

**Table 1.2: Dispersion constant, *c* in equation $\phi(v) = cv^{t+1} + O(v^{t+3})$.**

| $q$ | $c$ |
|---|---|
| 2 | $\left[\sigma_1^2 + 4\sigma_2 - 4\pi_1 - 4\pi_2 - 4/3\right]/8$ |
| 4 | $-\left[6\sigma_1\sigma_2 + 12\sigma_3 - 4\pi_1 - 12\pi_2 - 12\pi_3 - 8/15\right]/24$ |
| 6 | $[45\sigma_2^2 + 90\sigma_1\sigma_3 + 180\sigma_4 - 8\pi_1 - 60\pi_2 - 180\pi_3 - 180\pi_4 - 4/7]/360$ |
| 8 | $-[45\sigma_2\sigma_3 + 45\sigma_1\sigma_4 + 90\sigma_5 - 2\pi_1/7 - 4\pi_2 - 30\pi_3 - 90\pi_4 - 90\pi_5 - 4/315]/180$ |
| 10 | $[315\sigma_3^2 + 1260\sigma_6 + 630\sigma_1\sigma_5 + 630\sigma_2\sigma_4 - 8\pi_1/45 - 4\pi_2 - 56\pi_3$ $-420\pi_4 - 1260\pi_5 - 1260\pi_6 - 8/1485]/2520$ |

By expanding equation (1.65) and (1.66) as Taylor series, we can determine the dissipation order and dissipation constant of a method.

## 1.7 Analysis of phase-fitted and amplification-fitted

The analysis of phase-fitted (dispersion of order infinity) and amplification-fitted (dissipation of order infinity) are based on dispersion and dissipation quantities that have been discussed in Definition 1.3. Simos (2001) derived a modified phase-fitted RK method for Schrodinger equation and Papadopoulos (2009) and (2010) have derived a phase-fitted RKN method for solving oscillatory problems and a modified phase-fitted and amplification-fitted RKN method for radial Schrodinger equation.

The equation (1.63) and (1.64) led us to the following definition as shown by Papadopoulos (2010).

**Definition 1.4**

A method is said to have phase-fitted and amplification-fitted, if $\phi(v)=0$ and $\alpha(v)=0$ hold.

**Theorem 1.1**

We have phase-fitted $\phi(v)=0$ and amplification-fitted $\alpha(v)=0$. Then $R(v^2)-2\cos(v)=0$ and $S(v^2)-1=0$.

**Proof**

From equation (1.53), we have

$$\phi(v)=v-\cos^{-1}\left(\frac{R(v^2)}{2\sqrt{S(v^2)}}\right)=0$$

$$\cos(v)=\frac{R(v^2)}{2\sqrt{S(v^2)}} \Leftrightarrow 2\cos(v)=\frac{R(v^2)}{\sqrt{S(v^2)}} \tag{1.67}$$

For amplification-fitted,

$$\alpha(v)=1-\sqrt{S(v^2)}=0$$

$$S(v^2)-1=0$$

$$S(v^2)=1. \tag{1.68}$$

Substitute (1.68) in (1.67), we have phase-fitted as follow:

$$R(v^2) - 2\cos(v) = 0. \tag{1.69}$$

## 1.8 Objectives of the Thesis

In this study, we develop new and more efficient methods based on explicit RKN method for solving homogeneous and inhomogeneous problems. The new methods are tested for both constant and variable step size. The main objectives are

i. to construct explicit RKN methods with high order of dispersion and dissipation for solving oscillatory problems using constant step size.

ii. to investigate the effect of symplectic properties on explicit RKN with high order of dispersion.

iii. to construct embedded explicit RKN methods with high order of dispersion and dissipation for solving oscillatory problems using variable step size codes.

iv. to derive phase-fitted and amplification-fitted explicit RKN methods for the fourth and fifth order.

## 1.9 Outline of Thesis

In Chapter 1, a brief introduction on the development of numerical solution, basic theory on algebraic order of RKN method, dispersion order, dissipation order and local truncation error are discussed.

In Chapter 2 and 4, we discuss fifth order explicit RKN methods with high order of dispersion and dissipation for constant and variable step size. The stability region of the methods has been determined. The strategies for getting the new methods also been discussed. The result of the methods has been compared with methods that have been developed by Bettis (1979), Dormand et al.(1987) and Senu et al.(2009a) for solving oscillatory problem. In Chapter 4, we discuss about embedded pair of explicit RKN methods for variable step size where the higher order of the methods are based on Chapter 2. The new methods are compared with methods that have been developed by Bettis (1979), Dormand et al.(1987) and Senu et al.(2009a) which are also an embedded pair of explicit RKN methods.

We discuss symplectic explicit RKN method in Chapter 3. We derive third order symplectic RKN methods with three- and four-stage. We also consider high order of dispersion to get a more accurate result when dealing with periodic solutions. The numerical result has been obtained and compared with Van der Houwen and

Sommeijer (1987), Garcia (2002) and Senu et al.(2009c). Method derived by Garcia (2002) do not relate to dispersion properties. Van der Houwen and Sommeijer (1987) and Senu et al.(2009c) developed method with high order of dispersion and dissipation. Since symplectic properties already satisfied zero dissipative, thus we do not need to consider for dissipation order.

In Chapter 5, we derived phase-fitted and amplification-fitted explicit RKN methods with algebraic condition for order four and five. In fifth order method, we divide the chapter into two parts. In first part, we derived phase-fitted RKN methods, and in the second part we derived phase-fitted and amplification-fitted RKN methods. We compared our method with methods derived by Calvo and Sanz Serna (1993), Papakostas et al.(1999), Papadopoulos et al.(2009) and Senu et al.(2009b) for fourth order method. While for the fifth order methods, we compared with methods derived by Bettis (1979), Dormand (1996) and Senu et al.(2009a).

Finally in Chapter 6, we summarize and conclude our studies. Future studies are also suggested in this chapter.

## 1.10 Scope of Study

The main purpose of this research is to solve the second order ordinary differential equations (1.1) in which the solutions exhibit a pronounced oscillatory character. In this study we are focusing on solving problem (1.1) by using explicit Runge-Kutta-Nyström methods for oscillating problems with high order dispersion and dissipation. The research also covered the phase-fitted and amplification-fitted RKN methods with constant and variable step size mode.

# BIBLIOGRAPHY

Allen R.C. and Wing G.M. (1974). An invariant imbedding algorithm for the solution of inhomogeneous linear two-point boundary value problems, *Journal of Computational Physics;* 14(1), 40-48.

Bettis D.G, (1973). A Runge- Kutta-Nyström Algorithm, *Celestial Mechanics*, 8: 229-233.

Bettis D.G, (1979). Runge-kutta for oscillatory problems, *J.Appl. Math Phy.* 30 :699-704.

Brusa L. and Nigro L. (1980). A One-Step Method for Direct Integration of Structural Dynamic Equation, *int J. Numer. Method Engg.,*15: 685-699.

Butcher J.C. (2003). *Numerical Methods for Ordinary Differential Equations*(New York: Wiley).

Calvo M.P. and Sanz-Serna J.M. (1993). High-order symplectic Runge-Kutta-Nyström methods, *SIAM J.Sci. Comput.*, 14(5): 1237-1252.

Chawla, M. M., Rao, P.S. (1985). High-accuracy P-stable methods, *IMA Journal of Numerical Analysis.* 5: 215-220.

Dormand J.R. (1996). *Numerical Methods for Differential Equations a computational approach*; CRC Press, Inc.

Dormand J.R. and Prince P.J. (1980). A Family of Embedded Runge-Kutta Formulae, *J.Comp. and App.Math.*, 6:19-26.

Dormand J.R., El-Mikkawy M.E.A. and Prince P.J. (1987).*IMA J. Numer. Anal* .7: 235.

Fehlberg E. and Marshall G.C. (1972). Classical eight- and Lower Order Runge-Kutta Nyström Formulas with Stepsize control for Special Second Order Differential Equations. *NASA Technical Report,* (R-410).

Franco J.M., Gomez I. and Randez L., (2001). Four-stage symplectic and P-stable SDIRKN methods with dispersion of high order, *Numer. Algor.*, 26: 347-363.

Franco J.M., (2003). A 5(3) pair of explicit ARKN methods for numerical integration of perturbed oscillators, *J. Comp. Appl. Math.* 161: 283-293.

Garcia A., Martin P. and Gonzalez A.B (2002) New methods for oscillatory problems based on classical codes, *Appl. Numer. Math.,*42 : 141-157.

Garcia A., Martin P. and Gonzalez A.B (2002) High order Runge-Kutta-Nyström codes for the integration of oscillatory problems, *Appl. Numer. Math.,*48 : 13-25.

Hairer E., Norsett S.P. and Wanner G. (1993). *Solving Ordinary Differential Equations I, Nonstiff Problems.* Berlin, Heidelberg, New York, Springer-Verlag.

Lambert J. D. (1991). *Numerical Methods for Ordinary Differential Systems-The Initial Value Problem* (New York: Wiley)

Lambert J. D. and Watson I. A.(1976).Symmetric Multistip Methods for Periodic Initial Value Problems, *IMAJ. Appl.Math.*18(2): 189-202.

Lin-Yi Chou and Sharp P.W., (2000). On order 5 symplectic explicit Runge-Kutta-Nyström methods, *Journal of Applied Mathematics & Decision Sciences,* 4(2): 143-150.

Okunbor D. and Skeel R. D. (1992a). Explicit Runge-Kutta-Nyström method is canonica if and only if its adjoint is explicit, *SIAM Journal on Numerical Analysis,*29 :521-527.

Okunbor D., and Skeel R.D., (1992b). Explicit canonical methods for Hamiltonian systems, *Math. Comp.*, 59: 439-455.

Okunbor D., and Skeel R.D.,(1994). Canonical Runge-Kutta-Nyström methods of five and six, *Math. Comp.*, 51: 375-382.

Papadeorgiou G., Tsitourus Ch. And Papakostas S.N. (1993). Runge-Kutta Pairs for Periodic Initial Value Problem,*Computing*, 51:151-163.

Papadopoulos D.F., Anastassi Z.A. and Simos T.E. (2009). A phase-fitted Runge-Kutta-Nyström method for the numerical solution of initial value problems with oscillating solutions, *Computer Physics Communications*, 180: 1839-1846.

Papadopoulos D.F., Anastassi Z.A. and Simos T.E. (2010). A modified phase-fitted and amplification-fitted Runge-Kutta-Nyström method for numerical solution of radial Schrodinger equation, *J Mol Model*, 16: 1339-1346.

Papakostas S.N. and Tsitouras Ch. (1999).High-Phase-Lag-Order Runge—Kutta and Nyström Pairs. *SIAM J. Sci. Comput*, 21(2): 747-763.

Senu N., Suleiman M., Ismail F. and Othman M. (2008). Kaedah Runge-Kutta-Nyström tahap empat dengan serakan berperingkat tinggi untuk menyelesaikan masalah berkala; *Proceeding of Simposium Kebangsaan Sains Matematik ke-16*, 2-5 June 2008, Kota Bharu, Kelantan, 507-514 .

Senu N. and Suleiman M., (2009a). A 5(4) Pair Explicit Runge-Kutta-Nyström Method for Solving Oscillatory Problems, *International Journal of Computational Science*, 3(1): 53-68.

Senu N., Suleiman M. and Ismail F. (2009b). An embedded explicit Runge–Kutta–Nyström method for solving oscillatory problems,*Phys. Scr*. 80: 015005.

Senu N., Suleiman M., Ismail F. and Othman M. (2009c). A zero-dissipative Runge-Kutta-Nyström with Minimal Phase-lag Method for Solving Oscillatory Problems; *Proceeding of The 5th IMT-GT 2009 International Conference on Mathematics, Statistics, and their Applications*, 9-11 June 2009, Bukit Tinggi, Indonesia .

Simos T.E. and Vigo-Aguiar J. (2000). A new modified Runge-KuttaNyström method with phase-lag of order infinity for the numerical solution of the Schrodinger equation and related problems, *International Journal of Modern Physics C*,11(6): 1195-1208.

Simos T.E. and Vigo-Aguiar J. (2001). A modified phase-fitted Runge-Kutta method for numerical solution of the Schrodinger equation, *Journal of Mathematical Chemistry*, 30(1): 121-131.

Stiefel E. and Bettis D.G. (1969). Stabilization of Cowell's Method, *Numerische Mathematik*, 13(2): 154-175.

Thomas,R.M. (1984). Phase properties of high order, almost *P*-stable formulae, *BIT Numerical Mathematics*, 24(2): 225-238.

Van de Vyver H. (2007). A symplectic Runge-Kutta-Nyström method with minimal phase-lag, *Physic Letter A*, 367, 16-24.

Van de Vyver H. (2008). Fourth order symplectic integration with reduced phase error, *International Journal of Modern Physics C,* 14(8): 1257-1268.

Van de Vyver H., (2007). A 5(3) pair of explicit Runge-Kutta-Nyström method for oscillatory problems,*Math. Comput. Model*, 45: 708.

Van Der Houwen P.J. and Sommeijer B.P. (1987). Explicit Runge-Kutta(-Nyström) methods with reduced Phase Error For Computing Oscillating Solution, *Siam J. Number*. *Anal* 24(3): 595-617.