Optimized Low Dispersion and Low Dissipation Runge-Kutta Algorithms in Computational Aeroacoustics

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Abstract: A new explicit fourth-order six-stage Runge-Kutta scheme with low dispersion and low dissipation properties is developed. This new Runge-Kutta scheme is shown to be more efficient in terms of dispersion and dissipation properties than existing algorithms such as Runge-Kutta temporal schemes developed by Hu et al. (1996), Mead and Renaut (1999), Tselios and Simos (2005). We perform a spectral analysis of the dispersion and dissipation errors. Numerical experiments dealing with wave propagation are performed with these four temporal Runge-Kutta schemes, all coupled with a nine-point centred difference scheme of eight order. The variation of two types of error: the error rate with respect to the L_1 norm and the Total Mean Square Error, both with respect to the CFL are obtained for all the four different schemes and it is seen that low CFL numbers are in general more effective than larger CFL numbers.

Keywords: Runge-Kutta, dispersion, dissipation, CFL

1 Introduction

In Computational Aeroacoustics (CAA), the accurate prediction of the generation of sound is demanding due to the requirement for preservation of the shape and frequency of wave propagation and generation. It is well-known [11,23] that in order to conduct satisfactory computational aeroacoustics, numerical methods must generate the least possible dispersion and dissipation errors. In general, higher order schemes would be more suitable for CAA than the lower-order schemes since, overall, the former are less dissipative [13]. This is the reason why higher-order spatial discretisation schemes have gained considerable interest in computational aeroacoustics.

Since multidimensional finite-volume algorithms are generally more expensive in terms of numerical cost than finite-difference algorithms, the majority of CAA codes are based on the finite-difference methodology [8]. The trend within the field of CAA has been to employ higher-order accurate numerical schemes that have in some manner been optimized for wave propagation in order to reduce the number of grid points per wavelength while ensuring tolerable levels of numerical error. We now highlight some developments made in the construction of low dispersion and low dissipation Runge-Kutta algorithms.

Hu et al. [14] have constructed Runge-Kutta methods with low dispersion and low dissipation properties. They minimize the error between the exact and the numerical solution by determining the required coefficients. Stanescu and Habashi [21] propose a special Runge-Kutta scheme that can be written using minimum storage (i.e 2N-storage where N is the dimension of the first order differential system). Mead and Renaut [19] propose a six-stage fourth order Runge-Kutta method, in the context of Chebyshev pseudospectral discretization, with extended stability along the imaginary axis. Berland et al. [9] have constructed an explicit low-storage fourth-order six-stage Runge-Kutta scheme optimized in the Fourier space with a large stability range.

2 Organisation of paper

In section 3, we obtain estimates for the dispersion and dissipation errors in a six-stage fourth order Runge-Kutta scheme containing two parameters, β_5 and β_6. Section 4 highlights the salient features of some of our techniques

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of optimisation. In section 5, we use our techniques of optimisation to find optimal values of β_5 and β_6 and then perform a comparison of the spectral analysis of the dispersive and dissipative properties of the Runge Kutta schemes constructed by Hu et al. [14], Mead and Renaut [19], Tselios and Simos [25] with our new Runge-Kutta scheme. In section 6, we present the results of a numerical experiment dealing with a convective wave equation and a non-linear spherical wave problem using four different schemes and compare some types of errors. Section 7 highlights the main results of this paper.

3 Dispersion and Dissipation in Runge-Kutta Methods

We consider the time integration using Runge-Kutta algorithms of the differential equation

$$\frac{\partial u}{\partial t} = F(u,t),$$

where the operator, F is a function of the unknown, u and of time, t.

Hu et al. [14] proposed the following low-storage s-stage algorithm to compute the time integration from $u^n = u(n\Delta t)$ to $u^{n+1} = u[(n+1)\Delta t]$ namely,

$$u^{n+1} = u^n + \sum_{j=1}^{s} \beta_j (\Delta t)^j F^j(u). \tag{1}$$

where $F^j = F \circ ... \circ F$.

This can be rewritten as

$$u^0 = u^n, \tag{2}$$

$$u^\rho = u^n + \alpha_\rho \Delta t F(u^{\rho-1}), \tag{3}$$

and

$$u^{n+1} = u^s, \tag{4}$$

where $\rho = 1, 2, ..., s$.

For $F(u)$ linear and a six-stage algorithm, we have

$$u^{n+1} = u^n + \sum_{j=1}^{6} \prod_{\rho=7-j}^{6} \alpha_\rho (\Delta t)^j \ F^j(u), \tag{5}$$

where $\rho = 1, 2, ..., 6$ and $\prod_{\rho=7-j}^{6} \alpha_\rho = \beta_j$.
We note that $\beta_j = \frac{1}{j!}$ for $j = 1, 2, 3, 4$.

The scheme given by (5) is detailed as follows:

$$u^0 = u^n, \tag{6}$$

$$u^1 = u^n + \alpha_1 \Delta t F(u^0), \tag{7}$$

$$u^2 = u^n + \alpha_2 \Delta t F(u^1), \tag{8}$$

$$u^3 = u^n + \alpha_3 \Delta t F(u^2), \tag{9}$$

$$u^4 = u^n + \alpha_4 \Delta t F(u^3), \tag{10}$$

$$u^5 = u^n + \alpha_5 \Delta t F(u^4), \tag{11}$$

$$u^6 = u^n + \alpha_6 \Delta t F(u^5), \tag{12}$$

and

$$u^{n+1} = u^6. \tag{13}$$

Thus, we have the following relationships

$$\alpha_1 = \frac{\beta_6}{\beta_5},$$

$$\alpha_2 = \frac{\beta_5}{\beta_4}.$$

We consider the usual linear test equation, $u_t = \lambda u$ where $\lambda = x + yI$. The exact solution to this test equation can be easily obtained as

$$u(t + \Delta t) = \exp(\Delta t(x + yI)) \ u(t), \tag{14}$$

where Δt is the time step.

Using the notation of Albrecht [1], the Runge Kutta solution [19] has the following form:

$$u_{n+1} = (1 + (\lambda k)b^T e + (\lambda k)^2 \ b^T A e + ... + (\lambda k)^s \ b^T A^{s-1} e) \ u_n, \tag{15}$$

where $k = \Delta t$ and $e = (1, 1, 1, ..., 1) \in \Re^s$.

If $\beta_j = b^T A^{j-1} e$, then we can rewrite (3) as [19]

$$u_{n+1} = (1 + (\lambda k) \ \beta_1 + ... + (\lambda k)^s \beta_s) \ u_n, \tag{16}$$

or

$$u_{n+1} = (P_s + I \ F_s) \ u_n, \tag{17}$$

where,

$$P_s = 1 + k \ x\beta_1 + k^2 \ (x^2 - y^2) \ \beta_2 + k^3 \ (x^3 - 3xy^2) \ \beta_3 + \\ k^4(x^4 - 6x^2y^2 + y^4) \ \beta_4 + ... \tag{18}$$

and

$$F_s = k \ y\beta_1 + k^2 \ (2xy) \ \beta_2 + k^3 \ (3x^2y - y^3) \ \beta_3 + \\ k^4 \ (4x^3y - 4xy^3)\beta_4 + k^5(5x^4y - 10x^2y^3 + y^5) \ \beta_5 + ... \tag{19}$$

We next consider the following definition:

Definition 1 (Van Der Howen and Sommeijer [26])
The Runge Kutta scheme given by (16) is dissipative of order p if

$$\exp(xk) - |P_s + IF_s| = O(k^{p+1}), \qquad (20)$$

and dispersive of order q if

$$hy - \tan^{-1}\left(\frac{F_s}{P_s}\right) = O(k^{q+1}). \qquad (21)$$

In [26], Van Der Houven and Sommeijer consider the case when $x = 0$ (exact solution is non-dissipative). For a fourth-order six-stage method with $x = 0$, P_6 and F_6 can be written as

$$P_6 = 1 - \beta_2(yk)^2 + \beta_4(yk)^4 - \beta_6(yk)^6, \qquad (22)$$

$$F_6 = yk - \beta_3(yk)^3 + \beta_5(yk)^5, \qquad (23)$$

with $\beta_2 = \frac{1}{2}$, $\beta_3 = \frac{1}{6}$ and $\beta_4 = \frac{1}{24}$.

The dissipation and dispersion errors can be obtained as

$$E_A(yk) = 1 - |P_6 + I\,F_6|, \qquad (24)$$

and

$$E_\phi(yk) = yk - \tan^{-1}\left(\frac{F_6}{P_6}\right). \qquad (25)$$

We now describe how Tselios and Simos [25] have obtained their optimal parameters for β_5 and β_6 respectively.

3.1 Approach by Tselios and Simos [25]

If we expand (24) and (25) using Taylor series, we obtain an estimate of the dissipation and dispersion errors as [25]

$$E_A(yk) = (yk)^6\left(\frac{1}{144} - \beta_5 + \beta_6\right) +$$
$$(yk)^8\left(-\frac{1}{1152} + \frac{\beta_5}{6} - \frac{\beta_6}{2}\right) + (yk)^{10}\left(-\frac{(\beta_5)^2}{2} + \frac{\beta_6}{24}\right)$$
$$+ (yk)^{12}\left(\frac{1}{41472} + \frac{(\beta_5)^2}{2} + \right.$$
$$\left. \beta_5\left(-\frac{1}{144} - \beta_6\right) + \frac{\beta_6}{144}\right), \qquad (26)$$

and

$$E_\phi(yk) = (yk)^5\left(\frac{1}{120} - \beta_5\right) + (yk)^7\left(-\frac{1}{336} + \frac{\beta_5}{2} - \beta_6\right)$$
$$+ (yk)^9\left(-\frac{1}{5184} - \frac{\beta_5}{24} + \frac{\beta_6}{6}\right)$$
$$+ (yk)^{11}\left(\frac{1}{19008} + (\beta_5)^2 + \beta_5\left(-\frac{1}{72} - \beta_6\right)\right), \qquad (27)$$

where E_A and E_ϕ are the dissipation and dispersion errors respectively.

Estimates of the magnitude of the dissipation and dispersion errors have been obtained by Tselios and Simos [25] as follows:

$$|E_A(\beta_5, \beta_6)| = \left(\left(\frac{1}{144} - \beta_5 + \beta_6\right)^2\right.$$
$$+ \left(-\frac{1}{1152} + \frac{\beta_5}{6} - \frac{\beta_6}{2}\right)^2$$
$$+ \left(-\frac{(\beta_5)^2}{2} + \frac{\beta_6}{24}\right)^2 +$$
$$\left.\left(\frac{1}{41472} + \frac{(\beta_5)^2}{2} + \beta_5\left(-\frac{1}{144} - \beta_6\right) + \frac{\beta_6}{144}\right)^2\right)^{1/2} \qquad (28)$$

and

$$|E_\phi(\beta_5, \beta_6)| = \left(\left(\frac{1}{120} - \beta_5\right)^2 + \left(-\frac{1}{336} + \frac{\beta_5}{2} - \beta_6\right)^2\right.$$
$$+ \left(\frac{1}{5184} - \frac{\beta_5}{24} + \frac{\beta_6}{6}\right)^2 +$$
$$\left.\left(\frac{1}{19008} + (\beta_5)^2 + \beta_5\left(-\frac{1}{72} - \beta_6\right)\right)^2\right)^{1/2} \qquad (29)$$

We note that Tselios and Simos [25] minimize the quantity, $(E_A(\beta_5, \beta_6))^2 + (E_\phi(\beta_5, \beta_6))^2$ using the Levenberg Marquart method [20] and obtain

$$\beta_5 = 0.008267383750863793$$

and

$$\beta_6 = 0.00121166825454822479.$$

The coefficients proposed by Mead and Renaut [19] are $\beta_5 = 0.00556$ and $\beta_6 = 0.00093$.
Hu et al. [14] found that the optimal values of β_5 and β_6 are 0.00781005 and 0.0013214 respectively. They minimize the following integral,

$$\int_0^{\pi/2} |r - r_e|^2\, d(yk), \qquad (30)$$

where $r = \frac{u^{n+1}}{u^n} = 1 + z\beta_1 + \dots + z^s\ \beta_s$ and $r_e = \frac{u(t+k)}{u(t)} = \exp(k(x + y\,I))$.

In the following section, we describe some of our techniques of optimisation [2,4] and in section 5, we use these techniques to compute optimal values of β_5 and β_6.

4 Minimized Integrated Exponential Error for Low Dispersion and Low Dissipation

In this section, we describe briefly the technique of Minimized Integrated Exponential Error for Low Dispersion and Low Dissipation (**MIEELDLD**). This technique have been introduced in Appadu and Dauhoo [2], Appadu and Dauhoo [3]. We now give a resume of how we have derived this technique of optimisation.

Suppose the amplification factor of the numerical scheme when applied to the 1-D linear advection equation, given by

$$\frac{\partial u}{\partial t} + \beta \frac{\partial u}{\partial x} = 0, \tag{31}$$

is

$$\xi = A + IB.$$

Then the modulus of the Amplification Factor, (AFM) and the relative phase error, (RPE) are calculated as

$$AFM = |\xi|,$$

and

$$RPE = -\frac{1}{cw} \tan^{-1} \frac{B}{A},$$

where c and w are the CFL number and phase angle respectively.

For a scheme to have Low Dispersion and Low Dissipation, we require

$$|1 - RPE| + (1 - AFM) \longrightarrow 0.$$

The quantity, $|1 - RPE|$ measures dispersion error while $(1 - AFM)$ measures dissipation error. Also when dissipation neutralises dispersion optimally, we have,

$$\left| |1 - RPE| - (1 - AFM) \right| \to 0.$$

Thus on combining these two conditions, we get the following condition necessary for dissipation to neutralise dispersion and for low dispersion and low dissipation character to be satisfied:

$$\mathbf{eldld} = \left| |1 - RPE| - (1 - AFM) \right| +$$
$$(|1 - RPE| + (1 - AFM)) \longrightarrow 0. \tag{32}$$

Similarly, we expect

$$\mathbf{eeldld} = \exp \left(\left| |1 - RPE| - (1 - AFM) \right| \right) +$$
$$\exp(|1 - RPE| + (1 - AFM)) - 2 \longrightarrow 0, \tag{33}$$

in order for Low Dispersion and Low Dissipation properties to be achieved.

The measure, **eeldld** denote the exponential error for low dispersion and low dissipation. The reasons why we prefer **eeldld** over **eldld** is because the former is generally

more sensitive to perturbations [2].

We next explain how the integration process is performed in order to obtain the optimal parameter(s).

Only one parameter involved
If the CFL is the only parameter, we compute

$$\int_0^{w_1} \mathbf{eeldld} \, dw,$$

for a range of $w \in [0, w_1]$, and this integral will be a function of c. The optimal CFL is the one at which the integral quantity is closest to zero.

Two parameters are involved
We next consider a case where two parameters are involved and whereby we would like to optimise these two parameters.

Suppose we want to obtain an improved version of the Fromm's scheme which is made up of a linear combination of Lax-Wendroff (LW) and Beam-Warming (BW) schemes. Suppose we apply BW and LW in the ratio $\lambda : 1 - \lambda$. This can be done in two ways.

In the first case, if we wish to obtain the optimal value of λ at any CFL, then we compute

$$\int_0^{c_1} \int_0^{w_1} \mathbf{eeldld} \, dw \, dc, \tag{34}$$

which will be in terms of λ.

The value of c_1 is chosen to suit the region of stability of the numerical scheme under consideration while $w_1 \in [0, 1.1]$.

The second way to optimise a scheme made up of a linear combination of Beam-Warming and Lax-Wendroff is to compute the **IEELDLD** as $\int_0^{w_1} \mathbf{eeldld} \, dw$ and the integral obtained in that case will be a function of c and λ. Then a 3-D plot of this integral with respect to $c \in [0, c_1]$ and $\lambda \in [0, 1]$ enables the respective optimal values of c and λ to be located. The optimised scheme obtained will be defined in terms of both a CFL and the optimal value of λ to be used.

Considerable and extensive work on the technique of Minimised Integrated Exponential Error for Low Dispersion and Low Dissipation has been carried out in Appadu and Dauhoo [2], Appadu and Dauhoo [3], Appadu [4,5,6].

In Appadu and Dauhoo [2], we have obtained the optimal CFL for some explicit methods like Lax-Wendroff, Beam-Warming, Crowley, Upwind Leap-Frog and Fromm's schemes. In Appadu and Dauhoo [3], we have combined some spatial discretisation schemes with the optimised time discretisation method proposed by Tam and Webb [23] in order to approximate the 1-D linear advection equation. These spatial derivatives are: a

standard 7-point and 6th-order central difference scheme (ST7), a standard 9-point and 8th-order central difference scheme (ST9) and optimised spatial schemes designed by Tam and Webb [23], Lockard et al. [17], Zingg et al. [28], Zhuang and Chen [29] and Bogey and Bailly [10]. The results from some numerical experiments were quantified into dispersion and dissipation errors and we have found that the quality of the results is dependent on the choice of the CFL number even for optimised methods, though to a much lesser degree as compared to standard methods. Moreover, in Appadu [2], we have obtained the optimal CFL of some multi-level schemes in 1-D. These schemes are high order in space and time and have been designed by Wang and Liu [27]. We have also optimised the parameters in the family of Third Order schemes proposed by Takacs [22]. The optimal CFL of the 2-D CFLF4 scheme which is a composite method made up of Corrected Lax-Friedrichs and the two-step Lax-Friedrichs developed by Liska and Wendroff [16] has been computed and some numerical experiments have been performed such as: 2-D solid body rotation test [18], 2-D acoustics [15] and 2-D circular riemann problem [18]. We have shown that better results are obtained when the optimal parameters obtained using **MIEELDLD** are used.

The technique of MIEELDLD has been extended from Computational Fluid Dynamics framework to Computational Aeroacoustics and used to construct high-order methods [7] which approximate the 1-D linear advection equation. Modifications to the spatial discretization schemes designed by Tam and Webb [23], Lockard et al. [17], Zingg et al. [28] and Bogey and Bailly [10] have been obtained, and also a modification to the temporal scheme developed by Tam et al. [24] has been obtained. These novel methods obtained using MIEELDLD have in general better dispersive properties as compared to the existing optimised methods [7].

Since, in this work, we have estimates for the dissipation and dispersion errors, we do not work with the quantities, $|1 - RPE|$ and $(1 - AFM)$. Expressions for the dissipation and dispersion errors of the six-stage fourth-order Runge-Kutta scheme are given by (26) and (27) respectively where β_5 and β_6 are the two parameters. Hence, the measure, **eldld** given by (32) is equivalent to

$$M_1 = \left| |E_\phi| - |E_A| \right| + (|E_\phi| + |E_A|). \qquad (35)$$

For dissipation to neutralise dispersion and for low dispersion and low dissipation properties to be satisfied, we require

$$M_1 = \left| |E_\phi| - |E_A| \right| + (|E_\phi| + |E_A|) \longrightarrow 0. \qquad (36)$$

From (36), we can deduce that

$$M_2 = (|E_\phi| - |E_A|)^2 + (|E_\phi| + |E_A|)^2 \longrightarrow 0. \qquad (37)$$
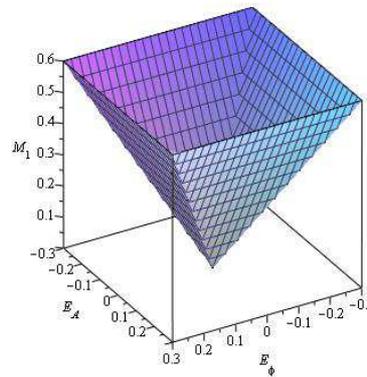

Fig. 1: Plot of the metric, M_1 vs E_ϕ vs E_A

The measure, **eeldld** given by (33) is equivalent to

$$M_3 = \exp||E_\phi| - |E_A|| + \exp\left(|E_\phi| + |E_A|\right) - 2 \longrightarrow 0. \qquad (38)$$

From (38), we can deduce that

$$M_4 = \exp\left(|E_\phi| - |E_A|\right)^2 + \exp\left(|E_\phi| + |E_A|\right)^2 - 2 \longrightarrow 0. \qquad (39)$$

We note that (36), (37), (38), (39) must be satisfied if we require dissipation to neutralise dispersion and also for low dispersion and low dissipation character to be satisfied.

We next obtain 3D plots of the four measures, all vs dispersion error vs dissipation error in Figs. (1, 2, 3, 4). Dispersion error can be negative if there is phase lag. It can be seen that the measure is zero only when dispersion error and dissipation error are both equal to zero for all the four measures.

The reason why we derive M_2 and M_4 is because we use a nonlinear programme (NLP) to compute the minimum of a real-valued objective function. Most of the algorithms used by NLP assume that the objective function and constraints are twice continuously differentiable. However, NLP will sometimes succeed even if these conditions are not met.

5 Finding optimal values of the two parameters in Runge-Kutta schemes

We now consider the dispersion and dissipation errors given by (26) and (27) respectively. The integrated error from the metric, M_1 is computed as
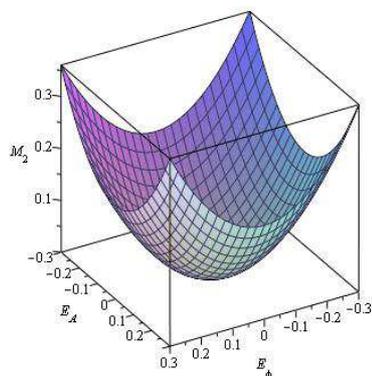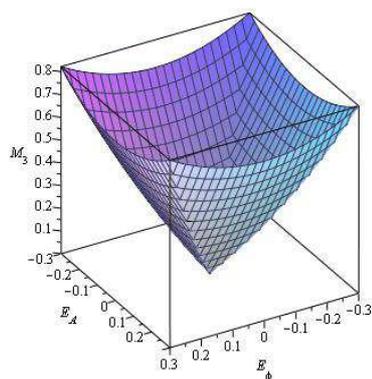
Fig. 2: Plot of the metric, M_2 vs E_ϕ vs E_A

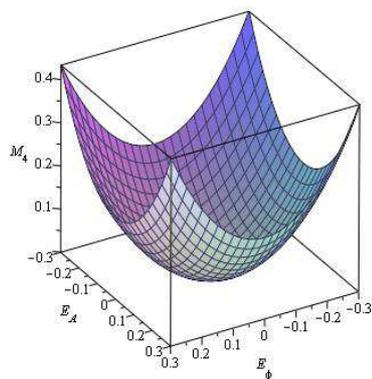**Fig. 3:** Plot of the metric, M_3 vs E_ϕ vs E_A

Fig. 4: Plot of the metric, M_4 vs E_ϕ vs E_A

$$\int_0^{1.1} ||E_\phi| - |E_A|| + |E_\phi| + |E_A| \, d(yk). \qquad (40)$$

A 3-D plot and contour plot of this integrated error vs $\beta_5 \in [0, 0.02]$ vs $\beta_6 \in [0, 0.0015]$ is shown in Fig. (5) and we can deduce that the approximate values for β_5 and β_6 are 0.008 and 0.00132 respectively.

The Integrated Error for the metric, M_2 is computed as

$$\int_0^{1.1} (|E_\phi| - |E_A|)^2 + (|E_\phi| + |E_A|)^2 \, d(yk), \qquad (41)$$

and a plot of this integrated error vs β_5 vs β_6 is shown in Fig. (6). We then use optimisation function to obtain the optimal values of β_5 and β_6 as 0.00813684557939976447 and 0.00136374541073363914 respectively.

A plot of the Integrated Error from M_3 vs β_5 vs β_6 is shown in Fig. (7). However, we cannot locate the optimal values of β_5 and β_6 accurately. It is for this reason precisely that we define the metric, M_4.

A plot of the integrated error from M_4 vs β_5 vs β_6 is shown in Fig. (8) and we obtain the optimal values of β_5 and β_6 as 0.00813684556860650062 and 0.00136374541912936944.
We observe that the optimal values of β_5 and β_6 obtained using the metrics, M_2 and M_4 agree to 10 decimal places. Hence, the values of β_5 and β_6 that we use for our new scheme are 0.0081368456 and 0.0013637454 respectively.

5.1 Comparison of known methods with new method

In our work, we shall take $\beta_5 = 0.0081368456$ and $\beta_6 = 0.0013637454$. Table (1) gives values for β_5 and β_6 for four temporal Runge-Kutta schemes namely; Hu et al., Mead and Renaut, Tselios and Simos and our new method. We use Eqs. (26) and (27) to obtain the plots of the dissipation and dispersion errors vs yk.

Figs. (9) and (10) shows the plot of the magnitude of the dispersion and dissipation errors vs yk for four temporal Runge-Kutta schemes.
With increase in yk, the magnitude of the dispersion error increases as expected. The scheme proposed by Mead and Renaut and Hu et al. have significantly more dispersion error than the other two schemes. The dispersion error from Tselios and Simos [25] is slightly smaller than the one by Appadu for $yk \in [0, 0.8]$ but for $yk > 0.8$, the dispersion error from Appadu is much less than the other three schemes.
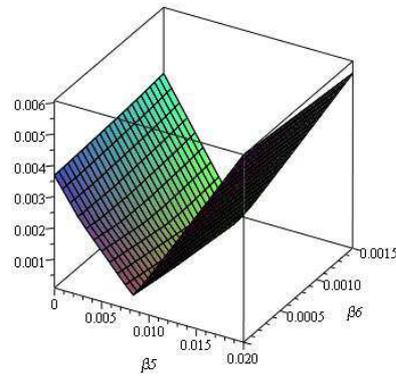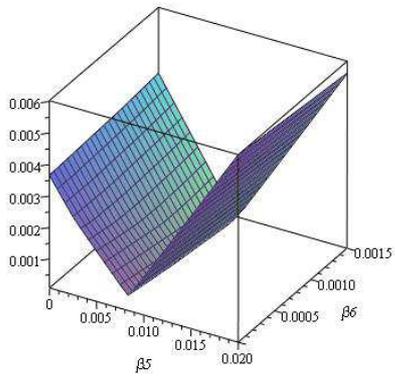
Fig. 5: Plot of Integrated Error from M_1 vs vs β_5 vs β_6.
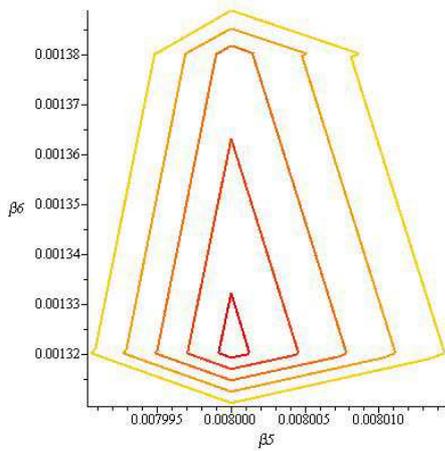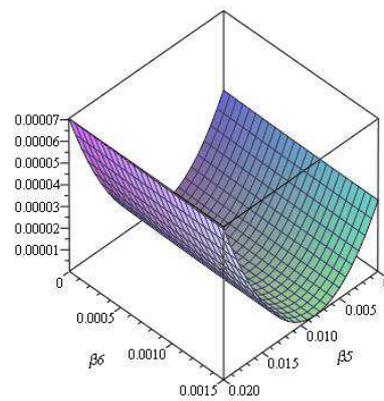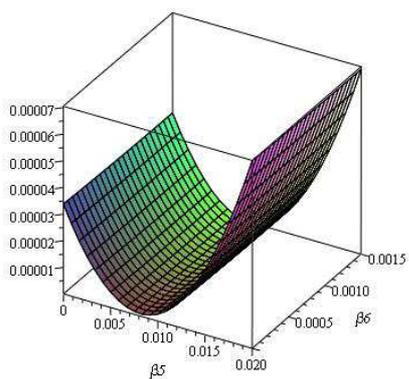

Fig. 6: Plot of Integrated Error from M_2 vs vs β_5 vs β_6.

Fig. 7: Plot of Integrated Error from M_3 vs vs β_5 vs β_6.

Fig. 8: Plot of Integrated Error from M_4 vs vs β_5 vs β_6.
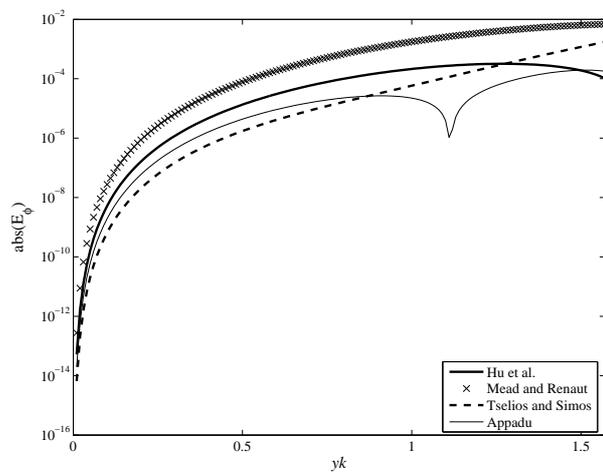

Fig. 9: Plot of the magnitude of the dispersion error on a logarithmic scale vs $yk \in [0, 1.5]$ for some temporal discretisation schemes.

Table 1: Comparing the coefficients of β_5 and β_6 for the four Runge Kutta schemes

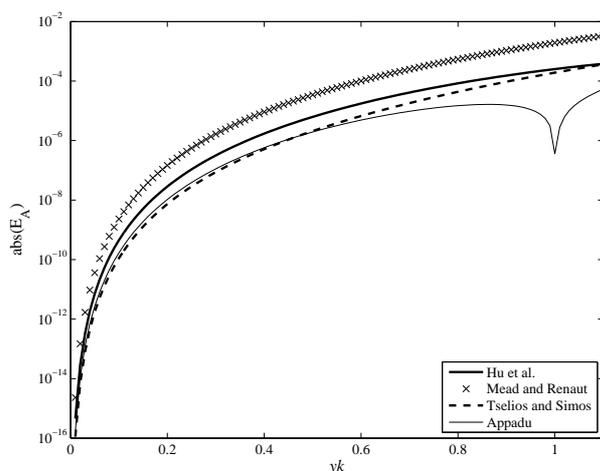| Method	β_5	β_6
Hu et al. [14]	0.00781005	0.00132141
Mead and Renaut [19]	0.00556	0.00093
Tselios and Simos [25]	0.0082673838	0.0012116682
Appadu	0.0081368456	0.0013637454

Fig. 10: Plot of the magnitude of the dissipation error on a logarithmic scale vs $yk \in [0, 1.1]$ for some temporal discretisation schemes.

The scheme proposed by Mead and Renaut [19] has the largest dissipation error followed by the one proposed by Hu et al. [14]. The scheme by Tselios and Simos, Appadu have almost the same dissipation error for $yk \in [0, 0.5]$ but for $yk > 0.5$, the scheme by Appadu has significantly less dissipation error.

6 Numerical Experiments

6.1 Convective Wave Equation

We consider the following partial differential equation:

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0. \tag{42}$$

At $t = 0$, we have a Gaussian profile, $u_0 = 0.5 \exp\left[-\left(\frac{x}{3}\right)^2\right]$ [25] and the domain extends from $x_{min} = -50$ to $x_{max} = t + 50$. The analytical solution is $u(x,t) = 0.5 \exp\left[-\left(\frac{x-t}{3}\right)^2\right]$.

A nine point centred difference scheme of eight order is used for the spatial discretization which is given by

$$\frac{\partial u}{\partial x} \approx \frac{1}{h}\left(-\frac{4}{5}(u_{i-1}^n - u_{i+1}^n) + \frac{1}{5}(u_{i-2}^n - u_{i+2}^n)\right.$$
$$\left. -\frac{4}{105}(u_{i-3}^n - u_{i+3}^n) + \frac{1}{280}(u_{i-4}^n - u_{i+4}^n)\right). \tag{43}$$

Our new method is compared with
(i) the fourth-order six-stage Runge-Kutta scheme of Hu et al [14].
(ii) the fourth-order six-stage Runge-Kutta scheme of Mead and Renaut [19].
(iii) the fourth-order six-stage Runge-kutta scheme of Tselios and Simos [25]

In all four cases, we have used a nine point centred difference scheme of eight order for the spatial discretization scheme.

Our aim is to obtain values of the error rate with respect to the L_1-norm and the Total Mean Square Error [22] which are computed as

$$E_{num} = h \sum_{i=1}^{N} |u_c - u_e|, \tag{44}$$

and

$$\frac{1}{N} \sum_{i=1}^{N} (u_c - u_e)^2, \tag{45}$$

where u_c and u_e are the computed and exact values, respectively and N is the number of spatial grid points. The Total Mean Square Error is equivalent to the sum of the dispersion and dissipation errors as shown by Takacs [22]. We then plot these two types of errors vs the CFL number and find out how these two errors vary with the CFL number. We consider two cases namely, $t = 400$ and $t = 1000$.

Case 1
We consider the case when time, $t = 400$, and spatial step, $h = 0.5$. Since, CFL$= k/h$, and $k = 400/n_{max}$, then

$$CFL = 800/n_{max}, \tag{46}$$

where n_{max} is the number of time steps.
We use some CFL numbers to satisfy (46) such that n_{max} is an integer. Once n_{max} has been determined, we can find the time step, k. The CFL numbers we consider and the corresponding values of n_{max} and k are shown in Table (2).

Fig. (11) shows the variation of the error rate vs CFL for four numerical schemes. The general tendency is that the error is not much affected by the choice of the CFL number except in the case of Mead and Renaut. We have

Table 2: Some values of CFL, n_{max} and k for time, $t = 400$ and spatial step, $h = 0.5$

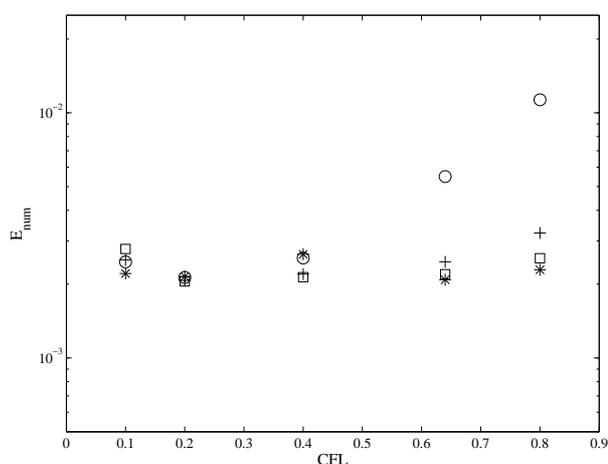| CFL	n_{max}	k
0.1	80000	0.05
0.2	4000	0.1
0.4	2000	0.2
0.64	1250	0.32
0.80	1000	0.40

Fig. 11: Error rate as a function of CFL, using Runge-Kutta scheme of Hu et al $'+'$, Mead and Renaut 'o', Tselios and Simos $'\square'$ and our new scheme, New $'*'$, all combined with a nine-point central difference scheme of eight order at time, $t = 400$ and spatial step, $h = 0.5$.

considered five CFL numbers namely 0.1, 0.2, 0.4, 0.64 and 0.8. At CFL 0.1, 0.64 and 0.8, our scheme is the most effective one. At CFL 0.4, the schemes by Tselios and Simos and Hu et al. are the most effective.

Fig. (12) shows the variation of the Total Mean Square Error vs the CFL number. The general tendency is that the error increases with increase in CFL number for the scheme by Mead and Renaut and Hu et al. Our scheme followed by Tselios and Simos are the most effective ones over the five values of CFL used.

Case 2

We consider the case when time, $t = 1000$ and $h = 0.5$. Values of CFL and the corresponding values of n_{max} and k are shown in Table (3). The difference is since the time has now been multiplied by 2.5, therefore the values of n_{max} are multiplied by 2.5, as compared to the values in Table (2).
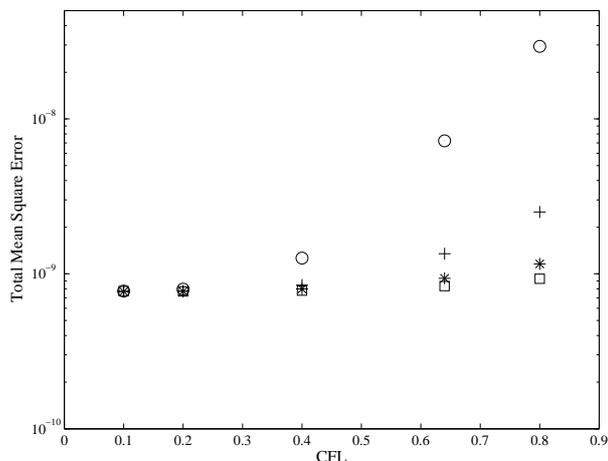

Fig. 12: Total Mean Square Error as a function of CFL, using Runge-Kutta scheme of Hu et al $'+'$, Mead and Renaut 'o', Tselios and Simos $'\square'$ and our new scheme, New $'*'$, all combined with a nine-point central difference scheme of eight order at time, $t = 400$ and spatial step, $h = 0.5$.

Table 3: Some values of CFL, n_{max} and k for time, $t = 1000$ and spatial step, $h = 0.5$

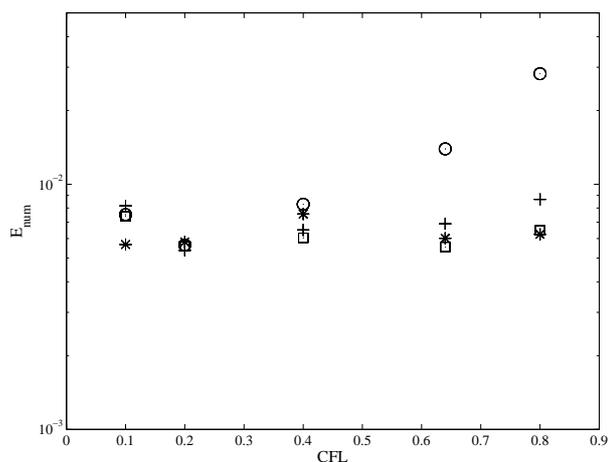| CFL	n_{max}	k
0.1	20000	0.05
0.2	10000	0.1
0.4	5000	0.2
0.64	3125	0.32
0.80	2500	0.40

Fig. 13: Error rate as a function of CFL using Runge-Kutta scheme of Hu et al $'+'$, Mead and Renaut $'o'$, Tselios and Simos $'\square'$ and our new scheme, New $'*'$, all combined with a nine-point central difference scheme of eight order at time, $t = 1000$ and spatial step, $h = 0.50$.

Fig. 14: Total Mean Square Error as a function of CFL using Runge-Kutta scheme of Hu et al $'+'$, Mead and Renaut $'o'$, Tselios and Simos $'\square'$ and our new scheme, New $'*'$, all combined with a nine-point central difference scheme of eight order at time, $t = 1000$ and spatial step, $h = 0.50$.
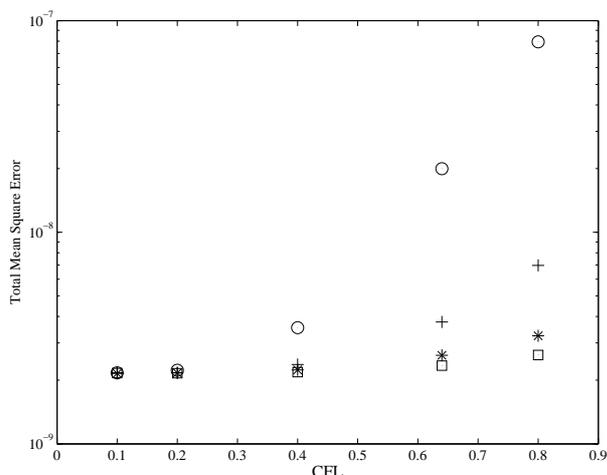
Fig. (13) shows the variation of the error rate vs CFL. The values of the error rate are much affected by the CFL number in the case of Runge-Kutta scheme proposed by Mead and Renaut. At CFL 0.1, 0.64 and 0.8, our proposed scheme is better. At CFL 0.4, the scheme by Tselios and Simos is slightly better. Over the five CFL numbers, our scheme is generally the best one followed by the scheme of Tselios and Simos.

Fig. (14) shows the variation of the Total Mean Square Error vs CFL. The values of the Total Mean Square Error are much affected by CFL in the case of Runge Kutta schemes by Hu et al., Mead and Renaut.

6.2 Spherical Wave Problem [12]

We consider the following problem

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial r} + \frac{u}{r} = 0, \qquad (47)$$

where $5 \leq r \leq 315$ and $t > 0$.

The initial condition is $u(r,0) = 0$ for $5 \leq r \leq 315$.

The boundary condition is $u(5,t) = \sin(\pi t/3)$ for $0 < t < 300$.

The analytic solution is given by

$u(r,t) = 0$ for $r > t + 5$ and
$u(r,t) = \frac{5}{r} \sin(\pi(t-r+5)/3)$ for $r \leq t+5$.

Since we have found from section 6.1 that low CFL numbers are preferred to minimise both dispersion and

dissipation errors, we shall use a small CFL for this experiment, say 0.1. We perform the numerical experiment at time, $t = 300$ at CFL=0.1 with time step 0.02 and spatial step 0.2. The error rate with respect to L_1 error and the Total Mean Square Error are compared in Table (4). The results are shown in Fig. (15). Once again, it is seen that the scheme by Appadu is the best one.
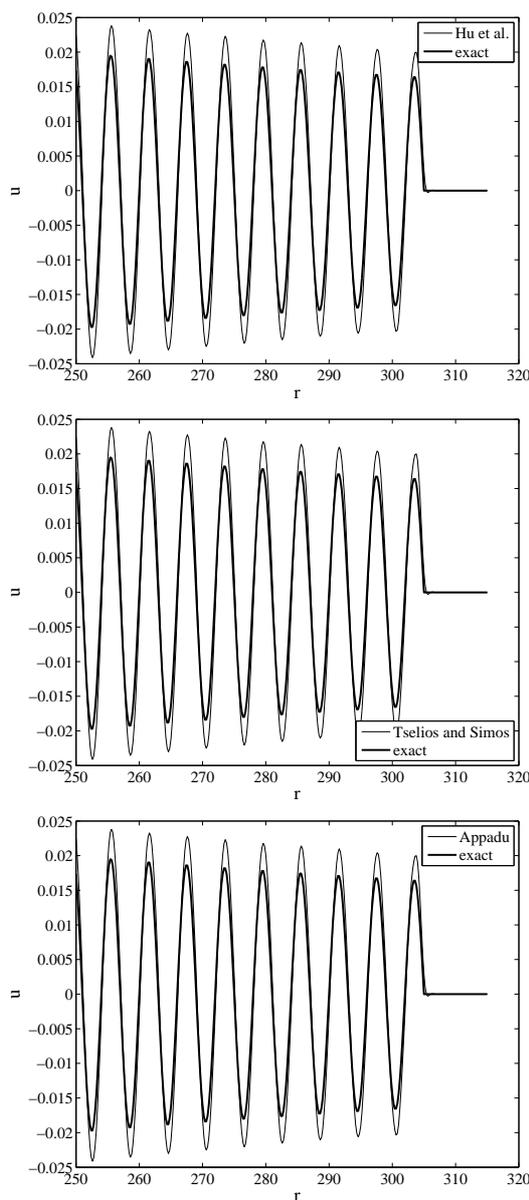

Fig. 15: Solution of the spherical wave problem with three temporal Runge-Kutta schemes, all coupled with with a nine-point centred difference scheme of eight order at time, $t = 300$ with spatial step 0.2 and time step 0.02.

Table 4: Spherical wave problem with spatial step 0.2 and time step 0.02

Method	Error rate - L_1 error	Total Mean Square Error
Hu et al.	3.081115	3.863205×10^{-4}
Tselios and Simos	3.081116	3.863204×10^{-4}
Appadu	3.081114	3.863198×10^{-4}

7 Conclusion

We have performed a spectral analysis of the dispersion and dissipation errors of four temporal Runge-Kutta schemes coupled with a nine-point centred difference scheme of eight order and seen that our proposed scheme has the best dispersive and dissipative character. Based on the plots of the error rate of the L_1 norm and the Total Mean Square Error vs CFL number for the convective wave equation, we conclude that our proposed scheme is better than the other three schemes when h is chosen as 0.50 at two different times, $t = 400$ and $t = 1000$. Also, our proposed scheme is the best one for the simulation of the spherical wave problem. These demonstrate that our technique of optimisation is effective to construct low dispersion and low dissipation Runge-Kutta schemes. Secondly, we observe that the general trend is that low CFL numbers are more efficient than larger CFL numbers in the case of optimized schemes as opposed to standard schemes.

One possible extension of this work is to take stability into consideration when we optimise the parameters which control the grade and balance of dispersion and dissipation. We will aim to construct low dispersion and low dissipation Runge-Kutta schemes with large range of stability.

Nomenclature

$I = \sqrt{(-1)}$
k: time step
h: spatial step
n: time level
β: advection velocity
c: CFL/Courant number
$c = \dfrac{\beta k}{h}$
w: phase angle in 1-D
$w = \theta h$
RPE: relative phase error per unit time step
AF: amplification factor
$AFM = |AF|$
LDLD: Low Dispersion and Low Dissipation
IEELDLD: Integrated Exponential Error for Low Dispersion and Low Dissipation
MIEELDLD: Minimised Integrated Exponential Error for Low Dispersion and Low Dissipation.

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