Closure Report

File Number : MTR/2017/000038

Project Title : Development of dispersion, dissipation characteristics preserving finite difference schemes for fluid flow problems.

Principal Investigator : Dr. Shuvam Sen

Tezpur University

Distt. sonitpur p.b.no.72 napaam, tezpur, Tezpur, Assam-784011

Total Sanctioned Amount : 0 (INR)

Total Released Amount : 5,60,000 (INR)

Start Date of the Project: 13 Jun, 2018

Date of completion: 12 Jun, 2021 (36 months)

Approved Objectives :

Not Available

Deviation made from original objectives (If Any) :

-

Ph.D. Produced/Likely to be Produced	: 1
Technical Personnel Trained	: 0
Total Expenditure	: 5,60,000 (INR)

Concise Research Accomplishment :

Accomplishments are summarized below: 1. The possibility of low-dissipation low-dispersion diagonally implicit R-K schemes has been thoroughly investigated. 2. In the process, an algorithm is derived to propose two, three, and four stage diagonally implicit R-K schemes with negligible dissipation and optimally low-dispersion characteristics. 3. We also document, probably for the first time, numerical dispersion and dissipation characteristics of two and three stage Gauss-Legendre methods, viz. IRK24 and IRK36. Their inherent potential beyond the order of accuracy is highlighted. 4. Weighted phase error reduction with targeted wavenumber space is advocated and is found suitable. We see that IRK24 and IRK36 relate to the limiting case of the strategy advocated in this study. As we work with A-stable schemes, it is noticed that no single implicit R-K scheme might be equally efficient across all step sizes. Subsequently, an algorithm is devised to come up with distinct classes of two and three stage implicit R-K methods and observed that different methods are best for a diverse range of time steps. 5. Further, as dispersion error reduction at times results in dissipation error growth and conversely, an independent study is conducted leading to a new three stage second order diagonally implicit scheme. Such a scheme carries an optimum balance of dissipation and dispersion accuracy is found better compared to the other three stage low-dissipation low-dispersion A-stable diagonally implicit schemes. 6. Moving to spatial discretization, we derive a family of upwind compact schemes with an optimally high dispersive order of accuracy. Appropriate boundary and near boundary closure schemes help maintain the global high accuracy of these schemes. The asymptotic stability analysis establishes the efficiency of the schemes for long time simulation. 7. Different numerical examples in one and two dimensions covering linear and non-linear propagation problems have been solved for verification studies of newly developed spatial and temporal schemes. 8. We also work with nonuniform grids and develop a scheme based on a comparatively smaller five-point stencil. It leads to an algebraic system of equations with constant coefficients. The scheme carries the flow variable and its gradients as unknown and is seen to report back truncation accuracy of order four for linear flow problems even in a nonuniform mesh. Temporally the scheme is second-order accurate. Both primitive and vorticity-streamfunction formulations of the Navier-Stokes equations, as well as the Boussinesq equations, have been successfully tackled using the proposed formulation.

Closure Details

Experimental/ Theoretical Investigation carried out

Please refer to the attached .pdf file (Other Information Document). This is done as I found it extremely difficult to write mathematical symbols and equations in this space. Hope it will be acceptable.

Detailed Analysis of result

Please refer to the attached .pdf file (Other Information Document). This is done as I found it extremely difficult to write mathematical symbols and equations in this space. Hope it will be acceptable.

Conclusions

At first, we concentrated on the development of temporal discretization procedures. A new class of A-stable diagonally implicit four-stage R-K methods with minimal dissipation and optimally low-dispersion error is proposed. These schemes obtained by minimizing both amplification and phase error are fourth-order accurate and are suitable for stiff systems. An algorithm is outlined and is used to develop diagonally implicit R-K methods of two, three, and four stages having low-dissipation low-dispersion virtues while retaining, to a large extent, inherent stability and high accuracy. Next, we extend the strategy for fully implicit R-K schemes. Here, we analyze dissipation and dispersion characteristics of the most accurate two and three-stage Gauss-Legendre implicit R-K methods. These methods are observed to carry minimum dissipation error along with the highest possible dispersive order in their respective classes and are inherently optimized to carry low phase error only at small wavenumber. As larger temporal step size is imperative in conjunction with implicit methods, it is noticed that a unique scheme might not be best across diverse temporal step sizes. We derive a class of minimum dissipation and optimally low-dispersion implicit R-K schemes by cutting down amplification error and maximum reduction of weighted phase error. They indeed carry better accuracy for relatively bigger and varied CFL numbers. Afterward, we explore the idea of simultaneous reduction of dissipation and dispersion error to come up with a new three-stage second-order diagonally implicit R-K method maintaining A-stability for the entire wavenumber range. Contrary to earlier efforts of complete reduction of amplitude error we look to allow small dissipation error and thereby enhance our leeway to substantially reduce dispersion error. Subsequently, we work for developing a new family of upwind compact schemes. These schemes sustain optimally attainable dispersive order of accuracy and carry virtues of minimized weighted phase error in L^2-norm over a complete wavenumber space. An integrated approach is followed whereby appropriate boundary closure schemes with the highest possible dispersive and overall accuracy are also developed. The asymptotic stability analysis with eigenvalue determination points to the long-time stability of the integrators. Finally, a new transformation-free compact formulation for the Navier-Stokes equations has been proposed. The scheme generalizes the idea of fourth-order implicit (5-5)CC formulation to nonuniform grid and carries wider appeal. Although, theoretically the scheme is only third-order accurate it is found to report higher convergence order for linear problems. The scheme is found to be suitable for both primitive variable and streamfunction-vorticity formulations. Diverse and appropriately designed numerical test cases help establish the efficiency and benefits of various schemes developed in this project.

Scope of future work

Possibility of future works are listed below: 1. In the future, we want to use the newly developed spatial and temporal schemes to simulate fluid flow problems mimicking physical situations. In particular, we are interested to explore flow around bluff bodies and fluid-structure interaction problems. 2. Further, we are interested to construct optimized Runge-Kutta methods for the solution of orbital problems like second order initial value problems. 3. We are also interested to derive high dispersive order accurate upwind compact finite difference schemes for higher order derivatives. 4. The schemes may be investigated for their potential in non-uniform grids as well. 5. Additionally, as the propagation problems involve an interplay between space and time, we shall like to approximate both spatial and temporal derivatives in a way related to each other as required by the dispersion relation of the governing PDE.

List of Publications (only from SCI indexed journals) :

Title of the Paper	List of Authors	Journal Details	Month & Year	Volume	Status	DOI No	Impact Factor
A new transformation free generalized (5,5)HOC discretization of transient Navier-Stokes/Boussinesq equations on nonuniform grids	Dharmaraj Deka, Shuvam Sen	INTERNATIONAL JOURNAL OF HEAT AND MASS TRANSFER (International)	Jun-2020	171 (21)	Published	doi.org/10.1016/j.ijheatmasstransfer.2020.120821	4.947
A new class of diagonally implicit Runge-Kutta methods with zero dissipation and minimized dispersion error	Subhajit Giri, Shuvam Sen	JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS (International)	Jun-2020	376 (23)	Published	https://doi.org/10.1016/j.cam.2020.112841	1.883

List of Papers Published in Conference Proceedings, Popular Journals :

Title of the Paper	List of Authors	Journal Details	Month & Year	Volume	Status	DOI No	Impact Factor
A New (3, 3) Low Dispersion Upwind Compact Scheme	Subhajit Giri, Shuvam Sen	Communications in Computer and Information Science (International)	Aug-2021	1345 (134-145)	Published	https://doi.org/10.1007/978-981-16-4772-7_10	

List of Patents filed/ to be filed :

Patent Title	Authors	Patent Type	Country/Agency Name	Patent Status	Application/Grant No.
Not Available					

Equipment Details :

Equipment Name	Cost (INR)	Procured	Make & Model	Utilization %	Amount Spent (INR)	Date of Procurement
Not Available						

Plans for utilizing the equipment facilities in future:

Not Available

File No. MTR/2017/000038

Principal Investigator: Dr. Shuvam Sen, Tezpur University
Project Title: Development of dispersion, dissipation characteristics preserving finite difference schemes for fluid flow problems

MATHEMATICAL RESEARCH IMPACT-CENTRIC SUPPORT SCHEME

Experimental/ Theoretical Investigation carried out
&
Detailed Analysis of result

1 Brief Review

To analyse a time advancing procedure it is often a good idea to start with initial value problem (IVP) of the form

$$\frac{du}{dt} = f(t,u), \quad u(t_0) = u_0. \tag{1.1}$$

The general R-stage Runge-Kutta (R-K) method can be defined as

$$u^{n+1} = u^n + \Delta t \sum_{r=1}^{R} b_r F_r \tag{1.2}$$

where

$$F_r = f\left(t^n + \Delta t c_r, u^n + \Delta t \sum_{s=1}^{R} a_{rs} F_s\right), \quad r = 1, 2, ..., R, \tag{1.3}$$

$$c_r = \sum_{s=1}^{R} a_{rs}, \qquad r = 1, 2, ..., R. \tag{1.4}$$

Using Butcher tableau [6] the above methods can be represented as

$$\begin{array}{c|c} \boldsymbol{c} & \boldsymbol{A} \\ \hline & \boldsymbol{b}^T \end{array} \tag{1.5}$$

where $\boldsymbol{A} = (a_{rs})_{R\times R}$, $\boldsymbol{b} = (b_r)_R^T$, $\boldsymbol{c} = (c_r)_R^T$. For explicit R-K scheme $\boldsymbol{A}$ is strictly lower triangular and for diagonally implicit schemes (DIRK) $\boldsymbol{A}$ is lower triangular with non-zero diagonal entries. At times a diagonally implicit scheme is further categorized as singly diagonally implicit (SDIRK) if its all diagonal entries are equal.

The consistency condition, which also guarantee first order accuracy, demands that

$$O(\Delta t) : \sum_{r=1}^{R} b_r = 1. \tag{1.6}$$

Some tedious derivation leads to the following order conditions [6]

$$O(\Delta t^2) \quad : \quad \sum_{r=1}^{R} b_r c_r = \frac{1}{2}, \tag{1.7}$$

$$O(\Delta t^3) \quad : \quad \sum_{r=1}^{R} b_r c_r^2 = \frac{1}{3}, \tag{1.8}$$

$$\sum_{r=1}^{R}\sum_{s=1}^{R} b_r a_{rs} c_s = \frac{1}{6}, \tag{1.9}$$

$$O(\Delta t^4) \quad : \quad \sum_{r=1}^{R} b_r c_r^3 = \frac{1}{4}, \tag{1.10}$$

$$\sum_{r=1}^{R}\sum_{s=1}^{R} b_r c_r a_{rs} c_s = \frac{1}{8}, \tag{1.11}$$

$$\sum_{r=1}^{R}\sum_{s=1}^{R} b_r a_{rs} c_s^2 = \frac{1}{12}, \tag{1.12}$$

$$\sum_{r=1}^{R}\sum_{s=1}^{R}\sum_{l=1}^{R} b_r a_{rs} a_{sl} c_l = \frac{1}{24}. \tag{1.13}$$

Eqs. (1.6)-(1.13) may not be independent. In fact, only two of the three Eqs. (1.11)-(1.13) are independent. Fifth and sixth order accuracy require satisfaction of additional nine and twenty conditions respectively [6].

2 Diagonally implicit R-K schemes with zero dissipation and optimally low dispersion error

Simulations in computational acoustics require highly accurate numerical schemes having low-dissipation low-dispersion characteristics in addition to large stability limits. A review of the literature reveals that most of the works have been done based on explicit R-K methods [2, 3, 5, 10, 16] barring a few.

As implicit R-K methods often lead to a full system of implicit non-linear equations and solutions of such a system at each time step is considered computationally expensive. Alexander [1] pointed out that a way out of this difficulty lies in designing diagonally implicit R-K schemes where the equations can be solved successively. During the last few years, we have seen renewed interest in diagonally implicit (DIRK) schemes as they offer the best compromise between computational efficiency and stability. In this connection, Najafi-Yazdi and Mongeau [12] proposed a three stage diagonally implicit A-stable low-dispersion low-dissipation R-K scheme. We further refer to the work of Nazari et al. [13] where three truly fourth order three stage diagonally implicit R-K schemes are investigated and optimized associated error function which is the ratio of numerical amplitude to the analytical amplitude is used to arrive at low-dissipation low-dispersion scheme. These schemes are presented in Table 1.

We propose a new class of A-stable diagonally implicit four stage R-K methods with minimal dissipation and optimally low dispersion error. These schemes obtained by mini-

Table 1: Fourth order three stage low-dissipation low-dispersion diagonally implicit R-K (LDDDIRK34) schemes.

Parameter	Schemes		
	Set1	Set2	Set3
b_1	1.351467260320785	0.006645466304608	0.667655846089925
b_2	−1.702414526538024	0.320198061838696	0.325888518017914
b_3	1.350947266217122	0.673156471856696	0.006455635892161
a_{11}	0.675592332328701	−0.851263454665540	0.678600761183237
a_{21}	1.351242940337120	0.221282760003727	−0.565323026062134
a_{22}	−0.851207182169909	0.675716813905398	0.672651748784065
a_{31}	1.351467260320785	−0.078577212831902	−8.404346586781380
a_{32}	−1.702697002012658	−0.272422066827441	11.106859072314800
a_{33}	0.675614858556262	0.675499639829671	−0.851256242766855

mizing both amplification and phase error enjoy fourth order of accuracy and are suitable for stiff systems. We outline here a generalized algorithm which is subsequently applied to propose two, three and four stage diagonally implicit R-K schemes. The algorithm is easy to implement and for three stage it is seen that the proposed algorithm advance the very same set of schemes as advocated by Nazari et al. [13] pointing out little scope of ambiguity in its application. A comparative study is carried out with other diagonally implicit schemes available in the literature by solving numerical test cases.

2.1 Dissipation and dispersion characteristics of implicit R-K schemes

Stability and phase-lag analysis of implicit R-K method can be done by using the test equation

$$\dot{u} = I\lambda u, \quad I = \sqrt{-1}. \tag{2.1}$$

Following Eq. (1.2), the solution at $(n+1)$-th time step is given by

$$u^{n+1} = \big(1 + I\sigma \boldsymbol{b}^T(\boldsymbol{I}_R - I\sigma\boldsymbol{A})^{-1}\mathbf{1}\big)u^n \tag{2.2}$$

where $\boldsymbol{I}_R$ is the identity matrix of order R, $\sigma = \lambda\Delta t$ and $\mathbf{1} = (1, 1, ..., 1)^T$ being a vector of length R.
The numerical amplification can be represented as

$$G_N(\sigma) = 1 + I\sigma\boldsymbol{b}^T(\boldsymbol{I}_R - I\sigma\boldsymbol{A})^{-1}\mathbf{1}. \tag{2.3}$$

Comparing with the exact amplification

$$G_E(\sigma) = e^{I\sigma}, \tag{2.4}$$

we see that for a numerically stable R-K scheme i.e. $|G_N(\sigma)| \leq 1$, the amplification (dissipation) and phase (dispersion) errors are represented by $a(\sigma) = 1 - |G_N(\sigma)|$ and $\phi(\sigma) = \sigma - \boldsymbol{arg}(G_N(\sigma))$ respectively.

2.2 Algorithm

In brief, we start by choosing an appropriate stage number R for the scheme and then appeal at least second order accuracy. We have to introduce additional conditions such that $|G_N(\sigma)|$ is unity throughout and insist requisite accuracy and make available free parameters. Then we formulate phase error in L^2-norm over wavenumber space and deduce constrained minimization conditions. Finally, we have to solve the entire system of equations to arrive at the proposed methods.

2.3 Two stage diagonally implicit schemes

In two stage diagonally implicit schemes $\boldsymbol{A} = (a_{rs})_{2\times 2}$ with $a_{12} = 0$. As such there are five free parameters $\{b_r, a_{rs} : 1 \leq s \leq r \leq 2\}$ which are to be determined. Three set of schemes are given in Table 2 termed as S2DD1, S2DD2 and S2DD3.

Table 2: Second order two stage low-dissipation low-dispersion diagonally implicit R-K (LDDDIRK22) schemes.

	Schemes		
Parameter	S2DD1	S2DD2	S2DD3
b_1	0.3000000000	-1.0000000000	0.5000000000
b_2	0.7000000000	2.0000000000	0.5000000000
a_{11}	0.2500000000	0.2500000000	0.2500000000
a_{21}	0.3571485714	0.1250000000	0.5000000000
a_{22}	0.2500000000	0.2500000000	0.2500000000

2.4 Three stage diagonally implicit schemes

Here $\boldsymbol{A} = (a_{rs})_{3\times 3}$ with $a_{12} = a_{13} = a_{23} = 0$ and as such there are nine free parameters $\{b_r, a_{rs} : 1 \leq s \leq r \leq 3\}$ which are to be determined such that the schemes enjoy not only high accuracy but also good dissipation and dispersion characteristics. Three set of schemes are given in Table 3 termed as S3DD1, S3DD2 and S3DD3. These methods closely resemble to the ones proposed by Nazari et al. [13] as given in Table 1.

2.5 Four stage diagonally implicit schemes

Finally, four stage diagonally implicit R-K schemes are considered. For such a case, out of twenty parameters $\{b_r, a_{rs} : 1 \leq s \leq r \leq 4\}$, only fourteen are free since $a_{12} = a_{13} = a_{14} = a_{23} = a_{24} = a_{34} = 0$ where $\boldsymbol{A} = (a_{rs})_{4\times 4}$. Four set of schemes are given in Table 4 termed as S4DD1, S4DD2, S4DD3 and S4DD4.

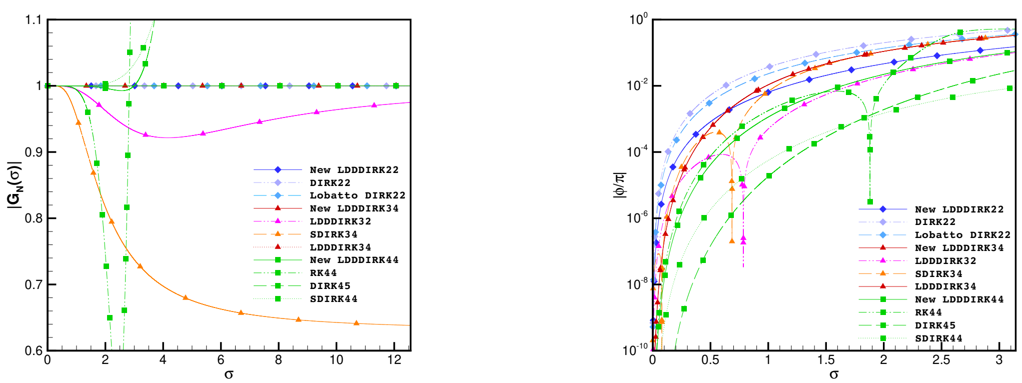
2.6 Comparison of numerical characteristics

We compare the numerical characteristics of diverse groups of schemes derived here with those available in the literature. Among two stage schemes, we consider Lobatto DIRK22 and DIRK22 schemes [6]. Among three stage schemes, low-dispersion low-dissipation

Table 3: Fourth order three stage low-dissipation low-dispersion diagonally implicit R-K (LDDDIRK34) schemes. Parameters closely resembles excogitation of Nazari et al. [13].

Parameter	Schemes		
	S3DD1	S3DD2	S3DD3
b_1	1.3512071855	0.0066398296	0.6729685779
b_2	-1.7024143710	0.3203915925	0.3203915925
b_3	1.3512071855	0.6729685779	0.0066398296
a_{11}	0.6756035959	-0.8512071919	0.6756035959
a_{21}	1.3512071919	0.2212466670	-0.5724538589
a_{22}	-0.8512071919	0.6756035959	0.6756035959
a_{31}	1.3512071811	-0.0786693505	-7.9733975150
a_{32}	-1.7024143730	-0.2725378414	10.6758118987
a_{33}	0.6756035959	0.6756035959	-0.8512071919

three stage diagonally implicit R-K (LDDDIRK32) method of Najafi-Yazdi and Mongeau [12], low-dissipation low-dispersion three stage fourth order diagonally implicit R-K (LDDDIRK34) method derived by Nazari et al. [13] and SDIRK34 [1] are considered. Among four stage methods we consider fourth order explicit R-K (RK44) method, a highly accurate diagonally implicit four stage fifth order R-K (DIRK45) [6]



(a) (b)

Figure 1: *Characteristics of various schemes: (a) Amplification factor, (b) Dispersion error in logarithmic scale.*

and the four stage fourth order singly diagonally implicit R-K (SDIRK44) method [8]. From Figs. 1(a) and (b) we have seen that among two stage scheme New LDDDIRK22 is best in terms of dissipation and phase error. Among three stage schemes, the characteristics completely overlap each other for the case of LDDDIRK34 proposed by Nazari et al. [13] and the newly developed LDDDIRK34. LDDDIRK32 [12] also display some dissipation error as shown in Fig. 1(a) but phase error is quite less shown in Fig. 1(b). RK44, SDIRK44 and DIRK45 become unstable at relatively small σ values. We could not find any four stage diagonally implicit method in the literature having stability for all σ values. In this connection, our newly developed method might just be a pioneering at-

Table 4: Fourth order four stage low-dissipation low-dispersion diagonally implicit R-K (LDDDIRK44) schemes.

	Schemes			
Parameter	S4DD1	S4DD2	S4DD3	S4DD4
b_1	−0.2238860718	0.4866215829	0.8165015748	−1.1182093314
b_2	0.4038240795	−1.3327297974	−0.0190097285	−2.0742229755
b_3	0.0727310064	0.4766400136	−0.0662717273	1.8622050279
b_4	0.7473309859	1.3694682009	0.2687798810	2.3302272790
a_{11}	−0.4632975659	0.3303348139	0.3303348139	0.3164813760
a_{21}	−0.5285039679	1.0068323624	2.3982625691	0.2899912957
a_{22}	0.3303348139	−0.4632975659	−0.4632975659	0.3164813760
a_{31}	0.9132692810	0.6222820844	0.1473423563	0.8010561189
a_{32}	−1.7043081356	−0.6710982512	−0.0034155910	−0.0416687644
a_{33}	0.3164813760	0.3164813760	0.3164813760	−0.4632975659
a_{41}	−0.3804715540	0.8838149227	2.3233817066	−0.5581638372
a_{42}	0.6348036654	−0.6615144252	−0.0574270290	−0.0352818382
a_{43}	0.1127051360	0.1447367505	−1.4752984758	0.9327760476
a_{44}	0.3164813760	0.3164813760	0.3164813760	0.3303348139

tempt. New LDDDIRK44 shows negligible dissipation error and phase error is decidedly less at least for small σ values which are visible in Figs. 1(a) and (b) respectively.

Although diverse numerical examples were tested during we present here only one problem for brevity.

2.7 Problem: Linear convection equation

The linear convection equation

$$u_t + u_x = 0 \tag{2.5}$$

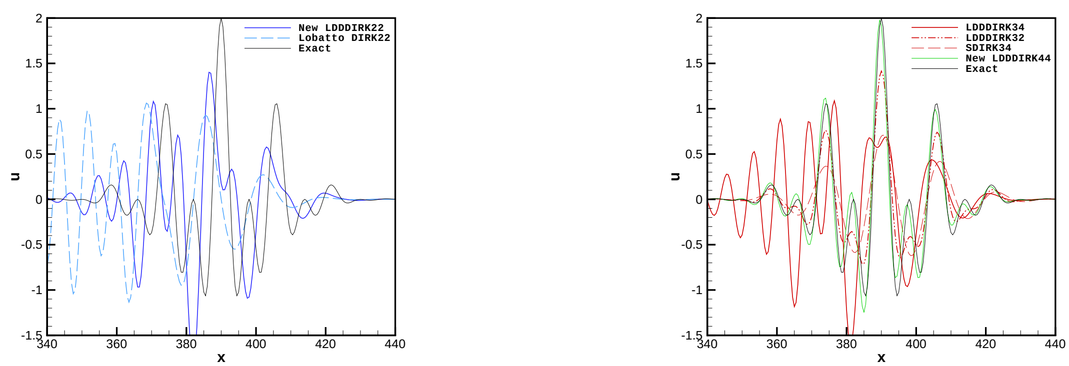
with initial condition

$$u(x,0) = e^{-\frac{(x-x_m)^2}{b^2}} \times [\cos(2\pi k_1(x-x_m)) + \cos(2\pi k_2(x-x_m))] \tag{2.6}$$

which is a combination of two waves of wavenumbers $2\pi k_1$ and $2\pi k_2$ is tested. Following Najafi-Yazdi and Mongeau [12] we take $x_m = 90$, $b = 20$, $k_1 = 0.125$ and $k_2 = 0.0625$ and compute solutions up to $t = 300$ for CFL numbers (N_c) from 0.5 to 2.0. Spatial discretization is carried out using sixth order five point Lele scheme [11] with $h = 0.5$. L^2-norm error for various schemes are given in Table 5. From Table 5, it is clear that the least error is reported for SDIRK44 and DIRK45 for $N_c = 0.5$, 1.0 and 1.5 which could be attributed to their low phase error at small σ values. But as N_c value increases these schemes suddenly lose stability in consonance with our earlier analysis and New LDDDIRK44 remains the best choice for computation. We also present our results in Fig. 2 for $N_c = 2.0$. Among two stage schemes, New LDDDIRK22 is clearly superior than Lobatto DIRK22 as seen in Fig. 2(a). DIRK22 does not converge at this N_c value. New LDDDIRK44 which carries the same accuracy as that of LDDDIRK34 [13] and SDIRK34 [1] but better dispersion characteristic generates significantly better result as seen in Fig. 2(b).

Table 5: Problem: L^2-norm error between numerical and exact solutions at $t = 300$.

Scheme	$N_c = 0.5$	$N_c = 1.0$	$N_c = 1.5$	$N_c = 2.0$
New LDDDIRK22	2.8400e-02	1.0990e-01	2.1891e-01	2.8387e-01
DIRK22	3.7762e-02	1.4291e-01	2.6006e-01	–
Lobatto DIRK22	1.0996e-01	2.8396e-01	1.9486e-01	2.8837e-01
LDDDIRK34	3.6062e-03	5.0853e-02	1.9504e-01	2.5039e-01
LDDDIRK32	4.6554e-03	1.9830e-02	4.5451e-02	7.7114e-02
SDIRK34	8.2628e-03	7.8975e-02	1.3682e-01	–
New LDDDIRK44	3.1447e-04	3.8421e-03	1.8295e-02	5.3904e-02
DIRK45	8.6713e-05	1.1398e-04	3.3721e-04	–
SDIRK44	5.8465e-05	1.0551e-04	7.5577e-04	–



(a) (b)

Figure 2: *Problem: Numerical solution at* $t = 300$ *computed with (a) two stage, (b) three and four stage schemes for* $N_c = 2.0$.

3 Fully implicit minimal dissipation low dispersion R-K schemes

The general R-K methods widely known as implicit R-K methods are more challenging vis-a-vis explicit ones. As pointed out by Butcher [6] there are compelling reasons to study them from a theoretical and practical point of view. One of the reasons for interest in implicit R-K schemes lies in their weak stability characteristics, which are superior to those of explicit schemes. Alexander [1] has noted in his work that for stiff problems only A-stable implicit R-K methods are useful. Explicit methods often suffer from stability limitations and as such small temporal step size becomes imperative. In numerical acoustics, small time steps lead to excessive computational cost. An A-stable implicit method allows one to compute with bigger step size thereby somewhat compensating for the additional time spent on each step. A R-stage implicit Gauss-Legendre method admits an order of accuracy as high as $2R$ as can be found in works of Butcher [6] and Alexander [1]. Nevertheless, it must be said that the ability to compute stiff problems that too with a relatively bigger time step is the main motivation for implicit R-K methods. Although good stability characteristics can be found in diagonally implicit R-K methods [8], it is amply clear that the phase-lag virtues of diagonally implicit schemes are a compromise between explicit and fully implicit methods.

In the current section, we analyze dissipation and dispersion characteristics of the most accurate two and three-stage Gauss-Legendre implicit R-K methods [6]. As larger temporal step size is imperative in conjunction with implicit R-K methods for physical problems, we interpret to derive a class of minimum dissipation and optimally low dispersion implicit R-K schemes which are obtained by cutting down amplification error and maximum reduction of weighted phase error, suggest better accuracy for relatively bigger CFL number. A potentially generalizable algorithm is used to design stable implicit R-K methods for a suitable time step with better accuracy virtues. As we focus on two and three-stage schemes a comprehensive comparison is carried out using numerical test cases. The idea developed in this section is relatively novel and new.

3.1 Summarized Methodology

The main steps that are to be followed in deriving low-dissipation low-dispersion schemes can be summarized as follows. First, we will start with an appropriate stage number $R = 2$ or 3. We introduce additional conditions such that $|G_N(\sigma)| = 1$ as discussed in this work. Then we look to impose the highest possible order of accuracy such that free parameters are available. We have to decide on appropriate weight kernel $e^{-\alpha\sigma^2}$ by keeping in mind period or wave number and time step. Phase error in L^2-norm over a suitable wave number space with the above chosen weight kernel is formulated. Subsequently, the minimization problem is dealt with for the corresponding point of minima. Finally, the resulting system of equations is solved to arrive at the method.

3.2 Two stage schemes

In two stage implicit schemes $\boldsymbol{A} = (a_{rs})_{2\times 2}$. We have used weighted phase error with a weight parameter α. We worked with four cases $\alpha = 0$, 4, 16, and $\alpha \to \infty$ to understand the effect of phase reduction which corresponds to S2A, S2B, S2C and S2D set of scheme. Two stage fourth order Gauss-Legendre scheme (IRK24) is found to belong to the S2D set of schemes. The corresponding schemes are given in Table 6.

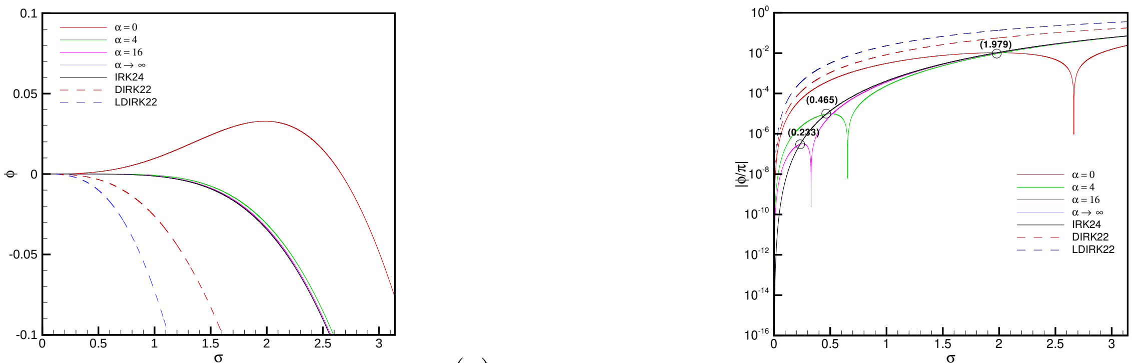
Table 6: Second order two stage low-dissipation low-dispersion implicit R-K schemes.

	Schemes				
Parameter	S2A	S2B	S2C	S2D	IRK24
b_1	0.5000000000	0.5000000000	0.6666666667	0.8367053706	0.5000000000
b_2	0.5000000000	0.5000000000	0.3333333333	0.1632946294	0.5000000000
a_{11}	0.2500000000	0.2500000000	0.2500000000	0.4183526852	0.2500000000
a_{12}	−0.0585699937	−0.0397174719	−0.0389376339	0.2091763426	−0.0386751346
a_{21}	0.5585699937	0.5397174719	0.5389376339	−0.2350933158	0.5386751346
a_{22}	0.2500000000	0.2500000000	0.2500000000	0.0816473148	0.2500000000

3.3 Comparison of numerical characteristics

The numerical phase difference of four different classes of scheme discussed above along with IRK24 is compared in Fig. 3(a). Additionally variation of phase error of two diagonally implicit second order schemes with optimized dissipation error viz. DIRK22 and

Lobatto DIRK22 [6] are also plotted. This figure amply demonstrated that there is no difference in the dispersive nature of the S2D scheme obtained using the asymptotic value of α and those of IRK24 and is indeed a member of a S2D family of schemes albeit with a higher order of accuracy. σ values at which phase variation graphs intersect is also shown in this figure. Fig. 3(b) makes it clear that with a varied choice of Δt distinct group of scheme might hold superiority with $T/\Delta t = 2\pi/\sigma$ and to the best of our knowledge is not documented in the literature.



(a) (b)

Figure 3: *(a) Phase difference and (b) dispersion error in logarithmic scale of various two stage schemes.*

3.4 Three stage schemes

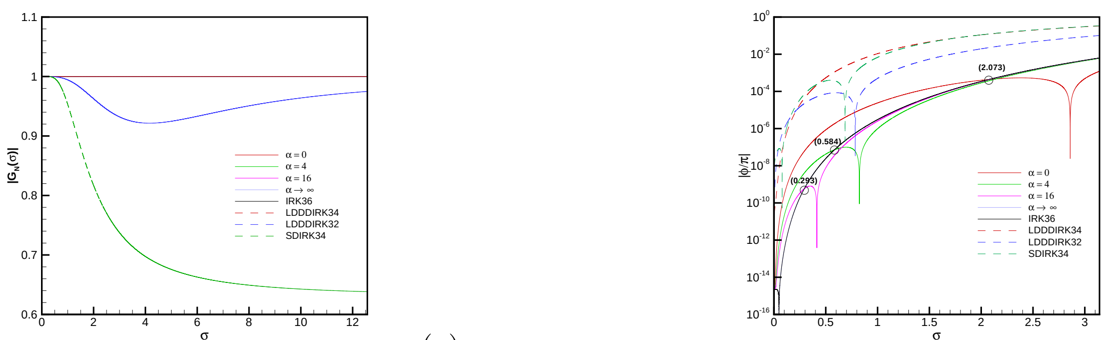
For three stage methods $\boldsymbol{A} = (a_{rs})_{3\times3}$, $\boldsymbol{b} = (b_r)_3$. Hence we are required to find as many as twelve free parameters $\{b_r, a_{rs} : 1 \leq r, s \leq 3\}$. As in two stage here again we work with four cases $\alpha = 0$, 4, 16, and $\alpha \to \infty$ to understand the effect of phase reduction which corresponds to S3A, S3B, S3C and S3D set of scheme. Three stage sixth order Gauss-Legendre scheme (IRK36) belongs to S3D set of schemes. The corresponding schemes are shown in Table 7.

3.5 Comparison of numerical characteristics

We compare the numerical characteristics of diverse groups of three stage schemes in Fig. 4(a) and (b) along with some diagonally implicit schemes available in the literature. As all methods studied here carry negligible dissipation errors as visible in Fig. 4(a), it is important to point out that no particular three stage R-K scheme might be superior globally i.e. across the entire range of Δt which is visible in Fig. 4(b). This inherent limitation noticed earlier in two stage fully implicit R-K methods is thus carried over to three stage methods as well. In our work, we have found a direct relation between dispersion error reduction and accuracy. It is seen that complete dispersion relation preservation across the entire wave number range is futile rather a targeted reduction with a specific region in mind yields dividend.

Table 7: Fourth order three stage low-dissipation low-dispersion implicit R-K schemes.

	Schemes				
Parameter	S3A	S3B	S3C	S3D	IRK36
b_1	0.4902164042	0.4968572595	0.4973158852	0.4974707660	0.2777777778
b_2	0.4902164042	0.4968572595	0.4973158852	0.4974707660	0.4444444444
b_3	0.0195671916	0.0062854810	0.0053682296	0.0050584680	0.2777777778
a_{11}	0.2267610814	0.2162822020	0.2155587380	0.2153144231	0.1388888889
a_{12}	0.0000000000	0.0000000000	0.0000000000	0.0000000000	−0.0359766675
a_{13}	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0097894440
a_{21}	0.5149632492	0.5384237709	0.5399915310	0.5405195031	0.3002631950
a_{22}	0.2396583441	0.2395278133	0.2395372403	0.2395409352	0.2222222222
a_{23}	0.0381882637	0.0120518190	0.0102807976	0.0096836713	−0.0224854172
a_{31}	0.7895342543	2.2933385501	2.6764782769	2.8373912650	0.2679883338
a_{32}	−0.8134251058	−2.3343956093	−2.7187053498	−2.8800130375	0.4804211120
a_{33}	0.0335805745	0.0441899847	0.0449040217	0.0451446417	0.1388888889



(a) (b)

Figure 4: *(a) amplification factor, (b) dispersion error in logarithmic scale.*

3.6 Problem: Periodic Test

In this test a periodical initial value problem represented by second order inhomogeneous ODE

$$\ddot{u} = -\kappa^2 u + (\kappa^2 - \omega^2)\sin(\omega t), \quad t \geq 0, \quad u(0) = u_0, \quad \dot{u}(0) = \bar{u}_0 \tag{3.1}$$

is numerically solved. This problem admit analytical solution

$$u(t) = u_0 \cos(\kappa t) + \frac{(\bar{u}_0 - \omega)\sin(\kappa t)}{\kappa} + \sin(\omega t). \tag{3.2}$$

With $\kappa > \omega$ the exact solution consists of a rapidly and a slowly varying function. For numerical computation two frequencies ω and κ are maintained at 10 and 15 respectively. With $u_0 = 0$ and $\bar{u}_0 = \omega$, the solution reduces to $u(t) = \sin(\omega t)$. Results obtained are arranged in Table 8. From the table also it is visible that for different values of Δt diverse schemes carry superior accuracy.

Table 8: Problem: Absolute error at point of maxima and relative CPU time (in parenthesis).

Scheme	Δt=0.016	Δt=0.032	Δt=0.064	Δt=0.128
S2A	1.6303e-3 (9.3)	6.3090e-3 (5.0)	2.2161e-2 (2.7)	5.4964e-2 (1.3)
S2B	7.5929e-5 (9.0)	2.1227e-4 (4.7)	**5.5976e-4**(2.3)	**2.2917e-2**(1.3)
S2C	1.3538e-5 (9.3)	**3.4885e-5** (4.7)	1.5168e-3 (2.3)	2.6517e-2 (1.0)
IRK24	**7.4294e-6** (9.3)	1.1798e-4 (4.7)	1.8392e-3 (2.7)	2.7734e-2 (1.3)
DIRK22	4.4369e-3 (8.0)	1.8065e-2 (4.0)	7.6434e-2 (2.3)	3.2599e-1 (1.3)
Lobatto DIRK22	6.7051e-3 (8.0)	2.8304e-2 (4.0)	1.2466e-1 (2.0)	2.8768e-1 (1.0)
S3A	5.0629e-7 (70.0)	7.9574e-6 (35.0)	1.1828e-4 (17.7)	1.3524e-3 (8.7)
S3B	3.6518e-8 (69.3)	4.8201e-7 (34.7)	**1.3072e-6** (17.7)	**3.5405e-4**(9.0)
S3C	7.6048e-9 (67.3)	**2.1913e-8** (35.0)	5.8897e-6 (24.0)	4.5921e-4 (9.3)
IRK36	**2.0722e-9** (67.3)	1.3199e-7 (34.7)	8.2968e-6 (18.0)	4.9438e-4 (9.0)
LDDDIRK34	4.4967e-4 (12.3)	6.4069e-3 (6.7)	7.6013e-2 (3.3)	4.7213e-1 (1.3)
LDDDIRK32	4.3874e-4 (12.7)	2.2474e-3 (6.3)	1.4103e-2 (3.0)	9.3179e-2 (1.7)
SDIRK34	6.7715e-4 (14.0)	2.6864e-3 (7.3)	1.9398e-2 (3.7)	3.0498e-2 (2.0)

4 Three stage low-dispersion low-dissipation diagonally implicit R-K method

In the previous sections, we concentrated on zero dissipation implicit R-K schemes. These schemes were subsequently optimized to reduce the dissipation error. In this section, we explore simultaneous reduction of dissipation and dispersion errors. Maintaining A-stability for the entire wave number range we look to allow small dissipation error thereby enhancing our leeway to substantially reduce dispersion error. Hu et al. [10] in their pioneering investigation on low-dissipation low-dispersion explicit R-K method allowed dissipation error $|a(\sigma)| \leq 0.001$ and argued to strive for dispersion error $|\phi(\sigma)| \leq 0.001$. Authors in their work successfully derived second order accurate four stage R-K methods with accuracy limit $\sigma = 0.85$. Nevertheless the scheme being explicit was found stable only upto $\sigma = 2.85$. Subsequently, Najafi-Yazdi and Mongeau [12] proposed a three stage diagonally implicit A-stable low-dispersion low-dissipation R-K scheme. Constrained by the stability criterion authors in [12] formulated a minimization problem to reduce the error between numerical and exact amplification over a chosen wave number range. Although theoretically second order accurate the main lacuna of the scheme was its failure to satisfy important relation between nodes (c_r) and weights (a_{rs}) viz. $c_r = \sum_{s=1}^{R} a_{rs}$, $r = 1, 2, ..., R$. The mathematical significance of this relation is thoroughly discussed by Nazari et al. [13].

Here, we propose a new A-stable diagonally implicit three stage R-K method with optimally low dispersion error and significantly less dissipation error. The scheme is obtained by minimizing weighted phase error and enjoy second order of accuracy. Comprehensive comparison with three stage diagonally implicit scheme (LDDDIRK32) proposed by Najafi-Yazdi and Mongeau [12] help reveal the efficiency of the newly developed scheme.

4.1 Procedure adopted

A step by step systematic procedure is adopted for deriving the method. For three stage diagonally implicit scheme we start by applying second order accuracy conditions. A weighted phase error is defined with weight parameter α via L^2-norm over the wave number space $[0, \pi]$. Mathematical simplification help express both the amplitude and phase of the scheme in three parameter space. A comprehensive study involving varied weight parameters reveal maximum attainable second order dispersive accuracy. The resultant A-stable scheme carries significantly lower dissipation error compared to its peers in the category. The proposed new class of schemes is given in Table 9 for different values of the weight parameter α. We shall like to advance the scheme correspond to $\alpha = 2048$ for its overall superiority.

Table 9: Second order three stage low-dispersion low-dissipation diagonally implicit R-K schemes.

	Schemes			
Parameter	$\alpha = 256$	$\alpha = 512$	$\alpha = 1024$	$\alpha = 2048$
b_1	0.4151165621	0.4202147347	0.4247546027	0.4283185727
b_2	1.9181190343	1.9362789404	1.9526018051	1.9640824901
b_3	−1.3332355964	−1.3564936751	−1.3773564078	−1.3924016028
a_{11}	0.3208720847	0.3238411715	0.3262148684	0.3276158396
a_{21}	0.1133619989	0.1103734980	0.1078120817	0.1057338409
a_{22}	0.3209344480	0.3239229484	0.3264843652	0.3285626060
a_{31}	−0.3407257524	−0.3441364642	−0.3468445023	−0.3482002424
a_{32}	0.3287816175	0.3416438725	0.3518066694	0.3581217210
a_{33}	0.3616434674	0.3541358796	0.3483009484	0.3443715544

4.2 Comparison of numerical characteristics

Fig. 5(a) and (b) shows the amplification (dissipation) and phase (dispersion) errors of the proposed new scheme ($\alpha = 2048$) along with the same information for the low-dispersion low-dissipation implicit scheme (LDDDIRK32) of Najafi-Yazdi and Mongeau [12] respectively. The proposed new scheme shows significantly reduced dispersion and dissipation error as compare to LDDDIRK32. As $|G_N(\sigma)| \leq 1$, the proposed scheme is unconditionally stable for all values σ.

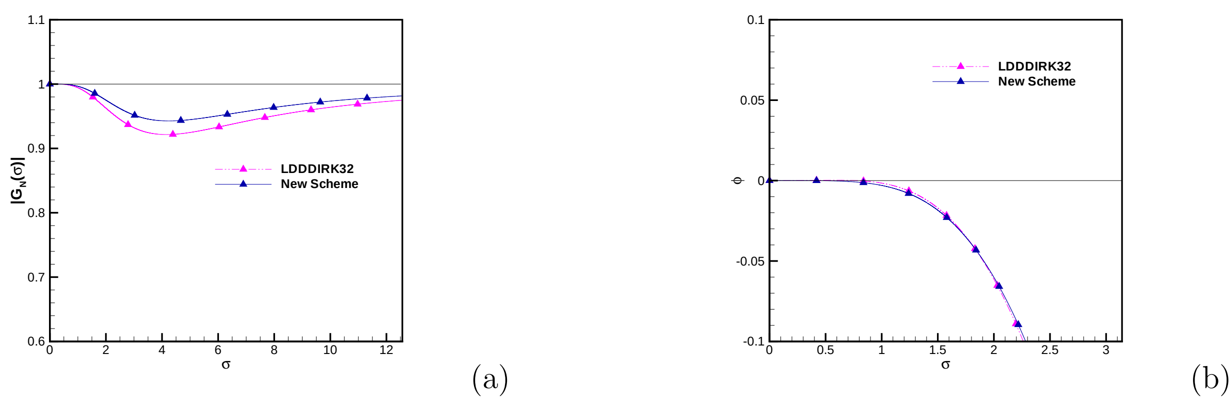


Figure 5: *Characteristics of schemes: (a) Amplification factor, (b) Phase difference.*

4.3 Problem: Convection equation with a non-linear source term

Here convection equation

$$u_t + u_x = f(u) \tag{4.1}$$

with a stiff non-linear source term $f(u) = u - u^2$ is considered following the works of Nazari et al. [13]. This equation which models non-equilibrium gas dynamics is chosen to test the efficiency of the newly developed schemes for non-linear problems. Computation is carried out using mesh $h = 0.05$ over a domain $[0, 25]$ with initial condition given by the discontinuous wave

$$u(x,0) = \begin{cases} 0, & x \leq 2 \\ 1, & 2 \leq x \leq 4 \\ 0, & x \geq 4 \end{cases} .$$

For this problem, we use the upwind scheme and compute for CFL numbers 0.125, 0.25 and 0.5. Errors obtained using different schemes at $t = 10.0$ have been compared in Table 10. From this table we see that the new scheme performs better than LDDDIRK32. In the absence of analytical solution error in L^2-norm is calculated relative to a reference solution obtained using IRK36 [6] method with a small CFL number $N_c = 0.001$. IRK36 is chosen for computing the reference solution for its overall superiority.

Table 10: Problem: L^2-norm error between numerical and reference solution.

Scheme	$N_c = 0.125$	$N_c = 0.25$	$N_c = 0.5$
New Scheme	4.4585e-06	1.6187e-05	5.1987e-05
LDDDIRK32	7.7381e-06	3.3322e-05	1.5494e-04

5 A class of optimally high dispersive order accurate upwind HOC schemes

Compact finite difference schemes providing improved representation of a range of scales for the evolution of first and second order derivatives can be traced to the works of Lele in 1992 [11]. In his work Lele [11], proposed finite difference approximations which were generalizations of Padé schemes. Tam and Webb in 1993 [15], while arguing for physically correct simulation, pointed out limitations of the higher order of accurate approximations for unsteady equations, especially in computational acoustics. They introduced the idea of low dispersion error methods and contended that the underlying finite difference scheme must bear nearly the same dispersion relation as that of the PDE itself. Tam and Webb [15] used Fourier-Laplace transform and minimized integrated wave number error to come up with a strategy to produce dispersion relation preserving schemes. But the work of Tam and Webb [15] was restricted to explicit approximations. In the year 1994, Haras and Ta'asan [9] also pointed out the limitations of higher order schemes vis-a-vis lower order ones, on the finite computational grid and proposed a general approach for designing implicit central finite difference schemes by minimizing the L^2-norm of the global error. It is important to note here that the differentiation operator used by the authors to define the L^2-norm relates to dispersion relation. Haras and Ta'asan [9] used different weight functions but the schemes so designed were limited to having formal order of accuracy two. Since then compact finite difference schemes have found wide use in simulations of complex flow fields [4, 5, 14, 17].

The development of upwind schemes using compact stencil was carried out by Zhong [17]. In developing these schemes emphasis was given to asymptotical stability in conjunction with appropriate boundary closure conditions. The author used eigenvalue analysis and the schemes were found to be less dissipative than conventional upwind schemes where upwind biased stencils are used. Sengupta et al. in 2003 [14], analyzed central and upwind compact schemes and demonstrated that improper treatment of near boundary stencil points can lead to the overall instability of the scheme by using matrix-spectral analysis. As a remedy, the authors suggested three optimal upwind biased compact schemes. Bhumkar et al. [4] have been able to derive a class of optimized upwind compact schemes having excellent dispersion relation preserving property. The schemes derived in [4] uses three to thirteen point stencil and are derived by minimizing dispersion error in the wave number range $[0, 7\pi/8]$. Nevertheless, the schemes do not carry optimum dispersive order of accuracy. Although effort of Bhumkar et al. [4] is praise worthy but closer analysis reveals that the schemes derived failed to attain the highest possible dispersive accuracy; further no effort was made to develop adequate boundary closure conditions.

In this work, we present a new algorithm to construct a family of optimized upwind compact finite difference schemes. The algorithm is based on the idea of constructing schemes on centred stencils with free parameters to prevent dispersion error growth. The schemes are made to carry optimal dispersive order of accuracy in both interior and boundary nodes. They are found to possess minimized weighted phase lag over the entire wave number range. The overall order of accuracy of the upwind schemes at interior nodes are single order less than the maximum permissible order in the central stencil. The focus here is on general and holistic approach integrating all nodal points. Hence an asymptotic stability analysis is used to determine the stability of the inner schemes coupled with newly developed boundary closure schemes. Finally, efficiency of the proposed schemes is documented by solving the numerical test cases of varied complexity to highlight computational efficiency, high accuracy and spectral resolution characteristics of the schemes.

Traditionally first order spatial derivative at the jth grid point with uniform grid spacing h is approximated as

$$u'_j = \frac{1}{h} \sum_{l=-N}^{N} a_l u_{j+l} \tag{5.1}$$

where u'_j is the numerical approximation of $(\partial u/\partial x)_j$ [5, 15]. But in case of compact discretization u'_j are implicitly linked to all nodal values and are generalizations of the Padé scheme. Following Zhong [17] compact approximation at the jth grid point can be written as

$$\sum_{l=-M}^{M} b_l u'_{j+l} = \frac{1}{h} \sum_{l=-N}^{N} a_l u_{j+l}. \tag{5.2}$$

This scheme uses a total of $2M + 1$ and $2N + 1$ grid points on left and right respectively. Compact schemes are implicit and use compact stencil with fewer points. Due to their compact nature, they are able to attain higher spectral resolution on a coarser mesh. The system is given by the Eq. (5.2) is often expressed in linear algebraic form

$$\begin{aligned} \boldsymbol{M}_1\boldsymbol{u}' &= \frac{1}{h}\boldsymbol{M}_2\boldsymbol{u} \\ \Rightarrow \qquad \boldsymbol{u}' &= \frac{1}{h}\boldsymbol{M}_1^{-1}\boldsymbol{M}_2\boldsymbol{u} \\ &= \frac{1}{h}\boldsymbol{C}\boldsymbol{u} \end{aligned} \tag{5.3}$$

In general M is kept fixed at 1 or 2 leading to $\boldsymbol{M}_1$ being banded, tri-diagonal [11,14,17] and penta-diagonal [11] system respectively. Note that $\boldsymbol{C} = \boldsymbol{M}_1^{-1}\boldsymbol{M}_2$ need not be compact.

5.1 Fourier analysis and dispersion error of semi-discretization

We set the coefficients of the leading truncation term of Taylor series of Eq. (5.2) as a free parameter ϱ. The effective equivalent wavenumber $[k_{eq}]$ is a function of k and can be written as

$$[k_{eq}]_j = \frac{I}{h}\sum_{l=1}^{N} C_{jl}e^{-Ik(x_l - x_j)}. \tag{5.4}$$

which implies

$$[k_{eq}]_j h = \Theta_{R_j}(kh) + I\Theta_{I_j}(kh). \tag{5.5}$$

For an efficient numerical scheme difference between the exact wave number k and the numerically estimated wavenumber $[k_{eq}]$ must be minimized over entire wavenumber range. This is proposed to be achieved by defining weighted dispersion error in L^2-norm as

$$\|DE_j\|_{L^2[-\pi,\pi]} = \left[\int_{-\pi}^{\pi} \left|k - \Theta_{R_j}(k)\right|^2 e^{-\alpha k^2} dk\right]^{1/2} \tag{5.6}$$

for all $1 \leq j \leq N$ where $\alpha \geq 0$ is some weight parameter. We define dispersive error of a compact scheme with equivalent wave number $[k_{eq}]_j$ as

$$\phi_j(k) = k - \Theta_{R_j}(k). \tag{5.7}$$

The above relation helps us to understand dispersive order of accuracy associated with a spatial discretization. From the definition it is clear that $\phi_j(0) = 0$. The following theorem relates dispersive order to the minimization of Eq. (5.6).

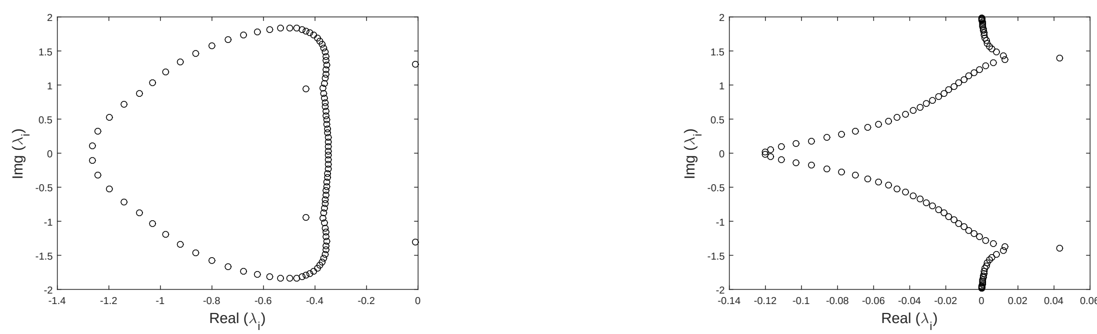
Theorem 5.1.1. *If $\phi_j(k)$ is analytic and carries zero as a root of multiplicity m with series expansion $\phi_j(k) = k^m(c_0 + c_1 k + c_2 k^2 + ...)$ then the weighted dispersion error $\|DE_j\|_{L^2}$ with $\alpha \to \infty$ is minimum for $c_0 = 0$.*

5.2 Semidiscrete eigenvalue and asymptotic stability analysis

In the previous section our focus was on low dispersive stable discretization at interior and boundary points simultaneously. In this section we explore long time behaviour of the discretization strategy. Carpenter et al. [7] in their study have shown that G-K-S stable (also known as Lax stable) semi-discrete scheme in conjunction with locally stable temporal scheme need not remain bounded for all times, even for a physically bounded solution. They found that for genuinely time dependent problems G-K-S stability of a discretization alone is not sufficient and such discretization strategy might require excessively large number of grids for long time simulation thereby negating the basic advantages of compact schemes. With the physical boundary condition imposed at the grid point $j = 1$ the semi discrete version of 1D convection equation can be expressed as

$$\frac{\partial \tilde{\boldsymbol{u}}}{\partial t} + \frac{c}{h}\tilde{\boldsymbol{C}}\tilde{\boldsymbol{u}} + \frac{c}{h}\tilde{\boldsymbol{M}}_1^{-1}\boldsymbol{B}g(t) = 0 \qquad (5.8)$$

where $\tilde{\boldsymbol{u}} = [u_2, u_3, ..., u_N]^T$ and $\boldsymbol{B}$ is the $N-1$ dimensional vector whose first N_R components describe dependence of the discretization on the boundary data. $\tilde{\boldsymbol{C}} = \tilde{\boldsymbol{M}}_1^{-1}\tilde{\boldsymbol{M}}_2$ with both $\tilde{\boldsymbol{M}}_1$ and $\tilde{\boldsymbol{M}}_2$ being matrices of dimension $N-1$. Further last $N-1-N_R$ rows of matrices $\tilde{\boldsymbol{M}}_1$ and $\tilde{\boldsymbol{M}}_2$ are same as those of $\boldsymbol{M}_1$ and $\boldsymbol{M}_2$ respectively. As argued by Carpenter et al. [7] $g(t)$ can be set to zero without any loss of generality. The asymptotic stability of the upwind schemes with numerical boundary closures is analyzed by computing the eigenvalues of the spatial discretization matrix $\tilde{\boldsymbol{C}}$ obtained in Eq. (5.8). It requires that the eigenvalues of $-\tilde{\boldsymbol{C}}$ contain no positive real part and is necessary for the stability of long time integration of the equation.



(a) (b)

Figure 6: *Eigenvalue spectra: (a) New LDC5U scheme with $N = 100$, (b) Sixth order Lele scheme closed with fifth order boundary and sixth order near boundary scheme with $N = 100$.*

Eigenvalue spectrum of the matrix $-\tilde{\boldsymbol{C}}$ associated with LDC5U discussed below could be found in Figs. 6(a) and 6(b) on grid 100. All eigenvalues carry negative real parts rendering the newly developed scheme asymptotically stable. This is in contrast to the optimally accurate sixth order Lele scheme where a pair of eigenvalues with large positive parts could be observed pointing its unsuitability for long time simulation.

5.3 Low-dispersion compact third order upwind (LDC3U) scheme

We have developed three point third order accuracy schemes for interior nodes $2 \leq j \leq N-1$ leaving free parameter ϱ for dispersion error reduction. The minimization of weighted dispersion error with asymptotic α value gives a minimum value of $\varrho = 0.7745966692$. The corresponding coefficients are given in Table 11. The scheme maintains highest the sixth order dispersive accuracy. We have also developed a sixth order dispersively accurate scheme with formal third order accuracy at the boundary points $j = 1,\ N$ as shown in Table 11.

Table 11: Coefficients of LDC3U scheme.

Parameter	$j = 1$	$2 \leq j < N$	$j = N$
b_{-1}	–	0.4436491673	2.1622776602
b_1	2.1622776602	0.0563508327	–
a_{-3}	–	–	0.0270462767
a_{-2}	–	–	−0.6622776602
a_{-1}	–	−1.1372983346	−1.9188611699
a_0	−2.5540925534	0.7745966692	2.5540925534
a_1	1.9188611699	0.3627016654	–
a_2	0.6622776602	–	–
a_3	−0.0270462767	–	–

5.4 Low-dispersion compact fifth order upwind (LDC5U) scheme

For five point fifth order accuracy schemes for all interior points $3 \leq j \leq N-2$, the minimum value of $\varrho = -2.3904572187$ for minimum dispersion error can be found. The schemes also maintain eighth order dispersive accuracy. The coefficients are given in Table 12. For boundary point $j = 1, N$ we have taken fifth order implicit boundary scheme. For other boundary points $j = 2$ and $N-1$ we have derived eighth order dispersively accurate scheme with formal fifth order accuracy.

Table 12: Coefficients of LDC5U scheme.

Parameter	$j = 1$	$j = 2$	$3 \leq j \leq N-2$	$j = N-1$	$j = N$
b_{-1}	–	0.1611048569	0.5325381016	0.5333708584	4.0000000000
b_1	4.0000000000	0.5333708584	0.1341285651	0.1611048569	–
a_{-4}	–	–	–	–	−0.0833333333
a_{-3}	–	–	–	0.0013904524	0.6666666667
a_{-2}	–	–	−0.0609785725	−0.0703870482	−3.0000000000
a_{-1}	–	−0.5411875471	−1.0433841354	−1.0166854292	−0.6666666667
a_0	−3.0833333333	−0.5444944779	0.5976143047	0.5444944779	3.0833333333
a_1	0.6666666667	1.0166854292	0.5121714201	0.5411875471	–
a_2	3.0000000000	0.0703870482	−0.0054230169	–	–
a_3	−0.6666666667	−0.0013904524	–	–	–
a_4	0.0833333333	–	–	–	–

5.5 Problem: Linear wave equation

The linear model equation [7] is described by

$$u_t + u_x = 0, \quad -1 \leq x \leq 1, \quad t \geq 0 \tag{5.9}$$

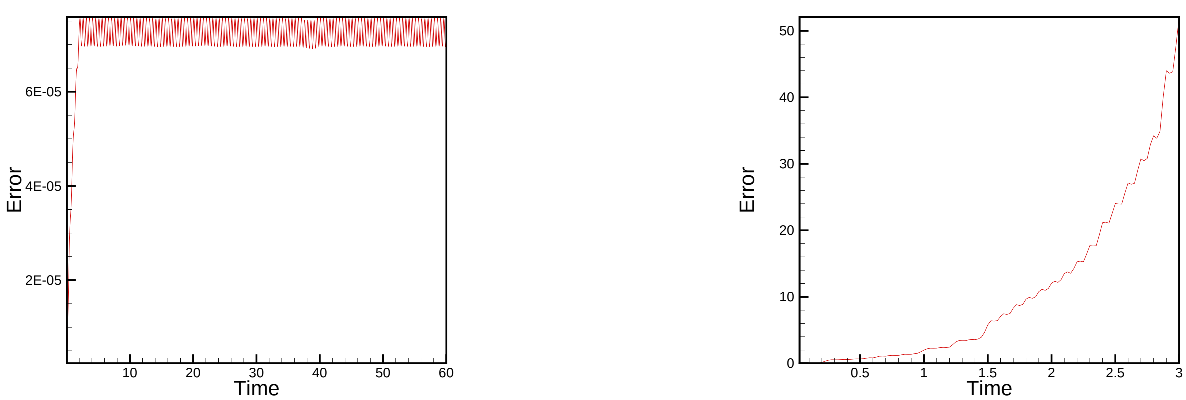
with the boundary and initial condition

$$\begin{aligned} u(-1,t) &= \sin 2\pi(-1-t), \\ u(x,0) &= \sin 2\pi x, \quad -1 \leq x \leq 1, \quad t \geq 0. \end{aligned} \tag{5.10}$$

The exact solution is given by

$$u(x,t) = \sin 2\pi(x-t), \quad -1 \leq x \leq 1, \quad t \geq 0. \tag{5.11}$$

We have used 41 grid points for computing the solution and computed upto time $t = 60$. Explicit RK44 is used for time advancing. For spatial discretization, we have used LDC3U and LDC5U. For all times the exact solution is a travelling sinusoidal wave of amplitude 1. Simulation was run at N_c values 0.25 and 0.5. In Fig. 7(a) we have plotted L^2-norm error with time at $N_c = 0.5$ for New LDC5U scheme. From this figure, we see that at early time error growth is registered but very quickly it settles down to periodic error variation with small amplitude. In Fig. 7(b) we have plotted L^2-norm error with time at $N_c = 0.5$ for sixth order Lele scheme with fifth order boundary and sixth order near boundary closure. Although theoretically, the scheme carries higher order of accuracy an unbounded error growth is registered. This relates well with the presence of eigenvalues with positive real part as documented in figure 6(b) implying the importance of asymptotic stability.



(a) (b)

Figure 7: *Problem: L^2-norm error with time for $N_c = 0.5$ (a) New LDC5U scheme, (b) Sixth order Lele scheme with fifth order boundary and sixth order near boundary closure.*

References

[1] Alexander, R. Diagonally implicit Runge-Kutta methods for stiff O.D.E.'s. *SIAM J. Numer. Anal.*, 14:1006-1021, 1977.

[2] Anastassi, Z. A. and Simos, T. E. An optimized Runge-Kutta method for the solution of orbital problems. *J. Comput. Appl. Math.*, 175:1-9, 2005.

[3] Berland, J., Bogey, C., and Bailly, C. Low-dissipation and low-dispersion fourth-order Runge-Kutta algorithm. *Comput. Fluids*, 35:1459-1463, 2006.

[4] Bhumkar, Y. G., Sheu, T. W. H., and Sengupta, T. K. A dispersion relation preseving optimized upwind compact difference scheme for high accuracy flow simulations. *J. Comput. Phys.*, 278:378-399, 2014.

[5] Bogey, C. and Bailly, C. A family of low dispersive and low dissipative explicit schemes for flow and noise computations. *J. Comput. Phys.*, 194:194-214, 2004.

[6] Butcher, J. *Numerical Methods for Ordinary Differential Equations*, John Wiley & Sons Ltd., 2nd edition, 2008.

[7] Carpenter, M. H., Gottlieb, D., and Abarbanel, S. Stable and accurate boundary treatments for compact, high-order finite-difference schemes. *Appl. Numer. Math.*, 12:55-87, 1993.

[8] Ferracina, L. and Spijker, M. N. Strong stability of singly-diagonally-implicit Runge-Kutta methods. *Appl. Numer. Math.*, 58:1675-1686, 2008.

[9] Haras, Z. and Ta'asan, S. Finite difference schemes for long time integration. *J. Comput. Phys.*, 114:265-279, 1994.

[10] Hu, F. Q., Hussaini, M. Y., and Manthey, J. L. Low-dissipation and low-dispersion Runge-Kutta schemes for computational acoustics. *J. Comput. Phys.*, 124:177-191, 1996.

[11] Lele, S. K. Compact finite difference schemes with spectral-like resolution. *J. Comput. Phys.*, 103:16-42, 1992.

[12] Najafi-Yazdi, A. and Mongeau, L. A low-dissipation and low-dispersion implicit Runge-Kutta scheme. *J. Comput. Phys.*, 233:315-323, 2013.

[13] Nazari, F., Mohammadian, A., and Charron, M. High-order low-dissipation low-dispersion diagonally implicit Runge-Kutta schemes. *J. Comput. Phys.*, 286:38-48, 2015.

[14] Sengupta, T. K., Ganeriwal, G., and De, S. Analysis of central and upwind compact schemes. *J. Comput. Phys.*, 192:677-694, 2003.

[15] Tam, C. K. W. and Webb, J. C. Dispersion-relation-preserving finite difference schemes for computational acoustics. *J. Comput. Phys.*, 107:262-281, 1993.

[16] Tselios, K. and Simos, T. E. Runge-Kutta methods with minimal dispersion and dissipation for problems arising from computational acoustics. *J. Comput. Appl. Math.*, 175:173-181, 2005.

[17] Zhong, X. High-Order Finite-Difference Schemes for Numerical Simulation of Hypersonic Boundary-Layer Transition. *J. Comput. Phys.*, 144:662-709, 1998.

– × –

RECURRING
GFR 12 – A
[(See Rule 238 (1))]
UTILIZATION CERTIFICATE (UC) FOR THE YEAR 2021-22
in respect of RECURRING
as on 12th June 2021 to be submitted to SERB
UC (Provisional/Audited)
(To be given separately for each financial year ending on 31st March)

1. Name of the grant receiving Organization: **Tezpur University**
2. Name of Principal Investigator(PI) : **Dr. Shuvam Sen**
3. SERB Sanction order no. & date : **MTR/2017/000038 dated 29th May 2018**
4. Title of the Project : ***Development of dispersion, dissipation characteristics preserving finite difference schemes for fluid flow problems***
5. Name of the SERB Scheme : **MTR – MATRICS** *(Mathematical Research Impact-Centric Support Scheme)*
6. Whether recurring or non-recurring grants: **Recurring**
7. Grants position at the beginning of the Financial year (Grants released by SERB)
   (i) Cash in Hand/Bank /Carry forward from previous financial year : **Rs. 29305/-**
   (ii) Others, If any : **NIL**
   (iii) Total : **Rs. 29305/-**
8. Details of grants received, expenditure incurred and closing balances: (Actuals)

Unspent Balance of Grants received previous years [figure as at Sl.No. 7(iii)]	Interest Earned thereon	Interest deposited back to the SERB	Grants received during the year			Total Available funds (1+2-3+4)	Expenditure incurred	Closing Balances (5-6)	Remark
1	2	3	4			5	6	7	8
			Sanction No. (i)	Date (ii)	Amount (iii)				
29,305/-	**NIL**	**NIL**	**NIL**	**NIL**	**NIL**	**29,305/-**	**28,590/-**	**715/-**	Closing balance correspond to total interest earned over 3 years

9. Component wise utilization of grants

Grants-in-aid-General	**Total**	**Remark**
Research Grant	**Rs. 16,994.00**	
Overhead	**Rs. 11,596.00**	
GRAND TOTAL	**Rs. 28,590.00**	

10. Details of grants position at the end of the year
    (i) Cash in Hand/Bank : **Rs. 715.00**
    (ii) Refunds to SERB, If any : NIL
    (iii) Balance (Carry forward to next financial year): **Rs. 715.00**

Signature Name: Dr. Shuvam Sen Principal Investigator(PI)	Signature with Seal Name: Finance Officer	Signature with Seal Name: Head of Organisation

Associate Professor
Department of Mathematical Sciences
Tezpur University

Finance Officer
Tezpur University

Registrar
Tezpur University

GFR 12 – A

[(See Rule 238 (1))]

UTILIZATION CERTIFICATE (UC) FOR THE YEAR 2021-22

in respect of *RECURRING*

as on 12th June 2021 to be submitted to SERB

Is the UC (Provisional/Audited)

(To be given separately for each financial year ending on 31st March)

Certified that I have satisfied that the conditions on which grants were sanctioned have been duly fulfilled/are being fulfilled and that I have exercised following checks to see that the money has been actually utilized for the purpose for which it was sanctioned:

(i) The main accounts and other subsidiary accounts and registers (including assets registers) are maintained as prescribed in the relevant Act/Rules/Standing instructions (mention the Act/Rules) and have been duly audited by designated auditors. The figures depicted above tally with the audited figures mentioned in financial statements/accounts.

(ii) There exist internal controls for safeguarding public funds/assets, watching outcomes and achievements of physical targets against the financial inputs, ensuring quality in asset creation etc. & the periodic evaluation of internal controls is exercised to ensure their effectiveness.

(iii) To the best of our knowledge and belief, no transactions have been entered that are in violation of relevant Act/Rules/standing instructions and scheme guidelines.

(iv) The responsibilities among the key functionaries for execution of the scheme have been assigned in clear terms and are not general in nature.

(v) The benefits were extended to the intended beneficiaries and only such areas/districts were covered where the scheme was intended to operate.

(vi) The expenditure on various components of the scheme was in the proportions authorized as per the scheme guidelines and terms and conditions of the grants-in-aid.

(vii) It has been ensured that the physical and financial performance under …………….. **(CRG/NPDF/ECR…..etc.)** (Name of the scheme has been according to the requirements, as prescribed in the guidelines issued by Govt. of India and the performance/targets achieved statement for the year to which the utilization of the fund resulted in outcomes given at Annexure

I duly enclosed.

(viii) The utilization of the fund resulted in outcomes given at Annexure – II duly enclosed (to be formulated by the Ministry/Department concerned as per their requirements/specifications.)

(ix) Details of various schemes executed by the agency through grants-in-aid received from the same Ministry or from other Ministries is enclosed at Annexure –II (to be formulated by the Ministry/Department concerned as per their requirements/specifications).

Date: 30.07.2021
Place: Tezpur

Signature Name: Dr. Shyam Sen Principal Investigator(PI)	Signature with Seal 9/8/21 Name: Finance Officer	Signature with Seal 9/8/21 Name: Head of Organisation

(Strike out inapplicable terms)

Associate Professor
Department of Mathematical Sciences
Tezpur University

Finance Officer
Tezpur University

Registrar
Tezpur University

Annexure-II

REQUEST FOR ANNUAL INSTALMENT WITH UP-TO-DATE STATEMENT OF EXPENDITURE

1. SERB Sanction Order No and date : **MTR/2017/000038 dated 29th May 2018**
2. Name of the PI : **Dr. Shuvam Sen**
3. Total Project Cost : **6,60,000/-**
4. Revised Project Cost (if applicable) : **Not Applicable**
5. Date of Commencement : **13th June, 2018**
6. Statement of Expenditure : Month wise expenditure incurred during current financial year 2021-22

Month & year	Expenditure incurred/ committed	Remark
April, 2021	NIL	
May, 2021	Rs. 25287.00	
June, 2021	Rs. 3303.00	
July, 2021	NIL	
August, 2021	NIL	
September, 2021	NIL	
October, 2021	NIL	
November, 2021	NIL	
December, 2021	NIL	
January, 2022	NIL	
February, 2022	NIL	
March, 2022	NIL	
Total	**Rs. 28,590.00**	

7. Grant received in each year

(a) 1st Year : **2,20,000/-**
(b) 2nd Year : **2,20,000/-**
(c) 3rd Year : **1,20,000/-**
(d) Interest, if any : **715/-**
(e) Total (a + b + c + d) : **5,60,715/-**

Statement of Expenditure

From (DOS*) 13-06-2018 to 12.06.2021, financial year 2020-21

Sr. No. (I)	Sanctioned Heads (II)	Total Funds Allocated (indicate sanctioned or revised) (III)	Expenditure Incurred: 1st Year (13th June 2018 to 31st March 2019) (IV)	Expenditure Incurred: 2nd Year (1st April 2019 to 31st March 2020) (V)	Expenditure Incurred: 3rd Year (1st April 2020 to 31st March 2021) (VI)	Expenditure Incurred: 4th Year (1st April 2021 to 12th June 2021) (VII)	Total Expenditure till 12th June 2021 (VIII = IV + V+ VI+VII)	Balance as on 12th June 2021 (IX = III –VIII)	Requirement of Funds	Remarks (if any)
1.	Research Grant	5,09,091.00	1,76,328.00	1,82,671.00	1,33,098.00	16,994.00	5,09,091.00	NIL	NIL	
2.	Overhead expenses	50,909.00	14,500.00	18,000.00	6,813.00	11,596.00	50,909.00	NIL	NIL	
3.	Interest earned	715.00	--	--	--	--	--	715.00	--	
4.	**Total**	5,60,715.00	1,90,828.00	2,00,671.00	1,39,911.00	28,590.00	5,60,000.00	715.00	NIL	Closing balance correspond to total interest earned over 3 years

Signature
Name: Dr. Shuvam Sen
Principal Investigator(PI)
Associate Professor
Department of Mathematical Sciences
Tezpur University

Signature with Seal
Name:
Finance Officer
Finance Officer
Tezpur University

Signature with Seal
Name:
Head of Organisation
Registrar
Tezpur University

*DOS – Date of Start of project

Note:

1. Expenditure under the sanctioned heads, at any point of time, should not exceed funds allocated under that head, without prior approval of SERB i.e. Figures in Column (IX) should not exceed corresponding figures in Column (III)
2. Utilization Certificate (Annexure III) for each financial year ending 31st March has to be enclosed along with request for carry-forward permission to the next financial year.