

A Framework for Multidimensional Analysis and Development of Numerical Schemes

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Abstract

Partial differential equations are found throughout engineering and sciences. Under the constraint of complex initial and boundary conditions, most of these complex equations do not have analytical solutions, and therefore require solution by numerical methods. In the context of this thesis, the goal is to examine the governing equations of fluid mechanics (Euler and Navier Stokes) which require both spatial and temporal discretization. Under the effects of numerical differencing, the numerical solution is subjected to both dispersion and dissipation error. These error can be identified and analyzed through spectral analysis method. The analysis of numerical schemes under a coupled spatial temporal framework in one dimensional wavespace is well understood. However, the extension of these methods to multidimensional wavespace and the spectral properties of a hybrid finite difference/Fourier spectral spatial discretization method in multidimensional space is not well understood. Furthermore, the extension of this multidimensional analysis framework to non-linear shock capturing schemes is not done before.

This dissertation introduces a generic method for the spectral analysis of linear and non linear finite difference schemes in multidimensional wavenumber space. The aim is to understand the properties of the coupled system for a series of representative spatial and temporal schemes. Theoretical predictions are then compared with numerical solutions based on model equations such as the advection, linearized Euler and linearized Navier Stokes equations. Finally, this framework is used to develop a spectrally optimized hybrid shock capturing scheme which switches between a linear and non linear scheme. Various canonical numerical examples were conducted in order to compare the spectral properties of the new scheme with existing numerical schemes.

For the one dimensional linearized Euler equation, it was shown that the dispersion rela-

tion belonging to the largest eigenvalue ($\omega = \bar{u} + a$) provides the limiting criteria for the stability limit as well as the onset of dispersion error. When the linear spectral analysis method is extended to the two dimensional wavespace, the dispersion and dissipation properties of the coupled schemes become a function of both the reduced wavenumber and the wave propagation angle. When the two dimensional linear spectral analysis method is extended to the two dimensional linearized Compressible Navier Stokes equations (LCNSE), viscous and acoustic effects are taken into account in addition to the convection effects. The addition of the acoustic term to the dispersion relation leads to a coupling of the resolution characteristic such that the group velocities in either spatial direction become a function of the wavenumber in both spatial directions. The two dimensional spectral analysis method was extended to non linear finite difference schemes based on a quasi-linear assumption. In this assumption, the contribution of the harmonic modes (as a result of the non linear differentiation) are neglected during the calculation of the modified wavenumber of the spatial scheme. Using the semi-discretized dispersion relation of the two dimensional advection and linearized Euler equations, the dispersion and dissipation property of a non linear scheme in two dimensional wavespace can be quantified. Using this framework, a non linear scheme, HYB-MDCD-TENO6 was developed based on the principle that the linear part of the scheme can be optimized for minimum dispersion and dissipation error. Furthermore, the non linear part of the scheme is only activated in the vicinity of a sharp gradient. Through a series of numerical experiments, it was found that the hybrid scheme optimized based on the linearized Euler equation tend to give slightly better results than the one optimized based on the advection equation in some of the numerical experiments. In all cases, it was found that the HYB-MDCD-TENO6 scheme provides better resolution than existing baseline TENO and WENO-JS schemes for the same grid size considered.

Declaration

This is to certify that

1. the thesis comprises only my original work towards the PhD,
2. due acknowledgement has been made in the text to all other material used,
3. the thesis is less than 100,000 words in length, exclusive of tables, maps, bibliographies and appendices.

A handwritten signature in black ink, appearing to read 'Raynold', written over a horizontal line.

Raynold Tan Yiyun, July 2020

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Preface

The two results chapters (Chapter 3 and 4) have either been presented in conferences or in the process of getting published:

Journal/Conference

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2. R. Tan, A. Ooi and R. Sandberg, "Multidimensional Analysis and Optimization of Non Linear Shock Capturing Schemes", *72nd Annual Meeting of the American Physical Society, Division of Fluid Dynamics*, November, 2019
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4. R. Tan, Jun Peng, A. Ooi and R. Sandberg, "Multidimensional Analysis and Optimization of Hybrid MDCD-TENO schemes", *Journal of Scientific Computing* (Under Review)

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Chapter 1

Introduction

Under the constraint of complex geometries, boundary or initial conditions, complex equations such as the governing equation of fluid mechanics do not have exact solutions and therefore require solution by numerical methods. The work presented in this thesis is largely motivated by the work in the field of fluid mechanics. However, the analysis framework to be presented is applicable to other hyperbolic partial differential equation. In the field of fluid mechanics, the two primary set of governing equations are the Euler and Navier-Stokes equations. The linearized version of the Euler and Navier-Stokes equation are used for the purpose of developing a unified framework in the analysis of numerical schemes. A physical representation of reality is usually modelled through the formulation of a set of governing equations (mathematical model). Regardless of the physical system being represented, one would like to match physical reality as much as possible. That said, this is strongly dependent on how much is known and understood about the real system. The process of defining a mathematical model from physical reality introduces an intrinsic model error. Going from the mathematical model to the numerical solution, numerical techniques involving spatial and temporal discretization methods are used. In this process, round off error, truncation error as well as aliasing error are introduced into the numerical solution. Round off errors occurred due to the computer's inability to handle unlimited number of significant digits. Truncation error arises as a result of replacing the exact mathematical expression for differential and integral operator with numerical approximations. Aliasing error occurs during the evaluation of the nonlinear terms of the governing equation. A schematic representation of this computational modelling process is shown in figure 1.1. A further point to note con-

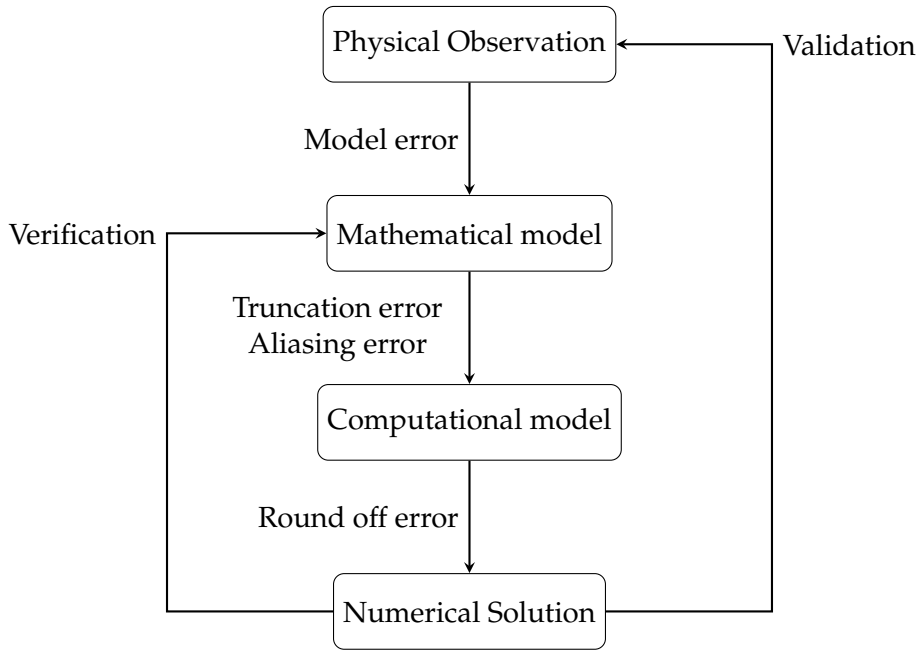


Figure 1.1: The steps to realizing a computational representation of a physical system

cerns the difference between verification and validation. Verification is concerned with the identification and removal of programming errors in a computer code. Its main purpose is to verify numerical algorithms. On the other hand, validation is concerned with the assessment of the numerical model with respect to the physical reality. Its main purpose is to evaluate the accuracy of the numerical model.

In this thesis, the work will mainly focus on the truncation error associated with the discretization error introduced through the numerical approximations. The truncation error which originates from both space and time discretization will manifest itself into the dispersion and dissipation error of the numerical schemes. In most of the analysis related to the governing equation of fluid mechanics, the advection equation represents the model equation. This is because the advection operator is omnipresent in these equations.

There are several methods available for spatially discretizing the domain. This includes finite difference, finite volume, finite element as well as spectral methods. The present work will focus on finite difference (FD) and Fourier spectral (FS) method. FS method can

provide the exact solution to a problem when a sufficiently refined grid is used. However, FS method is slower as compared to FD method of the same grid size. On the other hand, FD method have seen widespread use over many years due to its simplicity and speed as compared to other discretization method. Higher order FD methods have gained popularity in recent years due to the increased interest in applications related to computational turbulence and aeroacoustics. For the purpose of developing higher resolution method, the need for defining the accuracy of a scheme becomes paramount.

For high Reynolds number flows, energy spectrum is broadband. To represent these flow fields, adopted numerical schemes must be able to resolve a large range of length and time scales. Thus, one can immediately foresee the requirements for developing high accuracy schemes. The scheme should be accurate for a wide range of wave number (k) and circular frequency (ω). In the case of incompressible flow, one can generate truly high order scheme of any order. For compressible flow, this is not straight forward since the presence of various discontinuity and its associated Gibbs phenomena can lead to oscillations with over or undershoot of the solution in the vicinity of discontinuities. In this context, a numerical scheme is considered to be a high resolution scheme for compressible flow if the numerical method is at least second order accurate in the smooth part of the flow. In order to measure the accuracy of the scheme for every wave number, spectral analysis method is used. This provides more information about its accuracy as function of the wavenumber.

1.1 Previous work

1.1.1 1D Linear Spectral Analysis

One dimensional spectral analysis of spatial discretization method is well established and its earliest ideas date back to [Trefethen, 1982]. Fourier analysis of FD schemes in one dimensional wavenumber space has been extensively studied in majority of the literature such as [Tam and Webb, 1993, You et al., 2006, Sengupta et al., 2003, Sengupta and Dipankar, 2004, Sengupta et al., 2006, Kim and Lee, 1996, Lele, 1992, Pirrozoli, 2006, Pir-

rozoli, 2007, Li, 1997, Bogey and Bailly, 2004, Zingg, 2006, De and Eswaran, 2006, Zhong, 1998, Suman et al., 2017]. This analysis is based on the use of the semi-discretized numerical dispersion relation ($\omega_{semi}^* = U_{phase,exact} k^*$) of the one dimensional advection equation. k^* represents the modified wavenumber due to the spatial discretization scheme. When temporal discretization effect is taken into account, the fully (combined spatial and temporal) discretized numerical dispersion relation ($\omega_{full}^* = U_{phase,full}^* k$) is used to determine the spectral properties of the coupled (spatial and temporal) numerical schemes. $U_{phase,full}^*$ represents the numerical phase speed. The key difference being that the numerical phase speed, $U_{phase,full}^*$ is no longer a constant, but a function of the wavenumber. The analysis of numerical schemes under full discretization can be found in [Bhumkar et al., 2014], [Sengupta and Dipankar, 2004], [Sengupta et al., 2006] and [Sengupta et al., 2007], from which group velocities ($U_{grp,full}^*$), phase velocities ($U_{phase,full}^*$) and numerical amplification factor (Z) of the one dimensional advection equation was analysed for different combination of spatial and temporal discretization method. Phase velocity can be described as the speed for which a single mode of the wave travel in physical space. On the other hand, group velocity can be described as the wave-energy propagation speed. Assessment of schemes based on the one dimensional advection equation does not provide the full picture in term of their resolution characteristics especially when one considers solving Navier-Stokes equation in multidimensional space. This is because there exists other operators within the Navier-Stokes equation which can influence the resolution of the coupled numerical schemes. In particular, the diffusion operator is not taken into account. To rectify this differences, one dimensional full discretization analysis of the advection diffusion equation was investigated in [Suman et al., 2017]. The physical dispersion relation of the one dimensional advection diffusion equation is given by $\omega = U_{phase,exact} k - i\alpha k^2$, where $U_{phase,exact}$ and α is the physical phase speed and coefficient of viscosity respectively. In their analysis, it was shown that there are three main parameters measuring the accuracy of the scheme. They are the numerical phase speed, numerical group velocity and numerical diffusion coefficient. For the purpose of obtaining an accurate numerical solution equivalent to the physical solution, the ratio of $\frac{\alpha_{num}}{\alpha}$, $\frac{U_{phase,full}^*}{U_{phase,exact}}$ and $\frac{U_{grp,full}^*}{U_{grp,exact}}$ must be equal to 1.0.

1.1.2 2D Linear Spectral Analysis

When FD schemes are applied in multidimensional problems, a phenomenon known as numerical anisotropy is introduced. It is a phenomenon for which the resolution characteristics of the numerical scheme differs in different spatial directions. The resolution characteristic becomes a function of both the reduced wavenumber $k\Delta$ and the wave propagation angle, θ_w . Studies concerning multidimensional wavenumber analysis of numerical schemes can be found in [Li, 1997] and [Stegeman et al., 2012] but they were limited only to spatial discretization assumptions. Error due to temporal discretization were not considered. Analysis of numerical anisotropy under full discretization can be found in [Sengupta et al., 2011b]. The study assess the effect of changing grid aspect ratio and propagation angle on the solution of the linearized rotating shallow water equation and the two dimensional advection equation. It was conclusively shown that the use of wave aligned grid over grids with equal spacing in both directions leads to more accurate simulation results. In this thesis, a multidimensional wavenumber analysis under full discretization, similar to the approach outlined in [Sengupta et al., 2011b] is used.

In the case of the compressible Euler or Navier-Stokes equation, an additional operator exists which has an influence on the resolution of the numerical schemes when one considers multidimensional problems. This relates to the acoustic term found within its physical dispersion relation which is reported in [Tan et al., 2018], [Sescu, 2008] and [Stegeman et al., 2012]. The significance of this acoustic term stems from the coupling of wave number in both spatial directions, leading to the dependency of the group and phase velocities to the wave numbers in both spatial directions. In relation to the analysis to be presented in this thesis, the influence of the acoustic term on the resolution characteristic of a hybrid FD/FS method will be explored.

1.1.3 Non linear Spectral Analysis

The spectral analysis method discussed thus far is only valid for linear FD schemes. However, when non linear FD schemes are considered, analytical relations for the modified

wavenumber cannot be easily derived. Interest in the use of non linear schemes such as the Weighted Essentially Non Oscillatory (WENO) scheme stems from the need to accurately resolve flows with sharp gradients while preventing Gibbs phenomenon from occurring [Pirrozzoli, 2006]. The main disadvantage of such schemes is primarily related to its much larger numerical dissipation, which makes it unsuitable for the computation of turbulent flow. In order to determine the modified wavenumber of such schemes, non linear spectral analysis method should be employed. Currently, there exists two methods in the literature which deals with this and they can be found in [Pirrozzoli, 2006] and [Fauconnier and Dick, 2013]. They are termed as the Approximate Dispersion Relation (ADR) and the Non linear Spectral Analysis (NSA) method. The key differences between the ADR and NSA method lies in the initial condition used. ADR method relies on the extraction of a modified wavenumber from the convection of a sinusoidal wave with a certain wavenumber over a small distance. This quasi-linear method does not consider solutions that contain an entire spectrum of scales. Furthermore, the impact of the spurious modes, generated by the non linear schemes, and other non linear interactions during the evolution of a transported field is not considered. In contrast, the NSA method relies on the use of a large set of synthetic scalar fields with prescribed energy spectrum and random phase for its initial condition. The modified wavenumber extracted from this method does not neglect the spurious and harmonic modes generated from the non linear differentiation. The method also relies on the use of statistical technique to determine the mean modified wavenumber and its variance. This is achieved by determining the modified wavenumber for N realizations of the synthetic field $u(x)$, and calculating the mean modified wavenumber and the standard deviation [Fauconnier and Dick, 2013]. In this thesis, a variation of the ADR method developed by [Li et al., 2012] is used for determining the modified wavenumber of the non linear FD scheme. The method of [Li et al., 2012] is very similar to the ADR method but it does not take into account the temporal discretization in its formulation. In relation to the aim of this thesis, the non linear spectral analysis method proposed by [Li et al., 2012] is extended to multidimensional wave space.

1.1.4 Shock Capturing Finite Difference

For flows without discontinuities, spectral methods and compact schemes are readily used due to their superior spectral properties. Such schemes have the ability to accurately resolve a large range of wavenumber and circular frequency. For flows with discontinuities, there are restrictions to the use of schemes with very high spectral accuracy. Because of discontinuities and its associated Gibbs phenomenon, presence of numerical oscillation with over and under-shoot in the vicinity of discontinuity can make the entire numerical solution unstable. To overcome this issue, Total Variation Diminishing (TVD) schemes, Essentially Non Oscillatory (ENO) and Weighted Essentially Non Oscillatory (WENO) type schemes were introduced in [Harten, 1983], [Harten et al., 1987] and [Liu et al., 1994] to deal with this type of flow. TVD schemes are essentially a combination of upwind schemes with non linear flux limiters. At critical points near discontinuity, it degenerates to first order and produce excessive numerical dissipation. ENO schemes are based on the adaptive selection of stencils such that the smoothest stencil is selected for the evaluation of the numerical flux. WENO uses a weighted combination of sub stencils, in which each set of stencils represents a linear upwind scheme. Weighting applied on each set of stencils are calculated based on a set of smoothness indicators, from which the linear schemes are recovered in the smooth region of the flow and ENO property is utilized in the presence of discontinuity. These schemes were found to be robust but the schemes in their original form are too dissipative for turbulent flows. In addition, the dispersion properties of these schemes may not be optimal. Major efforts in the literature have been directed towards the development of high resolution shock capturing schemes with good shock capturing capabilities. More recently, the development of low dissipation shock capturing schemes can be found in the work of [Fu et al., 2016], who have developed modified version of the WENO scheme, known as the Targeted Essentially Non Oscillatory (TENOS) scheme. The scheme uses a cut off parameter which completely removes a sub scheme in its flux reconstruction when the normalized indicator exceeds a cut off value. A natural choice to achieve better resolution properties is to combine the TENOS/WENO/ENO schemes with another scheme which possess spectral like resolution to form a hybrid schemes. The development of such hybrid schemes can be found in

the works of [Adams and Shariff, 1996], [Pirroli, 2002], [Shen and Yang, 2007], [Costa and Don, 2007]. Most of these work concerns the hybridization of the WENO/ENO scheme with either a compact, central or spectral scheme to form a hybrid scheme. Key issues concerning hybrid schemes is the smooth transition from one scheme to another as the flow field changes from a smooth to discontinuous region.

Other than the hybridization of schemes, another approach which can improve the spectral properties of a shock capturing schemes is to use optimization technique. Optimization technique for explicit and implicit finite difference scheme can be found in the work of [Tam and Webb, 1993], [Kim and Lee, 1996], [Sun et al., 2011]. Most of these technique are usually based on the pioneering work of [Tam and Webb, 1993], who have devised the dispersion relation preserving schemes for computational acoustics. The key idea is to minimise the integrated sum of dispersive error across the relevant wavenumber range. Optimization technique applied to WENO schemes can be found in the work of [Sun et al., 2011]. The authors have devised the Minimum Dispersion and Controllable Dissipation (MDCD) scheme, from which the dispersion and dissipation properties of a linear scheme can be separately controlled through two independent parameters; γ_{disp} and γ_{diss} . By comparing the expression of the MDCD scheme to the WENO scheme, the weighting of each sub stencils of the WENO scheme can be expressed in terms of the two independent parameters. In the context of this thesis, a new shock capturing scheme based on the hybridization of the MDCD scheme with the TENO scheme is proposed. The formulation of the MDCD-TENO scheme is similar to the approach used in the MDCD-WENO scheme of [Sun et al., 2011]. Also, a multidimensional spectral optimization technique is used based on the non linear spectral analysis method developed in this thesis.

1.2 Motivation, Objectives and Scope

The main motivation of this work stems from the importance of resolving the frequency and wavenumber content in time-dependent numerical simulation such as large-eddy

simulation (LES), direct numerical simulations (DNS) and computational aeroacoustics (CAA). Therefore, the ability to clearly assess the resolution of the numerical method under a spatial temporal framework is important. This applies to both linear and non linear shock capturing finite difference schemes. It is perhaps more important to recognise the numerical defects when they occur. As for flows with discontinuities, there is always a need for schemes with high resolution and good shock capturing capabilities. Since classical shock capturing schemes offers too much numerical dissipation which damps away the high frequency and high wavenumber content of the flow, very fine resolution grid is necessary to capture the small scale structures. However, this is not always possible with current computational resources and the use of high order low dissipation shock capturing scheme can alleviate this issue. The objectives of this thesis are as follow:

- Establish a theoretical framework to assess the spectral accuracy of the numerical schemes under full discretization in both one and two dimensional wave space
- Understand the implication of temporal discretization on the resolution of the method
- Understand the implication of two dimensionality on the resolution of the method
- Understand the implication of using hybrid finite difference/Fourier spectral scheme on the resolution of the method
- Extend the analysis framework from the advection equation to the Linearized Euler and Linearized Navier-Stokes equation to better understand its implication on full Navier-Stokes equation
- Extend the analysis framework to non-linear shock capturing finite difference schemes
- Develop a nonlinear shock capturing scheme based on this framework and assess its performance on realistic cases.

For the first part of the thesis where linear finite difference schemes are assessed, the scope of the work is confined primarily to model equations and the use of simple periodic boundary conditions. The model equations considered are the advection, linearized Euler and linearized Navier-Stokes equations. For the second part of the thesis where

non linear finite difference schemes are assessed, more realistic test cases involving supersonic inlet/outlet, symmetry and wall boundary conditions are used. Idealized problems based on periodic boundary condition will be used initially to verify the non linear spectral analysis theory.

1.3 Outline

Chapter 2 of this thesis presents a literature review and theoretical background of the spectral analysis methods currently used in literature. This chapter will present some of the underlying theory of linear spectral analysis of one dimensional spatial finite difference discretization along with a brief overview of the various categories of finite differences schemes that have been developed in recent years. It will also present a few representative temporal discretization schemes that will be used in this study. One dimensional and two dimensional linear spectral analysis method under full discretization will be reviewed. Issues concerning the difference between implicit and explicit time marching schemes as well as the difference between stability and accuracy of the numerical solution will be explored. The effect of using higher order temporal schemes are discussed as well. Numerical examples are presented to verify the theory.

This is followed by chapter 3 where two dimensional spectral analysis under full discretization is extended to the linearized Euler and Navier-Stokes equations. The derivation of the dispersion relation for the linearized Euler and Navier-Stokes equations are presented. Anisotropy analysis of the full finite differences and hybrid Fourier Spectral/Finite difference schemes are compared and discussed. Different combinations of spatial and temporal discretization schemes are considered. Numerical examples are presented to verify the theory.

Chapter 4 of this thesis is concern with the two dimensional spectral analysis and development of non linear finite difference schemes. In the first part, a review of existing shock capturing finite difference schemes is presented. This is followed by one dimen-

sional and two dimensional non linear spectral analysis of these schemes. In the case of the non linear schemes, the analysis is restricted to semi-discrete analysis primarily because von Neumann linear stability analysis is not directly applicable to non linear schemes. The two dimensional spectral analysis method is then used to devised a new scheme based on spectral optimization technique. Finally, representative numerical examples were conducted to compare the performance of the new schemes with existing schemes.

Finally, chapter 5 of this thesis will summarize the main contribution of this work and present recommendations for future work.

Chapter 2

Theoretical framework

In this chapter, a summary of the existing literature on finite difference (FD) schemes, Fourier spectral methods as well as time advancement methods will be discussed. The basic concepts of linear spectral analysis on which the theory is built upon will be introduced. The analysis is then extended to full discretization analysis in both one and two dimensional wavenumber space.

FD schemes have been in use for many years due to its simplicity and speed of computation. The only drawback is that FD schemes are restricted to simple geometry. With the increased availability of computational resources, this has led to increased opportunities for application of FD methods to more expensive problems. In recent years, fully resolved computation of turbulent flow from low to moderate Reynolds number has become a possibility and similar advances have been made in establishing the field of computational aeroacoustics (CAA). Higher resolution finite difference methods have been developed for these application. Finite difference schemes can be mainly classified into a few different types; (i) standard explicit finite difference schemes derived from Taylor series expansion about a point. (ii) compact or implicit method [Adam, 1977] where the derivative information of the surrounding nodes are used in the calculation, (iii) Dispersion relation preserving (DRP) schemes [Tam and Webb, 1993] where the coefficients of each nodal points are optimized for reduced dispersion error, (iv) isotropy optimized schemes [Sescu, 2008] where nodal points from more than one spatial directions are used. Isotropy optimized schemes have an Isotropy Correction Factor (ICF) from which the ICF is optimized based on the condition that the group or phase velocities are the same on the cartesian coordinate axes (x and $x = y$ directions for two dimensions, x and $x = y = z$ directions for three dimensions).

2.1 Finite difference and Fourier spectral discretization

Generally speaking, standard finite difference schemes can be derived from Taylor series expansion [Ames, 1977]. The stencil can be centered, upwind biased or one sided. For central type schemes, there are equal number of nodes on either side of the node in question. The coefficients are equal but opposite in signs. Upwind biased schemes has more nodes in one direction than the other. One sided schemes has nodes in only one direction. Under the consideration of an uniform grid, the general expression of a first order derivative is given as:

$$\left(\frac{\partial \phi}{\partial x}\right)_i = \frac{1}{\Delta x} \sum_{l=-L}^{+L} a_l \phi_{i+l}, \quad (2.1)$$

where a_l are the coefficients representing the weighting that determines how much node $i + l$ contributes to the calculation of the derivative at node i . The coefficients a_l can be determined from a number of ways. By comparing equation (2.1) to the Taylor series expansion about a node i , one can deduce the coefficients. This general technique is outlined in many texts such as [Moin, 2001], [Ferziger and Peric, 2002], [Kopal, 1961]. Algorithms used for the generation of coefficients over non-uniform or arbitrary grid can be found in [Fornberg, 1988]. The use of one sided or upwind biased stencils leads to the introduction of numerical dissipation in the spatial discretization scheme. In some context, the numerical dissipation can be beneficial since there exists significant dispersion error in the high wavenumber range and it would be desirable to damp out the waves propagating at an incorrect speed. However, when one considers time accurate simulations such as large eddy simulations, direct numerical simulation of turbulence as well as computational aeroacoustics in which the propagation of waves are critical, the additional numerical dissipation from upwind schemes may not be desirable. A compromise in this aspect is to use high order upwind schemes such as those found in [Li, 1997], [Zhong, 1998], [Rai and Moin, 1991]. These schemes offer reduced numerical dissipation than low order upwind schemes and better stability and aliasing properties than central type schemes.

The formal order of a finite difference scheme is measured by the power of the leading order truncation error. As more surrounding nodes are included in the calculation of the finite difference derivatives, the formal order of the scheme will be higher. While the truncation error gives you an idea of the order of accuracy of the method, spectral analysis provides more information in terms of its accuracy as a function of the wavenumber spectrum. Before a detailed description of the different finite difference schemes is presented, the concept of spectral accuracy is described below.

2.1.1 Spectral accuracy of finite difference schemes

The information presented in this section can be found in [Vichnevetsky and Bowles, 1982], [Moin, 2001] and [Lele, 1992]. The process of discretizing a continuous variable inevitably leads to some degree of information loss. That is to say that the representation of the original curve by discrete points becomes poorer when fewer points are used. This discrepancy is a function of the wavenumber content of the original continuous data and the type of discretization scheme applied. Spectral analysis allow one to quantify this effect. In order to illustrate this, a plot of a wavelength being represented by different number of points is shown in figure 2.1.

The number of points on a single wavelength is a measure of the indicative resolution of the scheme. The minimum wavelength can be deduced directly from the number of points on a single wave. From this information, one can obtained the maximum wavenumber. This is expressed mathematically in equation (2.2). For the case of 2 points per wave, the equivalent reduced wavenumber, $k_x \Delta x$ is π . For the case of 4 points per wave, the equivalent reduced wavenumber, $k_x \Delta x$ is $\pi/2$. For the case of 8 points per wave, the equivalent reduced wavenumber, $k_x \Delta x$ is $\pi/4$. For a given grid size Δx , one can resolve the smallest wave of wavelength $2\Delta x$ which intersects the x-axis at three points. Hence, the minimum wavelength that is resolved by such a grid is given by $\lambda_{min} = 2\Delta x$. Therefore,

$$k_{max} = \frac{2\pi}{\lambda_{min}} = \frac{\pi}{\Delta x}. \quad (2.2)$$

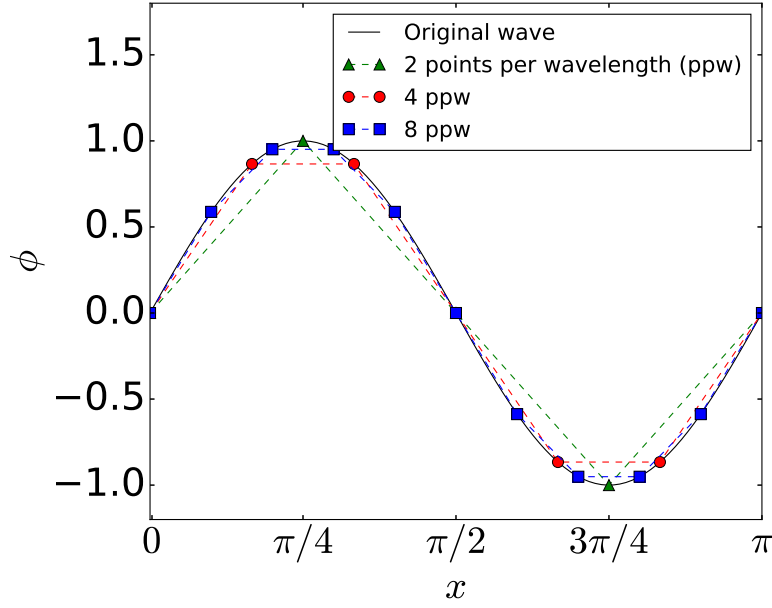


Figure 2.1: Illustrating the effect of discretization on a wave. Note that the first, last and mid points are not counted.

From this, one can see that the maximum physical reduced wavenumber is limited to $k_{max}\Delta x = \pi$. In the literature, this is known as the Nyquist limit. More information about this can be found in [Sengupta, 2013]. As mentioned previously, the truncation error from both the spatial and temporal discretization will manifest into dispersion and dissipation error. Dispersion refers to the transfer of energy away from its true wavelength. This will cause the propagating wave to become increasingly spread out as the numerical solution is propagated through time. Dissipation refers to the reduction in amplitude of the wave. In this context, the dissipation considered here is the numerical dissipation as oppose to the viscous dissipation of the real fluid. Numerical dissipation is completely artificial and is a result of the numerical scheme. To start off, we begin with the numerical approximation of a spatial derivative given in equation (2.1):

$$\left(\frac{\partial \phi}{\partial x}\right)_i = \frac{1}{\Delta x} \sum_{l=-L}^{+L} a_l \phi_{i+l}, \quad (2.3)$$

where ϕ_i written in terms of its Fourier transform is given as:

$$\phi_i = \frac{1}{2\pi} \int_{-\pi/\Delta x}^{\pi/\Delta x} \hat{\phi}(k_x) e^{ik_x x_i} dk_x. \quad (2.4)$$

Substituting equation (2.4) into (2.3) leads to:

$$\left(\frac{\partial \phi}{\partial x}\right)_i = \frac{1}{2\pi} \int_{-\pi/\Delta x}^{\pi/\Delta x} \left(\frac{1}{\Delta x} \sum_{l=-L}^{+L} a_l e^{ik_x x_l}\right) \hat{\phi}(k_x) e^{ik_x x_i} dk_x. \quad (2.5)$$

The numerical equivalent of the derivative of equation (2.4) is given as:

$$\left(\frac{\partial \phi}{\partial x}\right)_i = \frac{1}{2\pi} \int_{-\pi/\Delta x}^{\pi/\Delta x} ik_x^* \hat{\phi}(k_x) e^{ik_x x_i} dk_x. \quad (2.6)$$

where k_x is being replaced with k_x^* . k_x^* represents the modified wavenumber of the spatial discretization scheme. By comparing equation (2.6) to (2.5), it can be seen that modified wavenumber, k_x^* is related to the coefficients of the finite difference scheme via:

$$\begin{aligned} ik_x^* &= \frac{1}{\Delta x} \sum_{l=-L}^{+L} a_l e^{ik_x x_l}, \\ k_x^* \Delta x &= -i \sum_{l=-L}^{+L} a_l e^{ik_x x_l}. \end{aligned} \quad (2.7)$$

A relationship is now established between the modified wavenumber and the actual wavenumber. There are two main parameters associated with the modified wavenumber used to quantify the dispersion error from the spatial discretization scheme alone. This is the semi-discretized numerical phase and group velocities. The numerical phase and group velocity in this form do not take into account of the effect of the temporal discretization.

$$\begin{aligned} U_{phase,semi}^* &= \frac{k_x^* \Delta x}{k_x \Delta x}, \\ U_{grp,semi}^* &= \frac{\partial(k_x^* \Delta x)}{\partial(k_x \Delta x)}. \end{aligned} \quad (2.8)$$

As shown by [Trefethen, 1982], the speed of propagation of a computed signal is the

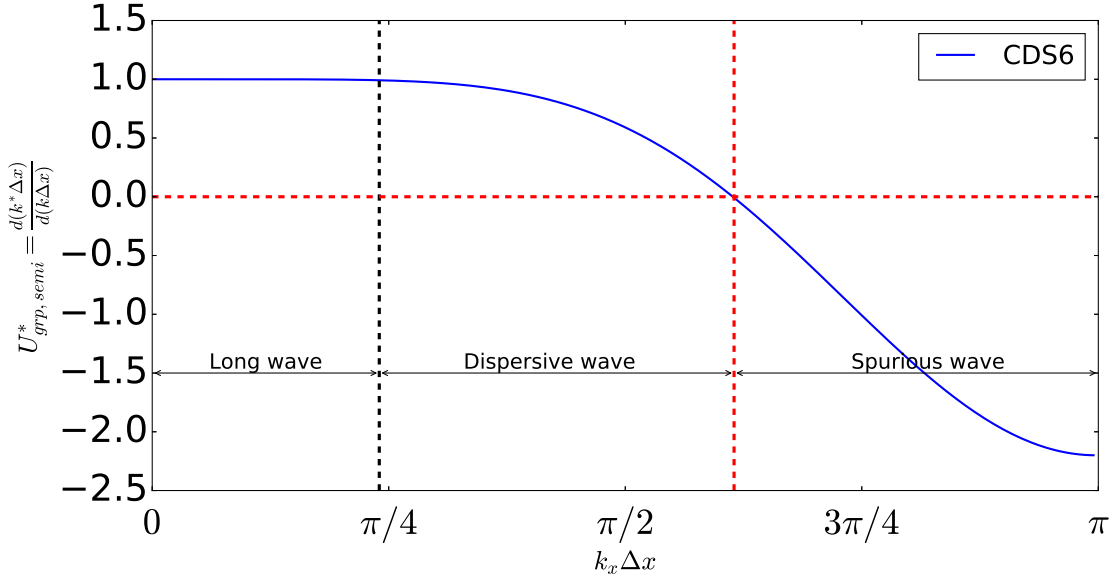


Figure 2.2: Illustrating the different categories of wave (long wave, dispersive wave and spurious wave) via the group velocity. The sixth order central difference scheme is shown (adapted from [Tam and Webb, 1993]).

numerical group velocity. Therefore, the key parameter used to quantify numerical dispersion is the numerical group velocity. Differences between numerical and physical phase speed can become significant when the numerical solution displays sharp spatial variation [Sengupta and Bhole, 2014]. Hence, phase error cannot be eliminated by grid refinement alone. Figure 2.2 shows the semi discretized numerical group velocity of the sixth order central difference (CDS6) scheme as a function of the reduced wavenumber, $k_x \Delta x$.

The group velocities can be split into three main categories of wave; namely the long wave, dispersive wave and spurious wave. The long wave represents the well resolved wave, for which the numerical group velocities remain close to 1.0. The dispersive wave represents the less well resolved waves and it travels at a slower speed. The spurious wave represents the poorly resolved wave for which the numerical group velocities is negative. In reality, the spurious wave represents the wave travelling in opposite direction to the physical wave. The real part of the modified wavenumber relates to the dispersion property while the imaginary part of the modified wavenumber relates to the dissipation property of the spatial discretization scheme. Mathematically, this is ex-

pressed as

$$\begin{aligned}\Re(k_x^* \Delta x) &= \sum_{l=-L}^{+L} a_l \sin(k_x x_l), \\ \Im(k_x^* \Delta x) &= - \sum_{l=-L}^{+L} a_l \cos(k_x x_l).\end{aligned}\tag{2.9}$$

This is illustrated in figures 2.3 and 2.4 for the second order central difference (CDS2) and second order backward difference (BDS2) scheme. Ideally, one would like to have a numerical method for which $k_x^*/k_x = 1.0$. However, one can see that at higher k , the derivative component of the CDS2 scheme are severely filtered (figure 2.3). Moreover, the use of one sided schemes such as the BDS2 scheme give rise to numerical dissipation (figure 2.4). The modified wavenumber of some representative finite difference schemes are described below.

2.1.2 Conventional finite difference schemes

For the purpose of comparison between a central and upwind biased schemes, we consider both the second order central difference (CDS2) and second order backward difference scheme (BDS2). The coefficients of the CDS2 scheme is given by: $a_{-1} = -\frac{1}{2}$ and $a_1 = \frac{1}{2}$. Its modified reduced wavenumber is given as:

$$\begin{aligned}(k_x^* \Delta x)_{CDS2} &= -i\left(-\frac{1}{2} \cos(k_x \Delta x) + i\frac{1}{2} \sin(k_x \Delta x) + \frac{1}{2} \cos(k_x \Delta x) + i\frac{1}{2} \sin(k_x \Delta x)\right), \\ &= -i(i \sin(k_x \Delta x)) = \underbrace{\sin(k_x \Delta x)}_{\Re(k_x^* \Delta x)},\end{aligned}\tag{2.10}$$

where Δx represents the uniform grid spacing. The coefficients of the BDS2 scheme is given by: $a_{-2} = \frac{1}{2}$, $a_{-1} = -2$ and $a_0 = \frac{3}{2}$. Its modified reduced wavenumber is given as:

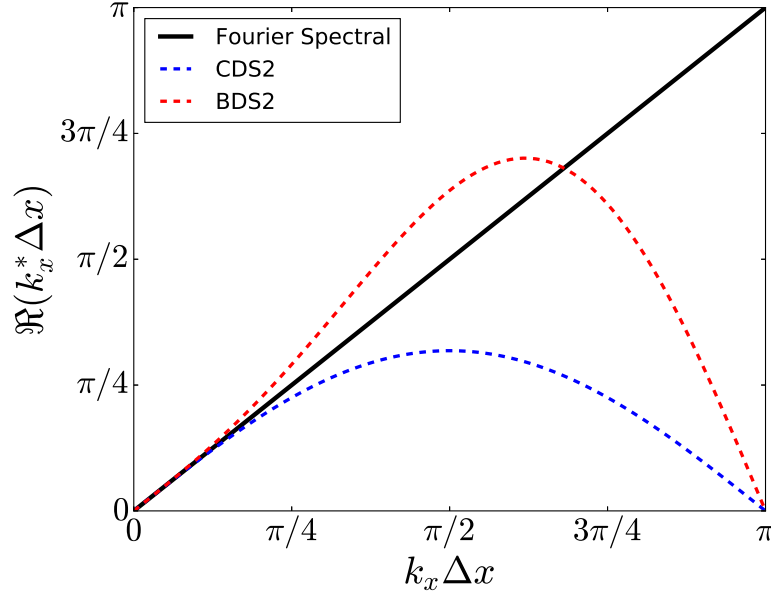


Figure 2.3: Dispersion property of the CDS2 and BDS2 scheme

$$\begin{aligned}
 (k_x^* \Delta x)_{BDS2} &= -i \left(\frac{1}{2} \cos(2k_x \Delta x) - i \frac{1}{2} \sin(2k_x \Delta x) - 2 \cos(k_x \Delta x) + i 2 \sin(k_x \Delta x) \right) \\
 &= \underbrace{2 \sin(k_x \Delta x) - \frac{1}{2} \sin(2k_x \Delta x)}_{\Re(k_x^* \Delta x)} + i \underbrace{\left(2 \cos(k_x \Delta x) - \frac{1}{2} \cos(2k_x \Delta x) - \frac{3}{2} \right)}_{\Im(k_x^* \Delta x)} \quad (2.11)
 \end{aligned}$$

For the BDS2 scheme, the modified reduced wavenumber has an imaginary component unlike the CDS2 scheme. In the case of the one dimensional convection equation, the numerical solution which accounts only for the spatial discretization effect is given by $\hat{\Phi}(k, t) = \hat{\Phi}(k, 0) e^{-i\bar{u}k_x^* t}$ [Sengupta, 2013]. Under the consideration of a positive phase velocity ($\bar{u}$), it can be seen that the use of a one sided biased scheme will introduce numerical dissipation into the numerical solution. The dispersion and dissipation property of the CDS2 and BDS2 schemes are shown in figures 2.3 and 2.4. In figure 2.3, the solid black line represents the ideal relation in which all frequencies up to the Nyquist limit are resolved, i.e. $\Re(k_x^* \Delta x) = k_x \Delta x$. Ideally, a spatial discretization scheme should try to match the solid black line as much as possible across the entire reduced wavenumber range.

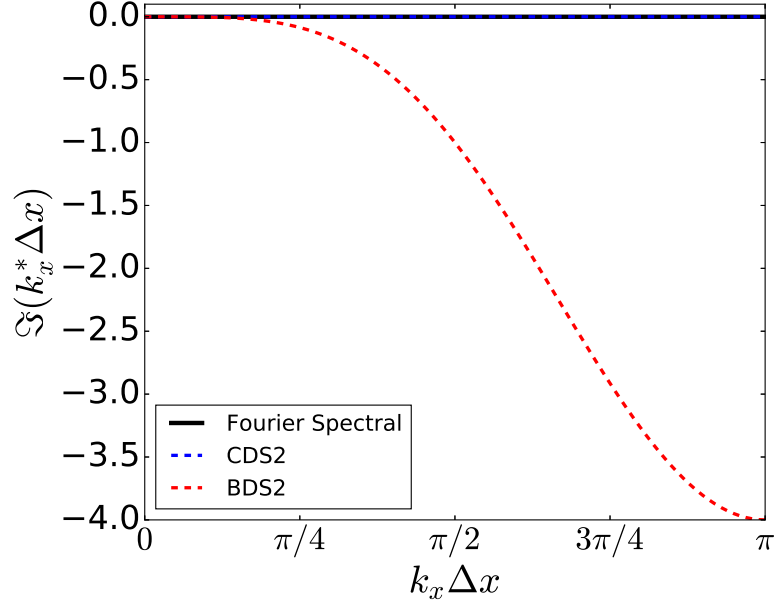


Figure 2.4: Dissipation property of the CDS2 and BDS2 scheme

The dispersion property of the BDS2 scheme in figure 2.3 has region where its modified wavenumber overshoots the ideal relation. Using such a scheme can lead to numerical solution whereby the waves are travelling at a faster numerical phase speed than the actual physical solution. Also, it can be seen in figure 2.4 that the CDS2 scheme is non dissipative unlike the BDS2 scheme. The solid black line in figure 2.4 represents the ideal relation in which there is no numerical dissipation, i.e. $\Im(k_x^* \Delta x) = 0$.

2.1.3 Compact difference schemes

Implicit compact difference scheme is introduced through the works of [Adam, 1977] and [Hirsh, 1975]. Subsequently, [Lele, 1992] developed a general approach to obtain compact schemes with formal order of accuracy up to 10th order. The notation of 'compact' refers to the reduced stencil width as compared to conventional finite difference scheme of the same order of accuracy. This has advantages in terms of the reduced number of ghost points needed for boundary condition and parallelization. However, the use of neighbouring derivative values to compute the derivative at the node of interest complicates the computational implementation. The general formulation of a compact scheme under

the consideration of uniform grid spacing is given by [Lele, 1992]:

$$\begin{aligned} & b_{-2}\Phi'_{i-2} + b_{-1}\Phi'_{i-1} + \Phi'_i + b_{+1}\Phi'_{i+1} + b_{+2}\Phi'_{i+2} \\ &= \frac{a_{-3}}{6\Delta x}\Phi_{i-3} + \frac{a_{-2}}{4\Delta x}\Phi_{i-2} + \frac{a_{-1}}{2\Delta x}\Phi_{i-1} + \frac{a_{+1}}{2\Delta x}\Phi_{i+1} + \frac{a_{+2}}{4\Delta x}\Phi_{i+2} + \frac{a_{+3}}{6\Delta x}\Phi_{i+3} \end{aligned} \quad (2.12)$$

For a given list of points, equation (2.12) can be written into a matrix system as follows:

$$[A]\Phi' = [B]\Phi. \quad (2.13)$$

The only unknown in this matrix system is Φ' . Depending on whether $b_{\pm 2}$ is equal to zero, matrix A can be either a pentadiagonal or tridiagonal matrix. If $b_{\pm 2} = b_{\pm 1} = 0$, then matrix A reduces to an identity matrix. In that case, the derivative can be computed explicitly just like conventional finite difference schemes. In the instance that matrix A is not an identity matrix, matrix inversion is required to solve the assembled system of equations. There are algorithms which take advantage of the diagonal structure of matrix A to solve equation (2.13) efficiently. Such algorithms are for instance the Thomas algorithm used for solving tridiagonal matrix. Similar to conventional finite difference scheme, the stencil of the compact scheme can be either central type or upwind biased, depending on the values of the coefficients in equation (2.12). Compact schemes with upwind biased stencils (known as the standard upwind compact difference scheme) can be found in [Fan, 2016]. The other type of 'upwind' compact schemes found in [Sengupta et al., 2003] has a centered stencil but comes with adjustable built in numerical dissipation. Comparatively speaking, the use of compact schemes are still computationally more expensive than conventional finite difference scheme of the same order of accuracy. The coefficients of the sixth order central compact scheme are as follows: $b_{\pm 2} = 0$, $b_{\pm 1} = \frac{1}{3}$, $a_{+2} = \frac{1}{36}$, $a_{-2} = -\frac{1}{36}$, $a_{+1} = \frac{7}{9}$, $a_{-1} = -\frac{7}{9}$. By applying a Fourier transform to both sides of equation (2.12), a general form of the modified wavenumber for compact scheme was derived in [Lele, 1992]. The modified wavenumber of the CCOM6 scheme is given as:

$$(k_x^*\Delta x)_{CCOM6} = \frac{\frac{14}{9} \sin(k_x\Delta x) + \frac{1}{18} \sin(2k_x\Delta x)}{1 + \frac{2}{3} \cos(k_x\Delta x)}. \quad (2.14)$$

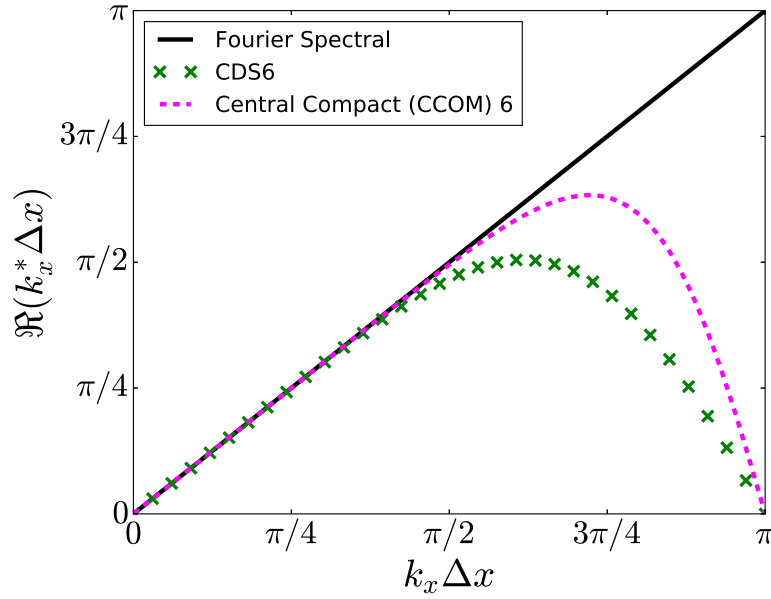


Figure 2.5: Dispersion property of the CDS6 and CCOM6 scheme

For the purpose of illustration, the dispersion property of the sixth order central compact scheme (CCOM6) is plotted alongside the sixth order central difference scheme (CDS6) in figure 2.5. It can be clearly seen that the CCOM6 scheme offers better spectral accuracy despite having the same order of accuracy.

2.1.4 Dispersion relation preserving schemes

As previously discussed, the truncation error of a numerical scheme is not the critical parameter which measures the performance of the finite difference scheme. What is of utmost importance is the spectral accuracy of the scheme in wavenumber space. Recognizing this, [Tam and Webb, 1993] took a conventional finite difference scheme and optimize its coefficients for optimal dispersion property at the expense of its formal order of accuracy. Similar approaches have been extended to compact difference schemes [Lele, 1992, Kim and Lee, 1996] as well as higher order central difference schemes [Bogey and Bailly, 2004]. The dispersion relation preserving (DRP) schemes that were developed in the literature have some degree of differences primarily because of the choices made in the range of wavenumber for which the dispersion error is minimized. The other

consideration is that the schemes can be optimized based on either the semi-discretized numerical dispersion or the fully discretized numerical dispersion relation. Use of the fully discretized numerical dispersion relation will take into account the optimization of the temporal discretization scheme as well [Sengupta et al., 2011a].

The major benefit of the DRP schemes is that improved spectral accuracy can be achieved without any increase in computing resources, unlike the compact schemes. For the purpose of illustration, the dispersion property of the fourth order DRP scheme (DRP4) of [Tam and Webb, 1993] is plotted alongside the 9 point optimized finite difference scheme (FDo9p) of [Bogey and Bailly, 2004]. These schemes are compared against conventional sixth and eighth order central difference schemes (CDS6, CDS8) having the same stencils respectively. This is presented in figure 2.11. The general form of the DRP or conventional FD schemes is given by equation (2.1). Their coefficients are shown in table 2.1.

Table 2.1: Coefficients of the different schemes ($a_0 = 0, a_{-j} = -a_j$):

Coeff.	DRP4	CDS6	FDo9p	CDS8
a_1	0.79926643	3/4	0.841570125482	4/5
a_2	-0.18941314	-3/20	-0.244678631765	-1/5
a_3	0.02651995	1/60	0.059463584768	4/105
a_4	-	-	-0.007650904064	-1/280

The modified wavenumber of these schemes can be obtained by using equation (2.7). It can be seen that the DRP schemes (DRP4, FDo9p) are able to achieve better spectral accuracy as compared to the conventional sixth and eighth order central difference schemes.

2.1.5 Isotropy optimized finite difference schemes

All of the finite difference schemes discussed thus far were developed in one dimension and then applied to multidimensional problems. There is some crucial considerations not taken into account when a method developed based on one dimensional analysis is used on multidimensional problems. In one dimensional space, the dispersion error of the FD scheme is translated into an error in the group velocity of the advecting wave. In multidimensional space, this will translate into directional error of the advecting wave.

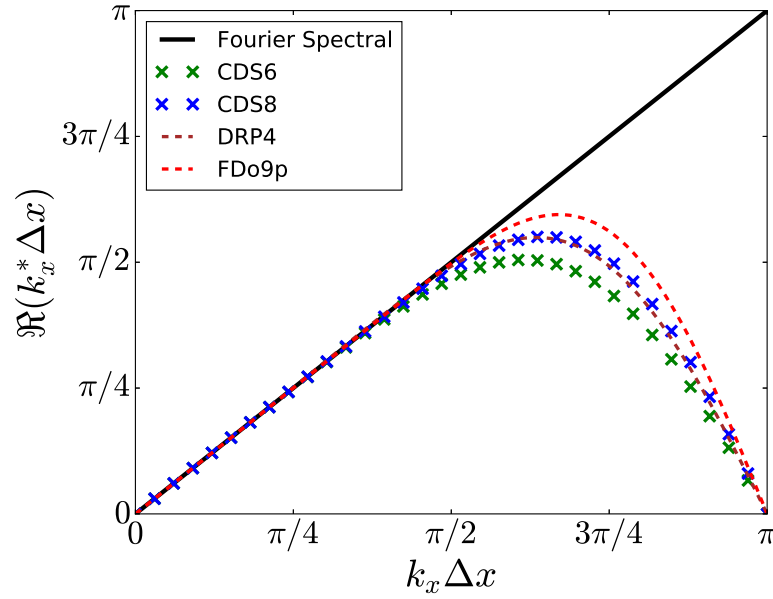


Figure 2.6: Dispersion property of the DRP schemes compared against conventional CDS6 and CDS8 schemes

In order to account for the anisotropy introduced in multidimensional problems, [Tam and Webb, 1993] developed a correction that could be used to account for the anisotropy. [Vichnevetsky and Bowles, 1982] noted the effect of applying different weighting to the surrounding nodes to influence the isotropic behaviour of the numerical scheme. [Sescu, 2008] built on this idea to develop a scheme that uses nodal points from more than one spatial direction. In particular, nodal points from the diagonal directions are used. The scheme is then optimized for isotropy by minimizing the difference in phase or group velocities along the x and $x = y$ directions. The idea is to obtain equal wave propagation speed along the main orthogonal direction so as to achieve isotropic behaviour in all directions. The fourth order isotropic optimized central difference scheme ($CDS4_{opt}$) is given as [Sescu, 2008]:

$$\begin{aligned}
\left(\frac{\partial \Phi}{\partial x}\right)_{i,j} \approx & \frac{1}{12\Delta x(1+\beta)} \left[\Phi_{i-2,j} - 8\Phi_{i-1,j} + 8\Phi_{i+1,j} - \Phi_{i+2,j} \right. \\
& + \frac{\beta}{2} (\Phi_{i-2,j-2} - 8\Phi_{i-1,j-1} + 8\Phi_{i+1,j+1} - \Phi_{i+2,j+2} - \Phi_{i+2,j-2} \\
& \left. + 8\Phi_{i+1,j-1} - 8\Phi_{i-1,j+1} + \Phi_{i-2,j+2}) \right], \tag{2.15}
\end{aligned}$$

$$\begin{aligned}
\left(\frac{\partial \Phi}{\partial y}\right)_{i,j} \approx & \frac{1}{12\Delta y(1+\beta)} \left[\Phi_{i,j-2} - 8\Phi_{i,j-1} + 8\Phi_{i,j+1} - \Phi_{i,j+2} \right. \\
& + \frac{\beta}{2} (\Phi_{i-2,j-2} - 8\Phi_{i-1,j-1} + 8\Phi_{i+1,j+1} - \Phi_{i+2,j+2} + \Phi_{i+2,j-2} \\
& \left. - 8\Phi_{i+1,j-1} + 8\Phi_{i-1,j+1} - \Phi_{i-2,j+2}) \right], \tag{2.16}
\end{aligned}$$

where β is the isotropy correction factor. It is found to be 0.26 for the fourth order central difference scheme [Sescu, 2008]. The modified wavenumber relation of the $CDS4_{opt}$ scheme is given as:

$$\begin{aligned}
(k_x^* \Delta x)_{CDS4_{opt}} = & \frac{1}{6(1+\beta)} \left\{ 8 \sin(k_x \Delta x) - \sin(2k_x \Delta x) + \frac{\beta}{2} \left(8 \sin(k_x \Delta x + k_y \Delta y) \right. \right. \\
& - \sin(2k_x \Delta x + 2k_y \Delta y) + 8 \sin(k_x \Delta x - k_y \Delta y) \\
& \left. \left. - \sin(2k_x \Delta x - 2k_y \Delta y) \right) \right\}, \tag{2.17}
\end{aligned}$$

$$\begin{aligned}
(k_y^* \Delta y)_{CDS4_{opt}} = & \frac{1}{6(1+\beta)} \left\{ 8 \sin(k_y \Delta y) - \sin(2k_y \Delta y) + \frac{\beta}{2} \left(8 \sin(k_x \Delta x + k_y \Delta y) \right. \right. \\
& - \sin(2k_x \Delta x + 2k_y \Delta y) - 8 \sin(k_x \Delta x - k_y \Delta y) \\
& \left. \left. + \sin(2k_x \Delta x - 2k_y \Delta y) \right) \right\}. \tag{2.18}
\end{aligned}$$

A schematic of the $CDS4_{opt}$ scheme stencils is illustrated in figure 2.7. It can be seen clearly that the nodal points in the diagonal direction are utilized in addition to the nodal points used in the x or y direction respectively.

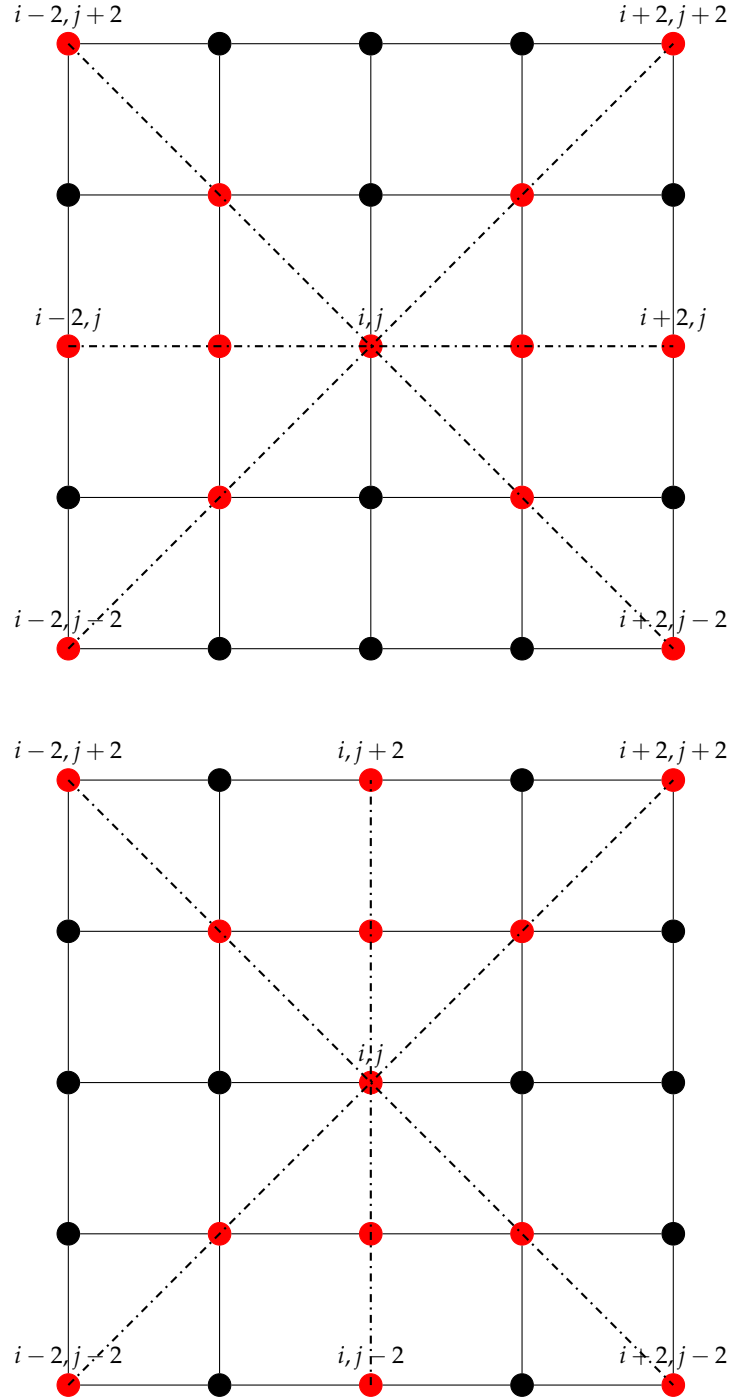


Figure 2.7: Schematic of $CDS4_{opt}$ stencils for x direction (Top) and y direction (Bottom) respectively

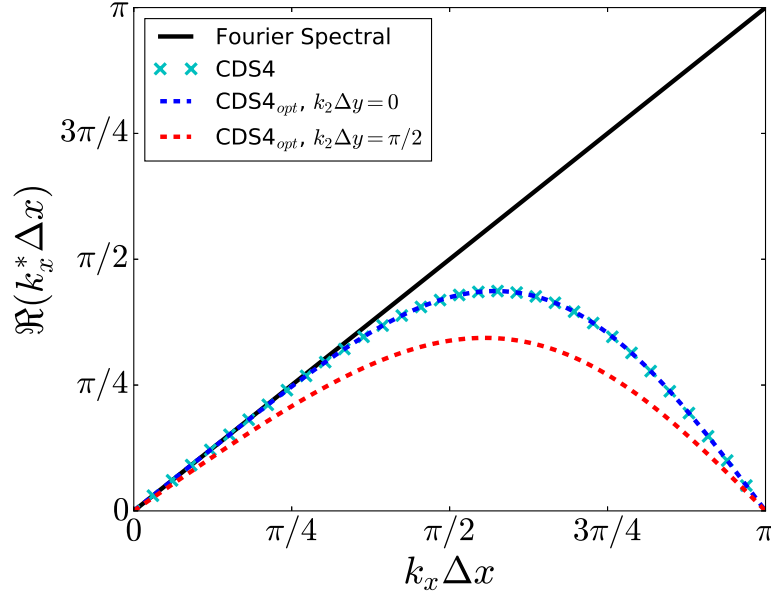


Figure 2.8: Dispersion property of the $CDS4_{opt}$ scheme compared against conventional CDS4 scheme

Unlike the FD schemes that have been discussed thus far, the modified wavenumber of the $CDS4_{opt}$ scheme is a function of the wavenumber in both spatial directions. This has consequences on the spectral properties of the numerical scheme especially when a multidimensional wavenumber analysis is considered. In one dimensional wavenumber analysis, the spectral property is influenced by the value of $k_y \Delta y$ chosen for the analysis. In order to illustrate this, the dispersion property of the $CDS4_{opt}$ is compared against conventional CDS4 scheme in figure 2.8.

It can be seen that the dispersion property of the $CDS4_{opt}$ scheme becomes the same as the conventional CDS4 scheme when $k_y \Delta y = 0$. When the value of $k_y \Delta y > 0$, the dispersion property of the $CDS4_{opt}$ scheme becomes poorer than conventional CDS4 scheme. Multidimensional wavenumber analysis of the $CDS4_{opt}$ scheme is presented in later sections.

2.1.6 Fourier spectral scheme

Last but not least, a discussion concerning Fourier spectral (FS) scheme is presented since the FS scheme is used in conjunction with the FD schemes in the later chapters. FS method was introduced by [Orszag, 1969]. Interest in the use of FS scheme arises primarily because of the perfect spectral accuracy ($k_x^* \Delta x = k_x \Delta x$) achievable by this method. However, its usage is limited to problems with periodic boundary condition as well as problems for which there are no discontinuities. This is related to the fact that a discontinuous function cannot be properly represented by a Fourier series. This give rise to the presences of Gibbs phenomenon near discontinuities. In this method, the governing equations are transformed into Fourier space using discrete Fourier transforms. Numerical solution is then advanced in time in Fourier space. Numerical solution is transformed back into physical space during the collection of data. A variable Φ written in terms of its discrete Fourier transform is given by

$$\Phi = \sum_{k=-N/2}^{N/2-1} \hat{\Phi}_k e^{ikx_j}. \quad (2.19)$$

A first order spatial derivative in Fourier space is given by

$$\mathcal{F}_k \left(\frac{\partial \Phi_j}{\partial x} \right) = \mathcal{F}_k \left(ik \sum_{k=-N/2}^{N/2-1} \hat{\Phi}_k e^{ikx_j} \right) = ik \hat{\Phi}_j, \quad (2.20)$$

where $j = 0 \dots N - 1$ represents the total number of points in a discretized domain. In the case for which there exists product (quadratic) terms in the governing equation, the application of discrete Fourier transform (DFT) directly to these product terms will lead to aliasing error. In order to resolve this issue, the 2/3 rule (or truncation method) is used [Canuto et al., 2006]. The basic idea is to set the amplitude of the coefficients for which $j > (2/3)N/2$ to zero before the inverse discrete Fourier transform (DFT^{-1}) is applied to the variables. Essentially, Fourier modes of the primitive variables greater than $N/3$ are truncated before they are transformed back to physical space. The rule is derived based on the condition that the aliased Fourier mode of the quadratic term should fulfil the condition $k_1 + k_2 - N < -k_{\max}$, where k_1 and k_2 represent the Fourier mode of the single term. Considering that the maximum values of k_1 and k_2 are $k_{\max}$, this would lead

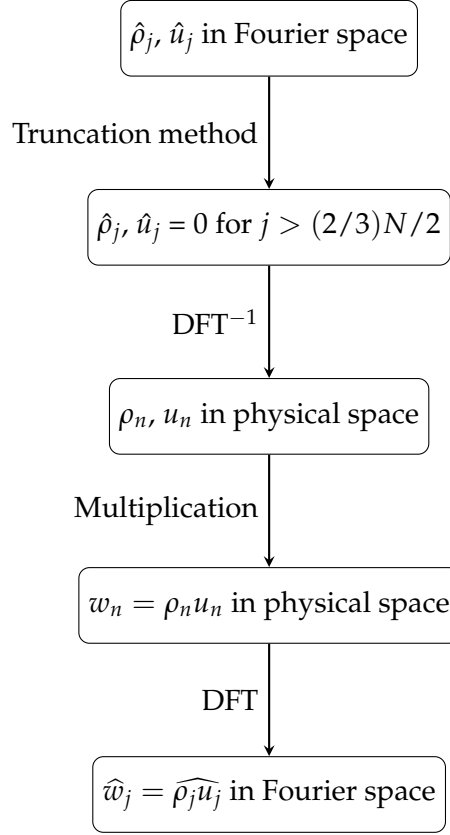


Figure 2.9: De-aliasing procedures for non linear terms at each time step

to the condition that $k_{max} < N/3$. The calculation procedure for a non linear term, ρu is illustrated in figure 2.9.

2.2 Temporal discretization methods

Temporal discretization methods can be classified mainly into explicit and implicit method. A range of representative temporal discretization method will be described. The schemes analyzed are considered as commonly used schemes in existing compressible and incompressible Navier-Stokes codes. In particular, the third order Runge Kutta (RK3) scheme is considered since it preserves the Total Variation Diminishing (TVD) property and is primarily used in chapter 4 of the thesis. The purpose is to introduce the temporal scheme, its numerical amplification factor and range of stability. Generally speaking, explicit method is more straight forward to implement and requires lesser computational

resources. On the other hand, implicit method requires more computational resources but are less affected by stability limitation.

2.2.1 Explicit Euler

The simplest time integration method is the explicit Euler method. This is a single step method. The scheme is given by

$$\Phi^{n+1} = \Phi^n + \left(\frac{\partial \Phi}{\partial t} \right)^n \Delta t, \quad (2.21)$$

where the superscript n refers to the index of the timestep, i.e. $t = n\Delta t$. Euler time integration method is simple to implement and uses little memory. However, the accuracy and region of stability is limited. Von Neumann stability analysis method [Moin, 2001] is used here to determine the stability region of the temporal scheme. The model equation for the temporal derivative is given by

$$\Phi' = \lambda \Phi, \quad (2.22)$$

where λ is a complex number with real and imaginary component. Using it within equation (2.21) leads to the amplification factor of the explicit Euler equation

$$\begin{aligned} \Phi^{n+1} &= \Phi^n + \lambda \Phi^n \Delta t \\ Z &= \frac{\Phi^{n+1}}{\Phi^n} = 1 + \lambda \Delta t. \end{aligned} \quad (2.23)$$

In order to ensure the stability of the numerical method, $|Z| \leq 1$, and therefore

$$|Z| = (1 + \lambda_{Re} \Delta t)^2 + (\lambda_{Im} \Delta t)^2 \leq 1. \quad (2.24)$$

This is the equation of a circle with radius 1, centered at (-1,0). The inequality sign implies that Z must lie inside the circle in order for the method to be stable. The stable region of the Explicit Euler scheme is plotted in a complex plane as shown in figure 2.10. Region within the blue contour line represents the stable region. The contour line demarcates

the location where the absolute stability is 1.0. For stability reason, the magnitude of the amplification factor must remain less than or equal to one in order for the solution to remain bounded and stable.

2.2.2 Third order Runge Kutta

The next commonly used explicit time integration scheme is the third order Runge Kutta scheme (RK3). The Runge Kutta methods are multi step methods and they offer improved accuracy and stability. The third order Runge Kutta scheme is given by:

$$\Phi^{n+1} = \Phi^n + \frac{1}{6}k_1 + \frac{2}{3}k_2 + \frac{1}{6}k_3 \quad (2.25)$$

where

$$\begin{aligned} k_1 &= \Delta t \mathcal{F}(\Phi^n, t^n) \\ k_2 &= \Delta t \mathcal{F}\left(\Phi^n + \frac{1}{2}k_1, t^n + \frac{\Delta t}{2}\right) \\ k_3 &= \Delta t \mathcal{F}(\Phi^n - k_1 + 2k_2, t^n + \Delta t). \end{aligned} \quad (2.26)$$

RK3 scheme is also known as a total variation diminishing (TVD) scheme since it preserves the TVD property [Sengupta, 2013] during the time integration. Using the model equation for the temporal derivative into equation (2.25), the numerical amplification factor of the RK3 scheme is given by:

$$Z = \frac{\Phi^{n+1}}{\Phi^n} = 1 + \lambda \Delta t + \frac{1}{2}(\lambda \Delta t)^2 + \frac{1}{6}(\lambda \Delta t)^3 \quad (2.27)$$

The stable region of the RK3 scheme is plotted in a complex plane as shown in figure 2.10. Region within the red contour line represents the stable region. The contour line demarcates the location where the absolute stability is 1.0.

2.2.3 Fourth order Runge Kutta

The fourth order Runge Kutta scheme (RK4) is given by:

$$\Phi^{n+1} = \Phi^n + \frac{1}{6}k_1 + \frac{1}{3}(k_2 + k_3) + \frac{1}{6}k_4 \quad (2.28)$$

where

$$\begin{aligned} k_1 &= \Delta t \mathcal{F}(\Phi^n, t^n) \\ k_2 &= \Delta t \mathcal{F}\left(\Phi^n + \frac{1}{2}k_1, t^n + \frac{\Delta t}{2}\right) \\ k_3 &= \Delta t \mathcal{F}\left(\Phi^n + \frac{1}{2}k_2, t^n + \frac{\Delta t}{2}\right) \\ k_4 &= \Delta t \mathcal{F}(\Phi^n + k_3, t^n + \Delta t) \end{aligned} \quad (2.29)$$

Using the model equation for the temporal derivative into equation (2.28), the numerical amplification factor of the RK4 scheme is given by:

$$Z = \frac{\Phi^{n+1}}{\Phi^n} = 1 + \lambda \Delta t + \frac{1}{2}(\lambda \Delta t)^2 + \frac{1}{6}(\lambda \Delta t)^3 + \frac{1}{24}(\lambda \Delta t)^4. \quad (2.30)$$

The stable region of the RK4 scheme is plotted in a complex plane as shown in figure 2.10. Region within the black contour line represents the stable region. The contour line demarcates the location where the absolute stability is 1.0. The stable region is demarcated by the location where the contour level remain below 1 for each respective scheme. This represents the region within the contour line of each temporal scheme. It can be seen that a higher order temporal scheme has a larger stable region. This allows for the use of a larger time step.

2.2.4 Implicit Euler

The implicit Euler time integration scheme is given by:

$$\Phi^{n+1} = \Phi^n + \left(\frac{\partial \Phi}{\partial t}\right)^{n+1} \Delta t. \quad (2.31)$$

Using the model equation for the temporal derivative into equation (2.31), the numerical amplification factor of the Implicit Euler scheme is given by:

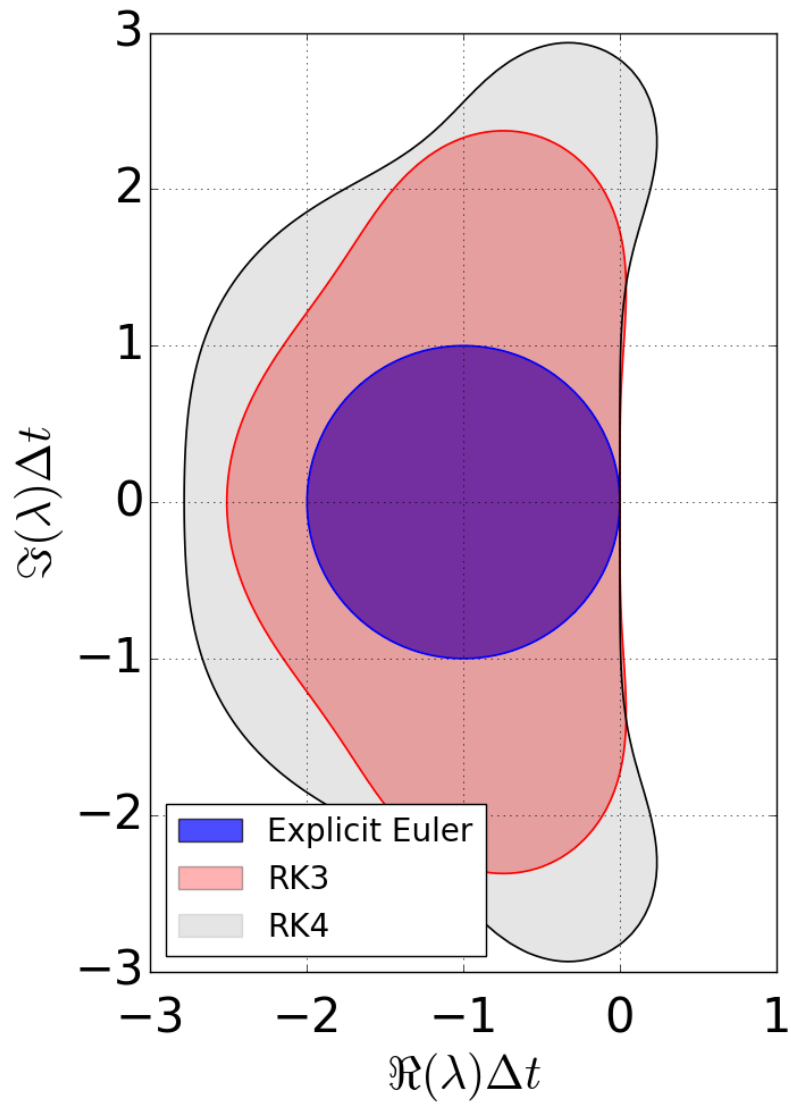


Figure 2.10: Stability region of the explicit Euler, RK3 and RK4 schemes. Stable region lies within the contour line of each scheme respectively.

$$\begin{aligned}\Phi^{n+1} &= \Phi^n + \lambda \Phi^{n+1} \Delta t \\ Z &= \frac{\Phi^{n+1}}{\Phi^n} = \frac{1}{1 - \lambda \Delta t}\end{aligned}\tag{2.32}$$

The condition for stability of the implicit Euler scheme can be re-written in terms of the real and imaginary part of λ as follows:

$$\begin{aligned}|Z| &= \frac{1}{(1 - \lambda_{Re} \Delta t)^2 + (\lambda_{Im} \Delta t)^2} \leq 1 \\ (1 - \lambda_{Re} \Delta t)^2 + (\lambda_{Im} \Delta t)^2 &> 1\end{aligned}\tag{2.33}$$

As with the explicit Euler scheme, this represents a circle of radius 1 centered at (1,0). The reverse in inequality sign implies that the stable region falls outside the circle. Therefore, the implicit Euler method is always stable as long as $\lambda_{Re} < 0$, no matter the chosen value of Δt . The stable region of the implicit Euler scheme is plotted in a complex plane as shown in figure 2.11.

2.2.5 Crank-Nicolson

The implicit Crank-Nicolson (CN) scheme is given by:

$$\Phi^{n+1} = \Phi^n + \frac{\Delta t}{2} \left[\left(\frac{\partial \Phi}{\partial t} \right)^{n+1} + \left(\frac{\partial \Phi}{\partial t} \right)^n \right].\tag{2.34}$$

It uses a combination of information from the current and future time step to compute the information in the next time step. Using the model equation for the temporal derivative into equation (2.34), the numerical amplification factor of the Implicit CN scheme is given by:

$$\begin{aligned}\Phi^{n+1} &= \Phi^n + \frac{\Delta t}{2} \lambda \Phi^n + \frac{\Delta t}{2} \lambda \Phi^{n+1} \\ Z &= \frac{\Phi^{n+1}}{\Phi^n} = \frac{(1 + \frac{\Delta t \lambda}{2})}{(1 - \frac{\Delta t \lambda}{2})}\end{aligned}\tag{2.35}$$

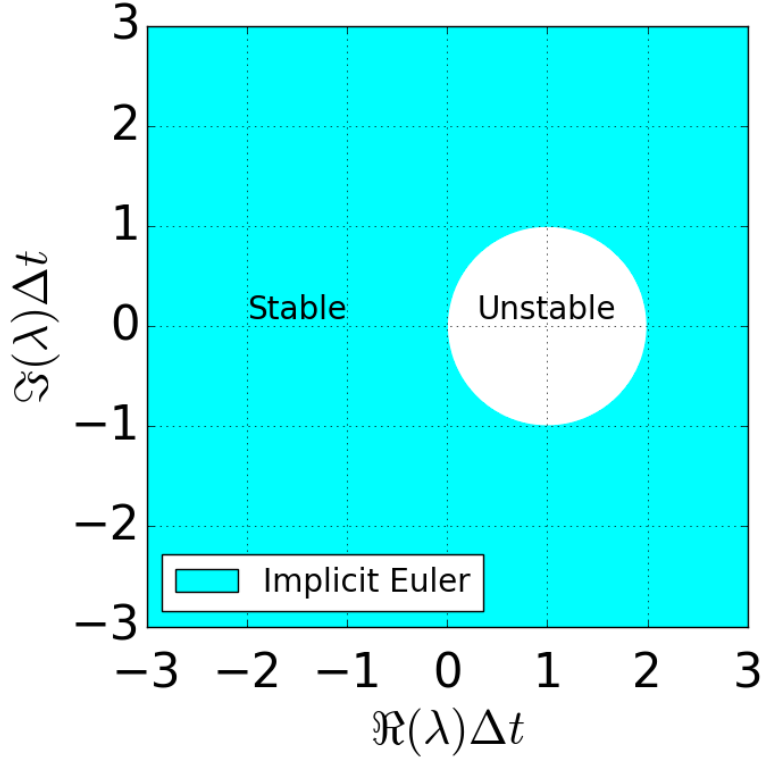


Figure 2.11: Stability region of the implicit Euler scheme. Stable region lies outside the circle according to equation (2.33).

The stable region of the implicit CN scheme is plotted in a complex plane as shown in figure 2.12. The stable region of the CN scheme is the entire left hand plane of the stability plot. The method is stable for any choice of Δt as long as $\lambda_{Re} < 0$. The implications of using implicit temporal schemes are further explored in the next section.

2.3 1D linear spectral analysis under full discretization

The accuracy of the spatial scheme determined through the use of Fourier analysis was established in the previous section. When it comes to assessing the accuracy of a numerical method, the accuracy of the spatial scheme is only part of the story. Assessing the spatial discretization in conjunction with the temporal discretization is critical in ensuring that the overall scheme is accurate and stable. For this purpose, we looked at the model 1D advection and linearized Euler equations.

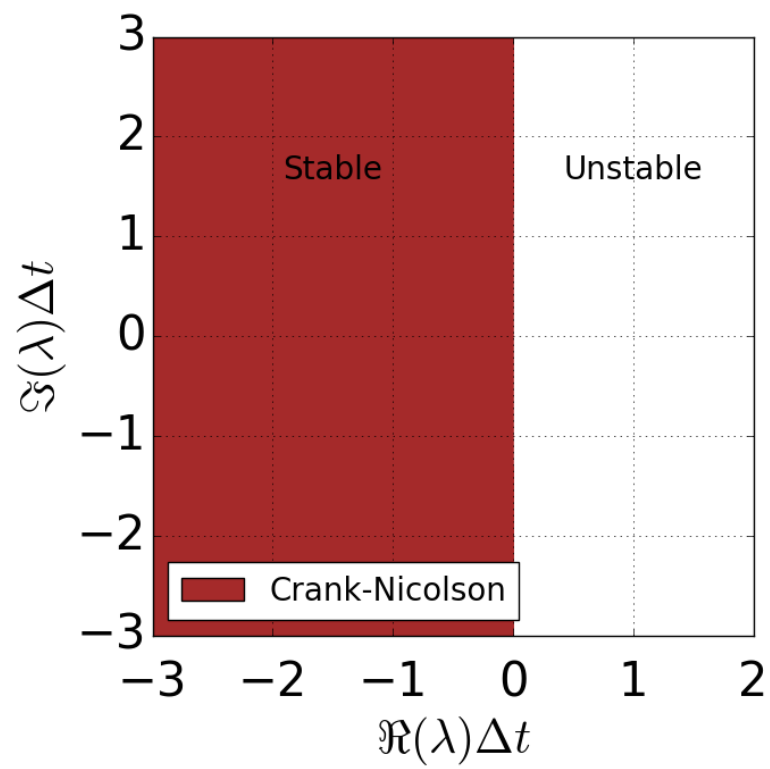


Figure 2.12: Stability region of the Crank-Nicolson scheme. Stable region lies on the left plane for $\lambda_{Re} < 0$.

2.3.1 1D Advection

We first begin with the linear model equation for inviscid flow. Equation (2.36) is a non-dispersive equation that convects the initial solution to the right at a group velocity, $\bar{u}$ equal to the phase speed at all times. In solving equation (2.36) numerically, the spatial and temporal derivatives are replaced by numerical approximation.

$$\frac{\partial \Phi}{\partial t} + \bar{u} \frac{\partial \Phi}{\partial x} = 0. \quad (2.36)$$

The field variable, Φ , is written in terms of its inverse Fourier transform:

$$\Phi(x, t) = \frac{1}{2\pi} \int_{-\pi/\Delta x}^{\pi/\Delta x} \hat{\Phi}(k_x, t) e^{ik_x x} dk_x. \quad (2.37)$$

Substituting equation (2.37) into (2.36) and noting that the introduction of the inverse Fourier transform of the field variable into the numerical approximation of the spatial derivative term introduces a modified wavenumber k_x^* [Vichnevetsky and Bowles, 1982], the resulting equation is:

$$\frac{\partial \hat{\Phi}(k_x, t)}{\partial t} = -i\bar{u}k_x^* \hat{\Phi}(k_x, t). \quad (2.38)$$

Equation (2.38) has a solution of the form:

$$\hat{\Phi}(k_x, t) = \hat{\Phi}(k_x, 0) e^{-i\bar{u}k_x^* t}. \quad (2.39)$$

By substituting equation (2.39) back into equation (2.37), the field variable Φ can be written as follows:

$$\Phi(x, t) = \int_{-\pi/\Delta x}^{\pi/\Delta x} \hat{\Phi}(k_x, 0) e^{i(k_x x - \bar{u}k_x^* t)} dk_x. \quad (2.40)$$

By comparing this to the exact solution:

$$\Phi(x, t) = \int_{-\pi/\Delta x}^{\pi/\Delta x} \hat{\Phi}(k_x, 0) e^{i(k_x x - \omega t)} dk_x. \quad (2.41)$$

The numerical dispersion relation is given by $\omega = \bar{u}k_x^*$. It can be seen that the numerical

dispersion relation in this form considers only the spatial discretization effect. Hence it will be denoted as ω_{semi}^* hereafter. The solution $\hat{\Phi}(k_x, t) = \hat{\Phi}(k, 0)e^{-i\bar{u}k_x^*t}$ is only true when there is no error in the time discretisation scheme. In reality, a numerical solution must be advanced through time using a temporal scheme and this will introduce temporal discretization error. In order to account for the temporal discretization effect, the numerical amplification factor of the temporal scheme is considered.

For the explicit Euler scheme, the solution at the next time step written in terms of the solution at the current time step in Fourier space is given by

$$\begin{aligned}\hat{\Phi}(k_x, t + \Delta t) &= \hat{\Phi}(k_x, t) + \left(\frac{\partial \hat{\Phi}}{\partial x}\right) \Delta t \\ &= \hat{\Phi}(k_x, t) - i\bar{u}k_x^* \hat{\Phi} \Delta t \\ &= [1 - \Delta t i\bar{u}k_x^*] \hat{\Phi}(k_x, t) \\ &= [1 - \Delta t i\omega_{semi}^*] \hat{\Phi}(k_x, t).\end{aligned}\tag{2.42}$$

Following this process, the analysis framework can be generalized to other temporal scheme such as the RK3, RK4 and CN scheme since $\frac{\partial \hat{\Phi}}{\partial x} = -i\omega_{semi}^* = -i\bar{u}k_x^*$. The fully discretized numerical amplification factor of the RK3, RK4 and CN scheme are given as

$$\hat{\Phi}(k_x, t + \Delta t) = \underbrace{\left[1 - \Delta t i\bar{u}k_x^* + \frac{(\Delta t i\bar{u}k_x^*)^2}{2} - \frac{(\Delta t i\bar{u}k_x^*)^3}{6}\right]}_{Z_{RK3}} \hat{\Phi}(k_x, t), \tag{2.43}$$

$$\hat{\Phi}(k_x, t + \Delta t) = \underbrace{\left[1 - \Delta t i\bar{u}k_x^* + \frac{(\Delta t i\bar{u}k_x^*)^2}{2} - \frac{(\Delta t i\bar{u}k_x^*)^3}{6} + \frac{(\Delta t i\bar{u}k_x^*)^4}{24}\right]}_{Z_{RK4}} \hat{\Phi}(k_x, t), \tag{2.44}$$

$$\hat{\Phi}(k_x, t + \Delta t) = \underbrace{\left[\frac{1 - \frac{\Delta t i\bar{u}k_x^*}{2}}{1 + \frac{\Delta t i\bar{u}k_x^*}{2}}\right]}_{Z_{CN}} \hat{\Phi}(k_x, t), \tag{2.45}$$

where:

$$\bar{u}k_x^*\Delta t = Rk_x^*\Delta x, \quad R = \frac{\bar{u}\Delta t}{\Delta x}. \quad (2.46)$$

R represents the CFL number. The solution, $\hat{\Phi}$ in the next instant is represented by the product of a complex number, Z and the solution of the previous timestep. Using this information and equation (2.37), the general solution of Φ considered after n time steps can be written as follows:

$$\Phi(x, t_0 + n\Delta t) = \frac{1}{2\pi} \int_{-\pi/\Delta x}^{\pi/\Delta x} Z^n \hat{\Phi}(k_x, 0) e^{ik_x x} dk_x, \quad (2.47)$$

where Z is a complex number which can be expressed in terms of its modulus and argument, $Z = |Z|e^{-i\psi}$. The resulting equation is

$$\Phi(x, t_0 + n\Delta t) = \frac{1}{2\pi} \int_{-\pi/\Delta x}^{\pi/\Delta x} |Z|^n \hat{\Phi}(k_x, 0) e^{i(k_x x - n\psi)} dk_x. \quad (2.48)$$

The general numerical solution to Equation (2.36) is given as

$$\Phi(x, t) = \frac{1}{2\pi} \int_{-\pi/\Delta x}^{\pi/\Delta x} |Z|^{t/\Delta t} \hat{\Phi}(k_x, 0) e^{i(k_x x - U_{phase,full}^* k_x t)} dk_x. \quad (2.49)$$

Instead of having a constant physical phase speed, $\bar{u}$ as in the case of an exact solution, the numerical solution is represented by a wavenumber dependent numerical phase speed, $U_{phase,full}^*$. This is because the numerical solution is dispersive. By comparing the numerical solution to the exact solution of the 1D advection equation:

$$\begin{aligned} \Phi(x, t) &= \frac{1}{2\pi} \int_{-\pi/\Delta x}^{\pi/\Delta x} |Z|^{t/\Delta t} \hat{\Phi}(k_x, 0) e^{i(k_x x - U_{phase,full}^* k_x t)} dk_x \\ &= \frac{1}{2\pi} \int_{-\pi/\Delta x}^{\pi/\Delta x} |Z|^{t/\Delta t} \hat{\Phi}(k_x, 0) e^{i(k_x x - \omega t)} dk_x, \end{aligned} \quad (2.50)$$

the numerical dispersion relation is given by $\omega = U_{phase,full}^* k_x$. The numerical dispersion relation in this form considers both space and time discretization and will be denoted as ω_{full}^* hereafter. It should be noted that $U_{phase,full}^*$ is a wavenumber dependent variable while k_x is an independent variable. The relation between ω_{full}^* and the numerical am-

plification factor, Z is established next. By comparing equation (2.50) to equation (2.48), it can be seen that ω_{full}^* of the 1D advection equation is related to the phase shift of the amplification factor via:

$$\begin{aligned}\omega_{full}^* t &= U_{phase,full}^* k_x n \Delta t = n \psi, \\ \omega_{full}^* &= U_{phase,full}^* k_x = \frac{\psi}{\Delta t}, \\ \frac{\omega_{full}^*}{k_x} &= U_{phase,full}^* = \frac{\psi}{k_x \Delta t}.\end{aligned}\tag{2.51}$$

The physical dispersion relation of the 1D advection is given by $\omega = \bar{u} k_x$ and the corresponding physical phase speed is calculated as $U_{phase,exact} = \frac{\omega}{k_x} = \bar{u}$. The normalized numerical phase speed can be expressed as follows:

$$\frac{U_{phase,full}^*}{U_{phase,exact}} = \frac{\psi}{\bar{u} k_x \Delta t} = \frac{\psi}{R k_x \Delta x}.\tag{2.52}$$

The normalized numerical group velocity based on full discretization consideration is obtained using the fully discretized numerical dispersion relation as follows:

$$\frac{U_{grp,full}^*}{U_{grp,exact}} = \frac{1}{\bar{u}} \frac{\partial \omega_{full}^*}{\partial k_x} = \frac{1}{\bar{u} \Delta t} \frac{\partial \psi}{\partial k_x} = \frac{1}{R \Delta x} \frac{\partial \psi}{\partial k_x},\tag{2.53}$$

where $\psi = -\tan^{-1} \left(\frac{\text{Im}(Z(\Delta t \omega_{semi}^*))}{\text{Real}(Z(\Delta t \omega_{semi}^*))} \right)$. It should be noted that $U_{grp,exact} = \frac{\partial \omega}{\partial k_x} = \bar{u}$ for the 1D advection equation. For group velocity calculated under full discretization, the fully discretized numerical dispersion relation is considered. As seen above, there are three error metrics to consider for the full discretization analysis. The numerical group and phase speed is related to the dispersion property while the numerical amplification factor is related to the dissipation property.

As shown by [Vichnevetsky and Bowles, 1982], the numerical dispersion relation for full discretization approaches those under semi-discretization consideration as $\Delta t \rightarrow 0$. Therefore, the semi-discretized numerical dispersion relation provides the effective limit

for the accuracy of the full discretization. We will now consider how the change in R influences the three different error metric; numerical amplification factor, numerical phase speed and numerical group velocity.

Effect of CFL number on numerical amplification factor

As seen from equation (2.43) to (2.46), the numerical amplification factor becomes a function of both the reduced wavenumber and R under full discretization. For illustration sake, figure 2.13 presents the numerical amplification factor of the RK4 scheme for a range of spatial schemes considered. The red contour region represents the unstable region where $|Z| > 1$. The critical CFL number, R_{crit} represents the CFL number for which $|Z| < 0.99$ for all wavenumber considered. Alternatively, one can also consider looking at 1D plot of numerical amplification factor versus reduced wavenumber for different R . This is shown in figure 2.14. R_{max} represents the maximum allowable CFL number for which the coupled spatial and temporal schemes start to exhibit amplification. In the case of the RK4 scheme, the allowable time step is calculated based on the condition that $|\Im(\lambda)|\Delta t < \sqrt{8}$ for purely imaginary λ (see stability plot of RK4 scheme, figure 2.10). For the model equation considered, $\lambda = -i\bar{u}k_x^*$. R_{max} is calculated as follows:

$$\Delta t = \frac{\sqrt{8}}{|\Im(\lambda)|} = \frac{\sqrt{8}}{\bar{u}k_x^*} \quad (2.54)$$

$$R_{max} = \frac{\bar{u}(\Delta t)_{max}}{\Delta x} = \frac{\sqrt{8}}{(k_x^* \Delta x)_{max}} \quad (2.55)$$

In figure 2.14, it can be seen that the use of central differencing scheme when coupled with the RK4 temporal scheme give rise to numerical dissipation with increasing R up to R_{max} at intermediate reduced wavenumber. Beyond R_{max} , numerical instability starts to occur for certain range of reduced wavenumber. Hence, the claim that the use of central difference scheme offers no numerical dissipation is only true when temporal discretization effects are not considered. However, it should be noted that at low reduced wavenumber range, there is hardly any numerical dissipation even when R is increased. It should be noted that R_{max} is only an indication of the maximum allowable CFL number

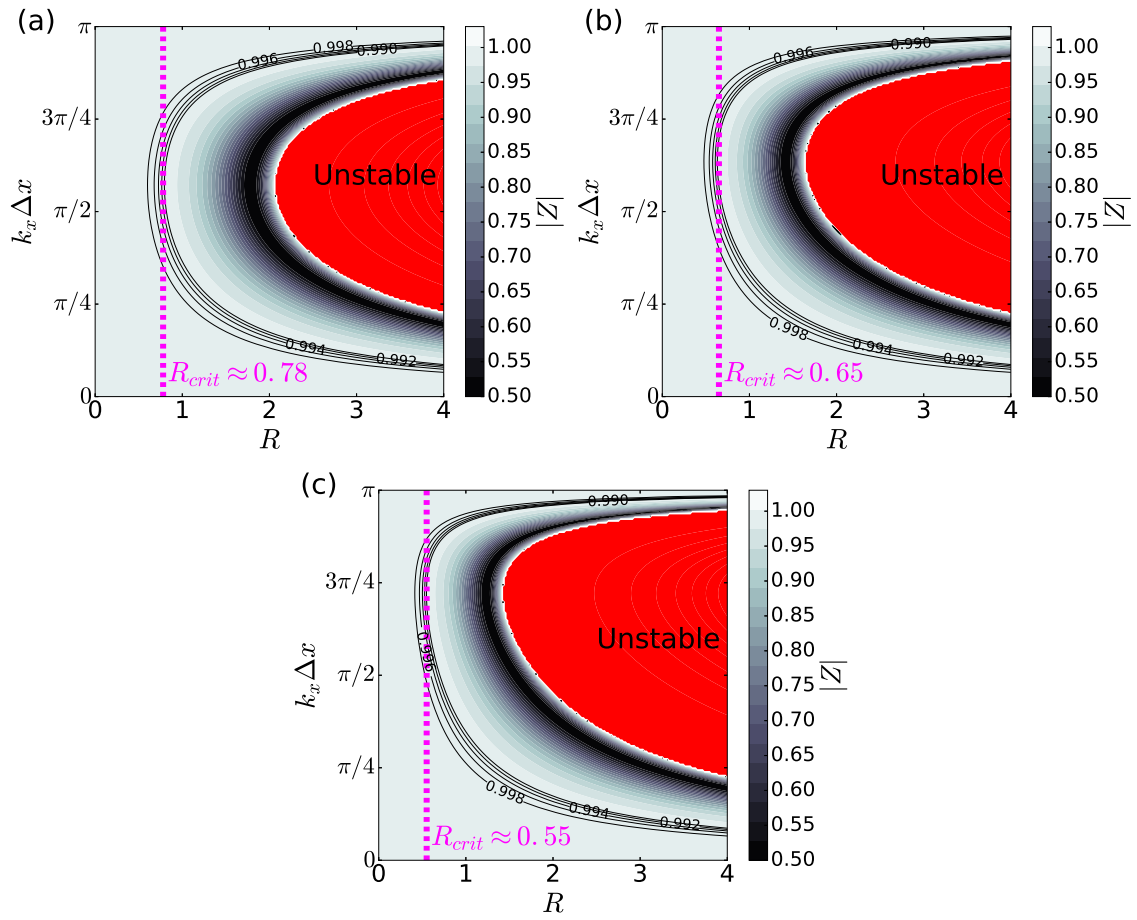


Figure 2.13: Effect of CFL number on the magnitude of the numerical amplification factor for (a) CDS4, (b) DRP4 and (c) CCOM6 with RK4 temporal scheme.

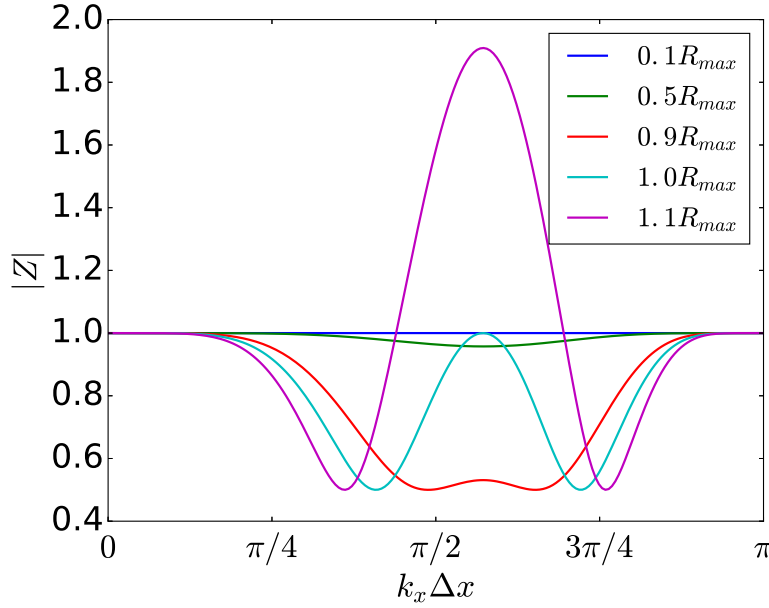


Figure 2.14: Effect of CFL number on the magnitude of the numerical amplification factor for CDS4 spatial and RK4 temporal scheme.

for numerical stability. It does not mean that there is no phase speed or group velocity error at R_{max} . It will be shown in subsequent sections that a change in R below R_{max} can lead to error in the numerical phase speed and numerical group velocity.

Effect of CFL number on numerical phase speed

We will now consider the effect of CFL number on numerical phase speed. For illustration sake, figure 2.15 presents the normalized numerical phase speed of the RK4 scheme for a range of spatial discretization schemes considered. Normalized values deviating from 1.0 provides an indication of the phase error.

Alternatively, one can also consider looking at 1D plot of normalized numerical phase speed versus reduced wavenumber for different R . This is shown in figure 2.16 for a range of spatial discretization scheme. For comparison sake, the results of the normalized numerical phase speed calculated based on semi discretization assumption are plotted alongside the normalized numerical phase speed calculated based on full discretization assumption. For $R = 0.1$, the normalized numerical phase speed of the CDS4, DRP4

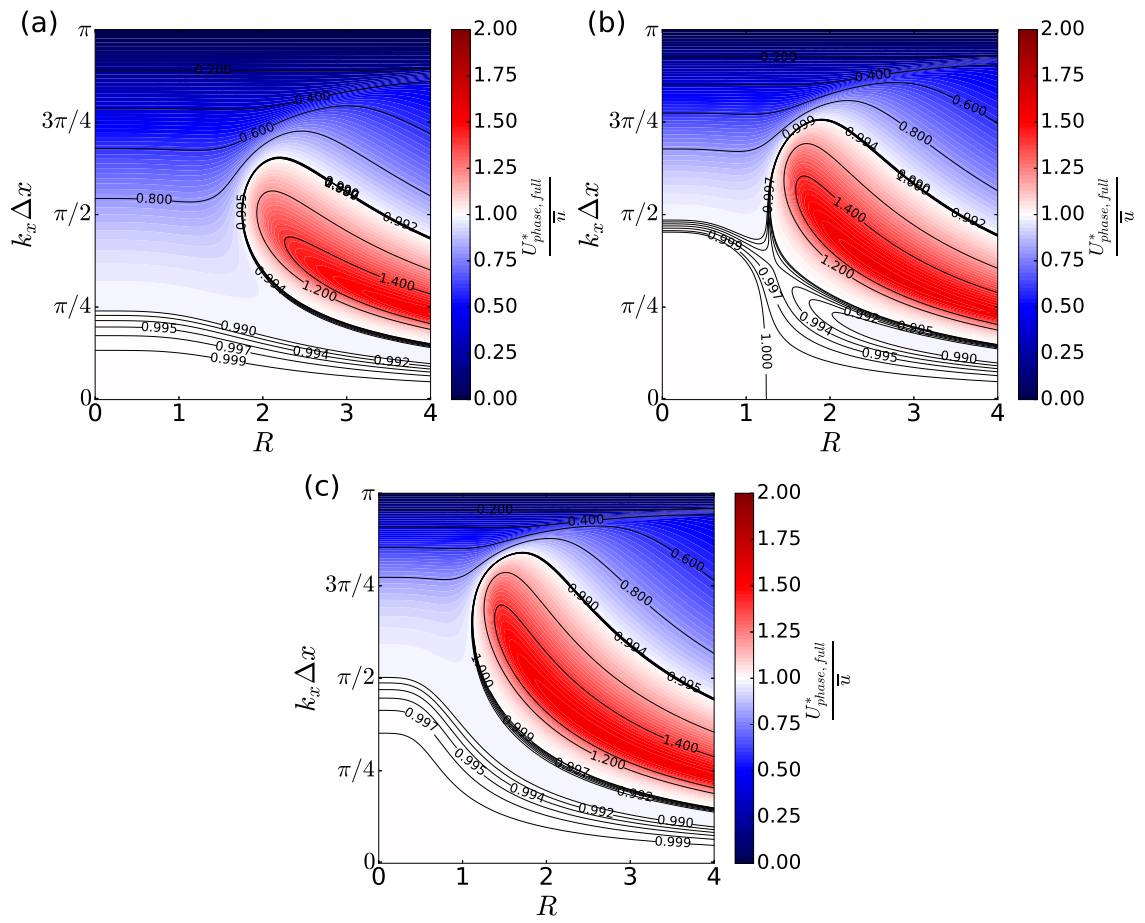


Figure 2.15: Effect of CFL number on the magnitude of the normalized numerical phase speed for (a) CDS4, (b) DRP4 and (c) CCOM6 with RK4 temporal scheme.

and CCOM6 scheme approaches those of the semi discretization assumption. When R increases, the normalized numerical phase speed calculated under full discretization becomes different from the normalized numerical phase speed calculated under semi discretization. Representative values of R are chosen for each scheme to illustrate the effect of varying R on the normalized numerical phase speed. In figure 2.16a, it can be seen that significant phase speed error (large overshoot/undershoot) exists for $R = R_{max} = 2.06$ at intermediate values of reduced wavenumber. Since R_{max} is only defined based on the value necessary for numerical stability, the numerical phase speed plot indicates that the numerical solution will exhibit significant phase error at intermediate reduced wavenumber despite being stable if $R = R_{max}$ is used. At low reduced wavenumber, there will be negligible phase error despite the change in R .

Effect of CFL number on numerical group speed

We will now consider the effect of CFL number on numerical group speed. For illustration sake, figure 2.17 presents the normalized numerical group speed of the RK4 scheme for a range of spatial discretization schemes considered. The hatched regions are denoted as the spurious wave region where the normalized group velocity $\frac{U_{grp,full}^*}{u}$ is lesser than zero. Spurious waves are essentially non-physical waves which arises due to numerical methods. They tend to be waves of higher wavenumber and they travel in opposite direction to the physical waves. Alternatively, one can also consider looking at 1D plot of normalized numerical group velocity versus reduced wavenumber for different R . This is shown in figure 2.18 for a range of spatial discretization scheme considered. Representative values of R are chosen for each scheme to illustrate the effect of varying R on the normalized numerical group velocity. The semi discretized group velocity represents the theoretical limit for the fully discretized numerical group velocity as $\Delta t \rightarrow 0$. It can be seen that as R reduces, the fully discretized numerical group velocity approaches the semi discretized numerical group velocity.

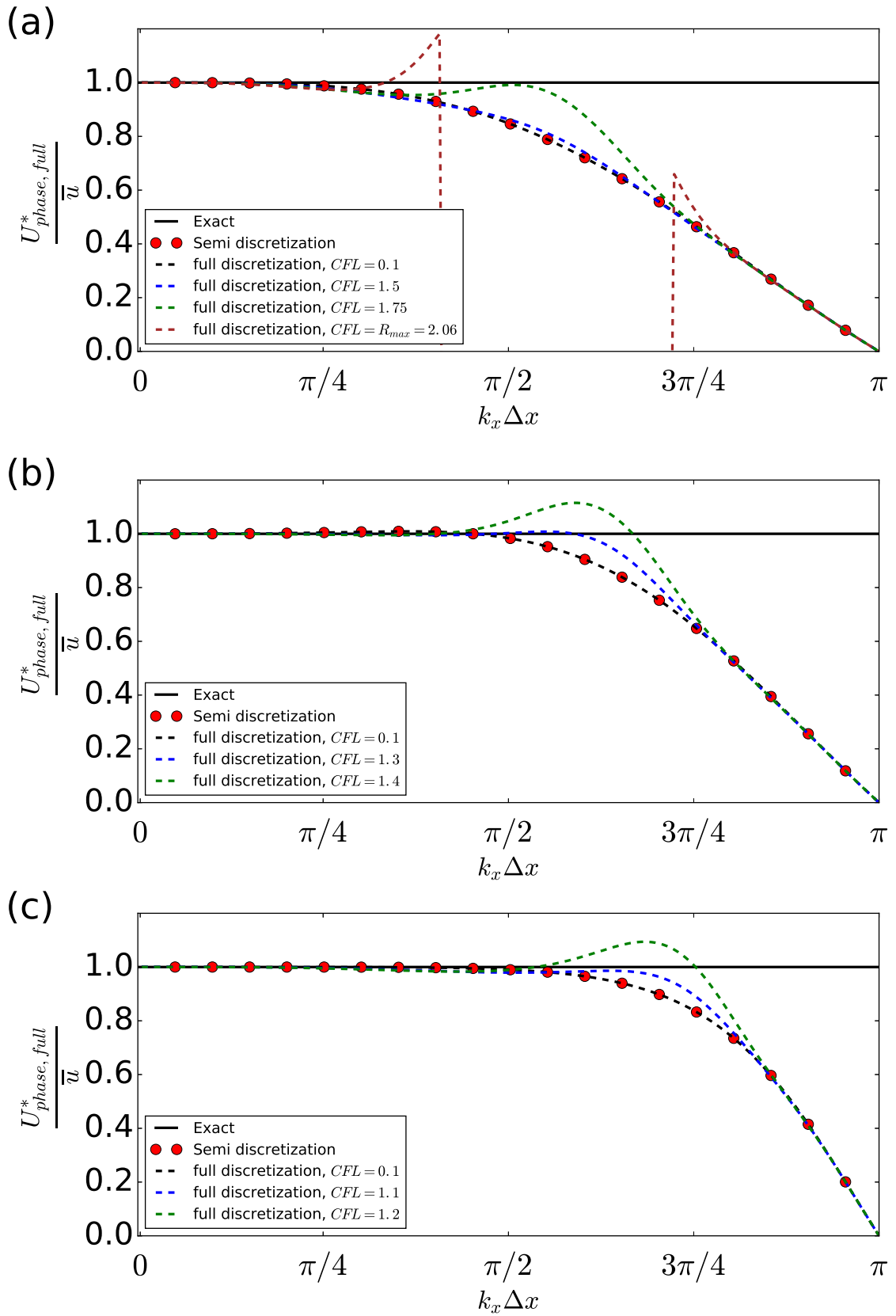


Figure 2.16: Effect of CFL number on normalized numerical phase speed for (a) CDS4, (b) DRP4 and (c) CCOM6 spatial and RK4 temporal scheme.

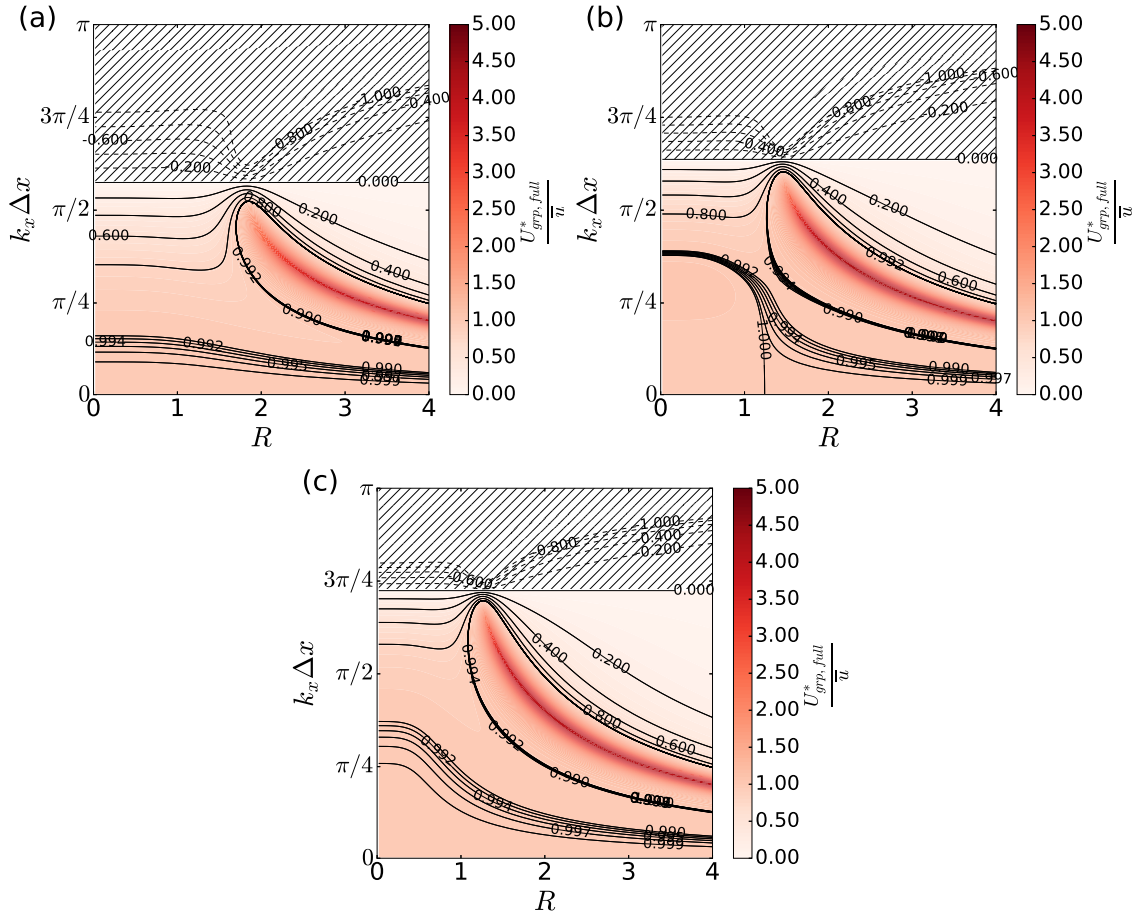


Figure 2.17: Effect of CFL number on the magnitude of the normalized numerical group speed for (a) CDS4, (b) DRP4 and (c) CCOM6 with RK4 temporal scheme.

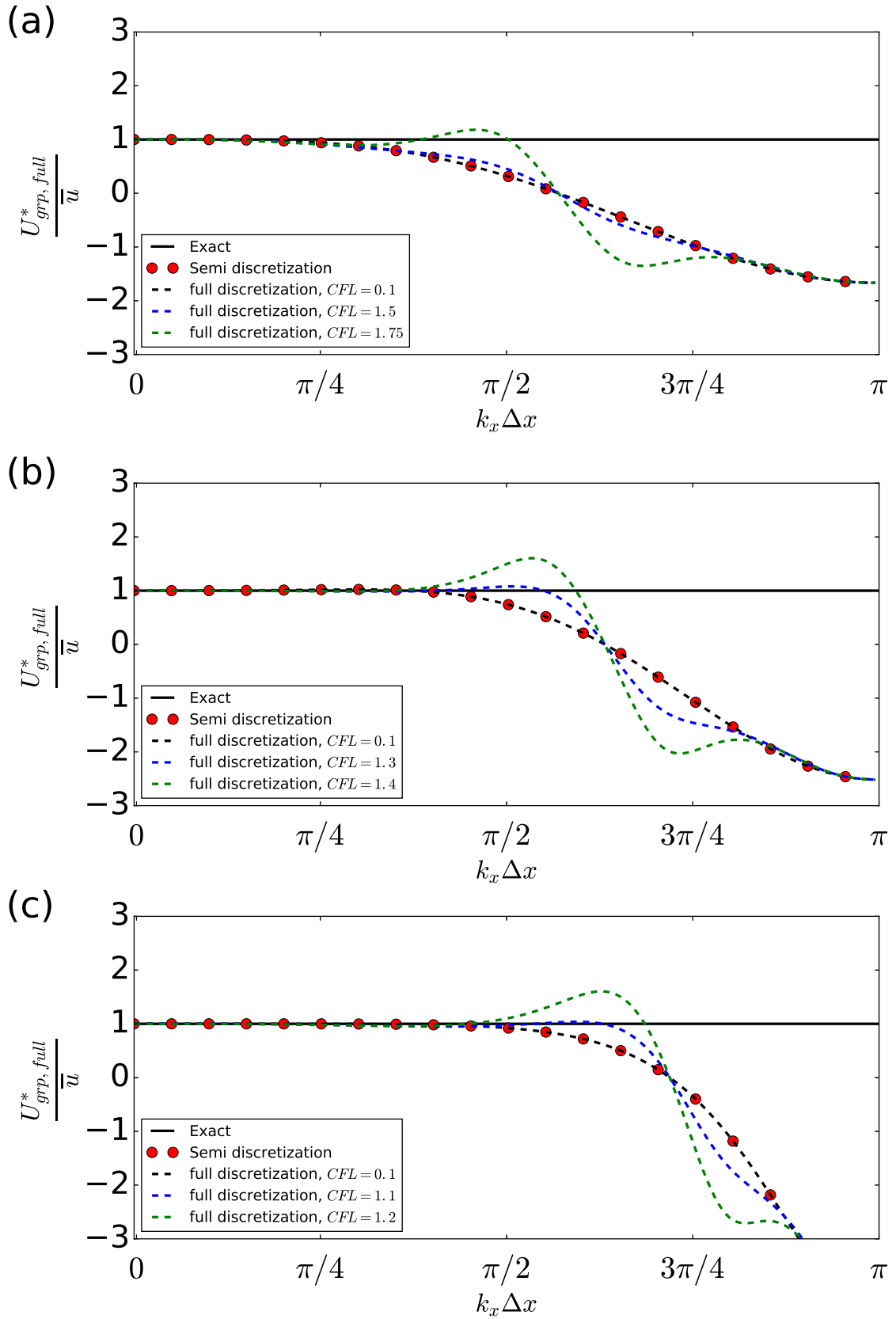


Figure 2.18: Effect of CFL number on normalized numerical group velocity for (a) CDS4, (b) DRP4 and (c) CCOM6 spatial and RK4 temporal scheme.

Effect of alternate temporal schemes on numerical amplification, group and phase velocity

In figures 2.13 to 2.18, we have seen that the effect of a change in CFL number not only has an impact on numerical stability but also the accuracy of the numerical solution. This is evident from the change in numerical phase and group velocity as R is varied. In this section, we will consider the impact of using alternate temporal discretization scheme on the stability and accuracy of the numerical solution. In particular, we will investigate the effect of using a lower order temporal scheme (RK3) and implicit temporal scheme (CN). Figures 2.19 to 2.21 illustrate the effect of using RK4, RK3 and CN temporal scheme on the numerical amplification, numerical phase speed and group velocity. In this comparison, the spatial discretization scheme (CDS4) is kept fixed.

When a lower order temporal scheme is used (RK4 to RK3), there is a shift in R_{crit} towards lower CFL number. Also, there is lesser numerical dissipation at higher CFL number. However, numerical instability starts to occur at a lower CFL number for the RK3 scheme as compared to the RK4 scheme. On the other hand, the implicit Crank-Nicolson scheme shows unconditional stability across the full range of R and $k_x \Delta x$. For both the normalized numerical phase speed and group velocity, there is significant changes in the variation of the phase speed and group velocities as a function of R . It is evident that a change in temporal discretization scheme has a significant impact on the dispersion error of the numerical solution especially at large values of R . To illustrate this better, we look at 1D plot of numerical amplification factor, numerical phase and group velocity versus reduced wavenumber for $R = 1.5$. This is shown in figure 2.22. For the RK3 scheme, numerical instability can occur at intermediate values of reduced wavenumber for $R = 1.5$. The immediate advantage of the implicit CN scheme can be seen from the fact that the amplification factor is neutrally stable across the full range of reduced wavenumber as compared to the explicit temporal schemes. However, the CN scheme suffers from significant dispersion error despite being stable. As compared to the RK4 temporal scheme, significant deviation in the numerical phase and group velocities from the semi-discretized results can be seen in figures 2.22b and 2.22c across the full range of reduced wavenumber.

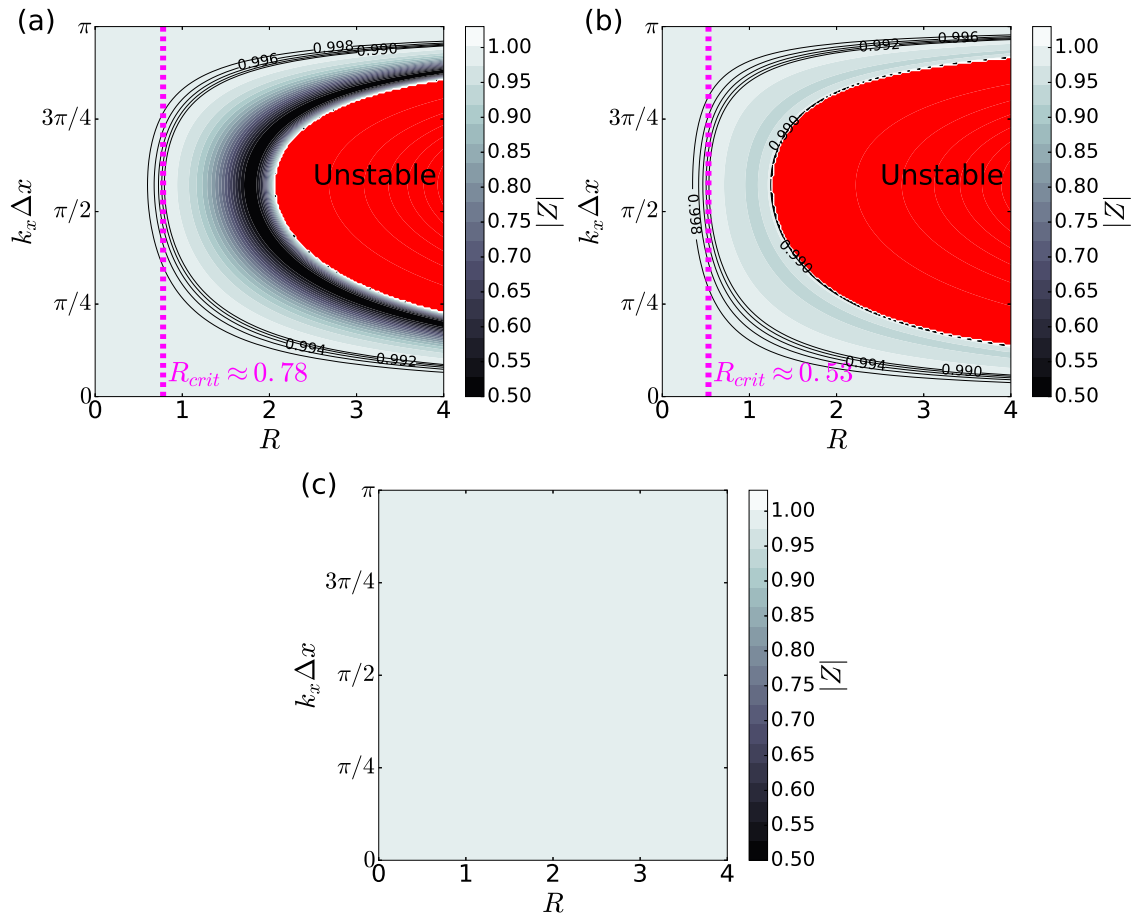


Figure 2.19: Effect of varying temporal schemes on the numerical amplification factor for (a) RK4, (b) RK3 and (c) CN temporal and CDS4 spatial scheme.

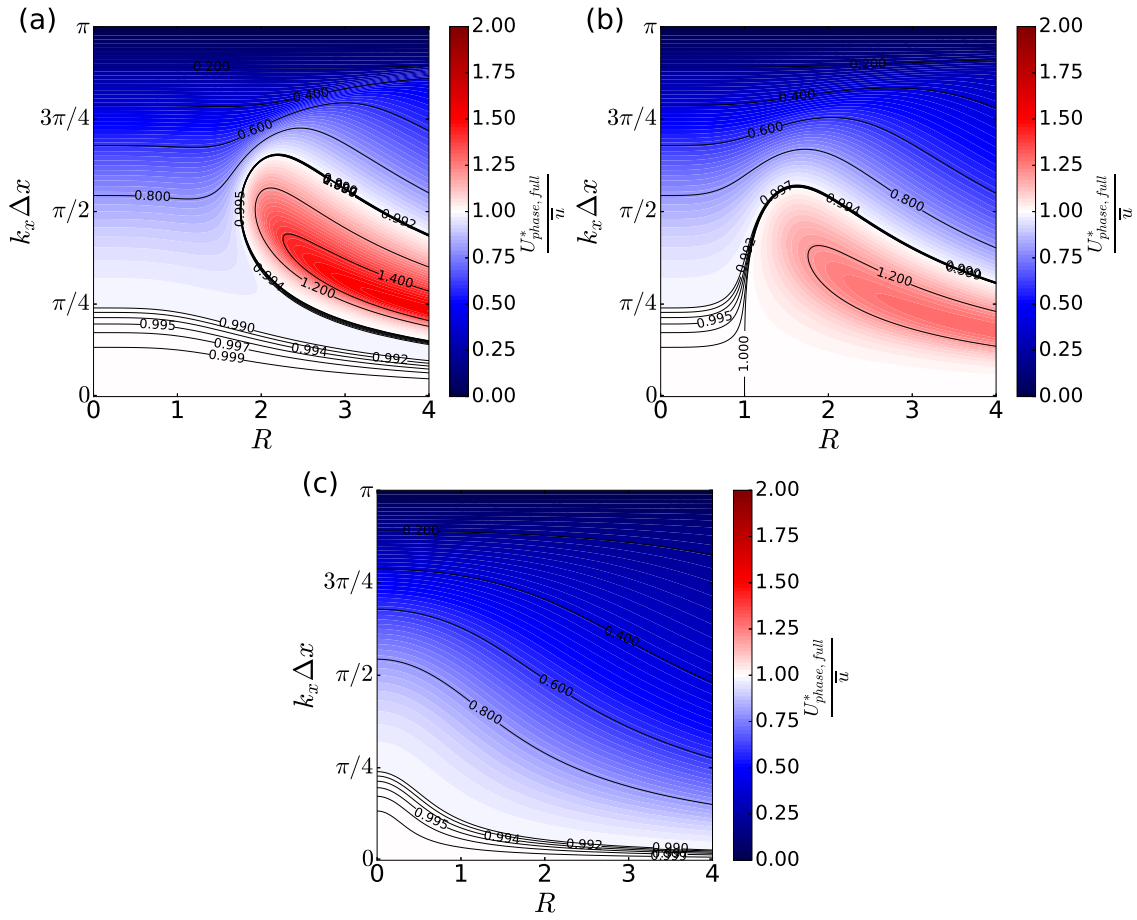


Figure 2.20: Effect of varying temporal schemes on the numerical phase speed for (a) RK4, (b) RK3 and (c) CN temporal and CDS4 spatial scheme.

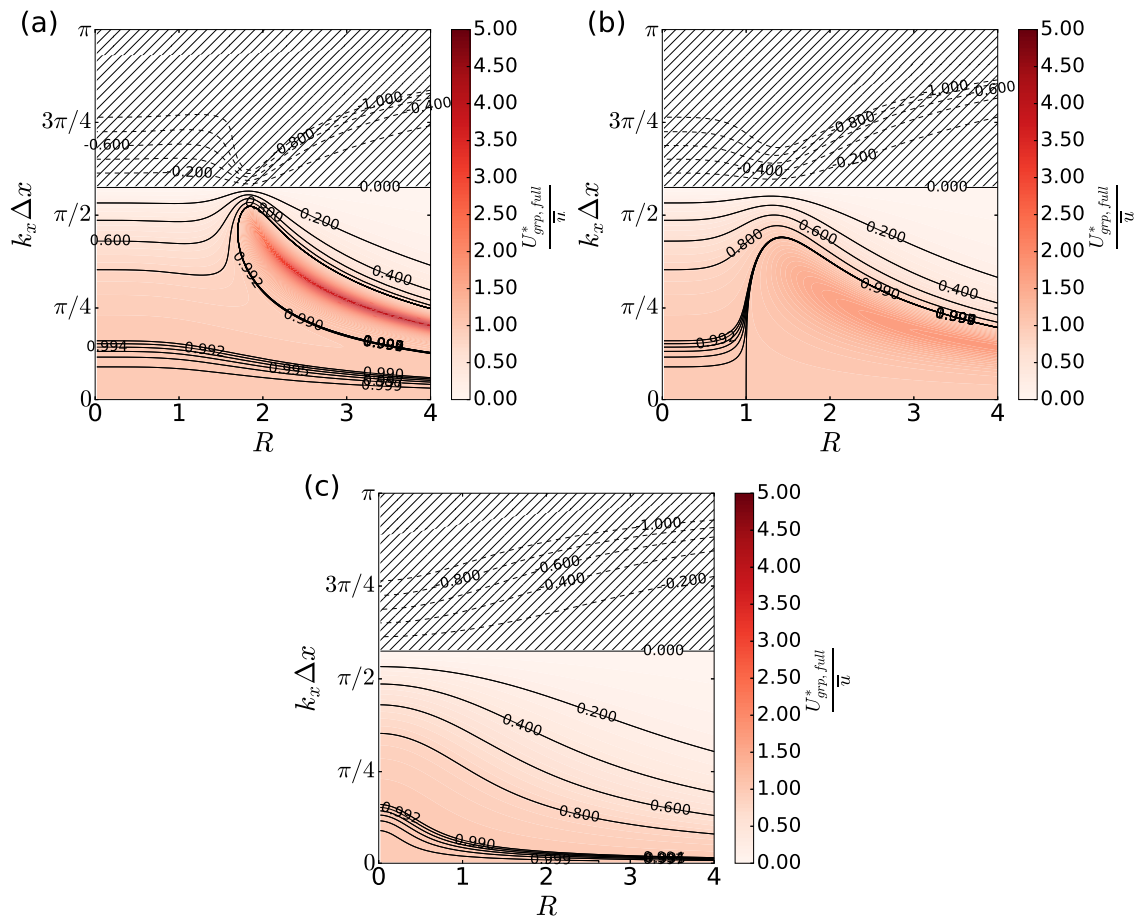


Figure 2.21: Effect of varying temporal schemes on the numerical group speed for (a) RK4, (b) RK3 and (c) CN temporal and CDS4 spatial scheme.

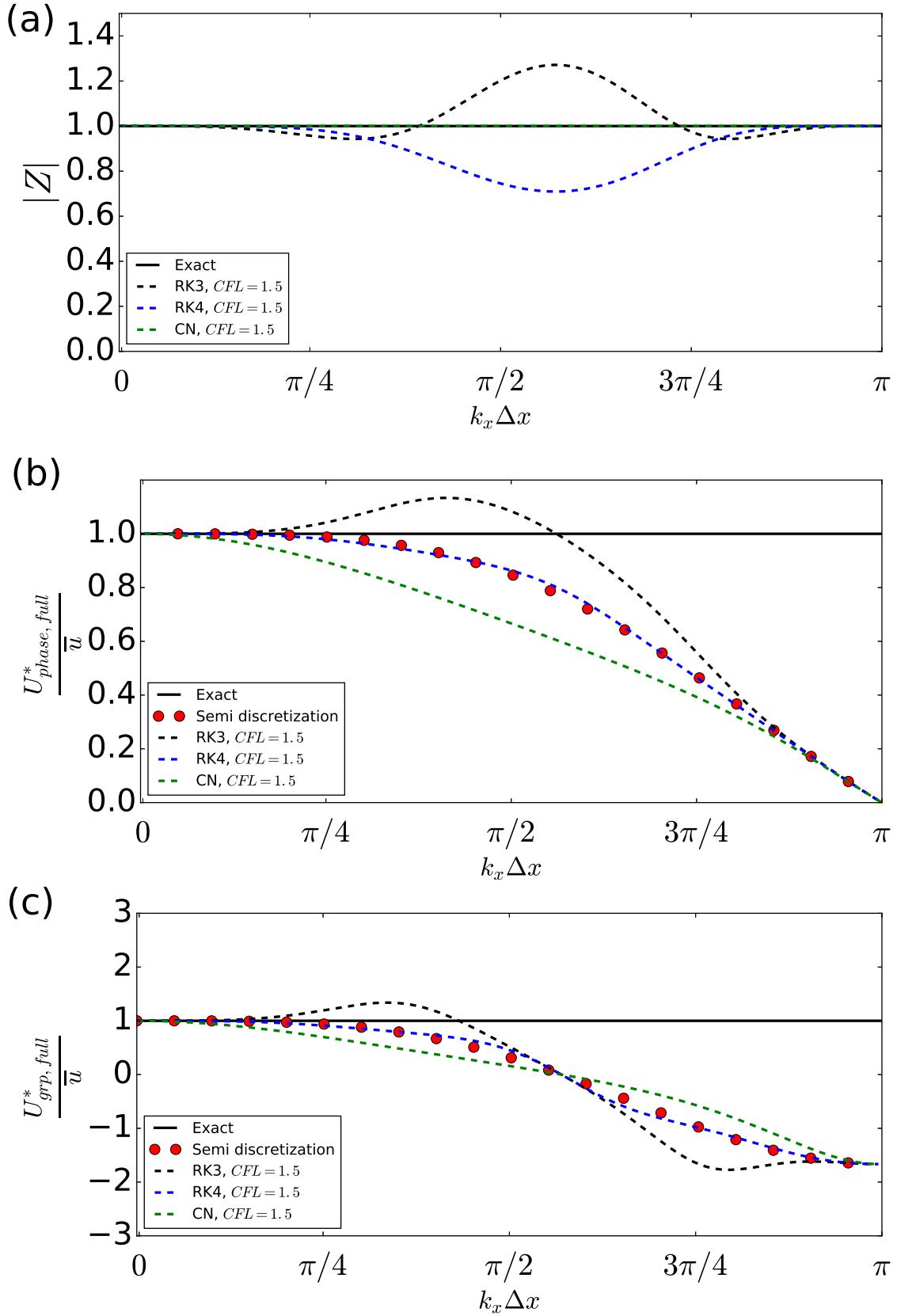


Figure 2.22: Effect of varying temporal schemes on the (a) numerical amplification factor, (b) numerical phase speed and (c) numerical group velocity for the CDS4 spatial scheme at $R = 1.5$.

2.3.2 1D linearized Euler

In this sub section, the analysis framework is extended to the one dimensional linearized Euler equations (LEE). Interest in the study of the linearized Euler equation stems from the fact that the Euler equation is a simplified form of the Navier Stokes equation neglecting the viscous effect. The use of the linearized Euler equations instead of the non linear Euler equations enable one to obtain exact solution based on the dispersion relation of the governing equation. This allows one to quantify the error of the numerical solution. The governing equation of the LEE is given as:

$$\begin{aligned}\frac{\partial \mathbf{U}'}{\partial t} + \frac{\partial \mathbf{E}}{\partial x} &= 0, \\ \frac{\partial \mathbf{U}'}{\partial t} + \frac{\partial \mathbf{E}}{\partial \mathbf{U}'} \frac{\partial \mathbf{U}'}{\partial x} &= 0,\end{aligned}\tag{2.56}$$

where

$$\mathbf{U}' = \begin{bmatrix} \rho' \\ u' \\ p' \end{bmatrix}, \quad \mathbf{E} = \begin{bmatrix} \bar{u}\rho' + \bar{\rho}u' \\ \bar{u}u' + p'/\bar{\rho} \\ \bar{u}p' + \bar{\rho}a^2u' \end{bmatrix}, \quad \frac{\partial \mathbf{E}}{\partial \mathbf{U}'} = \begin{bmatrix} \bar{u} & \bar{\rho} & 0 \\ 0 & \bar{u} & \frac{1}{\bar{\rho}} \\ 0 & \bar{\rho}a^2 & \bar{u} \end{bmatrix}.\tag{2.57}$$

ρ , u , p and a represent the density, x component of velocity, pressure and speed of sound. In order to determine the dispersion relation, a Fourier Laplace transform is applied to the governing equation. The Fourier Laplace transform of $\mathbf{U}'$ is given as:

$$\hat{\mathbf{U}}' = \frac{1}{2\pi} \int_0^\infty \int_{-\infty}^\infty \mathbf{U}' e^{i(k_x x - \omega t)} dk_x dt.\tag{2.58}$$

By substituting equation (2.58) into (2.56) and noting the following relations:

$$\begin{aligned}\frac{\partial \hat{\mathbf{U}}'}{\partial t} &= -i\omega \frac{1}{2\pi} \int_0^\infty \int_{-\infty}^\infty \mathbf{U}' e^{i(k_x x - \omega t)} dk_x dt, \\ \frac{\partial \hat{\mathbf{U}}'}{\partial x} &= ik_x \frac{1}{2\pi} \int_0^\infty \int_{-\infty}^\infty \mathbf{U}' e^{i(k_x x - \omega t)} dk_x dt,\end{aligned}\tag{2.59}$$

the resulting equation can be written as follows [Sescu, 2008, Stegeman et al., 2012]:

$$\begin{bmatrix} \omega - \bar{u}k_x & -\bar{\rho}k_x & 0 \\ 0 & \omega - \bar{u}k_x & -\frac{k_x}{\bar{\rho}} \\ 0 & -\bar{\rho}a^2k_x & \omega - \bar{u}k_x \end{bmatrix} \hat{\mathbf{U}} = 0. \quad (2.60)$$

Solving for the eigenvalue problem will lead to the physical dispersion relation of the 1D LEE [Sescu, 2008, Stegeman et al., 2012]:

$$\left. \begin{array}{l} \omega_1 = \bar{u}k_x \\ \omega_{2,3} = \bar{u}k_x \pm ak_x \end{array} \right\} \omega = \bar{u}k_x + \alpha ak_x, \quad \alpha = 0, 1, -1. \quad (2.61)$$

α takes on the value of 0 or ± 1 . The corresponding semi discretized numerical dispersion relation (ω_{semi}^*) can be obtained by replacing k_x with k_x^* . The first eigenvalue corresponds to the entropy mode while the next two eigenvalues corresponds to the acoustic mode. The entropy wave convects at the mean velocity, $\bar{u}$ and its dispersion relation is the same as the 1D advection equation. The acoustic wave convects at the speed $\bar{u} + a$ or $\bar{u} - a$.

Using a similar procedure to the 1D advection, the semi discretized dispersion relation is introduced into the numerical amplification factor of the temporal scheme so as to obtain the fully discretized numerical amplification factor, numerical phase and group velocity. For illustration sake, the RK4 temporal scheme is used in this analysis. The numerical amplification factor of the RK4 temporal scheme written in terms of ω_{semi}^* is given as:

$$Z_{RK4} = 1 + (-i\Delta t\omega_{semi}^*) + \frac{(-i\Delta t\omega_{semi}^*)^2}{2} + \frac{(-i\Delta t\omega_{semi}^*)^3}{6} + \frac{(-i\Delta t\omega_{semi}^*)^4}{24}, \quad (2.62)$$

where

$$\Delta t\omega_{semi}^* = R_a(M_x + \alpha)k_x^*\Delta x, \quad \bar{u} = M_x a \quad R_a = \frac{a\Delta t}{\Delta x}. \quad (2.63)$$

R_a is the CFL number defined in terms of the speed of sound. M_x is the Mach number in the x direction. The numerical group and phase velocity calculated under full discretization is related to the fully discretized numerical amplification factor via the phase shift,

ψ :

$$U_{phase,full}^* = \frac{\omega_{full}^*}{k_x} = \frac{\psi}{k_x \Delta t}. \quad (2.64)$$

The physical phase speed is given by:

$$U_{phase,exact} = \frac{\omega}{k_x} = a(M_x + \alpha). \quad (2.65)$$

The normalized numerical phase speed is given by:

$$\frac{U_{phase,full}^*}{U_{phase,exact}} = \frac{\psi}{R_a(M_x + \alpha)k_x \Delta x}. \quad (2.66)$$

The corresponding normalized numerical group velocity is given by:

$$\frac{U_{grp,full}^*}{U_{grp,exact}} = \frac{1}{U_{grp,exact}} \frac{\partial \omega_{full}^*}{\partial k_x} = \frac{1}{a(M_x + \alpha)} \frac{1}{\Delta t} \frac{\partial \psi}{\partial k_x} = \frac{1}{R_a(M_x + \alpha)} \frac{\partial \psi}{\partial k_x \Delta x}, \quad (2.67)$$

where the physical group velocity, $U_{grp,exact}$ is given by $\frac{\partial \omega}{\partial k_x} = a(M_x + \alpha)$.

For illustration sake, the numerical amplification factor, normalized numerical group and phase velocities of the different modes (entropy and two acoustic modes) are plotted in figures 2.23 to 2.25. The RK4 temporal and CDS4 spatial discretization scheme is used for this analysis. The speed of sound, a is taken to be 1.0 and M_x is set to 1.5 for this analysis. In figure 2.23, it can be seen that the critical CFL number, R_{crit} is primary decided based on the smallest R_{crit} among the three different modes. This correspond to the acoustic mode 1 where it has the maximum convection speed among the three different modes. For acoustic mode 2, there is no unstable region for the range of R considered. In figure 2.25, the critical wavenumber for which the normalized numerical group velocity becomes negative remains the same for the three different modes. However, there is significant changes in the normalized group velocities at higher R . This shows that the effect of R on the dispersion error of the different modes is different. Acoustic mode 1 displays the most changes in the normalized group velocities with increasing R . Acoustic mode 2 displays the least changes in the normalized group velocities with increasing R .

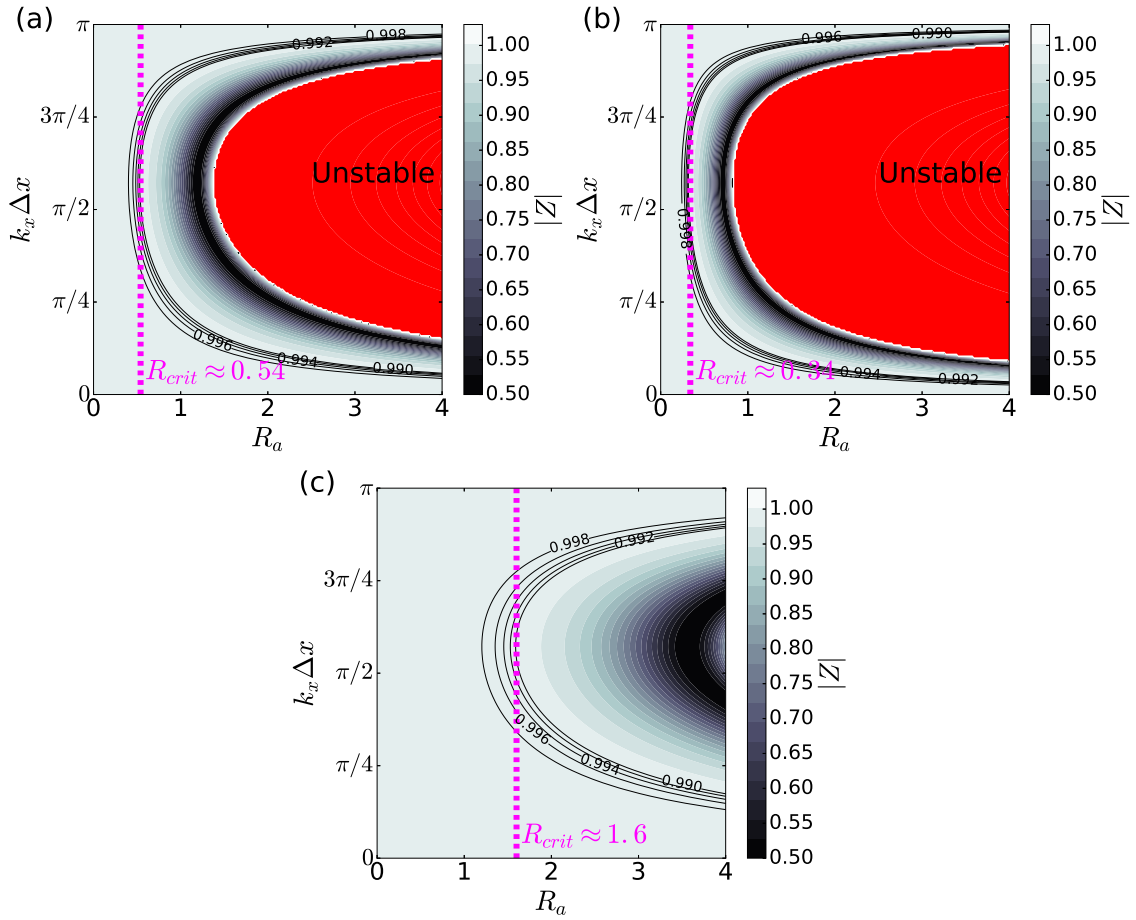


Figure 2.23: Numerical amplification factor of (a) entropy mode ($\alpha = 0$), (b) acoustic mode 1 ($\alpha = 1$) and (c) acoustic mode 2 ($\alpha = -1$) for RK4 temporal and CDS4 spatial scheme. $a = 1$, $M_x = 1.5$.

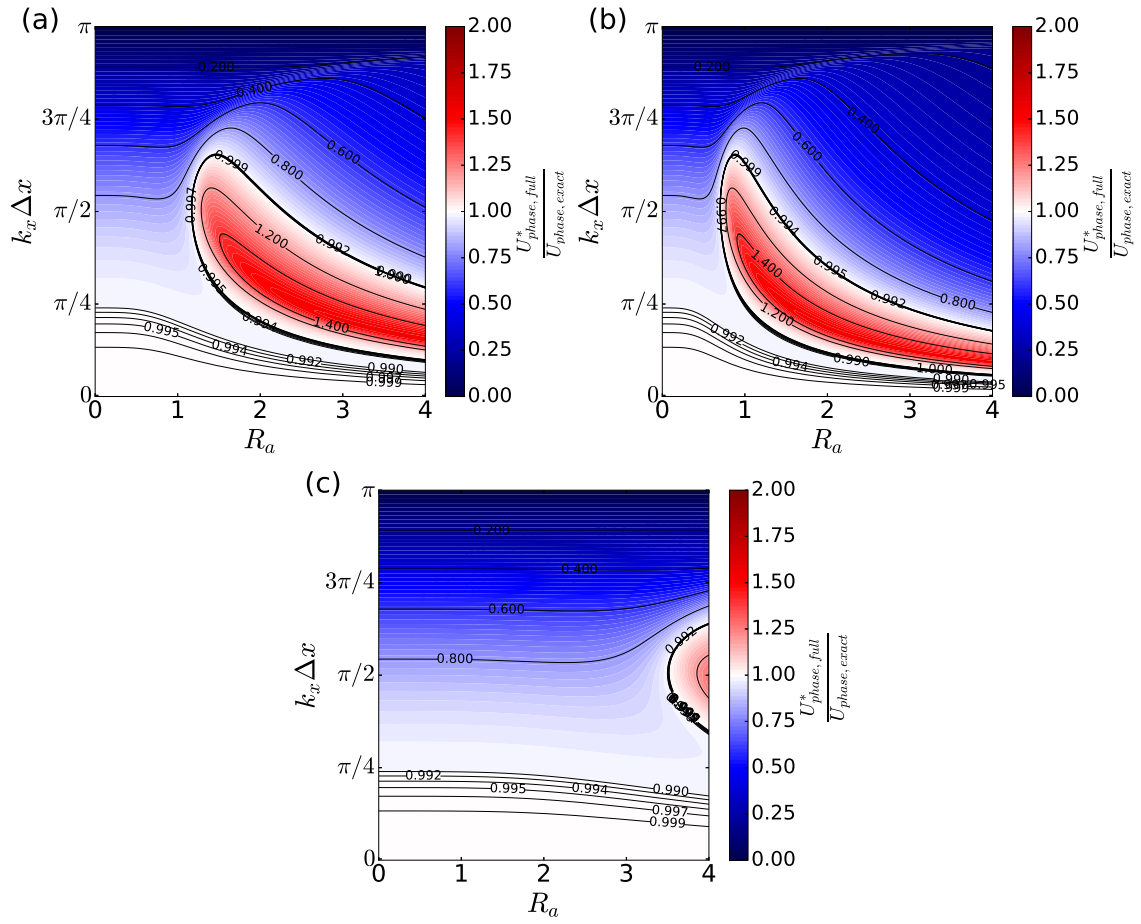


Figure 2.24: Normalized numerical group velocity of (a) entropy mode ($\alpha = 0$), (b) acoustic mode 1 ($\alpha = 1$) and (c) acoustic mode 2 ($\alpha = -1$) for RK4 temporal and CDS4 spatial scheme.

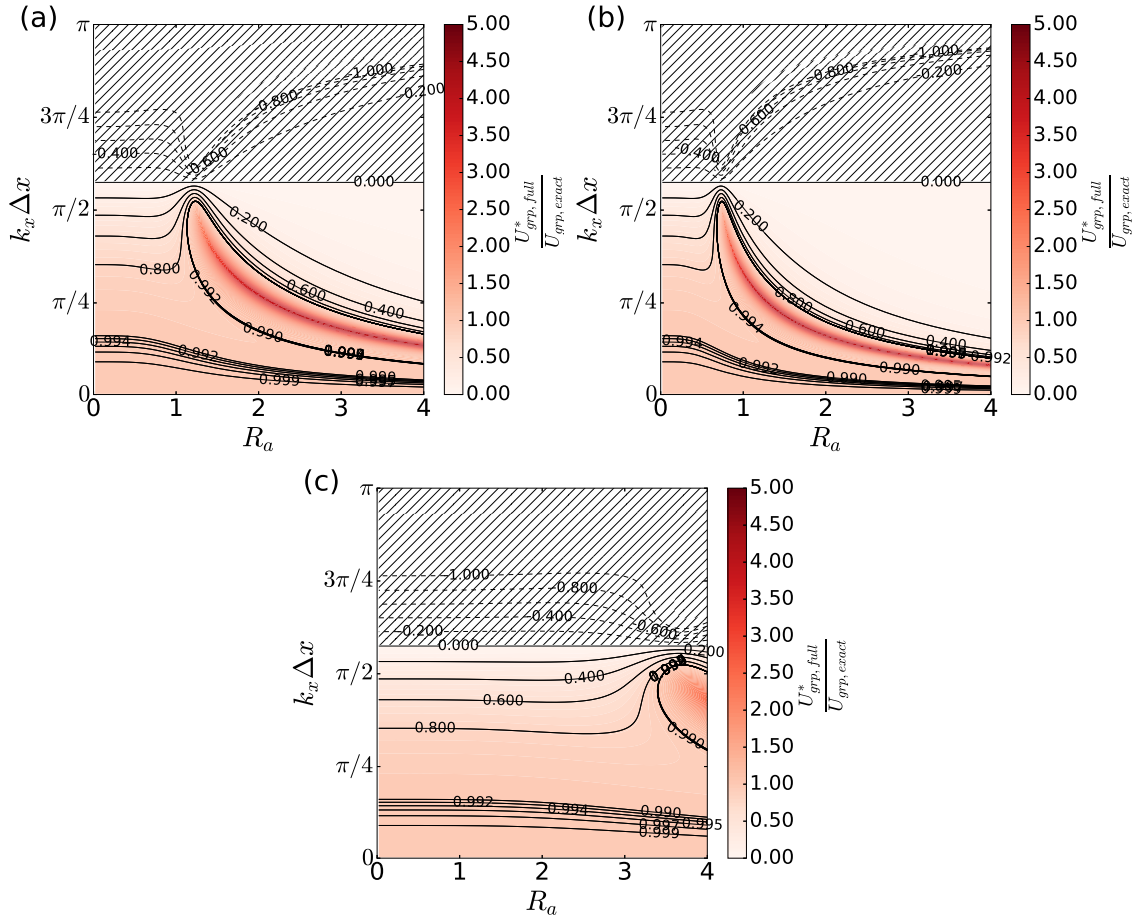


Figure 2.25: Normalized numerical group velocity of (a) entropy mode ($\alpha = 0$), (b) acoustic mode 1 ($\alpha = 1$) and (c) acoustic mode 2 ($\alpha = -1$) for RK4 temporal and CDS4 spatial scheme.

Table 2.2: Initial conditions and schemes for 1D advection

Case No.	$k_x \Delta x$	R	Spatial Scheme	Temporal Scheme
1	$\pi/16$	0.1	CDS4	RK4
2	$3\pi/8$	0.1	CDS4	RK4
3	$3\pi/4$	0.1	CDS4	RK4
4	$\pi/16$	$0.5R_{max}$	CDS4	RK4
5	$3\pi/8$	$0.5R_{max}$	CDS4	RK4
6	$3\pi/4$	$0.5R_{max}$	CDS4	RK4
7	$3\pi/8$	0.5	CDS4	CN
8	$3\pi/4$	0.5	CDS4	CN
9	$3\pi/8$	1.5	CDS4	CN
10	$3\pi/4$	1.5	CDS4	CN

2.3.3 Numerical experiments

In order to verify the analytical predictions, numerical results of the 1D advection and LEE are compared against these predictions.

1D advection

For the 1D advection equation, periodic boundary conditions are applied on both ends of the domain. The initial condition used is a single mode Gaussian modulated pulse, $\Phi(x, 0) = e^{-0.5x^2} \sin(k_x x)$. k_x is deduced from the reduced wavenumber used for the initial condition. This is shown in table 2.2. A uniformly spaced grid with 500 points across the entire domain is used. The computational domain is taken to be $[-\pi, \pi]$ and the solutions are compared at $t = 1$. The convection speed, $\bar{u}$ of the governing equation is taken to be 1.0. Three different sets of numerical experiments were conducted. The first set of experiment (cases 1,2,3) was to verify if the propagating wave is travelling according to the group or phase velocity. The second set of experiment (cases 4,5,6) was to verify the effect of an increase in R on the numerical solution. The third set of experiment (cases 7,8,9) was to compare the numerical solution for different R when a different temporal discretization scheme is used.

Numerical results corresponding to the first set of experiments are illustrated in figure 2.26. The analytical group velocity results in figure 2.26 correspond to those in figure

2.17a. Firstly, it can be seen that the position of the wave packets (numerical solution) correspond to those predicted by the numerical group velocity. The black dotted line in figure 2.26 represents the position of the wave packet at $t = 1$ predicted by the numerical group velocity. Secondly, it can be seen that with increasing $k_x \Delta x$, the group velocity first becomes smaller and then negative. The wave packet propagates at either a slower speed or in opposite direction. Numerical results corresponding to the second set of experiments with a larger R are illustrated in figure 2.27. As compared to figures 2.26b and 2.26c, it can be seen that the amplitude of the wave packets at $t = 1$ become much smaller for the cases representing $k_x \Delta x = 3\pi/8, 3\pi/4$ in figures 2.27b and 2.27c. Numerical group velocities for the different reduced wavenumber remain approximately the same when R is increased from 0.1 to $0.5R_{max}$. Figure 2.28 showcases the numerical solution for the case when a CN temporal scheme is used. The effect of using different R was compared. It can be seen that with the use of larger R , the numerical solution has a larger dispersion error (lower group velocity). This is evident from the shift in the position of the wave packets at $t = 1$ for different reduced wavenumber considered.

1D linearized Euler

For the 1D LEE equation, periodic boundary conditions are applied on both ends of the domain. The initial condition used is a single mode Gaussian modulated pulse, $p(x, 0) = e^{-0.5x^2} \sin(k_x x)$ on the pressure variable. k_x is deduced from the reduced wavenumber used for the initial condition. The initial condition used is shown in table 2.3. A uniformly spaced grid with 1000 points across the entire domain is used. The computational domain is taken to be $[-10, 10]$ and the solutions are compared at $t = 2$. With reference to the analytical solutions shown in figures 2.23 to 2.25, the same parameters are used for the numerical solution. M_x and a are set to 1.5 and 1.0 respectively. One set of numerical experiments was conducted. The aim was to illustrate the solution of the different modes as compared to the 1D advection equation which has only one wave mode.

In the case of the pressure initial condition, the resulting numerical solution of the pressure variable would have two wave fronts propagating in opposite direction. This is illustrated in figure 2.29. Each of these wave front corresponds to one of the acoustic

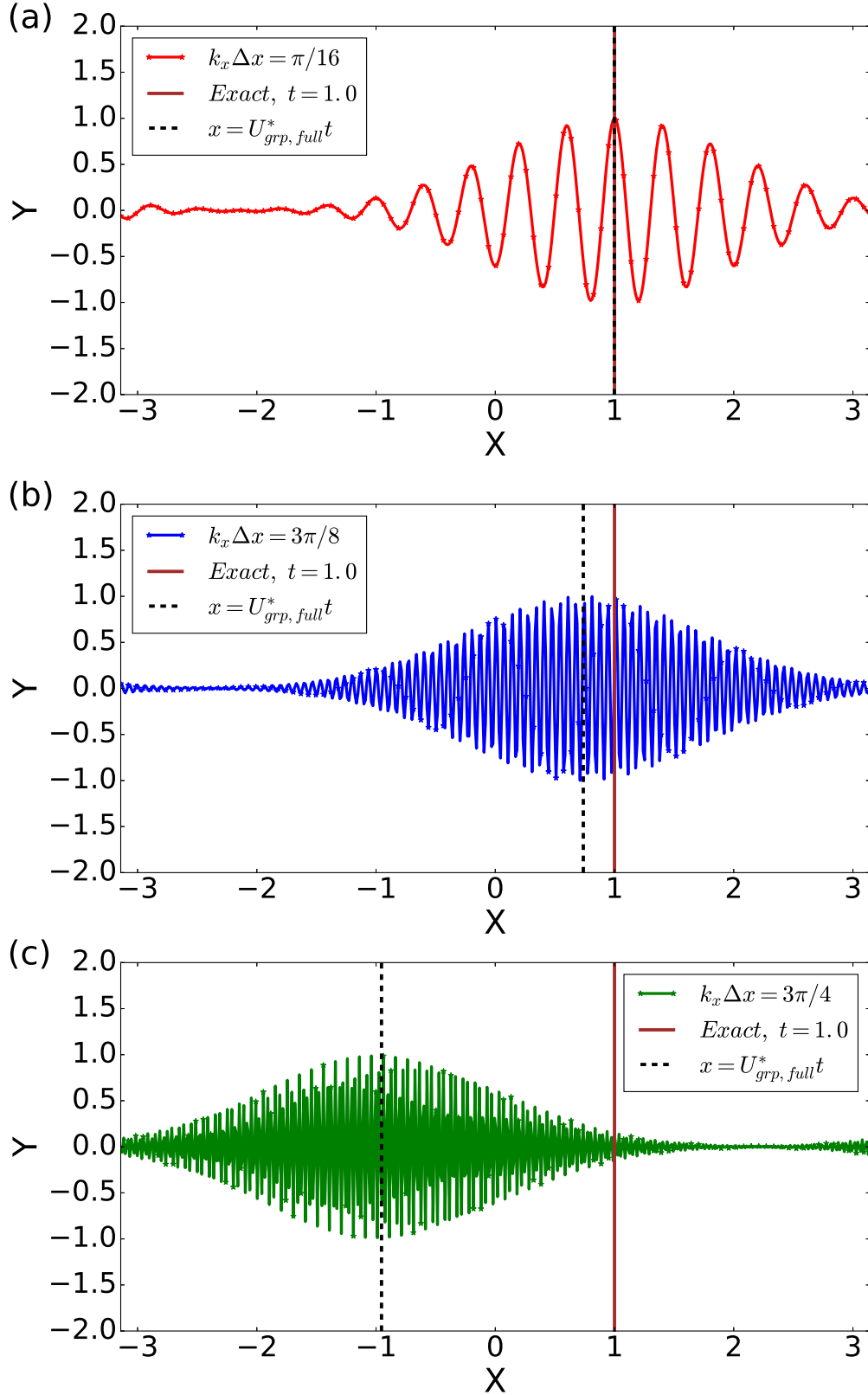


Figure 2.26: Illustrating the propagation of waves according to their group velocity. (a) $k_x \Delta x = \pi/16$, (b) $k_x \Delta x = 3\pi/8$ and (c) $k_x \Delta x = 3\pi/4$. $R = 0.1$. The brown line represents the exact position of the wave packet at $t = 1$. The black dotted line represents the position of wave packet computed from the analytical group velocity. They represent cases 1 to 3 of table 2.2.

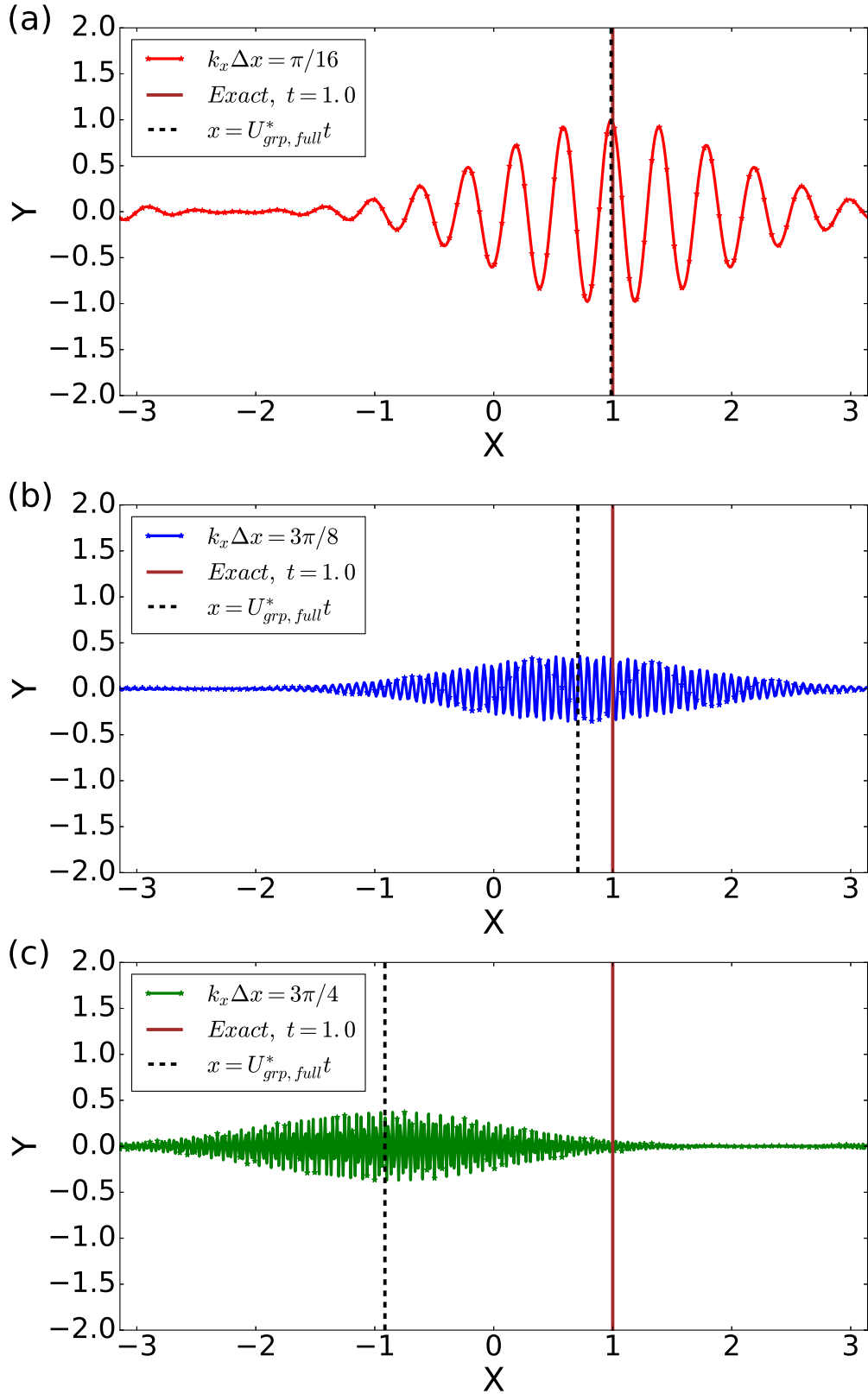


Figure 2.27: Illustrating the propagation of waves according to their group velocity. (a) $k_x \Delta x = \pi/16$, (b) $k_x \Delta x = 3\pi/8$ and (c) $k_x \Delta x = 3\pi/4$. $R = 0.5R_{max}$. The brown line represents the exact position of the wave packet at $t = 1$. The black dotted line represents the position of wave packet computed from the analytical group velocity. They represent cases 4 to 6 of table 2.2.

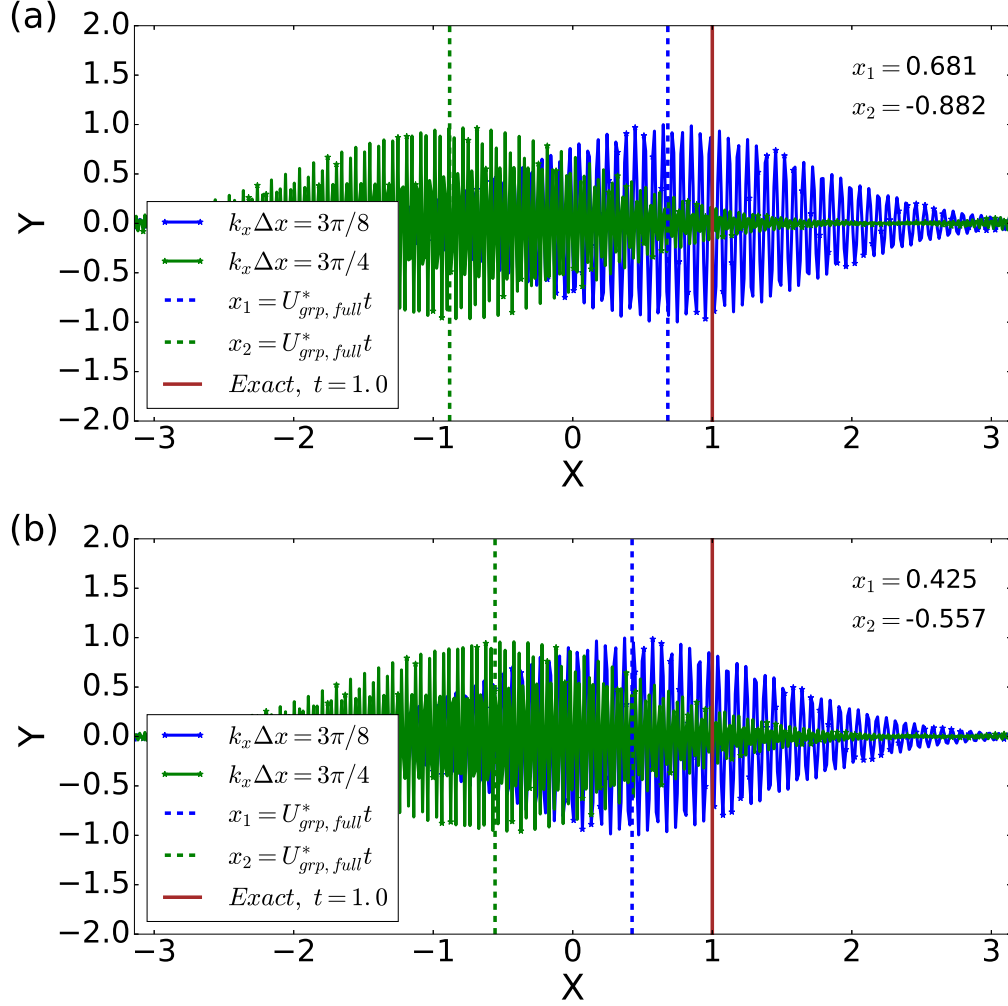


Figure 2.28: Illustrating the propagation of waves according to their group velocity. (a) $R = 0.5$ and (b) $R = 1.5$. The brown line represents the exact position of the wave packet at $t = 1$. The blue and green dotted lines represent the position of wave packet computed from the analytical group velocity. They represent cases 7 to 10 of table 2.2.

Table 2.3: Initial conditions and schemes for 1D LEE.

Case No.	$k_x \Delta x$	R_a	Spatial Scheme	Temporal Scheme
1	$\pi/8$	0.5	CDS4	RK4
2	$2\pi/8$	0.5	CDS4	RK4
3	$7\pi/8$	0.5	CDS4	RK4

modes. ω_2 and ω_3 represent the right and left going wave respectively.

For $k_x \Delta x = \pi/8$, the wave front belonging to acoustic mode 1 propagates to the right while the wave front belonging to acoustic mode 2 propagates to the left. The final position of both wave packets are very close to the exact solution. For $k_x \Delta x = 2\pi/8$, the wave front belonging to acoustic mode 1 travels at slower speed and experienced a reduction in its amplitude. The wave front belonging to acoustic mode 2 remains very close to the position of its exact solution at $t = 2$ with no change in amplitude. When $k_x \Delta x$ is increased to $7\pi/8$, the wave front belonging to acoustic mode 1 travels in the opposite direction (towards the left instead of the right) and experiences a reduction in its amplitude as well. The wave front belonging to acoustic mode 2 travels to the left at a faster speed, deviating away from the position of its exact solution. No change in the amplitude of the wave front belonging to acoustic mode 2 was found at $t = 2$.

2.4 2D linear spectral analysis under full discretization - Advection

In this section, the analysis framework is extended to multidimensional wavenumber space. The two-dimensional advection equation is used to illustrate the implication of multidimensionality on the resolution characteristic of the coupled numerical schemes. In two-dimensional wavenumber space, the resolution of the numerical scheme becomes a function of the wavenumber and the wave propagation angle. In this context, the wave propagation angle represents the orientation of the wave front with respect to the grid. It does not necessary coincides with the angle of the convection velocity ($\theta_a = \tan^{-1}(\frac{\bar{v}}{\bar{u}})$). This is illustrated in figure 2.30.

We begin with the derivation of the dispersion relation of the two dimensional advection equation. The two dimensional advection equation is given by

$$\frac{\partial \Phi}{\partial t} + \bar{u} \frac{\partial \Phi}{\partial x} + \bar{v} \frac{\partial \Phi}{\partial y} = 0. \quad (2.68)$$

The field variable Φ written in terms of its inverse two dimensional Fourier transform is given by

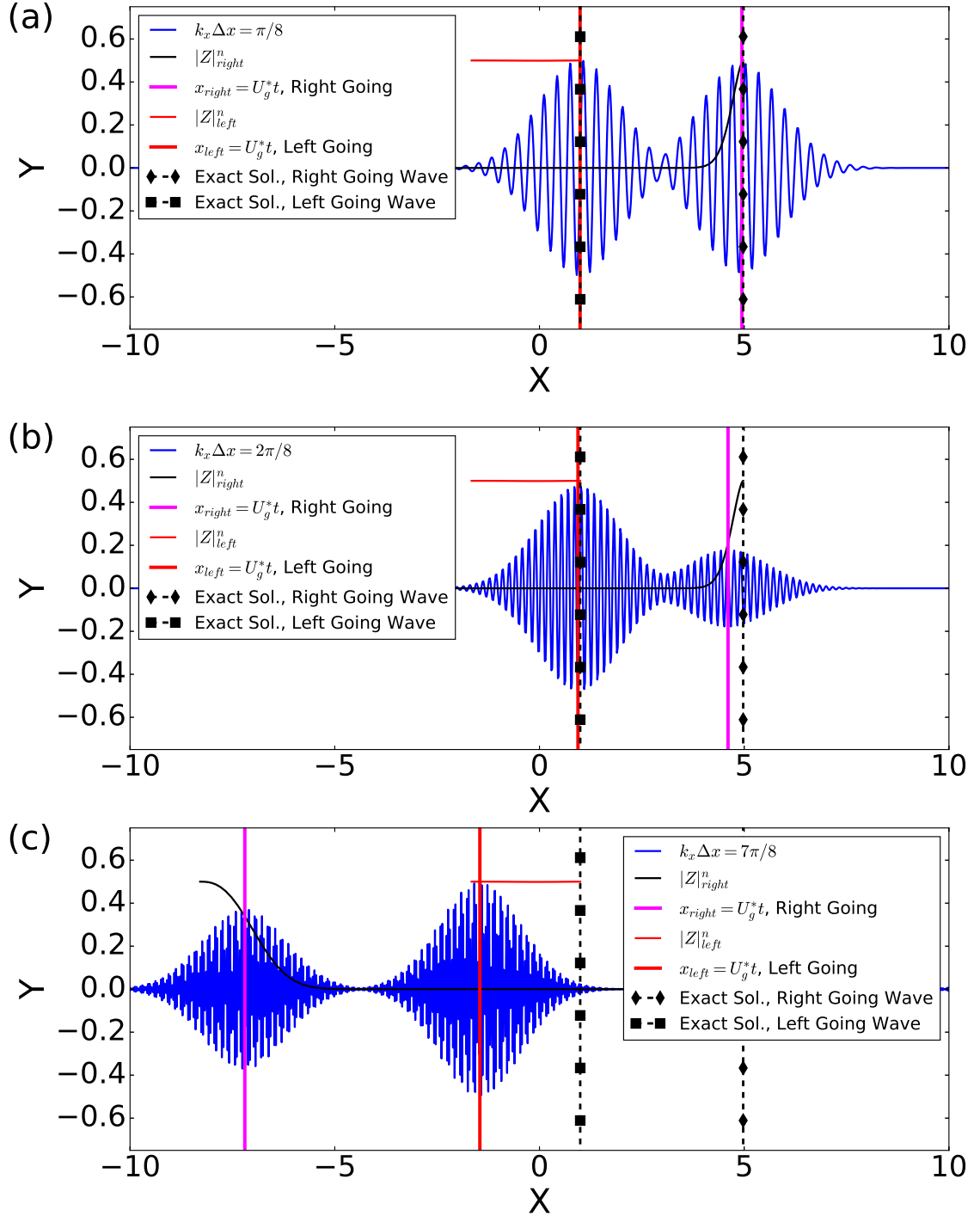


Figure 2.29: Illustrating the propagation of pressure waves according to their group velocity. (a) $k_x \Delta x = \pi/8$, (b) $k_x \Delta x = 2\pi/8$ and (c) $k_x \Delta x = 3\pi/4$. $R_a = 0.5$. Black dotted lines with symbols represent the exact solution of the right and left going waves at $t = 2$. The magenta and red lines represent the position of wave packet computed from the analytical group velocity. They represent cases 1 to 3 of table 2.3.

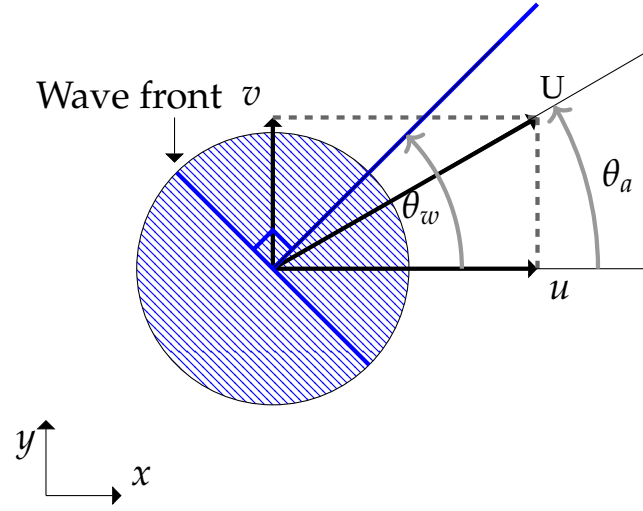


Figure 2.30: Illustration of wave propagation angle (θ_w) and convection angle ($\theta_a = \tan^{-1}(\frac{\bar{v}}{\bar{u}})$).

$$\Phi(x, y, t) = \frac{1}{(2\pi)^2} \int_{-\pi/\Delta x}^{\pi/\Delta x} \int_{-\pi/\Delta x}^{\pi/\Delta x} \hat{\Phi}(k_x, k_y, t) e^{ik_x x} e^{ik_y y} dk_x dk_y. \quad (2.69)$$

By substituting equation (2.69) into (2.68) and noting that the numerical approximation of the spatial derivatives will introduce a modified wavenumber, k_x^* and k_y^* , the resulting equation is

$$\frac{\partial \hat{\Phi}(k_x, k_y, t)}{\partial t} = -i(\bar{u}k_x^* + \bar{v}k_y^*) \hat{\Phi}(k_x, k_y, t). \quad (2.70)$$

Equation (2.70) has a solution of the form

$$\hat{\Phi}(k_x, k_y, t) = \hat{\Phi}(k_x, k_y, 0) e^{-i(\bar{u}k_x^* + \bar{v}k_y^*)t}. \quad (2.71)$$

By substituting equation (2.71) back into equation (2.69), the field variable Φ can be written as

$$\Phi(x, y, t) = \frac{1}{(2\pi)^2} \int_{-\pi/\Delta x}^{\pi/\Delta x} \int_{-\pi/\Delta x}^{\pi/\Delta x} \hat{\Phi}(k_x, k_y, 0) e^{i(k_x x + k_y y - \bar{u}k_x^* t - \bar{v}k_y^* t)} dk_x dk_y. \quad (2.72)$$

By comparing this to the exact solution,

$$\Phi(x, y, t) = \frac{1}{(2\pi)^2} \int_{-\pi/\Delta x}^{\pi/\Delta x} \int_{-\pi/\Delta x}^{\pi/\Delta x} \hat{\Phi}(k_x, k_y, 0) e^{i(k_x x + k_y y - \omega t)} dk_x dk_y, \quad (2.73)$$

the semi discretized numerical dispersion relation is given by $\omega = \bar{u}k_x^* + \bar{v}k_y^*$. The numerical dispersion relation in this form considers only the spatial discretization effect. Hence it will be denoted as ω_{semi}^* hereafter. The solution $\hat{\Phi}(k_x, k_y, t) = \hat{\Phi}(k_x, k_y, 0) e^{-i(\bar{u}k_x^* + \bar{v}k_y^*)t}$ is only true when the semi-discretized equation is propagated exactly through time. In reality, a numerical solution must be advanced through time using a temporal scheme and this will introduce temporal discretization error. In order to account for the temporal discretization effect, the numerical amplification factor of the temporal scheme is considered. Similar to the 1D advection case, the semi discretized numerical dispersion relation is used within the numerical amplification factor to obtain the phase shift. With the phase shift, one can obtain the fully discretized numerical phase and group velocity. The physical dispersion relation of the 2D advection equation is given by $\omega = \bar{u}k_x + \bar{v}k_y$. The physical phase and group velocities are given by:

$$U_{phase,exact} = \frac{\omega}{k_x} = \bar{u} + \bar{v} \frac{k_y}{k_x}, \quad V_{phase,exact} = \frac{\omega}{k_y} = \bar{u} \frac{k_x}{k_y} + \bar{v}, \quad (2.74)$$

$$U_{grp,exact} = \frac{\partial \omega}{\partial k_x} = \bar{u}, \quad V_{grp,exact} = \frac{\partial \omega}{\partial k_y} = \bar{v}. \quad (2.75)$$

The fully discretized numerical phase and group velocities are computed from the fully discretized numerical dispersion relation as follows:

$$U_{phase,full}^* = \frac{\omega_{full}^*}{k_x} = \frac{\psi}{k_x \Delta t}, \quad V_{phase,full}^* = \frac{\omega_{full}^*}{k_y} = \frac{\psi}{k_y \Delta t} \quad (2.76)$$

$$U_{grp,full}^* = \frac{\partial \omega_{full}^*}{\partial k_x} = \frac{1}{\Delta t} \frac{\partial \psi}{\partial k_x}, \quad V_{grp,full}^* = \frac{\partial \omega_{full}^*}{\partial k_y} = \frac{1}{\Delta t} \frac{\partial \psi}{\partial k_y}, \quad (2.77)$$

where

$$\psi = -\tan^{-1} \left(\frac{\text{Im}(Z(\Delta t \omega_{semi}^*))}{\text{Real}(Z(\Delta t \omega_{semi}^*))} \right). \quad (2.78)$$

Table 2.4: Parameters and schemes used for 2D advection

Case No.	R	Spatial Scheme	Temporal Scheme
1	0.1	CDS4	RK4
2	0.1	DRP4	RK4
3	0.1	CDS4 _{opt}	RK4
4	0.1	CCOM6	RK4
5	0.5	CDS4	RK4
6	0.5	CDS4	RK3
7	0.5	CDS4	CN

We will now present the numerical amplification factor, normalized numerical phase and group velocities of some representative numerical schemes in multidimensional wavenumber space. The effect of varying temporal scheme and R on the resolution of the coupled spatial and temporal numerical schemes is presented. In this comparison, $R_x = R_y = R$ and the grid spacing is set to equal in both directions ($\Delta x = \Delta y$). In order to obtain different values of reduced wavenumber on different spatial directions, the grid spacing is kept constant while the values of k_x and k_y are varied based on the initial conditions. Studies concerning error analysis of non uniform grid spacings are beyond the scope of this thesis and readers are referred to [Babucke and Kloker, 2009] for more information. The same spatial scheme is used in both spatial directions. Table 2.4 showcases the parameters and schemes used for each case.

2.4.1 Comparison of different spatial discretization schemes

Since $R = 0.1$ is a sufficiently low value and central type spatial schemes are used for the comparison, the numerical amplification factor would remain almost 1.0 for all wavenumber combination. Therefore, it is not plotted. The plot of the normalized numerical phase and group velocities for the different spatial schemes are shown in figures 2.31 to 2.38. They correspond to cases 1 to 4 in table 2.4. For the CDS4, DRP4 and CCOM6 spatial scheme, it can be seen that the normalized group velocities ($\frac{U_{grp,full}^*}{U_{grp,exact}^*}$ and $\frac{V_{grp,full}^*}{V_{grp,exact}^*}$) vary in only one wavenumber direction. In contrary, the normalized group velocities of the CDS4_{opt} scheme varies in both wavenumber directions. This is expected since the

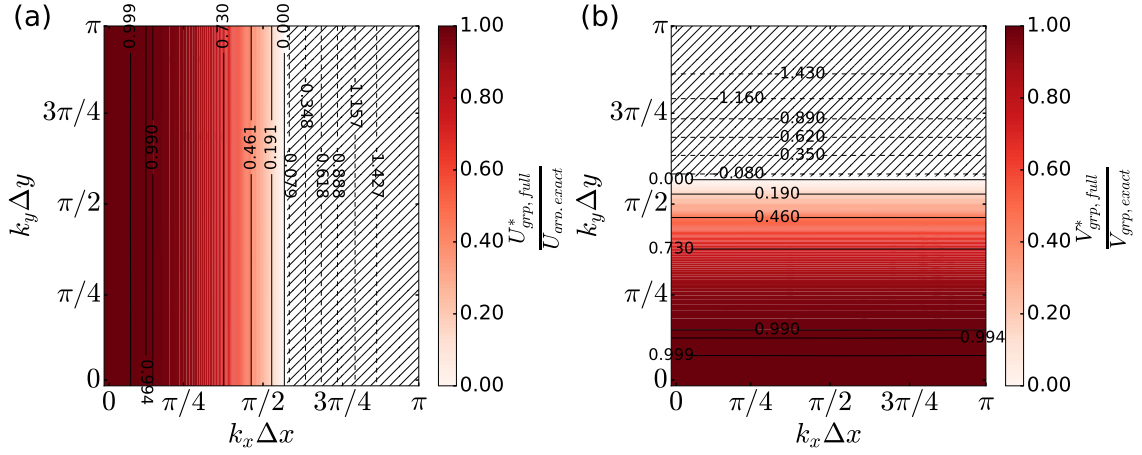


Figure 2.31: Normalized numerical group velocities (a) $\frac{U_{grp,full}^*}{U_{grp,exact}}$ and (b) $\frac{V_{grp,full}^*}{V_{grp,exact}}$ for CDS4 spatial and RK4 temporal scheme. $R = 0.1$

modified wavenumber of the $CDS4_{opt}$ scheme is a function of the wavenumber in both spatial directions. This is less obvious in the comparison of the respective phase velocities plots. However, it is noted that the $CDS4_{opt}$ scheme displays much more phase error even at low reduced wavenumber.

2.4.2 Effect of a change in CFL number

For the sake of brevity, only one type of spatial scheme is used here to showcase the effect of an increase in R in multidimensional wavenumber space. In order to illustrate this, case 1 (figure 2.31) is compared against case 5 (figure 2.39). With increasing R , the normalized numerical group velocity begins to show variation in both k_x and k_y directions unlike the baseline line case ($R = 0.1$) where the normalized numerical group velocity showcases variation in either k_x or k_y direction.

The numerical amplification factor of the cases representing $R = 0.1$ and $R = 0.5$ are plotted in figure 2.41. For $R = 0.1$, the numerical amplification remain approximately 1.0 across all wavenumber combination. When R is increased from 0.1 to 0.5, the numerical amplification factor becomes lesser than 1 especially at intermediate wavenumber range.

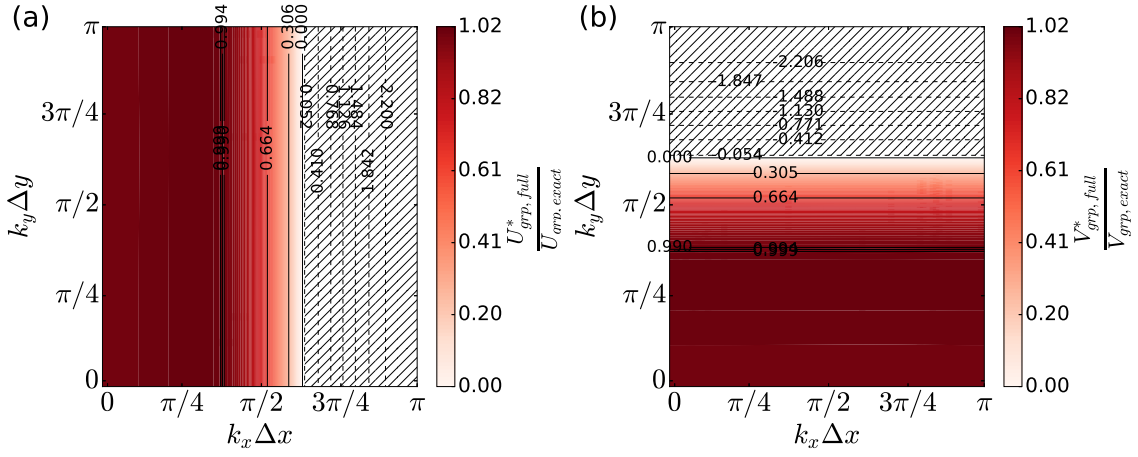


Figure 2.32: Normalized numerical group velocities (a) $\frac{U_{grp,full}^*}{U_{grp,exact}}$ and (b) $\frac{V_{grp,full}^*}{V_{grp,exact}}$ for DRP4 spatial and RK4 temporal scheme. $R = 0.1$

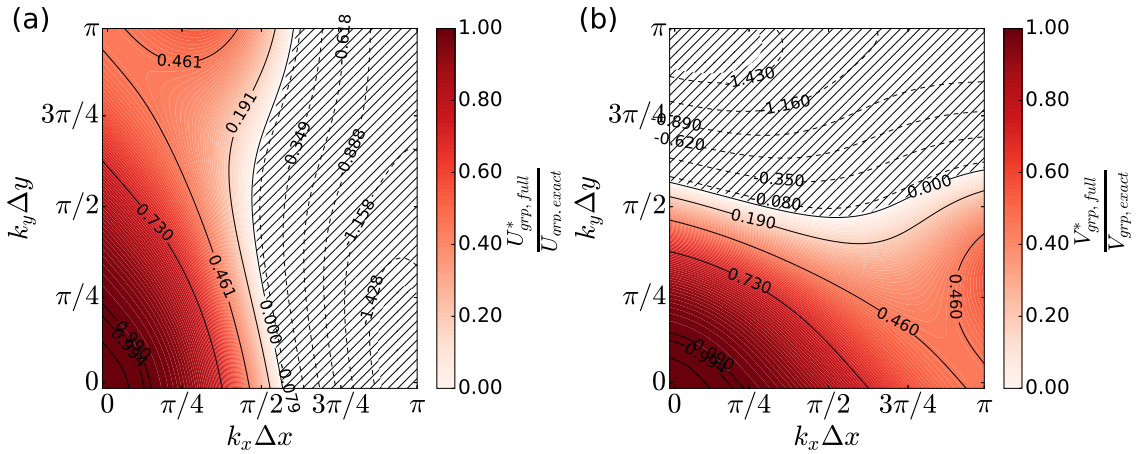
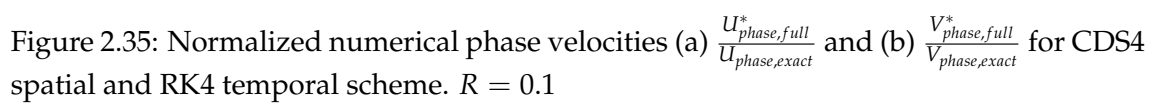
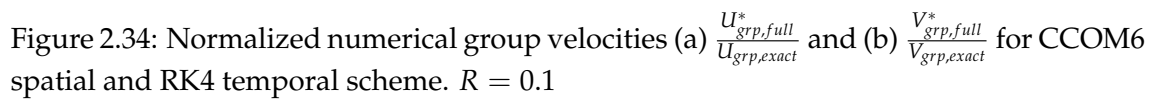


Figure 2.33: Normalized numerical group velocities (a) $\frac{U_{grp,full}^*}{U_{grp,exact}}$ and (b) $\frac{V_{grp,full}^*}{V_{grp,exact}}$ for CDS4_{opt} spatial and RK4 temporal scheme. $R = 0.1$



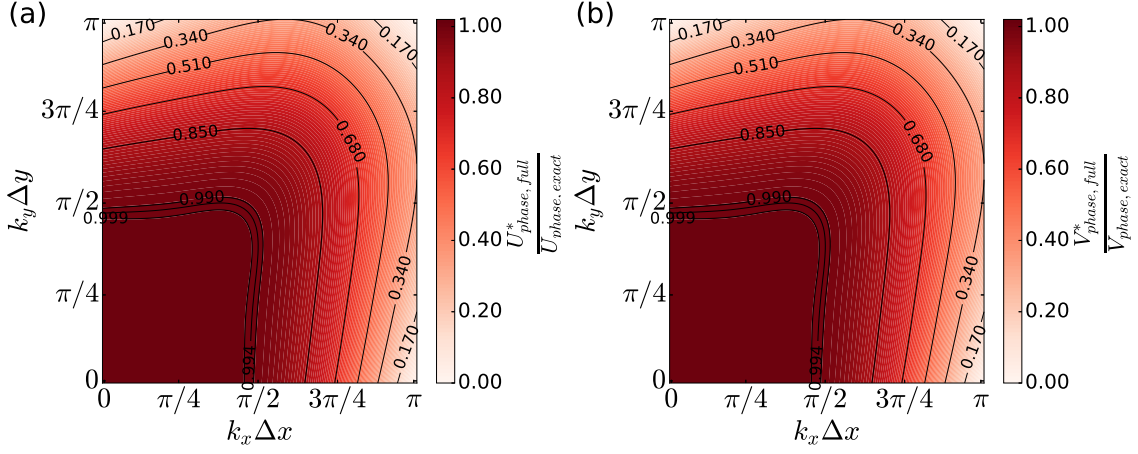


Figure 2.36: Normalized numerical phase velocities (a) $\frac{U_{phase,full}^*}{U_{phase,exact}}$ and (b) $\frac{V_{phase,full}^*}{V_{phase,exact}}$ for DRP4 spatial and RK4 temporal scheme. $R = 0.1$

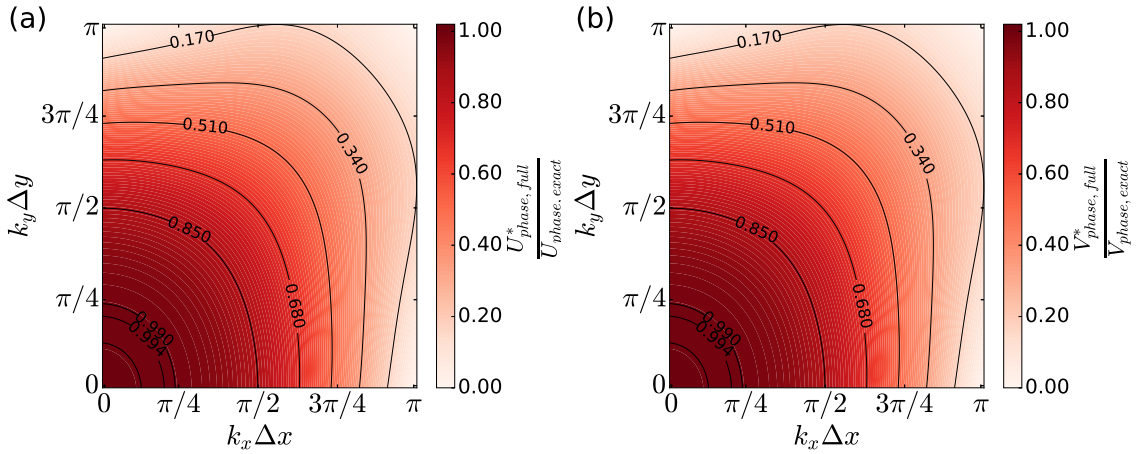
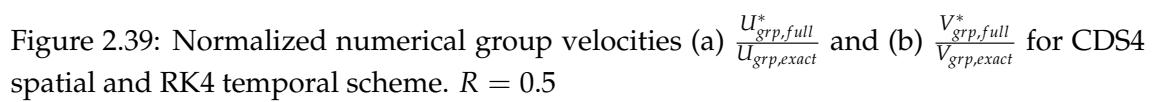
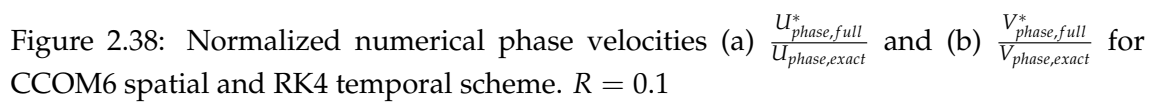


Figure 2.37: Normalized numerical phase velocities (a) $\frac{U_{phase,full}^*}{U_{phase,exact}}$ and (b) $\frac{V_{phase,full}^*}{V_{phase,exact}}$ for CDS4_{opt} spatial and RK4 temporal scheme. $R = 0.1$



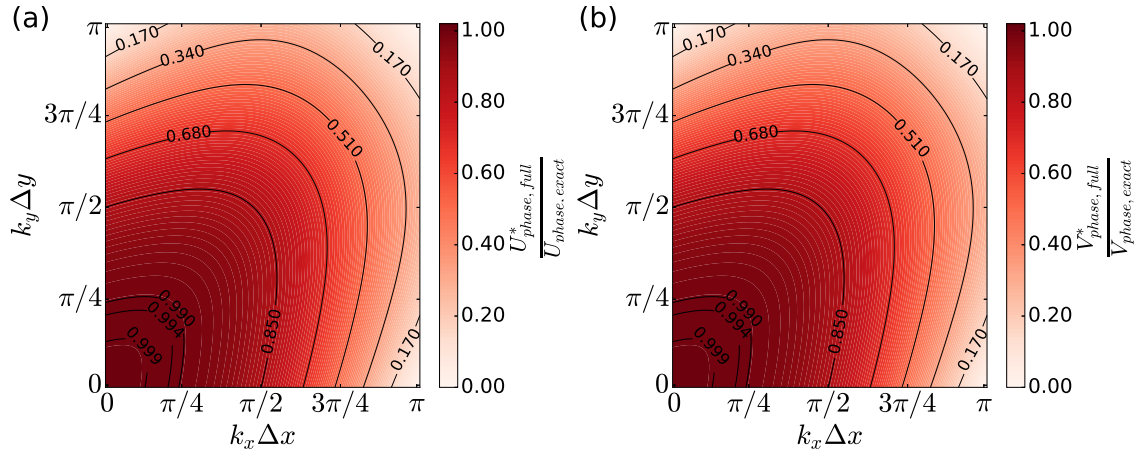


Figure 2.40: Normalized numerical phase velocities (a) $\frac{U_{\text{phase,full}}^*}{U_{\text{phase,exact}}^*}$ and (b) $\frac{V_{\text{phase,full}}^*}{V_{\text{phase,exact}}^*}$ for CDS4 spatial and RK4 temporal scheme. $R = 0.5$

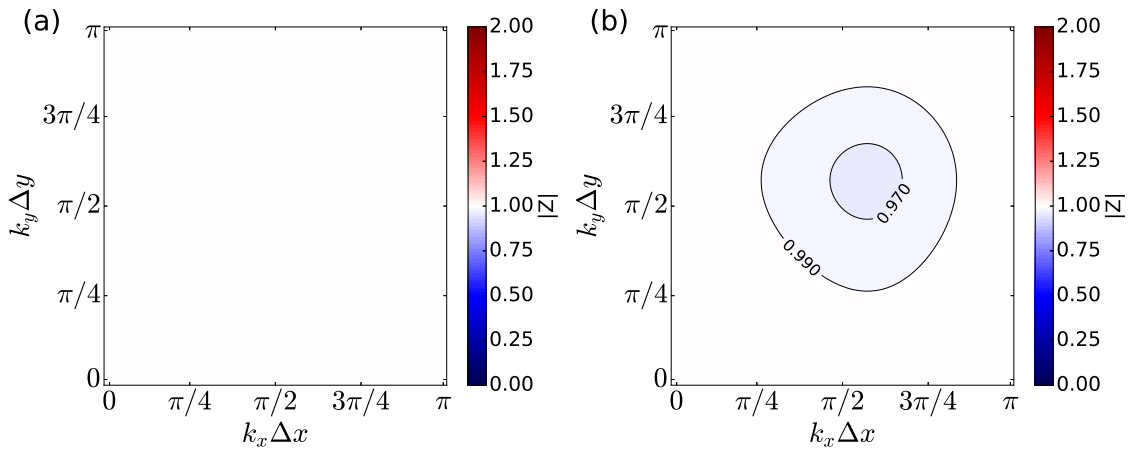


Figure 2.41: Numerical amplification factor of cases with (a) $R = 0.1$ and (b) $R = 0.5$ for CDS4 spatial and RK4 temporal scheme.

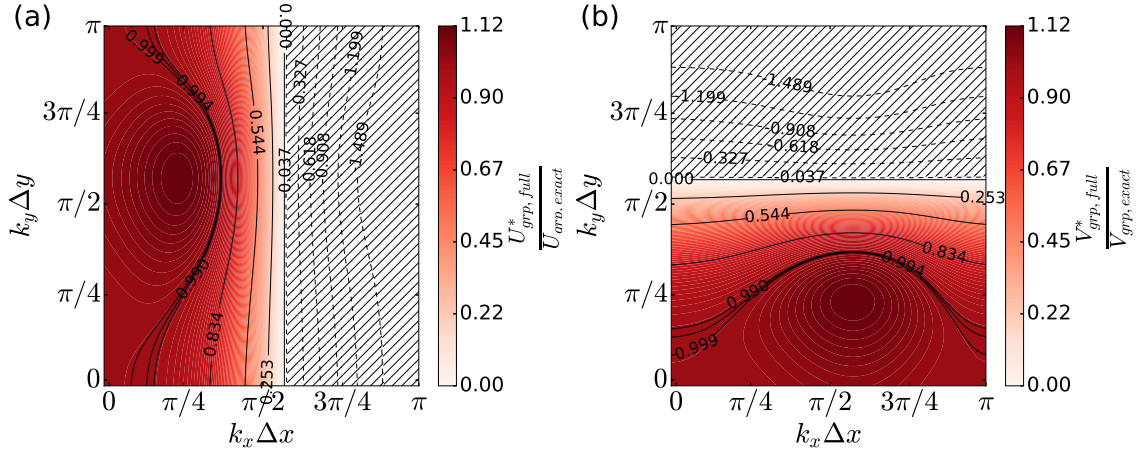


Figure 2.42: Normalized numerical group velocities (a) $\frac{U_{grp,full}^*}{U_{grp,exact}}$ and (b) $\frac{V_{grp,full}^*}{V_{grp,exact}}$ for CDS4 spatial and RK3 temporal scheme. $R = 0.5$

2.4.3 Effect of a change in temporal discretization schemes

In order to illustrate the effect of a change in temporal scheme in multidimensional wavenumber space, case 5 (figure 2.39) is compared against cases 6 (figure 2.42) and 7 (figure 2.43) at a larger R value of 0.5. It can be seen that when the temporal scheme is switched to a lower order scheme (RK4 to RK3), there is notably more dispersion error at the low wavenumber range. This is evident from the larger deviation in normalized group velocity from 1.0 at the low wavenumber range. When an implicit temporal scheme is used instead, there is even more dispersion error at the low wavenumber range as compared to the explicit RK3 and RK4 temporal scheme. Again, this is evident from the larger deviation in normalized group velocity at the low wavenumber range.

Similar trends can be observed in the numerical phase speed plots (figures 2.44 and 2.45). Observable differences in the numerical phase speed can be found at the low wavenumber range when different temporal schemes are used. At the high wavenumber range, the numerical phase speed plots remain the same for the three different temporal schemes.

The numerical amplification factor of the cases representing RK4, RK3 and CN temporal schemes are plotted in figure 2.46. It can be seen that when the temporal scheme is changed to a lower order scheme (RK3), larger numerical dissipation across a larger wavenumber range is present for the same R . When the temporal scheme is changed to an implicit CN scheme, the numerical amplification factor remains neutrally stable across

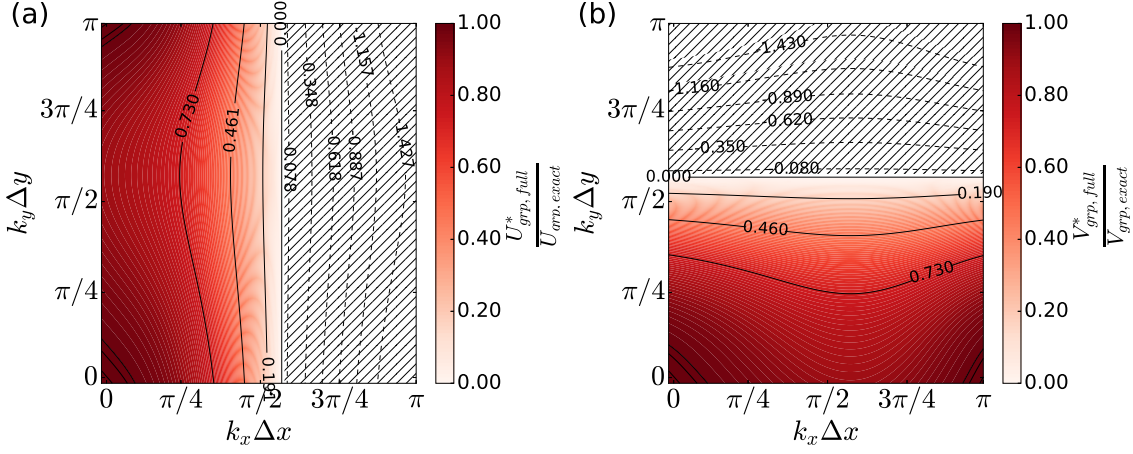


Figure 2.43: Normalized numerical group velocities (a) $\frac{U_{grp,full}^*}{U_{grp,exact}}$ and (b) $\frac{V_{grp,full}^*}{V_{grp,exact}}$ for CDS4 spatial and CN temporal scheme. $R = 0.5$

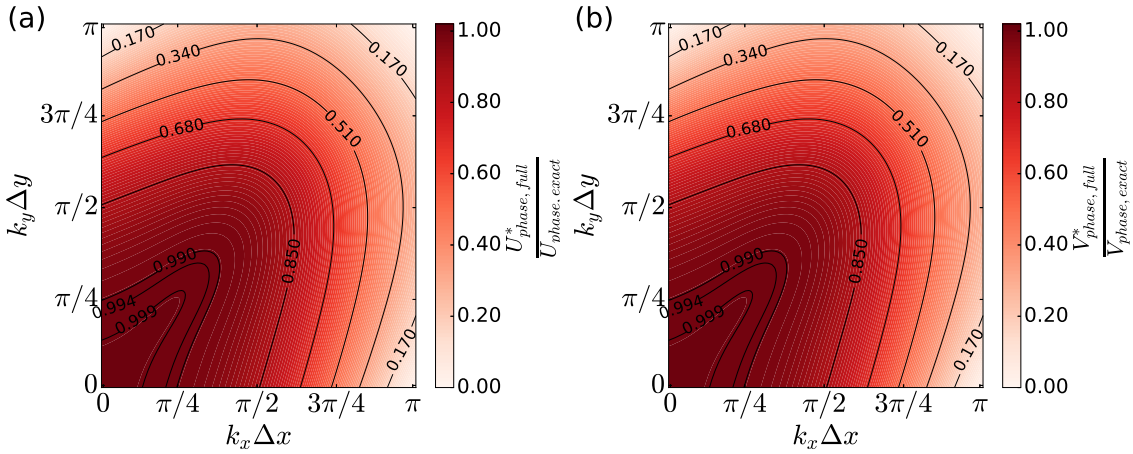


Figure 2.44: Normalized numerical phase velocities (a) $\frac{U_{phase,full}^*}{U_{phase,exact}}$ and (b) $\frac{V_{phase,full}^*}{V_{phase,exact}}$ for CDS4 spatial and RK3 temporal scheme. $R = 0.5$

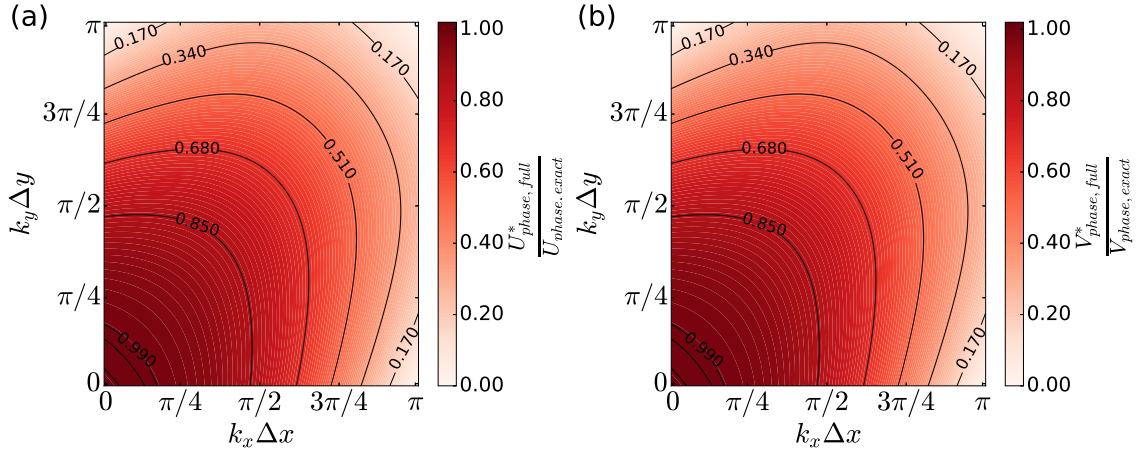


Figure 2.45: Normalized numerical phase velocities (a) $\frac{U_{phase,full}^*}{U_{phase,exact}}$ and (b) $\frac{V_{phase,full}^*}{V_{phase,exact}}$ for CDS4 spatial and CN temporal scheme. $R = 0.5$

all wavenumber range.

2.4.4 Numerical experiments

For the purpose of verifying the analytical predictions, numerical simulations were conducted to compare the results. Same as the 1D numerical tests, the position of the wave packets at $t = 1$ are compared against the solution predicted by the analysis framework. The initial conditions are as follows: $\Phi(x, y, 0) = e^{-0.5(x^2+y^2)} \sin(k_x x + k_y y)$, where $k_x = k \cos(\theta_w)$ and $k_y = k \sin(\theta_w)$. θ_w represents the orientation of the wave front with respect to the grid. The computational domain is taken to be $[-8, 8] \times [-8, 8]$. A uniformly spaced grid with 300 points across the entire domain in each spatial direction is used. The initial condition, parameters and schemes used for each case is presented in table 2.5. The convection velocity is set to $\bar{u} = \bar{v} = 1.0$.

Three set of numerical experiments were conducted. The first set is to verify the results of the analytical prediction. The comparison between the first and second set of numerical experiments was to illustrate the effect of a change in R . Finally, the comparison between the second and third set of numerical experiments was to illustrate the effect of a change in temporal scheme from RK4 to RK3. These numerical results are illustrated in figure 2.47.

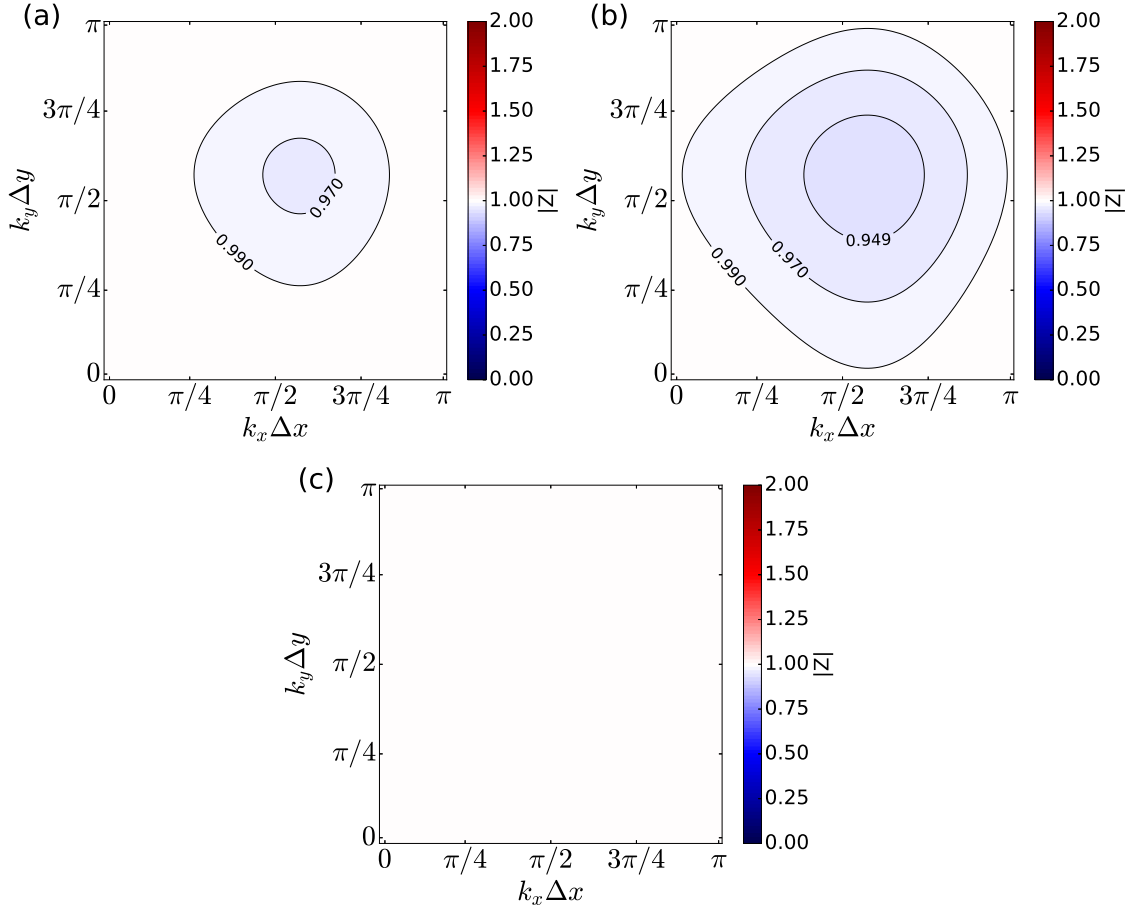


Figure 2.46: Numerical amplification factor of cases with (a) RK4, (b) RK3 and (c) CN temporal scheme and CDS4 spatial scheme for $R = 0.5$. It should be noted that the depth of the shade is proportional to the amplitude.

Table 2.5: Initial conditions, parameters and schemes used for 2D advection

Case No.	$k\Delta x$	$\theta_w [^\circ]$	R	Spatial Scheme	Temporal Scheme
1	$\frac{\pi}{8}$	30	0.1	CDS4	RK4
2	$\frac{3\pi}{8}$	30	0.1	CDS4	RK4
3	$\frac{3\pi}{4}$	30	0.1	CDS4	RK4
4	$\frac{\pi}{8}$	30	0.5	CDS4	RK4
5	$\frac{3\pi}{8}$	30	0.5	CDS4	RK4
6	$\frac{3\pi}{4}$	30	0.5	CDS4	RK4
7	$\frac{\pi}{8}$	30	0.5	CDS4	RK3
8	$\frac{3\pi}{8}$	30	0.5	CDS4	RK3
9	$\frac{3\pi}{4}$	30	0.5	CDS4	RK3

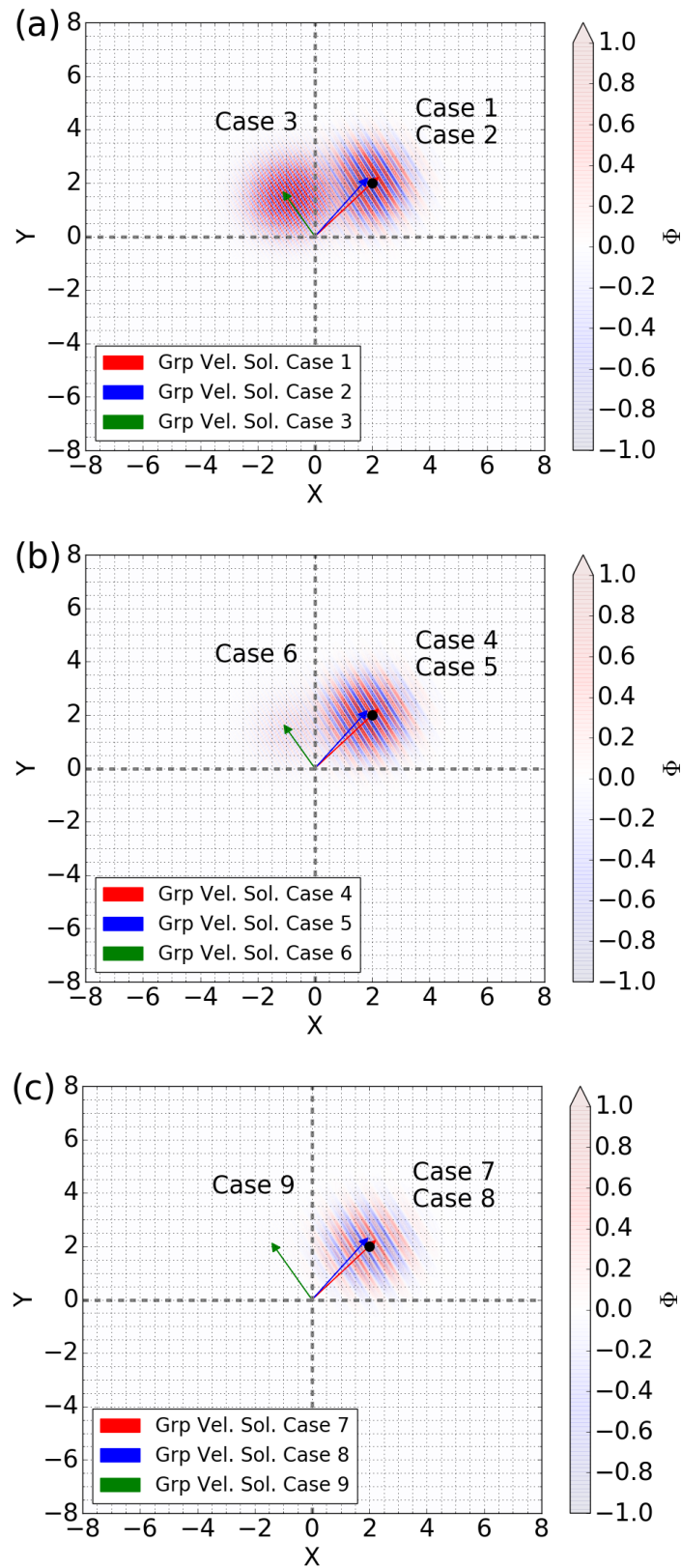


Figure 2.47: Numerical results of wave packet at $t = 1$ (a) Cases 1,2,3 (b) Cases 4,5,6 and (c) Cases 7,8,9. Arrows indicate position of wave packet computed by analytical group velocity at $t = 1$. Black dot represents the exact solution.

Firstly, it can be seen that the position of the wave packets are well predicted by the numerical group velocity results in figure 2.47. The arrow heads represent the position of the wave packets predicted by the numerical group velocity at $t = 1$ for the different cases. Secondly, when R is increased from 0.1 to 0.5, the amplitude of the numerical solution become smaller especially for the case where $k\Delta = 3\pi/4$ (Case 3 versus Case 6). This is consistent with what is found in the 1D advection example where the amplitude of the numerical solution is smaller at intermediate reduced wavenumber. The position of the wave packets remain approximately the same when R is increased from 0.1 to 0.5. This imply negligible change in the dispersion error. When the temporal scheme is changed from RK4 to RK3 with $R = 0.5$, the amplitude of the numerical solution become even smaller, implying larger numerical dissipation. Also, the position of the wave packet for cases 7, 8 and 9 are shifted a little as compared to cases 4, 5 and 6 respectively, implying a small change in the dispersion error.

2.5 Chapter summary

This chapter has covered much of the background theory for which the following chapters will be built upon. Namely, it has introduced the finite difference (FD) method and summarised the different types of linear FD schemes; introduced the concept of spectral accuracy as a way to assess the accuracy of the spatial discretization scheme; introduced a series of implicit and explicit temporal discretization method and finally, present the full discretization analysis framework in both one and two dimensional wavenumber space. For the full discretization analysis of the 1D advection equation, a comparison of explicit and implicit temporal discretization scheme was made at a intermediate value of $R = 1.5$. Although the implicit CN temporal scheme is unconditionally stable across all time steps, the use of intermediate CFL number give rise to a much larger dispersion error at intermediate and large wavenumber as compared to the RK4 and RK3 scheme. When the governing equation is changed from the 1D advection to the 1D Linearized Euler Equations (LEE), the dispersion relation composed of three different modes; one entropy and two acoustic modes. A comparison of the amplification factor of the three

different modes shows that the dispersion relation belonging to the largest eigenvalue ($\omega = \bar{u} + a$, acoustic mode) provides the limiting criteria for the stability limit. This is evident in the plot of group and phase velocities as well. When the analysis is extended to the two dimensional wavenumber space, the dispersion and dissipation properties of the coupled schemes become a function of the reduced wavenumber and the wave propagation angle. For a sufficiently low value of $R = 0.1$, the group velocities of the CDS4, DRP4, CCOM6 varies in one spatial direction only. In the case of the CDS4_{opt} scheme, the group velocities varies in both spatial direction since the modified wavenumber is a function of the wavenumber in both spatial directions.

With respect to the practical usage of numerical schemes investigated, it is recommended to use the CDS4 and DRP4 scheme when discretising the convective terms of the Navier-Stokes. This has advantage in terms of the ease of numerical implementation and the faster speed of computation. Although it is possible to use the CCOM6 scheme which has better spectral accuracy (for the same stencil width considered), the speed of computation is generally slower as compared to explicit spatial discretization method. As for the temporal discretization, it is recommended to use explicit temporal schemes such as RK3 and RK4 for the convective terms, which give much less dispersion error at low/intermediate reduced wavenumber at intermediate CFL values. In the case of viscous simulation, the time step is mainly limited by the much smaller grid size required at region within the boundary layer. Due to the unconditional stability of implicit temporal schemes, the use of schemes such as CN for the diffusive term allows for a larger CFL value to be used. However, the implicit CN scheme introduces much more dispersion error at intermediate CFL value. Hence, the use of much larger CFL value than required is not recommended.

Chapter 3

Multidimensional analysis of hybrid Fourier-spectral/finite-difference schemes

In this chapter, the two dimensional linear spectral analysis method is extended to the two dimensional linearized Euler/Navier Stokes equations. Assessment of numerical schemes based on the advection equation only considers the convection contribution. By extending it to the linearized compressible Euler/Navier Stokes equation (LCNSE), viscous and acoustic effects are also taken into account. In particular, the case of using hybrid finite difference/Fourier spectral scheme in multidimensional space is analyzed to understand its effect on the anisotropy of the numerical scheme.

3.1 Spectral analysis of 2D linearized compressible Navier-Stokes equation (LCNSE)

As shown in chapter 2, the fully discretized numerical group and phase velocities are calculated from the phase shift of the fully discretized numerical amplification factor. To obtain the fully discretized numerical amplification factor, the dispersion relation of the governing equation considered should be first derived. The primitive form of the two dimensional compressible Navier-Stokes equations[[Abarbanel and Gottlieb, 1981](#)] is given by

$$\frac{\partial \mathbf{U}}{\partial t} + A_1 \frac{\partial \mathbf{U}}{\partial x} + A_2 \frac{\partial \mathbf{U}}{\partial y} - B_1 \frac{\partial^2 \mathbf{U}}{\partial x^2} - B_2 \frac{\partial^2 \mathbf{U}}{\partial y^2} - B_3 \frac{\partial^2 \mathbf{U}}{\partial x \partial y} = \mathbf{0}, \quad (3.1)$$

where

$$\begin{aligned}
\mathbf{U} &= \begin{bmatrix} \rho \\ u \\ v \\ p \end{bmatrix} \quad \mathbf{A}_1 = \begin{bmatrix} u & \rho & 0 & 0 \\ 0 & u & 0 & \frac{1}{\rho} \\ 0 & 0 & u & 0 \\ 0 & \rho a^2 & 0 & u \end{bmatrix} \quad \mathbf{A}_2 = \begin{bmatrix} v & 0 & \rho & 0 \\ 0 & v & 0 & 0 \\ 0 & 0 & v & \frac{1}{\rho} \\ 0 & 0 & \rho a^2 & v \end{bmatrix} \\
\mathbf{B}_1 &= \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{4}{3} \frac{\mu}{\rho} & 0 & 0 \\ 0 & 0 & \frac{\mu}{\rho} & 0 \\ -\frac{\gamma \mu p}{P_r \rho^2} & 0 & 0 & \frac{\gamma \mu}{P_r \rho} \end{bmatrix} \quad \mathbf{B}_2 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{\mu}{\rho} & 0 & 0 \\ 0 & 0 & \frac{4}{3} \frac{\mu}{\rho} & 0 \\ -\frac{\gamma \mu p}{P_r \rho^2} & 0 & 0 & \frac{\gamma \mu}{P_r \rho} \end{bmatrix} \quad \mathbf{B}_3 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{3} \frac{\mu}{\rho} & 0 \\ 0 & \frac{1}{3} \frac{\mu}{\rho} & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}.
\end{aligned} \tag{3.2}$$

ρ , p , a , u and v represent the density, pressure, speed of sound as well as the velocity components in the x and y directions, respectively. Firstly, linearization of the two dimensional compressible Navier Stokes equations is carried out by applying a perturbation to the mean flow, $\mathbf{U} = \mathbf{U}_0 + \mathbf{U}'$ and assuming that the perturbation, $\mathbf{U}'$ is sufficiently small. This assumption allows one to neglect all non linear terms associated with either the squared of perturbed quantities or products of the perturbed quantities and perturbed gradients since these terms would be even smaller. Secondly, it is assumed that the mean flow is homogeneous, which allows one to neglect all mean spatial gradients. Thirdly, the mean flow is considered to be weakly compressible, which means that an isothermal assumption (no temperature gradients) is used on the energy equation. Finally, the fluid medium is considered to be mono-atomic and hence bulk viscosity is taken to be zero. After subtracting the mean flow terms from the expanded equations, the 2D Linearized compressible Navier Stokes equations can be written as follows [Marie et al., 2009]:

$$\frac{\partial \mathbf{U}'}{\partial t} + \overline{A}_1 \frac{\partial \mathbf{U}'}{\partial x} + \overline{A}_2 \frac{\partial \mathbf{U}'}{\partial y} - \overline{B}_1 \frac{\partial^2 \mathbf{U}'}{\partial x^2} - \overline{B}_2 \frac{\partial^2 \mathbf{U}'}{\partial y^2} - \overline{B}_3 \frac{\partial^2 \mathbf{U}'}{\partial x \partial y} = \mathbf{0}, \tag{3.3}$$

where

$$\mathbf{U}' = \begin{bmatrix} \rho' \\ u' \\ v' \\ p' \end{bmatrix} \quad \overline{\mathbf{A}}_1 = \begin{bmatrix} \bar{u} & \bar{\rho} & 0 & 0 \\ 0 & \bar{u} & 0 & \frac{1}{\bar{\rho}} \\ 0 & 0 & \bar{u} & 0 \\ 0 & \bar{\rho}a^2 & 0 & \bar{u} \end{bmatrix} \quad \overline{\mathbf{A}}_2 = \begin{bmatrix} \bar{v} & 0 & \bar{\rho} & 0 \\ 0 & \bar{v} & 0 & 0 \\ 0 & 0 & \bar{v} & \frac{1}{\bar{\rho}} \\ 0 & 0 & \bar{\rho}a^2 & \bar{v} \end{bmatrix} \quad (3.4)$$

$$\overline{\mathbf{B}}_1 = \bar{v} \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{4}{3} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad \overline{\mathbf{B}}_2 = \bar{v} \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \frac{4}{3} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad \overline{\mathbf{B}}_3 = \bar{v} \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{3} & 0 \\ 0 & \frac{1}{3} & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}.$$

In equation (3.4), $\bar{v} = \frac{\bar{u}}{\bar{\rho}}$. Field variables denoted with $(..)'$ represent the perturbed field while those with $(\overline{..})$ represent the time averaged mean field. A Fourier-Laplace transform of $\mathbf{U}'$ is given by:

$$\widehat{\mathbf{U}}'(k_x, k_y, \omega) = \frac{1}{(2\pi)^3} \int_0^\infty \int_{-\infty}^\infty \int_{-\infty}^\infty \mathbf{U}' e^{i(k_x x + k_y y - \omega t)} dx dy dt, \quad (3.5)$$

where the components of the wavenumber and frequency are denoted as k_x , k_y and ω respectively. By substituting equation (3.5) into equation (3.3):

$$\begin{aligned} \frac{\partial \widehat{\mathbf{U}}'}{\partial t} &= -i\omega \widehat{\mathbf{U}}', \quad \frac{\partial \widehat{\mathbf{U}}'}{\partial x} = ik_x \widehat{\mathbf{U}}', \quad \frac{\partial \widehat{\mathbf{U}}'}{\partial y} = ik_y \widehat{\mathbf{U}}', \\ \frac{\partial^2 \widehat{\mathbf{U}}'}{\partial x^2} &= -(k_x)^2 \widehat{\mathbf{U}}', \quad \frac{\partial^2 \widehat{\mathbf{U}}'}{\partial y^2} = -(k_y)^2 \widehat{\mathbf{U}}', \quad \frac{\partial^2 \widehat{\mathbf{U}}'}{\partial x \partial y} = -k_x k_y \widehat{\mathbf{U}}'. \end{aligned} \quad (3.6)$$

Equation (3.3) can be re-written as:

$$\mathbf{I}\omega \widehat{\mathbf{U}} = \underbrace{(k_x \overline{A}_1 + k_y \overline{A}_2 - i(k_x)^2 \overline{B}_1 - i(k_y)^2 \overline{B}_2 - i(k_x k_y) \overline{B}_3)}_{\mathbf{C}} \widehat{\mathbf{U}}, \quad (3.7)$$

where $\mathbf{I}$ represents the identity matrix and

$$\mathbf{C} = \begin{bmatrix} k_x \bar{u} + k_y \bar{v} & k_x \bar{\rho} & k_y \bar{\rho} & 0 \\ 0 & k_x \bar{u} + k_y \bar{v} - \frac{4}{3} i \bar{v} (k_x)^2 - i \bar{v} (k_y)^2 & -\frac{1}{3} i \bar{v} k_x k_y & \frac{k_x}{\bar{\rho}} \\ 0 & -\frac{1}{3} i \bar{v} k_x k_y & k_x \bar{u} + k_y \bar{v} - i \bar{v} (k_x)^2 - \frac{4}{3} i \bar{v} (k_y)^2 & \frac{k_y}{\bar{\rho}} \\ 0 & \bar{\rho} a^2 k_x & \bar{\rho} a^2 k_y & k_x \bar{u} + k_y \bar{v} \end{bmatrix}. \quad (3.8)$$

Solving for the four eigenvalues of $\mathbf{C}$ leads to the following solution:

$$\begin{aligned} \omega_1 &= k_x \bar{u} + k_y \bar{v} - i \nu |\mathbf{k}|^2 + |\mathbf{k}| a, \\ \omega_2 &= k_x \bar{u} + k_y \bar{v} - i \frac{4}{3} \nu |\mathbf{k}|^2 - |\mathbf{k}| a, \\ \omega_3 &= \omega_4 = k_x \bar{u} + k_y \bar{v}, \end{aligned} \quad (3.9)$$

where $|\mathbf{k}| = \sqrt{(k_x)^2 + (k_y)^2}$. The first two eigenvalues represent the dispersion relation for the acoustic waves while the last two eigenvalues represent the dispersion relation for the entropy and vortical waves respectively. The velocity components can be expressed in terms of the product of the speed of sound and Mach number of respective spatial directions. The resulting dispersion relation of the different modes can be re-written as:

$$\begin{aligned} \omega_1 &= k_x M_x a + k_y M_y a - i \nu |\mathbf{k}|^2 + |\mathbf{k}| a, \\ \omega_2 &= k_x M_x a + k_y M_y a - i \frac{4}{3} \nu |\mathbf{k}|^2 - |\mathbf{k}| a, \\ \omega_3 &= \omega_4 = k_x M_x a + k_y M_y a. \end{aligned} \quad (3.10)$$

For the dispersion relation belonging to the acoustic modes ($\omega_{1,2}$), the first two term on the right hand side represent the advection contribution. The third and fourth term represent the diffusive and acoustic contribution respectively. For the dispersion relation of the entropy and vortical modes ($\omega_{3,4}$), it only comprises of the advection contribution.

3.1.1 Physical group and phase velocities of the LCNSE

For the purpose of having a reference solution for comparison and normalization sake, the physical group and phase velocity are computed. The calculation of the physical group and phase velocities for one of the acoustic modes (ω_1) are demonstrated below:

$$\begin{aligned} U_{grp,exact} &= \frac{\partial \omega_1}{\partial k_x} = M_x a - i2\nu k_x + \frac{ak_x}{\sqrt{k_x^2 + k_y^2}}, \\ V_{grp,exact} &= \frac{\partial \omega_1}{\partial k_y} = M_y a - i2\nu k_y + \frac{ak_y}{\sqrt{k_x^2 + k_y^2}}, \end{aligned} \quad (3.11)$$

$$\begin{aligned} U_{phase,exact} &= \frac{\omega_1}{k_x} = M_x a + \frac{k_y M_y a}{k_x} - \frac{i\nu |\mathbf{k}|^2}{k_x} + \frac{|\mathbf{k}|a}{k_x}, \\ V_{phase,exact} &= \frac{\omega_1}{k_y} = \frac{k_x M_x a}{k_y} + M_y a - \frac{i\nu |\mathbf{k}|^2}{k_y} + \frac{|\mathbf{k}|a}{k_y}. \end{aligned} \quad (3.12)$$

3.1.2 Numerical group and phase velocities of the LCNSE

In this section, numerical group and phase velocities computed under full discretization consideration will be presented. As before, the results presented here are demonstrated for only one of the acoustic modes (ω_1). The procedure is applicable to the other modes in equation (3.10). In order to obtain the group velocities under full discretization, the numerical amplification factor is introduced. The corresponding semi-discretized numerical dispersion relation ($\omega_{semi,1,2,3,4}^*$) can be obtained by replacing the wavenumber in the above physical dispersion relations with the modified wavenumber, $k_{x,y}^* = k_{x,y}$. The semi-discretized numerical dispersion relation ($\omega_{semi,1}^*$) of the LCNSE is substituted into the numerical amplification factor of the *RK4* scheme, where:

$$\Delta t \omega_{semi,1}^* = \Delta t (k_x^* M_x a + k_y^* M_y a - i\nu |\mathbf{k}^*|^2 + |\mathbf{k}^*|a) \quad (3.13)$$

and defining the grid spacing, CFL number and cell Reynolds number in terms of the speed of sound:

$$R_a = \frac{a\Delta t}{\Delta x}, \quad Re_a = \frac{a\Delta}{\nu}, \quad \Delta = \Delta x = \Delta y, \quad (3.14)$$

$$\begin{aligned} \Delta t \omega_{semi,1}^* &= R_a \left(M_x k_x^* \Delta + M_y k_y^* \Delta - i \frac{\nu}{a\Delta} |\mathbf{k}^* \Delta|^2 + |\mathbf{k}^* \Delta| \right) \\ &= R_a \left(M_x k_x^* \Delta + M_y k_y^* \Delta - i \frac{1}{Re_a} |\mathbf{k}^* \Delta|^2 + |\mathbf{k}^* \Delta| \right). \end{aligned} \quad (3.15)$$

Numerical group and phase velocities under full discretization are computed from the fully discretized numerical dispersion relation (ω_{full}^*) as follows:

$$U_{grp,full}^* = \frac{\partial \omega_{full}^*}{\partial k_x} = \frac{1}{\Delta t} \frac{\partial \psi}{\partial k_x}, \quad V_{grp,full}^* = \frac{\partial \omega_{full}^*}{\partial k_y} = \frac{1}{\Delta t} \frac{\partial \psi}{\partial k_y}, \quad (3.16)$$

$$\begin{aligned} U_{phase,full}^* &= \frac{\omega_{full}^*}{k_x} = \frac{\psi}{k_x \Delta t}, \quad V_{phase,full}^* = \frac{\omega_{full}^*}{k_y} = \frac{\psi}{k_y \Delta t}, \\ \psi &= -\tan^{-1} \left(\frac{\text{Im}(Z(\Delta t \omega_{semi,1}^*))}{\text{Real}(Z(\Delta t \omega_{semi,1}^*))} \right). \end{aligned} \quad (3.17)$$

An inspection of equation (3.15) shows that the numerical amplification factor, group and phase velocities under full discretization are dependent on the following factors:

- CFL number (R_a); as R_a increases, the magnitude of the amplification factor as well as the region of stability in the two dimensional wavenumber plane changes. Beyond a certain value of R_a , dispersion error may be introduced as well, reflecting changes in the group and phase velocities.
- Mach number; a change in the Mach number regime not only affects the amplitude of the amplification factor but also the characteristics of the anisotropy map at different Mach number. At low Mach number, the acoustic and viscous terms dominate over the convective term. On the other hand, the convective term dominates over the viscous and acoustic terms at high Mach number.
- Viscous effects are related to the cell Reynolds number, Re_a . As Re_a reduces, viscous

effects become more dominant.

3.2 Anisotropy analysis in 2D wavenumber space - full finite difference

In this section, analytical solutions of numerical amplification factor, numerical group and phase velocities for full discretization are plotted and compared for different combinations of spatial discretization schemes. In particular, the focus of this analysis will look at how the resolution characteristic of the coupled numerical scheme in multidimensional wavenumber space changes when different spatial and temporal discretization schemes are used. Also, the effect of CFL number and cell Reynolds number on the spectral properties of the coupled scheme is investigated. Since the dispersion error is mainly affected by the hyperbolic term of the Navier Stokes equation, the analysis presented here will use the linearized Euler equations. Only in the specific instance where viscous effect are considered, the linearized compressible Navier Stokes equation is used.

The parameters and type of schemes used for each case are listed in table 3.1. The speed of sound, a is taken to be 1.0 for all cases. In order to demonstrate the coupling effect in the group velocities, M_y is kept zero to illustrate the contribution of the acoustic term solely for V_{grp}^* . It should be pointed out that the coupling effect of the numerical schemes in two spatial directions is independent of the change in Mach number. A change in Mach number only influences the magnitude of the group velocities. This is reflected in equations (3.15), (3.16) and (3.17).

3.2.1 Physical phase and group velocity solution

In this sub section, the plots of the two physical acoustic modes are compared. These plots are generated based on the exact solution of group and phase velocities given in equations (3.11) and (3.12). The physical viscosity is taken to be zero. The exact group and phase velocity solutions of the two acoustic modes are plotted in figures 3.1 and 3.2. These plots correspond to cases 1a and 1b in table 3.1. Since M_x is kept to 0.5 and M_y is

Table 3.1: Table representing parameter values and numerical schemes for various cases. The abbreviation, CDS4/CDS4 implies that the CDS4 scheme is used in the x and y spatial directions respectively.

Case	Convective schemes	Viscous schemes	Temporal schemes	R_a	Re_a	Solution Type
1a (baseline)	FS/FS	-	-	-	∞	Exact, ω_1^*
1b (baseline)	FS/FS	-	-	-	∞	Exact, ω_2^*
2a	CDS4/CDS4	-	RK4	0.1	∞	Numerical, ω_1^*
2b	DRP4/DRP4	-	RK4	0.1	∞	Numerical, ω_1^*
2c	CCOM6/CCOM6	-	RK4	0.1	∞	Numerical, ω_1^*
2d	CDS4 _{opt} /CDS4 _{opt}	-	RK4	0.1	∞	Numerical, ω_1^*
3a	CDS4/CDS4	-	RK4	0.5	∞	Numerical, ω_1^*
3b	DRP4/DRP4	-	RK4	0.5	∞	Numerical, ω_1^*
3c	CCOM6/CCOM6	-	RK4	0.5	∞	Numerical, ω_1^*
3d	CDS4 _{opt} /CDS4 _{opt}	-	RK4	0.5	∞	Numerical, ω_1^*
4a	CDS4/CDS4	-	RK3	0.5	∞	Numerical, ω_1^*
4b	DRP4/DRP4	-	RK3	0.5	∞	Numerical, ω_1^*
4c	CCOM6/CCOM6	-	RK3	0.5	∞	Numerical, ω_1^*
4d	CDS4 _{opt} /CDS4 _{opt}	-	RK3	0.5	∞	Numerical, ω_1^*
5a (baseline)	FS/FS	-	RK4	0.1	∞	Numerical, ω_1^*
5b	FS/FS	CDS4/CDS4	RK4	0.1	500	Numerical, ω_1^*
5c	FS/FS	CDS4/CDS4	RK4	0.1	100	Numerical, ω_1^*
5d	FS/FS	CDS4/CDS4	RK4	0.1	50	Numerical, ω_1^*
6a (baseline)	FS/FS	FS/FS	RK4	0.1	200	Numerical, ω_1^*
6b	FS/FS	CDS4/CDS4	RK4	0.1	200	Numerical, ω_1^*
6c	FS/FS	DRP4/DRP4	RK4	0.1	200	Numerical, ω_1^*
6d	FS/FS	CCOM6/CCOM6	RK4	0.1	200	Numerical, ω_1^*
6e	FS/FS	CDS4 _{opt} /CDS4 _{opt}	RK4	0.1	200	Numerical, ω_1^*

kept to 0 for this analysis, $U_{grp,exact}$ is generally greater than $V_{grp,exact}$ primarily because of the convection term $M_x a$ within the dispersion relation. A comparison of figures 3.1a and 3.1b shows that the group velocities of the two acoustic modes are generally in opposite direction for most of the wavenumber combinations. For the acoustic mode ω_2 , $V_{grp,exact}$ and $U_{grp,exact}$ is negative for the full range of wavenumber combinations. This is in contrast to the acoustic mode ω_1 , where the group velocities are positive for the full range of wavenumber combinations. In physical space, this would imply that there would be two different wave front travelling in opposite directions as the solution is marched in time. An important feature of the exact solution for the two acoustic modes is that the

group velocities only vary as a function of the wave propagation angle, θ_w (see figure 3.1). For the solutions of the entropy mode, $U_{grp,exact}$ and $V_{grp,exact}$ are equal to 0.5 and 0.0, respectively for all wavenumber combinations (not plotted). This corresponds to the convection velocity used in these cases. The physical phase speed plots display similar trend (see figure 3.2). For acoustic mode ω_1 , $U_{phase,exact}$ and $V_{phase,exact}$ are positive for the full range of wavenumber combinations. For acoustic mode ω_2 , $U_{phase,exact}$ and $V_{phase,exact}$ are negative for the full range of wavenumber combinations. In the remaining parts of this chapter, we will focus mainly on acoustic mode 1. This is because the critical mode of the Linearised Euler equations is the acoustic mode with the largest eigenvalue. As shown in the previous chapter (see figures 2.23, 2.24 and 2.25), this mode is the most critical since it provides the maximum allowable CFL number for numerical stability and it exhibits the largest change in the dispersion property when the CFL number is varied.

3.2.2 Comparison of different spatial discretization scheme - Convection term

In order to assess the effect of the spatial discretization on numerical anisotropy of the convection term, a comparison of the normalized group velocities using different combinations of spatial discretisation schemes was carried out. The parameters used for the plots in figure 3.3a to 3.3d correspond to cases 2a to 2d of table 3.1. In order to examine the error solely from the spatial discretization, the CFL number is kept sufficiently small ($R_a = 0.1$) to minimise the effect of the temporal discretization error. For these comparisons, the numerical amplification factor of the different schemes remain approximately 1.0 across all wavenumber combination, hence they are not plotted. Normalized numerical group and phase velocity plots belonging to the acoustic mode (ω_1^*) for different combinations of spatial discretization methods are presented in figures 3.3 and 3.4. Both the group and phase velocities are related to the dispersion of the numerical scheme. However, the error in phase velocities can become significant when the numerical solution display sharp spatial variation regardless of the grid refinement [Sengupta and Bhole, 2014]. On the other hand, the error in group velocities reduces with increasing grid refinement. Hence, phase velocity is another important element in understanding the error dynamics of linear system. For the normalized group velocities, a significantly

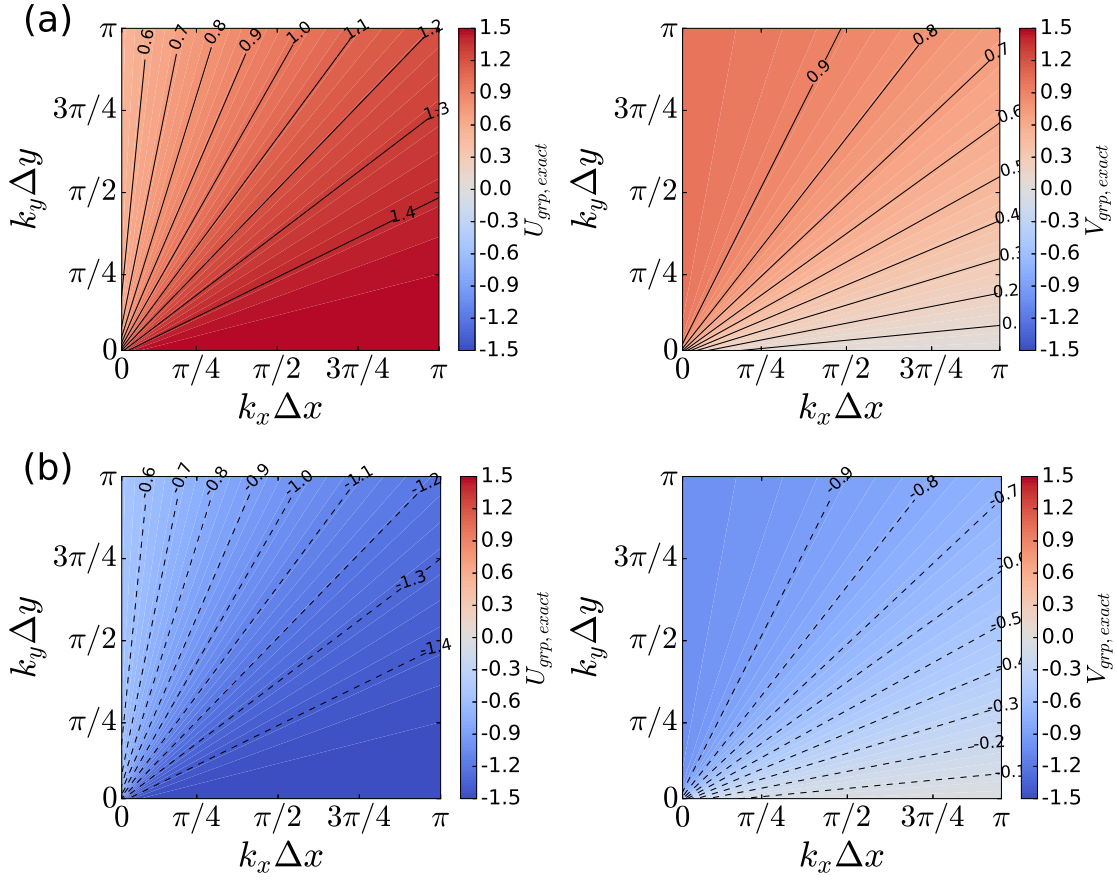


Figure 3.1: Comparison of physical group velocities ($U_{grp,exact}$, $V_{grp,exact}$) for solution of different modes, (a) acoustic mode (ω_1^*), (b) acoustic mode (ω_2^*). They represent cases 1a and 1b of table 3.1. All contour plots are ranged from -1.0 to 1.5 for comparison sake.

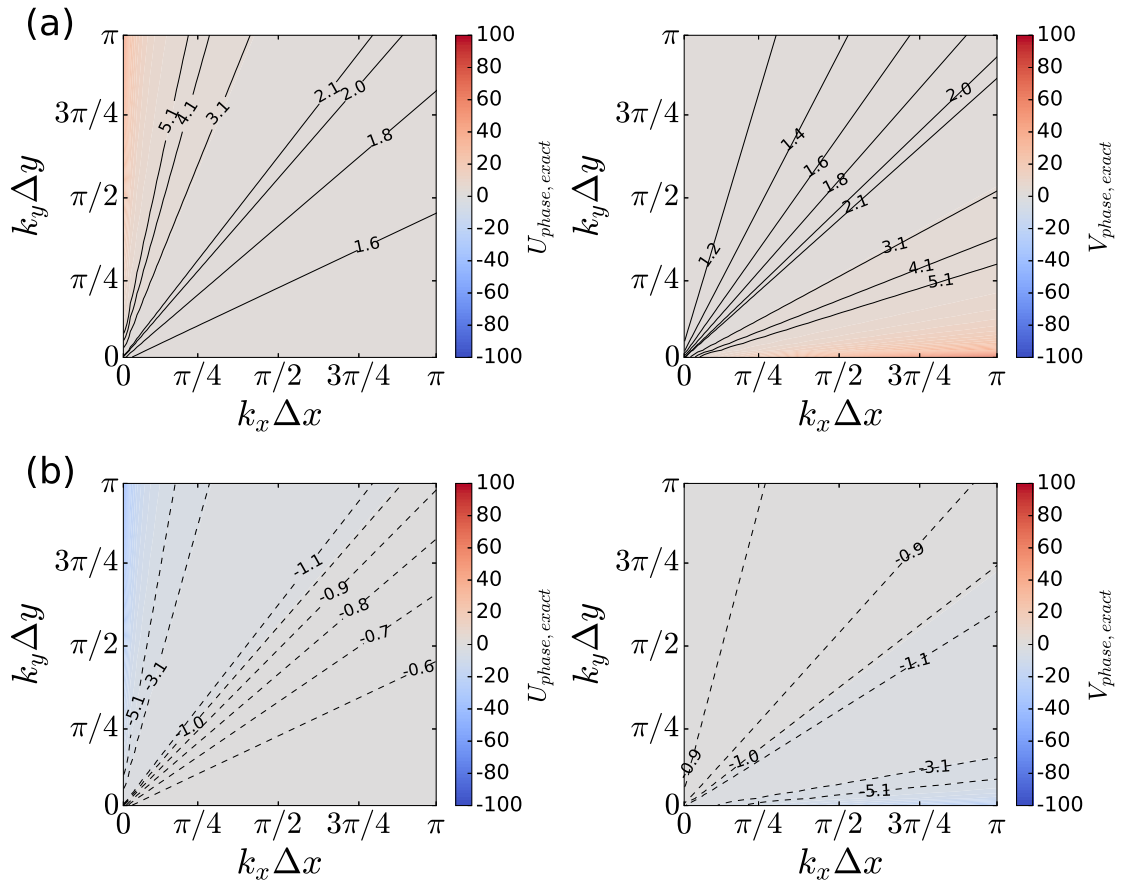


Figure 3.2: Comparison of physical phase velocities ($U_{phase, exact}$, $V_{phase, exact}$) for solution of different modes, (a) acoustic mode (ω_1^*), (b) acoustic mode (ω_2^*). They represent cases 1a and 1b of table 3.1. All colour contour plots are range from -100 to 100 for comparison sake.

different $\frac{V_{grp,full}^*}{V_{grp,exact}}$ was found for the $CDS4_{opt}/CDS4_{opt}$. Negative values of $\frac{V_{grp,full}^*}{V_{grp,exact}}$ was found even at low $k_y\Delta y$. The implication of this is that the numerical waves propagates in the opposite y direction even when the grid is refined (low values of $k_y\Delta y$) in the y direction. Also, the $CDS4_{opt}/CDS4_{opt}$ was found to have much more dispersion error at low and intermediate wavenumber for both $\frac{U_{grp,full}^*}{U_{grp,exact}}$ and $\frac{V_{grp,full}^*}{V_{grp,exact}}$ as compared to the other schemes. Similar comparisons between the group velocities of the $CDS4_{opt}$ scheme and the optimal upwind compact scheme (OUCS3) scheme can be found in [Sengupta et al., 2011b] where the $CDS4_{opt}$ scheme display much more dispersion error at low reduced wavenumber in both spatial directions. This implies that the numerical waves propagates at a slower speed with respect to the exact solution even when the grid is refined in both spatial directions.

3.2.3 Effect of a change in CFL number

In this sub section, the effect of a change in R_a will be explored. In particular, we will look at how the numerical amplification factor, normalized numerical group and phase velocities change when R_a is increased from 0.1 to 0.5. For this purpose, figures 3.3 and 3.4 are compared against figures 3.5 and 3.6. As R_a is changed from 0.1 to 0.5, the normalized group and phase velocities of the $CDS4/CDS4$ and $CDS4_{opt}/CDS4_{opt}$ scheme remain almost unchanged. However, this is not the case for the $DRP4/DRP4$ and $CCOM6/CCOM6$ scheme. Some minor differences in the normalized group and phase velocities were found at the low and intermediate wavenumber region for both $\frac{U_{phase,full}^*}{U_{phase,exact}}$ and $\frac{V_{phase,full}^*}{V_{phase,exact}}$. This implies a small increase in dispersion error arising from the temporal discretization scheme. The reduced wavenumber for which noticeable dispersion error can be found is shifted towards lower wavenumber when R_a is changed from 0.1 to 0.5. The comparison of the numerical amplification factor for $R_a = 0.1$ and $R_a = 0.5$ is plotted in figure 3.7. For $R_a = 0.1$, all the different spatial schemes have negligible numerical dissipation. When R_a is increased from 0.1 to 0.5, all the different spatial schemes experienced some numerical dissipation especially at intermediate wavenumber. Since the spatial schemes used all have central type stencils and are inherently non dissipative, the numerical dissipation comes solely from the temporal discretization scheme. Among the

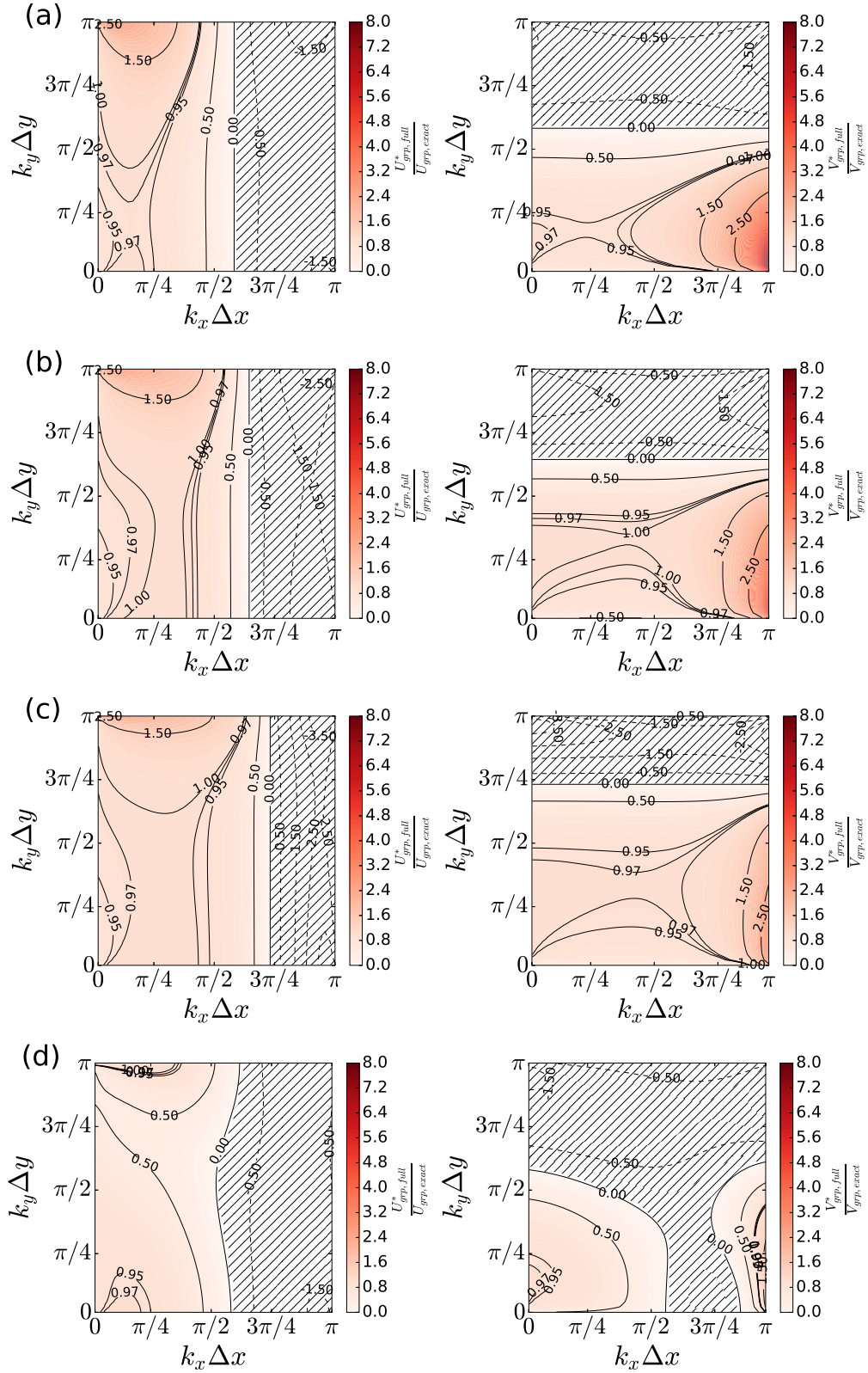


Figure 3.3: Comparison of normalized numerical group velocities ($\frac{U_{grp,full}^*}{U_{grp,exact}^*}$, $\frac{V_{grp,full}^*}{V_{grp,exact}^*}$) under different spatial discretization method for convective terms; (a) CDS4/CDS4, (b) DRP4/DRP4, (c) CCOM6/CCOM6 and (d) CDS4_{opt}/CDS4_{opt}. $R_a = 0.1$ and RK4 temporal scheme. They represent cases 2a to 2d of table 3.1. All colour contour plots are ranged from 0.0 to 8. Hatched region represents the spurious wave region where $\frac{U_{grp,full}^*}{U_{grp,exact}^*}, \frac{V_{grp,full}^*}{V_{grp,exact}^*} < 0$. They represent solutions for ω_1^* .

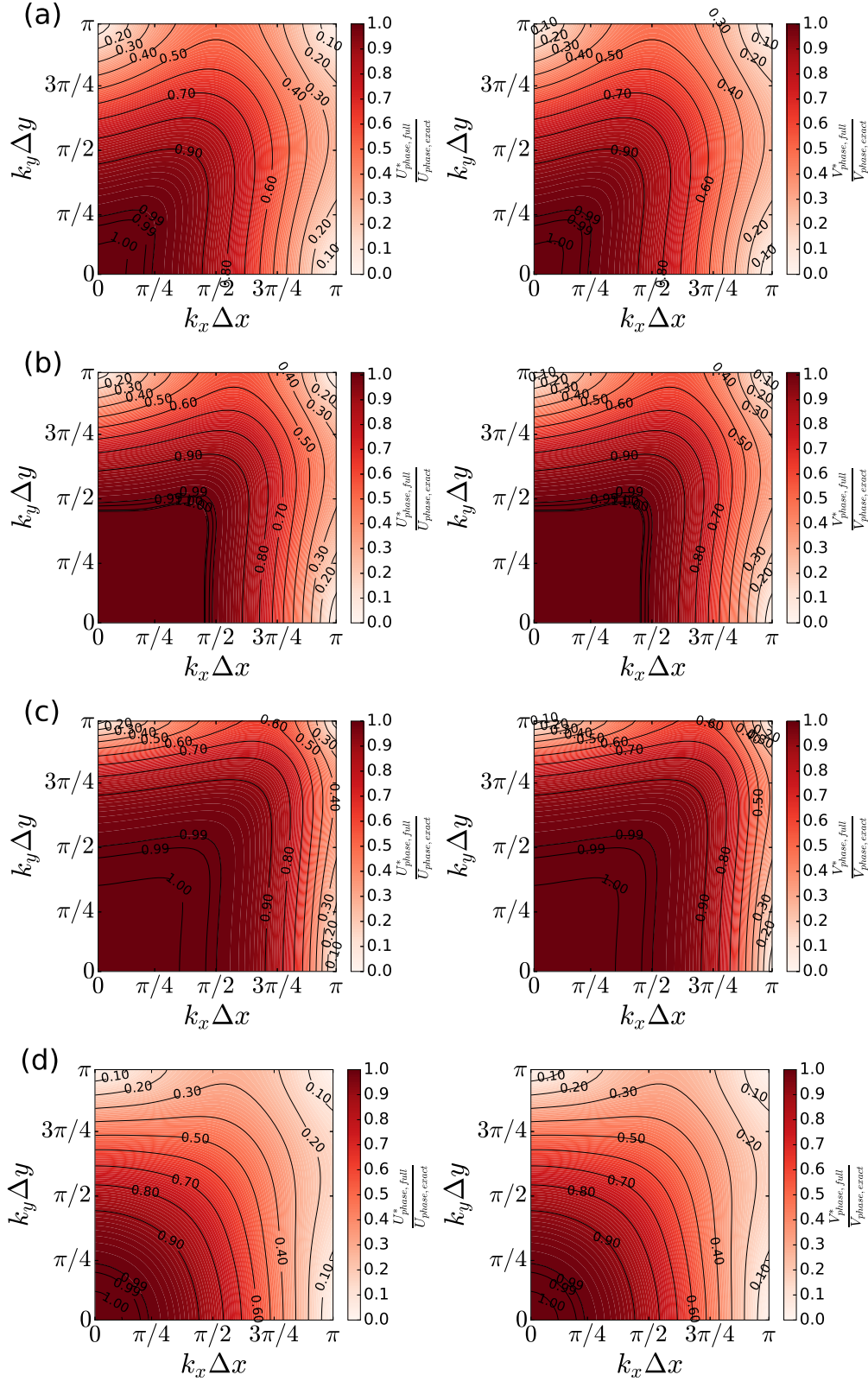


Figure 3.4: Comparison of normalized numerical phase velocities ($\frac{U_{\text{phase,full}}^*}{U_{\text{phase,exact}}^*}, \frac{V_{\text{phase,full}}^*}{V_{\text{phase,exact}}^*}$) under different spatial discretization method for convective terms; (a) CDS4/CDS4, (b) DRP4/DRP4, (c) CCOM6/CCOM6 and (d) CDS4_{opt}/CDS4_{opt}. $R_a = 0.1$ and RK4 temporal scheme. They represent cases 2a to 2d of table 3.1. All colour contour plots are ranged from 0.0 to 1.0. They represent solutions for ω_1^* .

different schemes, both the CCOM6/CCOM6 and DRP4/DRP4 scheme have the most numerical dissipation at intermediate wavenumber for $R_a = 0.5$. The CDS4_{opt}/CDS4_{opt} scheme has the least numerical dissipation for $R_a = 0.5$.

3.2.4 Comparison of different temporal discretization scheme

In this subsection, the effect of a change in temporal discretization scheme is assessed. In particular, we will consider how the numerical amplification factor, normalized numerical group and phase velocities change when the temporal scheme is changed from the RK4 to RK3 temporal scheme at $R_a = 0.5$. For this purpose, figures 3.5 and 3.6 are compared against figures 3.8 and 3.9. Noticeable differences in the normalized group and phase velocities can be seen for the CDS4/CDS4, DRP4/DRP4 and CCOM6/CCOM6 scheme. These differences imply an increase in the dispersion error. As for the CDS4_{opt}/CDS4_{opt} scheme, the plot of the normalized group and phase velocities remain approximately the same for both the RK4 and RK3 temporal scheme. The comparison of the numerical amplification factor for the RK4 and RK3 temporal scheme at $R_a = 0.5$ is plotted in figure 3.10. For both the CDS4/CDS4 and the CDS4_{opt}/CDS4_{opt} scheme, increased numerical dissipation is found at intermediate wavenumber when the temporal scheme is changed from RK4 to RK3. For the DRP4/DRP4 and CCOM6/CCOM6 scheme, reduced numerical dissipation is found at intermediate wavenumber when the temporal scheme is changed from RK4 to RK3. Moreover, the CCOM6/CCOM6 scheme has a region of reduced wavenumber (red coloured region) for which the amplification factor becomes greater than 1.0, implying numerical instability.

3.2.5 Effect of a change in cell Reynolds number

For the analysis considered here, the dispersion relation of the LCNSE is used. The FS and CDS4 spatial scheme is used for the convective and viscous term of the LCNSE respectively. The RK4 temporal scheme is used. For sufficiently low R_a where temporal discretization effects can be neglected, the viscous term in the dispersion relation does not contribute to the numerical group or phase velocities. Under the consideration of

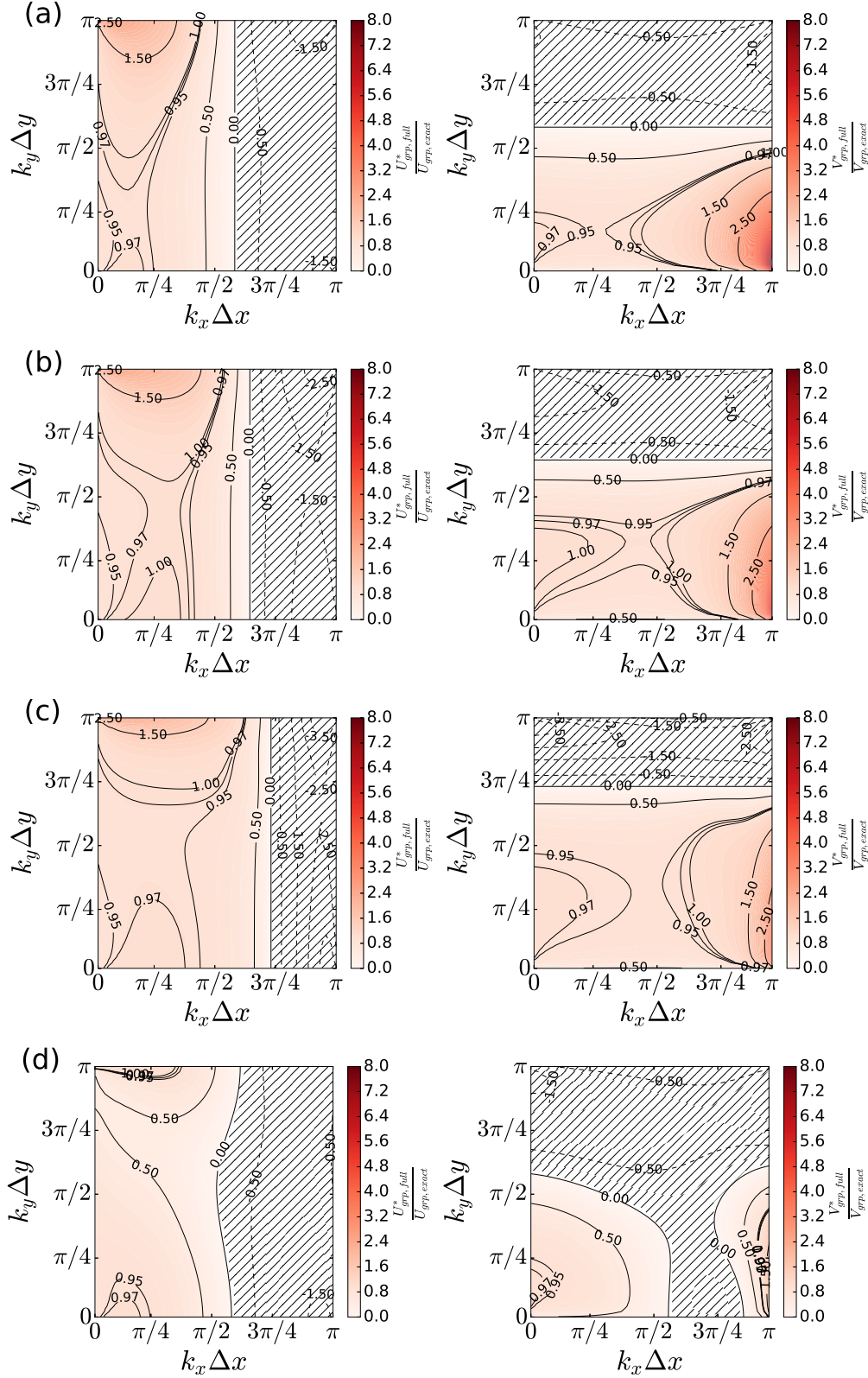


Figure 3.5: Comparison of normalized numerical group velocities ($\frac{U_{grp,full}^*}{U_{grp,exact}}, \frac{V_{grp,full}^*}{V_{grp,exact}}$) under different spatial discretization method for convective terms; (a) CDS4/CDS4, (b) DRP4/DRP4, (c) CCOM6/CCOM6 and (d) CDS4_{opt}/CDS4_{opt}. $R_a = 0.5$ and RK4 temporal scheme. They represent cases 3a to 3d of table 3.1. All colour contour plots are ranged from 0.0 to 8. Hatched region represents the spurious wave region where $\frac{U_{grp,full}^*}{U_{grp,exact}}, \frac{V_{grp,full}^*}{V_{grp,exact}} < 0$. They represent solutions for ω_1^* .

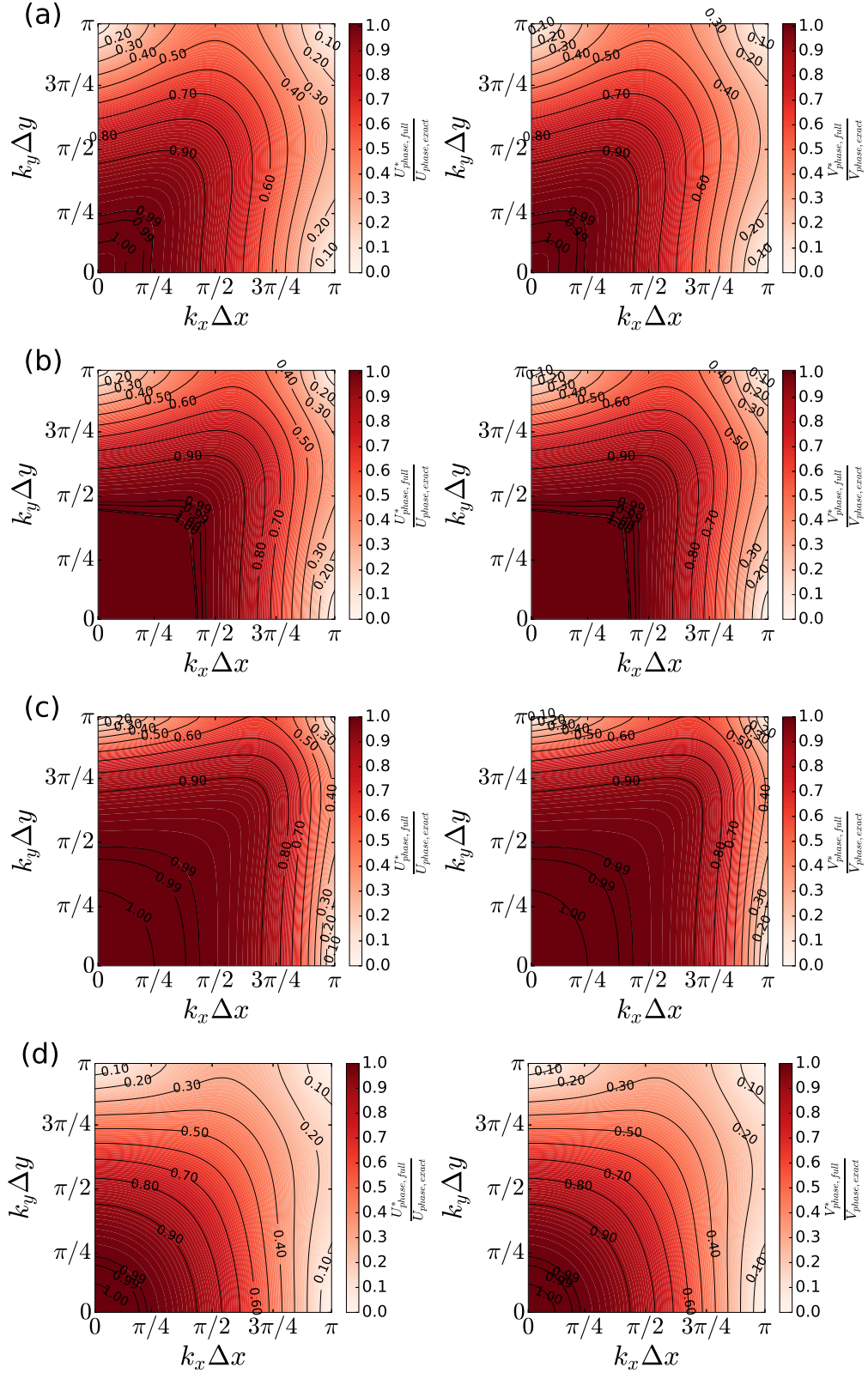


Figure 3.6: Comparison of normalized numerical phase velocities ($\frac{U_{\text{phase,full}}^*}{U_{\text{phase,exact}}}$, $\frac{V_{\text{phase,full}}^*}{V_{\text{phase,exact}}}$) under different spatial discretization method for convective terms; (a) CDS4/CDS4, (b) DRP4/DRP4, (c) CCOM6/CCOM6 and (d) CDS4_{opt}/CDS4_{opt}. $R_a = 0.5$ and RK4 temporal scheme. They represent cases 3a to 3d of table 3.1. All colour contour plots are ranged from 0.0 to 1.0. They represent solutions for ω_1^* .

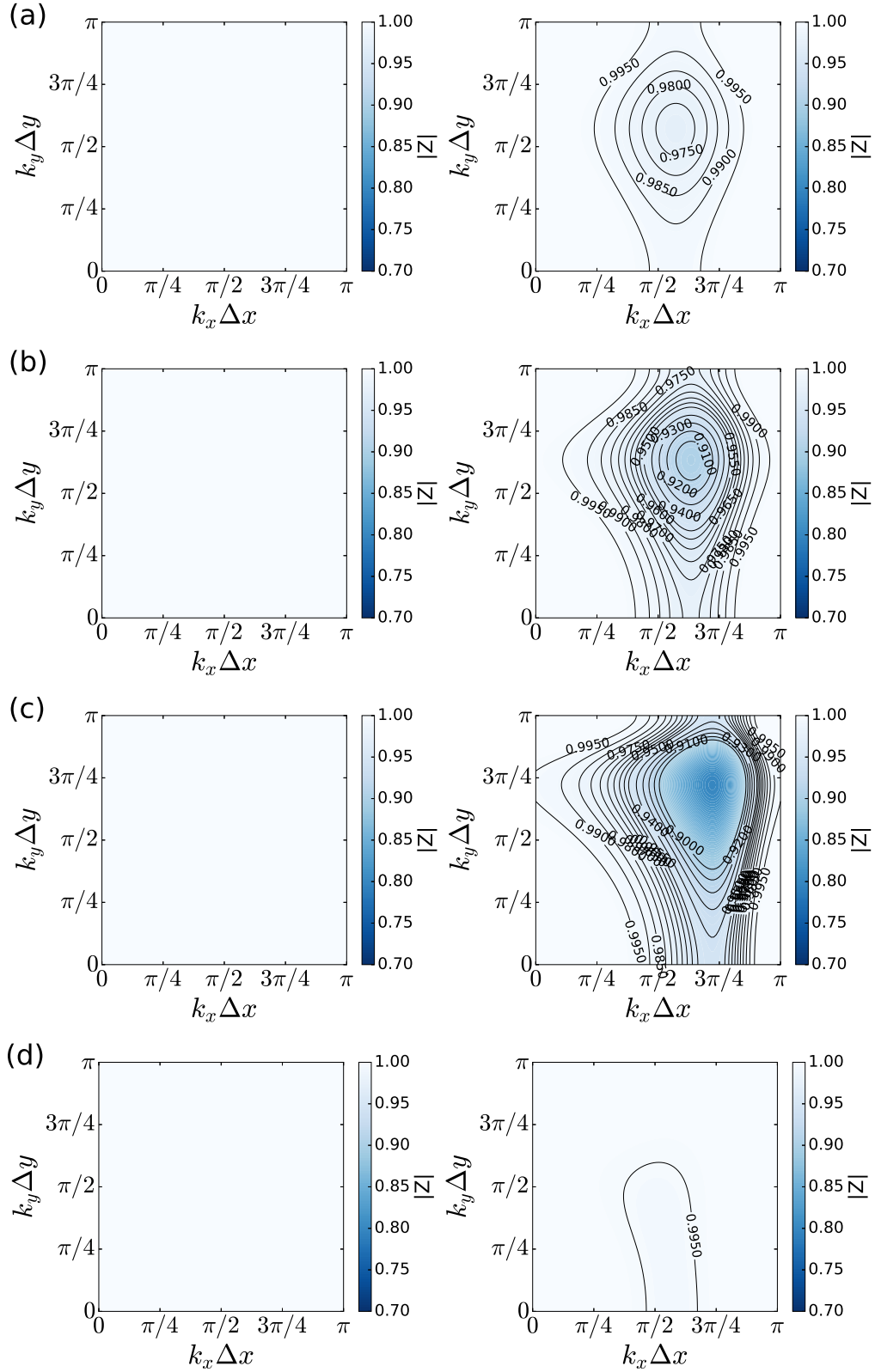


Figure 3.7: Comparison of numerical amplification factor, $|Z|$ between $R_a = 0.1$ (left) and $R_a = 0.5$ (right) for different spatial discretization method for convective terms; (a) CDS4/CDS4, (b) DRP4/DRP4, (c) CCOM6/CCOM6 and (d) CDS4_{opt}/CDS4_{opt}. RK4 temporal scheme. They represent cases 2a to 2d and 3a to 3d of table 3.1. All colour contour plots are ranged from 0.7 to 1.0. They represent solutions for ω_1^* .

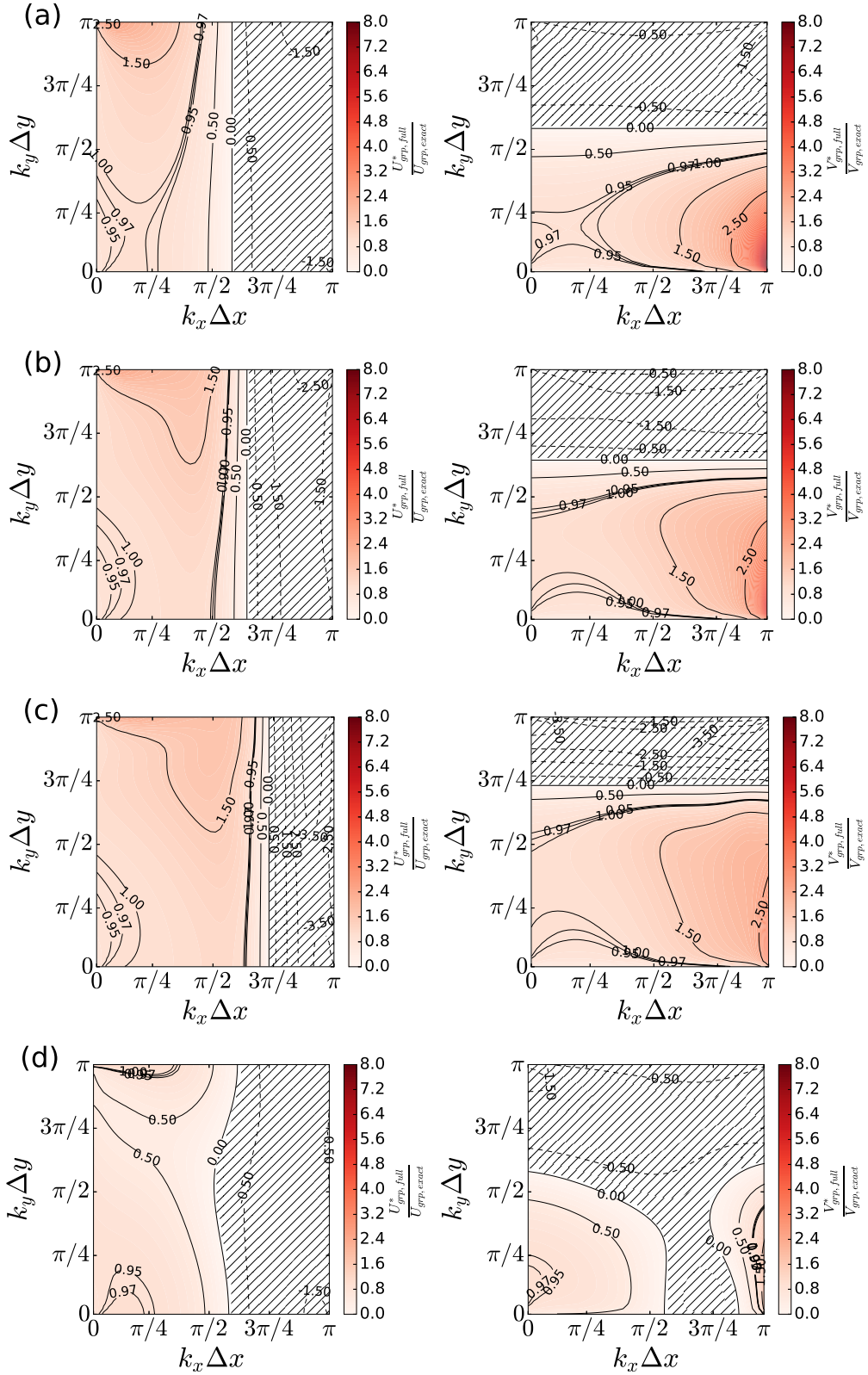


Figure 3.8: Comparison of normalized numerical group velocities ($\frac{U_{grp,full}^*}{U_{grp,exact}}, \frac{V_{grp,full}^*}{V_{grp,exact}}$) under different spatial discretization method for convective terms; (a) CDS4/CDS4, (b) DRP4/DRP4, (c) CCOM6/CCOM6 and (d) CDS4_{opt}/CDS4_{opt}. $R_a = 0.5$ and RK3 temporal scheme. They represent cases 2a to 2d of table 3.1. All colour contour plots are ranged from 0.0 to 8. Hatched region represents the spurious wave region where $\frac{U_{grp,full}^*}{U_{grp,exact}}, \frac{V_{grp,full}^*}{V_{grp,exact}} < 0.0$. They represent solutions for ω_1^* .

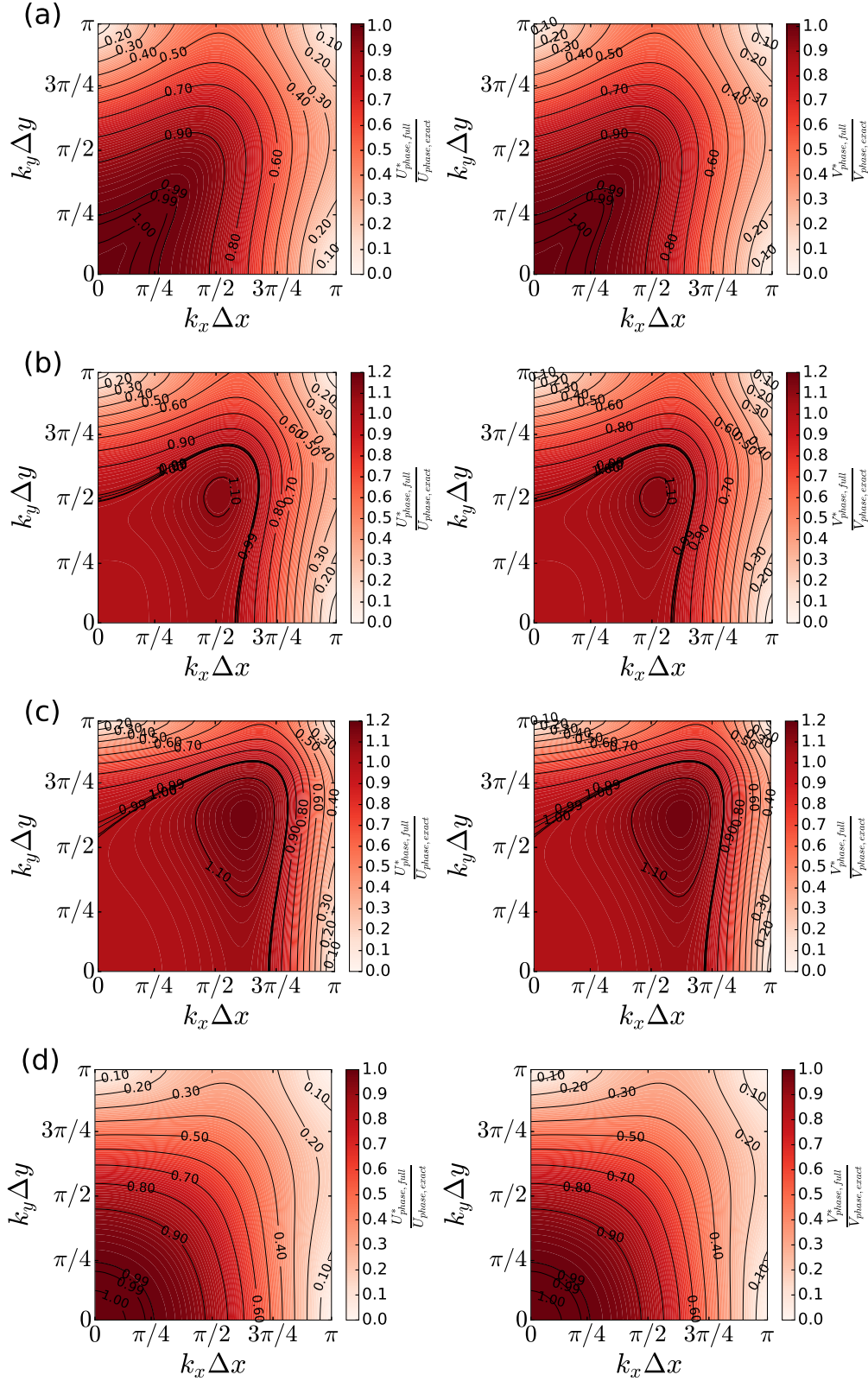


Figure 3.9: Comparison of normalized numerical phase velocities ($\frac{U_{phase,full}^*}{U_{phase,exact}}$, $\frac{V_{phase,full}^*}{V_{phase,exact}}$) under different spatial discretization method for convective terms; (a) CDS4/CDS4, (b) DRP4/DRP4, (c) CCOM6/CCOM6 and (d) CDS4_{opt}/CDS4_{opt}. $R_a = 0.5$ and RK3 temporal scheme. They represent cases 2a to 2d of table 3.1. All colour contour plots are ranged from 0.0 to 1.0 except for the DRP4/DRP4 and CCOM6/CCOM6 scheme where it is ranged from 0.0 to 1.2. They represent solutions for ω_1^* .

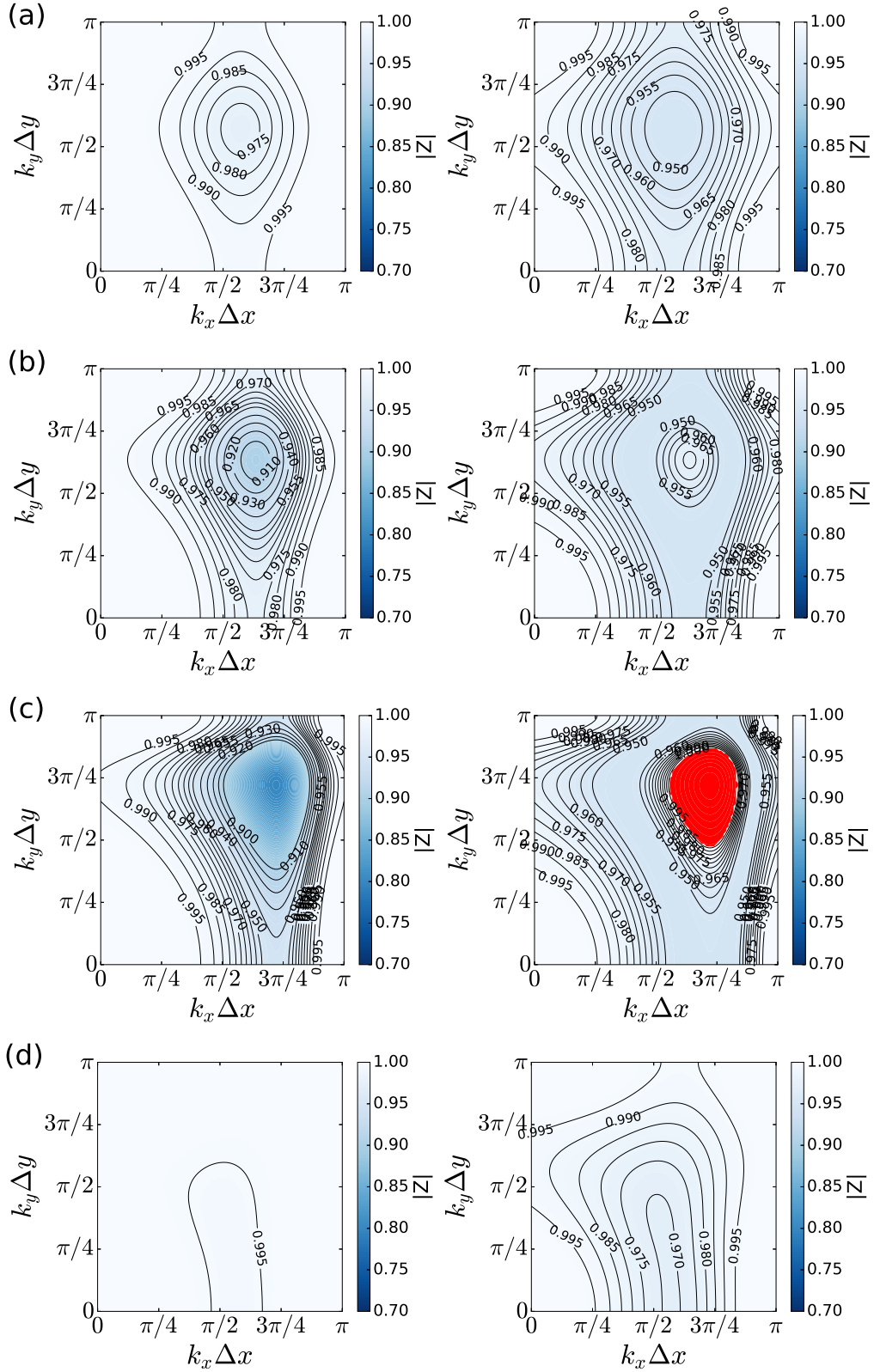


Figure 3.10: Comparison of numerical amplification factor, $|Z|$ between RK4 (left figures) and RK3 (right figures) temporal scheme for different spatial discretization method for convective terms; (a) CDS4/CDS4, (b) DRP4/DRP4, (c) CCOM6/CCOM6 and (d) CDS4_{opt}/CDS4_{opt}. $R_a = 0.5$. They represent cases 2a to 2d of table 3.1. All colour contour plots are ranged from 0.7 to 1.0. They represent solutions for ω_1^* .

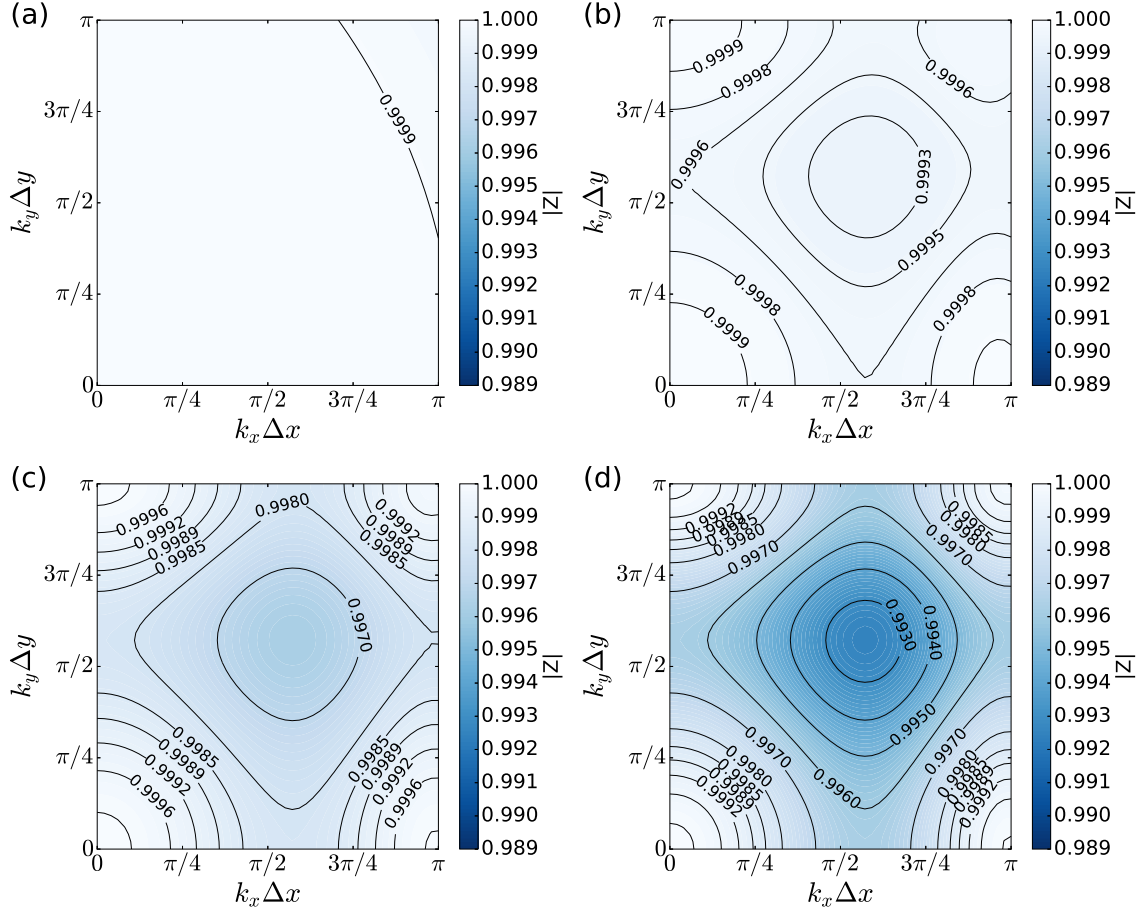


Figure 3.11: Comparison of numerical amplification factor, $|Z|$ under different cell Reynolds number; (a) $Re_a = \infty$, (b) $Re_a = 500$, (c) $Re_a = 100$ and (d) $Re_a = 50$. CDS4/CDS4 spatial scheme is used for both the convective and viscous term. $R_a = 0.1$ and RK4 temporal scheme. They represent cases 5a to 5d of table 3.1. All colour contour plots are ranged from 0.989 to 1. They represent solutions for ω_1^* .

spatial discretization effects only, the numerical group and phase velocities are calculated from only the real part of the semi discretized dispersion relation. Therefore, the imaginary viscous term has no influence on the dispersion property. Taking this into account, a comparison is made to study the effect of increasing cell Reynolds number on the numerical amplification factor only. In figure 3.11, increased numerical dissipation is found especially at intermediate wavenumber region as Re_a is reduced from $Re_a = \infty$ to $Re_a = 50$. This is expected since a reduction in Re_a implies an increase in magnitude of the viscous diffusion term.

3.2.6 Comparison of different spatial discretization scheme - Diffusion term

For the analysis considered here, the dispersion relation of the LCNSE is used. The FS spatial scheme is used for the convective term of the LCNSE. The RK4 temporal scheme is used. The spatial discretization scheme of the viscous term is varied to study its effect on the numerical amplification factor. In order to illustrate this differences better, $Re_a = 200$ was used in this analysis. The results are shown in figure 3.12. The baseline case is represented by the case for which the FS/FS scheme is used for the viscous term (figure 3.12a). The use of the FS/FS scheme would provide the true physical diffusion. It can be seen that the CCOM6/CCOM6 case (figure 3.12d) represents the case having the closest numerical dissipation to the true physical diffusion since the CCOM6 scheme has the best spectral accuracy as compared to the other FD schemes.

3.3 Anisotropy analysis in 2D wavenumber space - hybrid finite difference/ Fourier spectral

In this section, the specific case of using a hybrid finite difference/ Fourier spectral spatial discretization method is compared against a full finite difference spatial discretization method. Interest in the comparison between full finite difference method and hybrid finite difference/ Fourier spectral method stems from the widespread use of hybrid finite difference/ Fourier spectral spatial discretization method in large scale direct numerical simulation of canonical flows such as pipe or channel flow with periodic boundary conditions in the horizontal directions [Bodart et al., 2009]. Also, it is commonly assumed that the use of hybrid spectral/finite difference method tend to be more accurate than full finite difference method. The aim of this subsection is to understand the implication of using hybrid finite difference/ Fourier spectral discretization on the resolution characteristic of the coupled numerical schemes. As will be shown in this section, this is not necessarily true under all circumstances and it is strongly dependent on the reduced wavenumber and wave propagation angle. In this section, we will investigate how the resolution of the scheme varies as a function of the wave propagation angle. The list of cases with hybrid schemes used in this analysis is presented in table 3.2. Cases 1 and 2 of

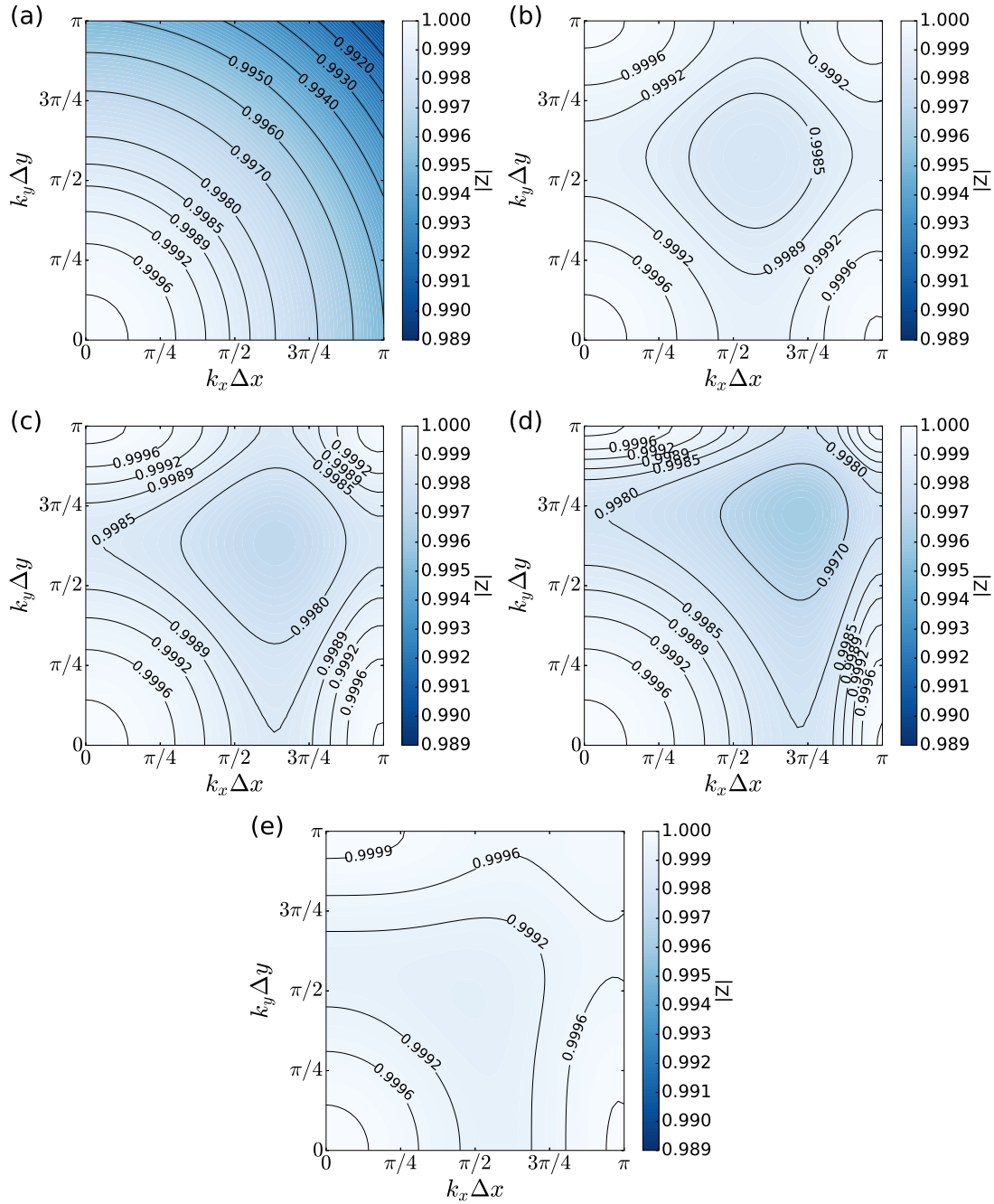


Figure 3.12: Comparison of numerical amplification factor, $|Z|$ under different spatial discretization scheme for the viscous term; (a) FS/FS, (b) CDS4/CDS4, (c) DRP4/DRP4, (d) CCOM6/CCOM6, and (e) CDS4_{opt}/CDS4_{opt}. $Re_a = 200$. FS/FS spatial scheme is used for the convective term. $R_a = 0.1$ and RK4 temporal scheme. They represent cases 6a to 6e of table 3.1. All colour contour plots are ranged from 0.989 to 1. They represent solutions for ω_1^* .

Table 3.2: Table representing parameter values and numerical schemes for various cases with hybrid schemes. The abbreviation, CDS4/CDS4 implies that the CDS4 scheme is used in the x and y spatial directions respectively.

Case	Convective schemes	Viscous schemes	Temporal schemes	R_a	Re_a	Solution Type
1a	CDS4/FS	-	RK4	0.1	∞	Numerical, ω_1^*
1b	DRP4/FS	-	RK4	0.1	∞	Numerical, ω_1^*
1c	CCOM6/FS	-	RK4	0.1	∞	Numerical, ω_1^*
1d	CDS4 _{opt} /FS	-	RK4	0.1	∞	Numerical, ω_1^*
2a	FS/FS	CDS4/FS	RK4	0.1	200	Numerical, ω_1^*
2b	FS/FS	DRP4/FS	RK4	0.1	200	Numerical, ω_1^*
2c	FS/FS	CCOM6/FS	RK4	0.1	200	Numerical, ω_1^*
2d	FS/FS	CDS4 _{opt} /FS	RK4	0.1	200	Numerical, ω_1^*

table 3.2 are compared against cases 1 and 6 of table 3.1.

3.3.1 Effect of a change in spatial discretization scheme - Convection term

Figures 3.13 and 3.14 present the normalized numerical group velocities and phase velocities of the cases using hybrid schemes (FD/FS) for the convective terms. For the comparison of the normalized group and phase velocities with the full FD discretization cases, figures 3.13 and 3.14 is compared against figures 3.3 and 3.4. Comparison of the numerical amplification factor is not considered since $|Z|$ will remain very close to 1.0 in either cases. To better illustrate the comparison of the dispersion property between a hybrid and full FD discretization, we look at 1D plot of numerical group velocity ($V_{grp,full}^*$) as a function of wave propagation angle (θ_w) for different reduced wavenumber. Results are compared to reference FS/FS spatial discretization scheme for the different spatial discretization scheme considered. This is presented in figures 3.15 to 3.17 for $k\Delta = 0.3\pi, 0.6\pi, 0.9\pi$. At low reduced wavenumber ($k\Delta = 0.3\pi$), the numerical group velocity ($V_{grp,full}^*$) of the different spatial schemes closely matches the FS/FS solution for the full range of wave propagation angle except for the CDS4_{opt}/CDS4_{opt} and CDS4_{opt}/FS scheme. Small deviation in the numerical group velocity from the FS/FS solution was found at large wave propagation angle. At intermediate reduced wavenumber ($k\Delta = 0.6\pi$), the numerical group velocity ($V_{grp,full}^*$) of the DRP4/DRP4, DRP4/FS, CCOM6/CCOM6 and

CCOM6/FS schemes closely matches the FS/FS solution for the full range of wave propagation angle. Except for the CDS4/CDS4, CDS4/FS, CDS4_{opt}/CDS4_{opt} and CDS4_{opt}/FS case, there is either small or large deviation in the numerical group velocity from the FS/FS solution. The CDS4_{opt}/CDS4_{opt} scheme show the poorest dispersion property among all the different schemes considered. At large reduced wavenumber ($k\Delta = 0.9\pi$), the numerical group velocity ($V_{grp,full}^*$) of the different spatial schemes show either small or large deviation from the FS/FS solution for the full range of wave propagation angle. For the CDS4, DRP4 and CCOM6 schemes, the comparison of group velocity between the full FD and its hybrid discretization counterpart can be split into three distinct region. At low wave propagation angle, the full FD and hybrid discretization scheme share the same numerical group velocity. At intermediate wave propagation angle, a region exists for which the numerical group velocity of the full FD discretization become closer to the FS/FS solution. At large wave propagation angle, the numerical group velocity of the hybrid discretization cases become closer to the FS/FS solution. This is expected since the resolution of the scheme will become close to that of the FS scheme as the wave propagation angle approaches the direction where the FS method is used. For the CDS4_{opt}/CDS4_{opt} scheme (figure 3.17d), group velocity become negative at large wave propagation angle, indicating the presence of spurious wave. Comparison of numerical group velocity between the full FD and its hybrid counterpart show significant difference across the full range of wave propagation angle. From a physical perspective, if the grid is sufficiently refined in both spatial directions, then the wave would propagate at the correct speed and direction irrespective of the type of spatial discretization methods employed and wave propagation angle considered. However, differences in the solutions of the different discretization method become obvious once the grid become sufficiently coarse. To better understand the comparison of the dispersion property between a hybrid and full FD scheme, the integrated sum of the error between the numerical group velocity $V_{grp,full}^*$ or $U_{grp,full}^*$ and the exact solution across all wavenumbers for a range of wave propagation angle is examined. This is illustrated in figures 3.18 and 3.19 for both $V_{grp,full}^*$ and $U_{grp,full}^*$ respectively. In figures 3.18, it can be seen that the CCOM6/CCOM6 and CCOM6/FS scheme have the least integrated error across all wave propagation an-

gle. For the CDS4, DRP4 and CCOM6 scheme, there exists a range of intermediate wave propagation angle for which the integrated error of the full FD schemes is smaller than the hybrid scheme. For the CDS4_{opt} scheme, the integrated error of the full FD scheme is smaller than the hybrid scheme only at low wave propagation angle. Some general observations can be made about figures 3.18. As θ_w approaches zero, the integrated error between $V_{grp,exact}$ and $V_{grp,full}^*$ approaches zero. This is because only the group velocity in the x spatial direction needs to be considered when $\theta_w = 0$. The second observation is that the integrated error between $V_{grp,exact}$ and $V_{grp,full}^*$ of the FD/FD cases increases with increasing θ_w . This is because $V_{grp,full}^*$ becomes increasingly negative with respect to the exact solution. As for the integrated error between $U_{grp,full}^*$ and $U_{grp,exact}$, large values of integrated error for the FD/FD and FD/FS cases can be seen at low values of θ_w . This is primarily due to the large dispersion error from the FD scheme used in the x direction. As θ_w approaches $\pi/2$, the error goes towards zero since $k_x\Delta$ approaches the low reduced wavenumber region. The FD/FD cases in figures 3.19a to 3.19c are almost similar to a symmetry reflection of the FD/FD cases in figures 3.18a to 3.18c about the line $\theta_w = \pi/4$ with the exception that the plots are shifted upward due to the difference in $U_{grp,exact}$ and $V_{grp,exact}$. For $\theta_w = 0$, it is expected to have maximum error in the integrated error between U_{grp} and $U_{grp,exact}$. For $\theta_w = \pi/2$, it is expected to have maximum error in the integrated error between $V_{grp,exact}$ and $V_{grp,full}^*$.

3.3.2 Effect of a change in spatial discretization scheme - Diffusion term

Figure 3.20 presents the comparison of the numerical amplification factor of the cases using full FD and hybrid (FD/FS) discretization for the diffusion terms. In this comparison, R_a is kept to a sufficiently low value of 0.1 such that the effect of the viscous term on the dispersion property of the coupled numerical schemes can be neglected. In this case, the effect of using different spatial discretization method for the diffusion term only affects the numerical dissipation of the coupled schemes. The figures on the left of figure 3.20 represent the cases for which a full FD discretization is used on the viscous term. The figures on the right of figure 3.20 represent the cases for which a hybrid FD/FS discretization is used on the viscous term. It can be seen that the use of FS scheme in the y spatial

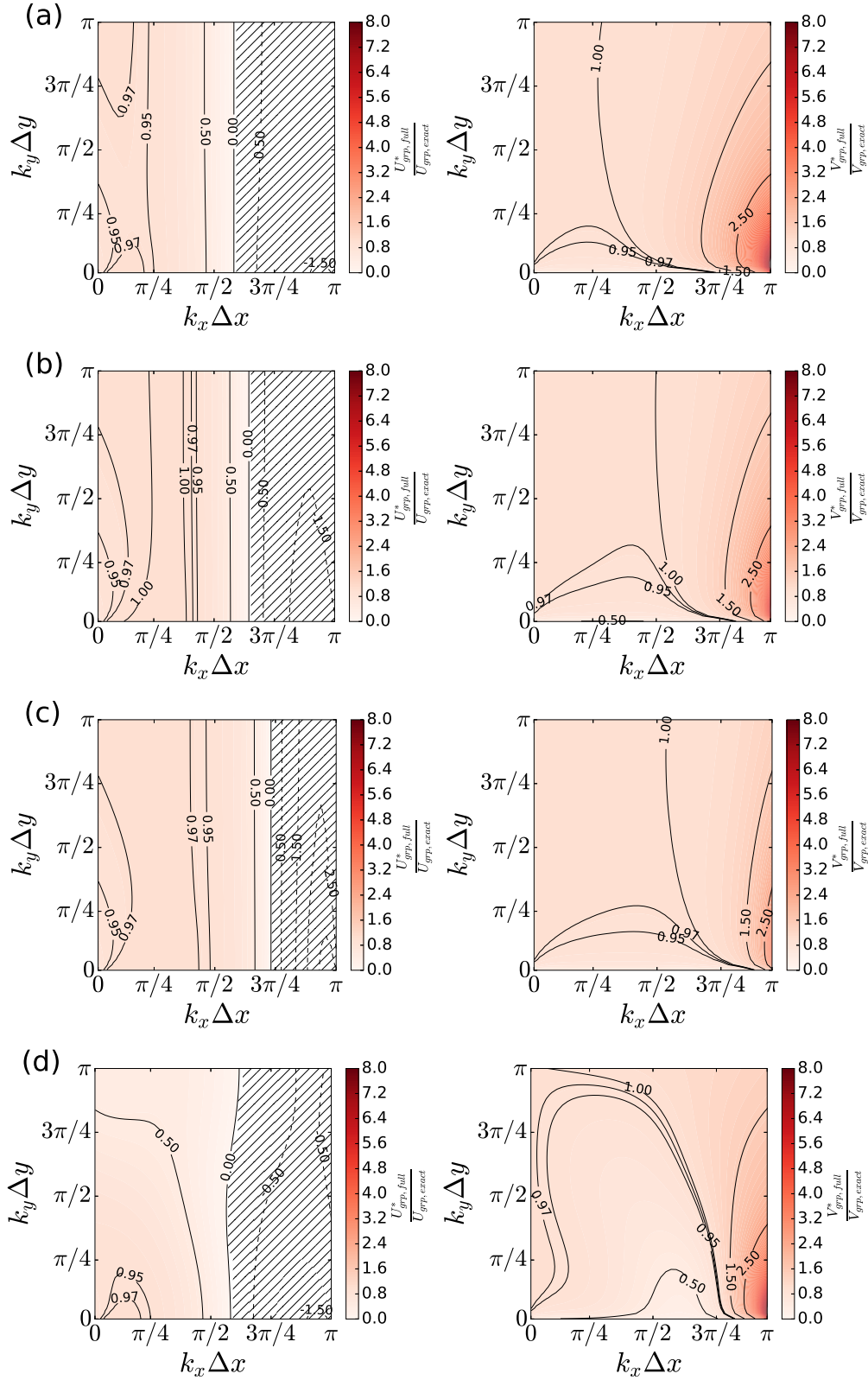


Figure 3.13: Comparison of normalized numerical group velocities ($\frac{U_{grp,full}^*}{U_{grp,exact}}, \frac{V_{grp,full}^*}{V_{grp,exact}}$) under different hybrid spatial discretization method for convective terms; (a) CDS4/FS, (b) DRP4/FS, (c) CCOM6/FS and (d) CDS4_{opt}/FS. $R_a = 0.1$ and RK4 temporal scheme. They represent cases 1a to 1d of table 3.2. All colour contour plots are ranged from 0.0 to 8. Hatched region represents the spurious wave region where $\frac{U_{grp,full}^*}{U_{grp,exact}}, \frac{V_{grp,full}^*}{V_{grp,exact}} < 0$. They represent solutions for ω_1^* .

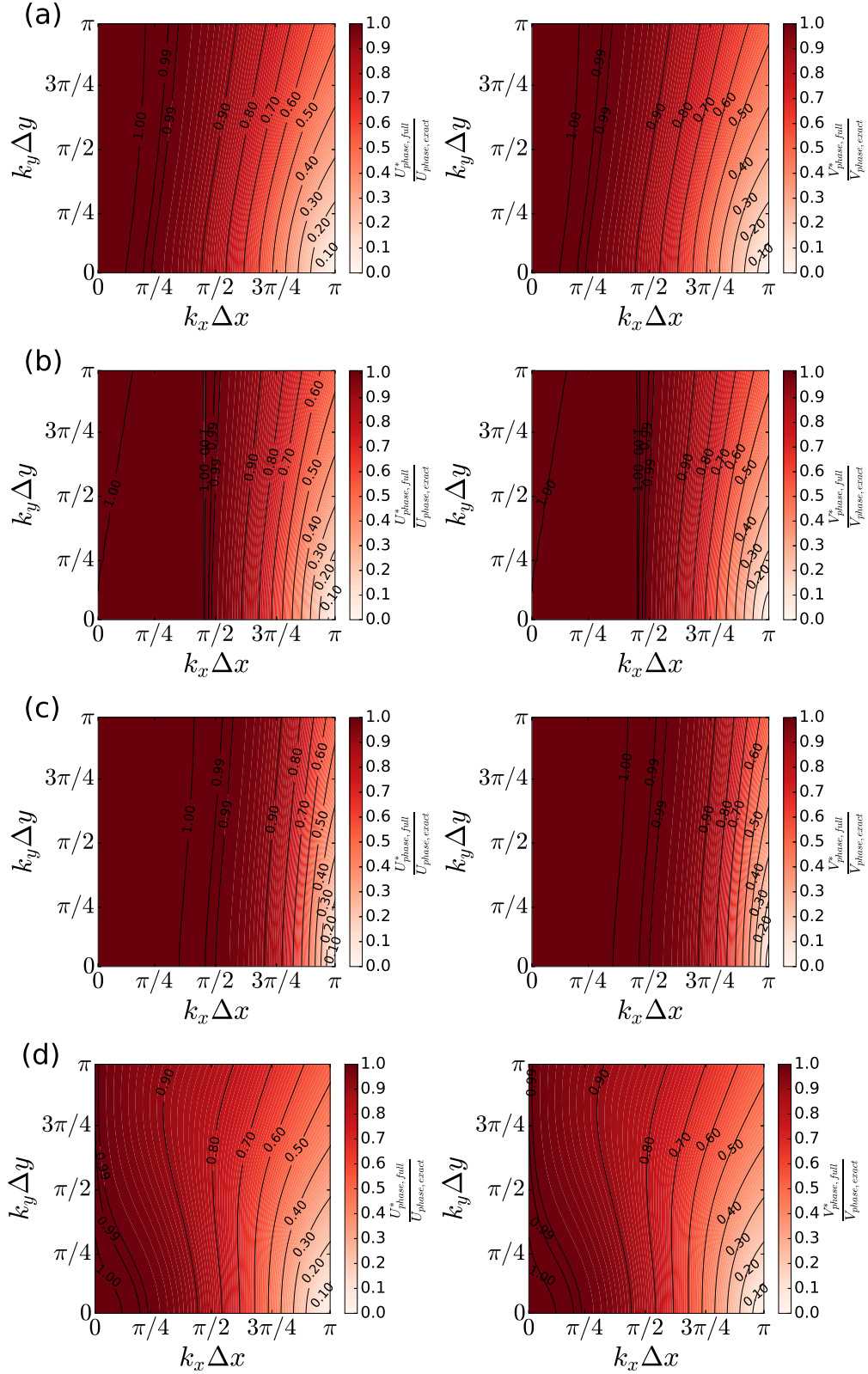


Figure 3.14: Comparison of normalized numerical phase velocities ($\frac{U_{\text{phase,full}}^*}{U_{\text{phase,exact}}}$, $\frac{V_{\text{phase,full}}^*}{V_{\text{phase,exact}}}$) under different hybrid spatial discretization method for convective terms; (a) CDS4/FS, (b) DRP4/FS, (c) CCOM6/FS and (d) CDS4_{opt}/FS. $R_a = 0.1$ and RK4 temporal scheme. They represent cases 1a to 1d of table 3.2. All colour contour plots are ranged from 0.0 to 1.0. They represent solutions for ω_1^* .

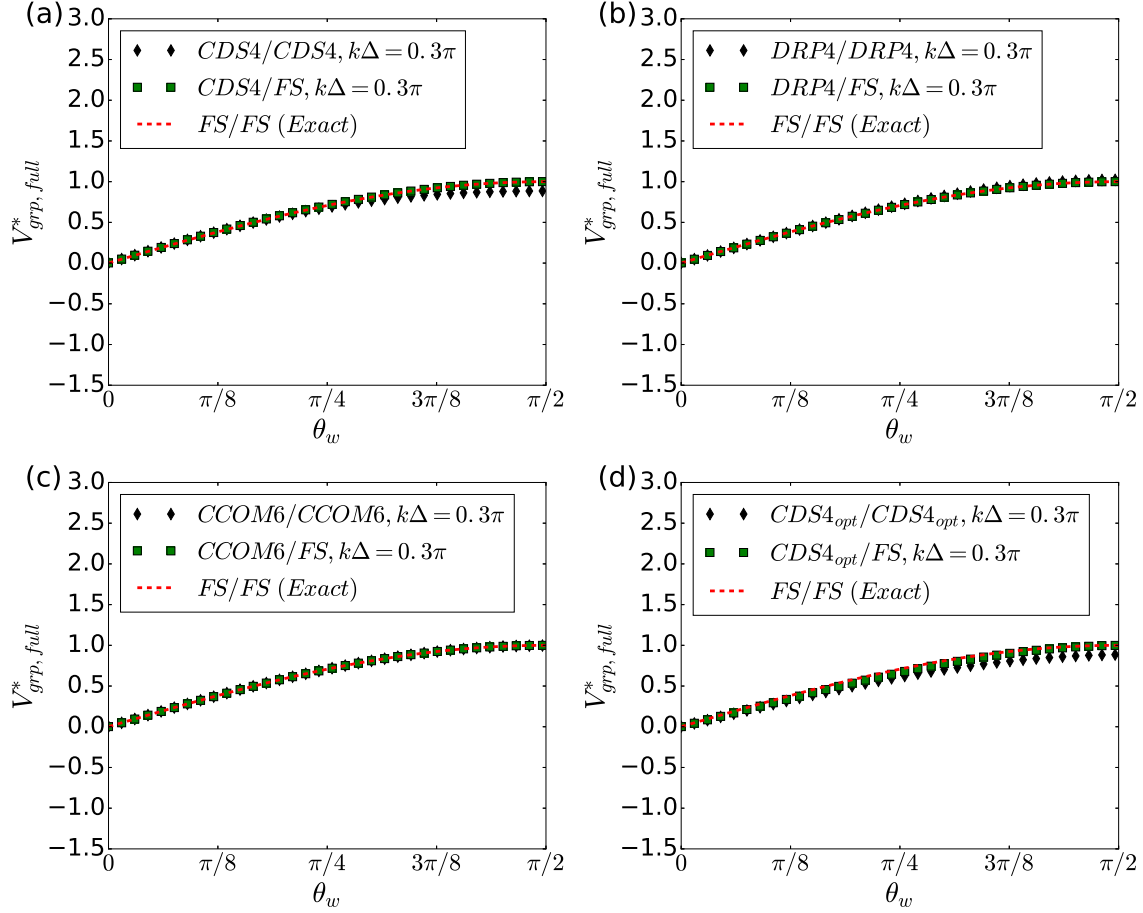


Figure 3.15: Comparison of numerical group velocities ($V_{grp,full}^*$) between full FD and hybrid discretization for convective terms; (a) CDS4/CDS4 vs. CDS4/FS, (b) DRP4/DRP4 vs. DRP4/FS, (c) CCOM6/CCOM6 vs. CCOM6/FS and (d) CDS4_{opt}/CDS4_{opt} vs. CDS4_{opt}/FS. $k\Delta = 0.3\pi$ where $k = \sqrt{k_x^2 + k_y^2}$. $R_a = 0.1$ and RK4 temporal scheme. They represent cases 1a to 1d of table 3.2. They represent solutions for ω_1^* .

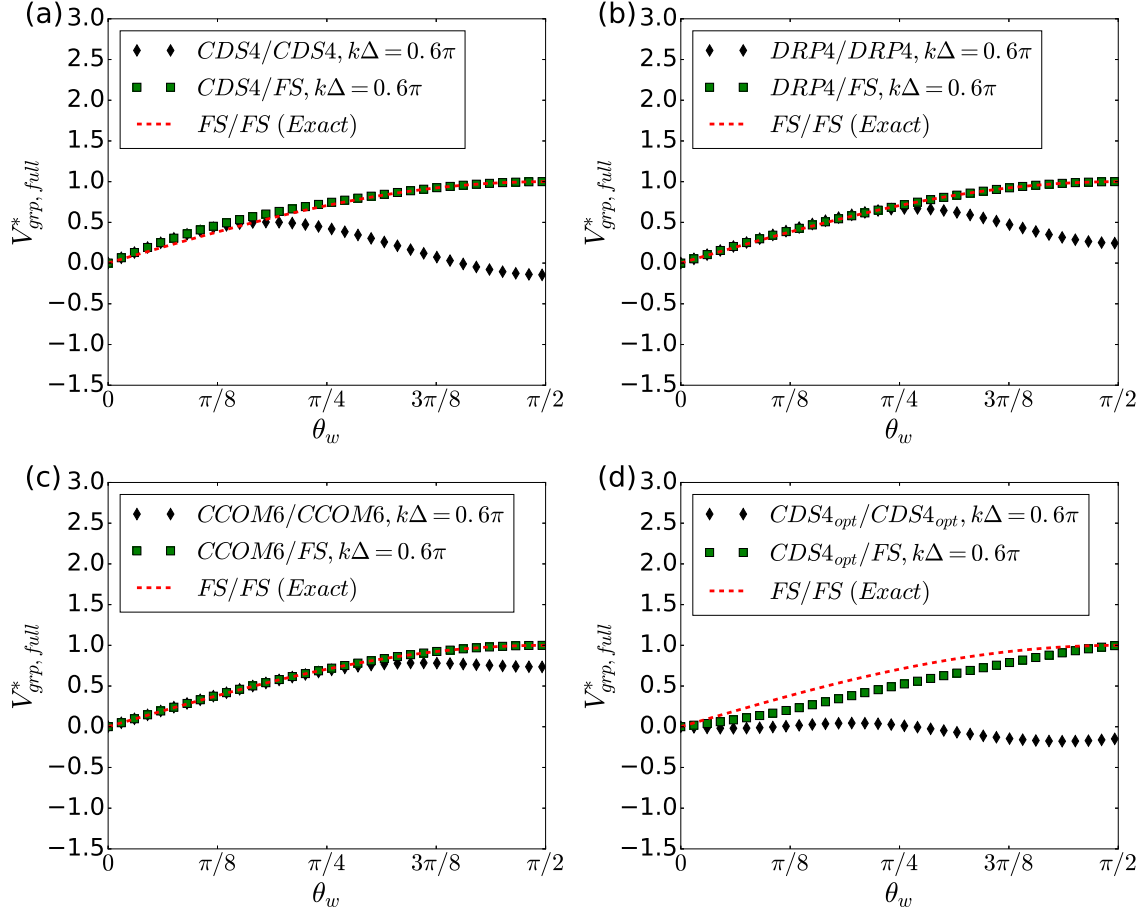


Figure 3.16: Comparison of numerical group velocities ($V_{grp,full}^*$) between full FD and hybrid discretization for convective terms; (a) CDS4/CDS4 vs. CDS4/FS, (b) DRP4/DRP4 vs. DRP4/FS, (c) CCOM6/CCOM6 vs. CCOM6/FS and (d) CDS4_{opt}/CDS4_{opt} vs. CDS4_{opt}/FS. $k\Delta = 0.6\pi$ where $k = \sqrt{k_x^2 + k_y^2}$. $R_a = 0.1$ and RK4 temporal scheme. They represent cases 1a to 1d of table 3.2. They represent solutions for ω_1^* .

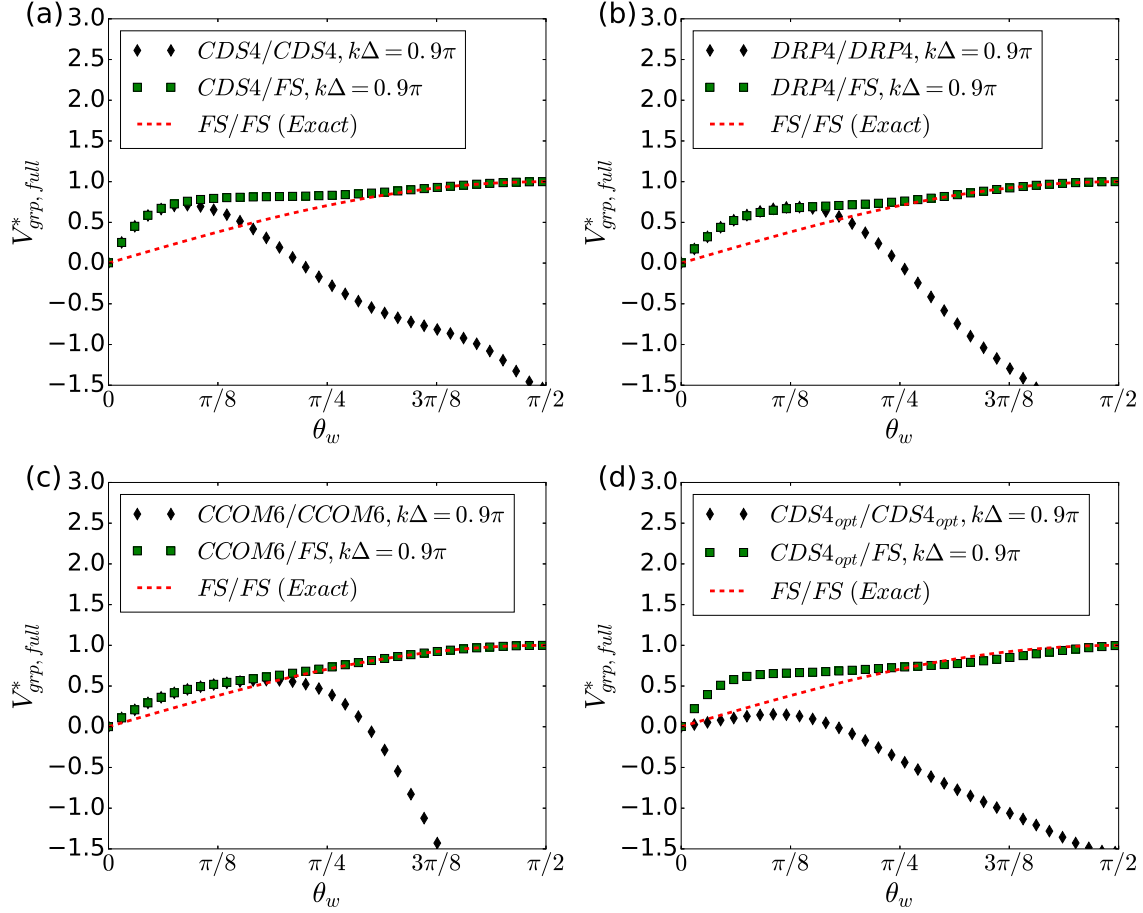


Figure 3.17: Comparison of numerical group velocities ($V_{grp,full}^*$) between full FD and hybrid discretization for convective terms; (a) CDS4/CDS4 vs. CDS4/FS, (b) DRP4/DRP4 vs. DRP4/FS, (c) CCOM6/CCOM6 vs. CCOM6/FS and (d) CDS4_{opt}/CDS4_{opt} vs. CDS4_{opt}/FS. $k\Delta = 0.9\pi$ where $k = \sqrt{k_x^2 + k_y^2}$. $R_a = 0.1$ and RK4 temporal scheme. They represent cases 1a to 1d of table 3.2. They represent solutions for ω_1^* .

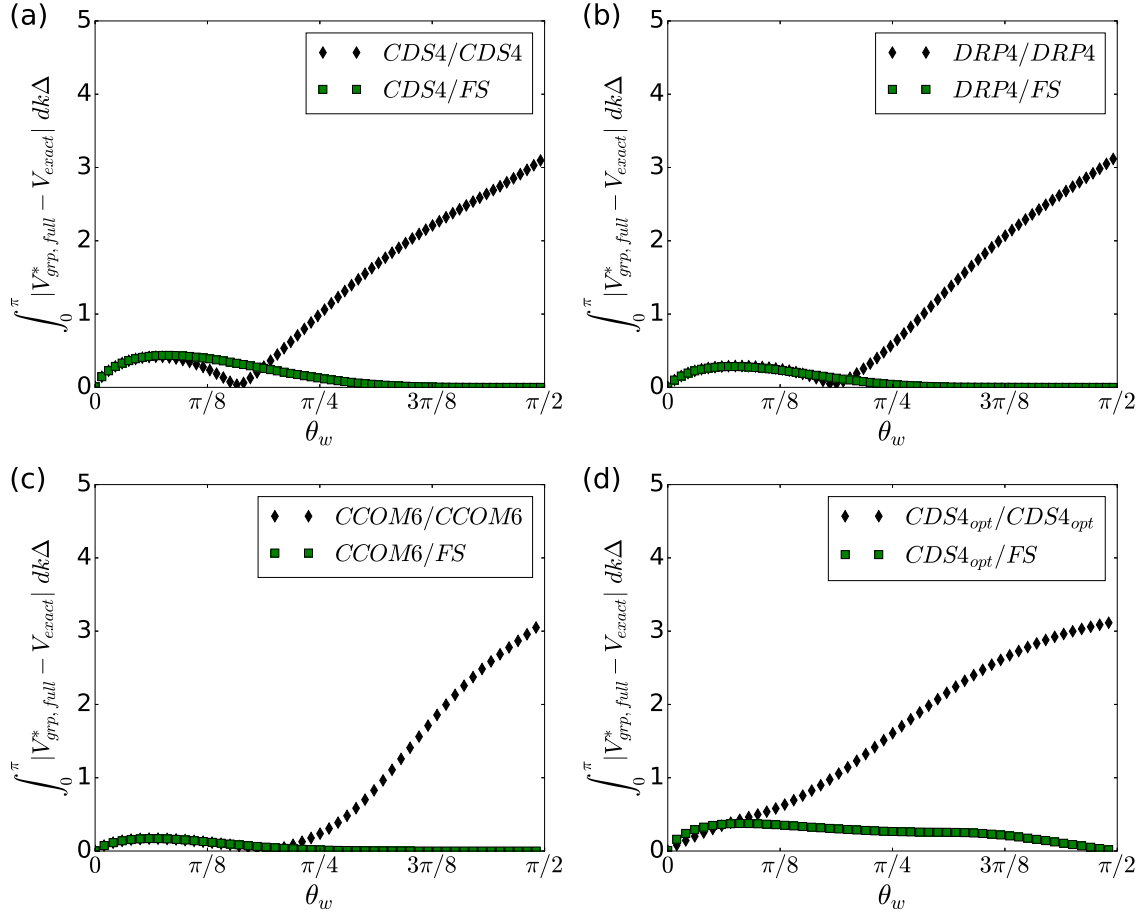


Figure 3.18: Comparison of integrated error in group velocities across all wavenumbers between full FD and hybrid discretization for convective terms ($\int_0^\pi |V_{grp,full}^* - V_{exact}| dk\Delta$); (a) CDS4/CDS4 vs. CDS4/FS, (b) DRP4/DRP4 vs. DRP4/FS, (c) CCOM6/CCOM6 vs. CCOM6/FS and (d) CDS4_{opt}/CDS4_{opt} vs. CDS4_{opt}/FS. $R_a = 0.1$ and RK4 temporal scheme. They represent cases 1a to 1d of table 3.2. They represent solutions for ω_1^* .

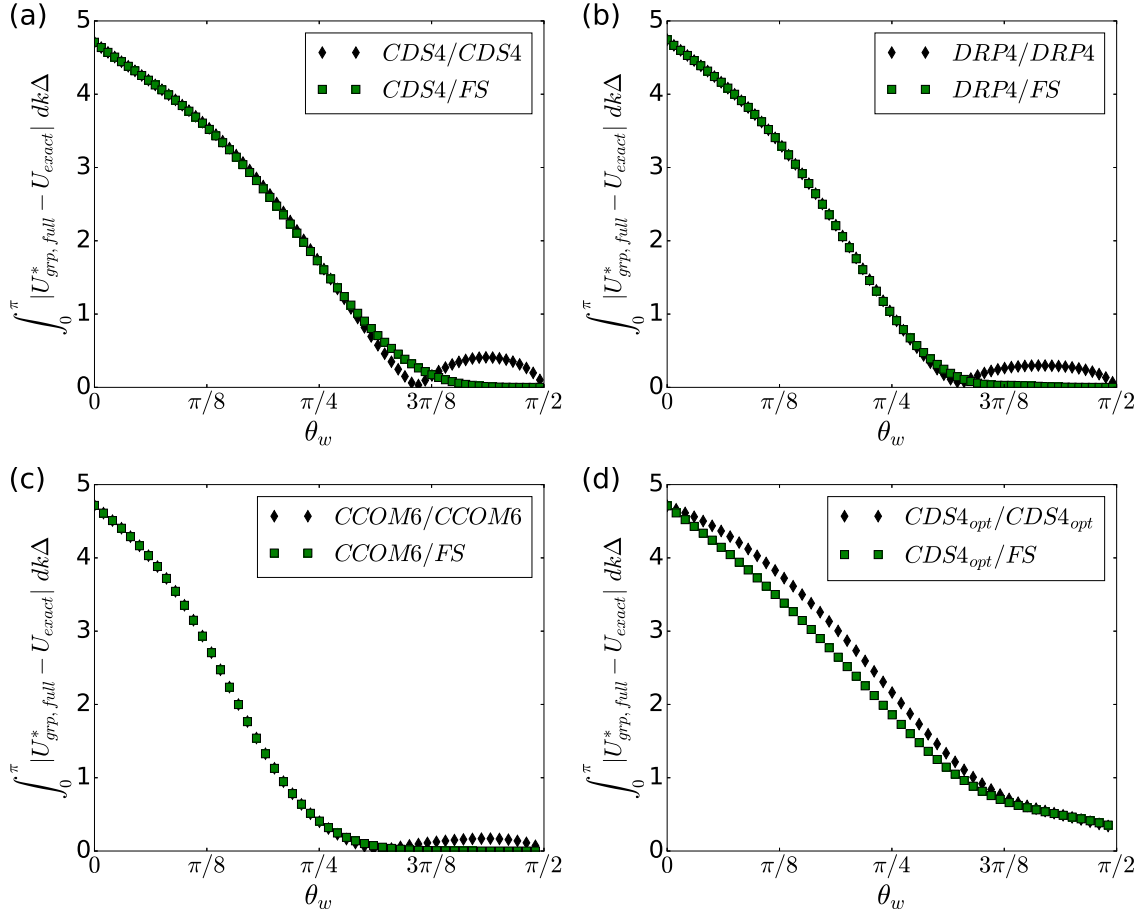


Figure 3.19: Comparison of integrated error in group velocities across all wavenumber between full FD and hybrid discretization for convective terms ($\int_0^\pi |U_{grp,full}^* - U_{exact}| dk\Delta$); (a) CDS4/CDS4 vs. CDS4/FS, (b) DRP4/DRP4 vs. DRP4/FS, (c) CCOM6/CCOM6 vs. CCOM6/FS and (d) CDS4_{opt}/CDS4_{opt} vs. CDS4_{opt}/FS. $R_a = 0.1$ and RK4 temporal scheme. They represent cases 1a to 1d of table 3.2. They represent solutions for ω_1^* .

direction leads to higher numerical dissipation at region of large $k_y \Delta y$ for all the different spatial schemes considered. Also, a comparison of the different schemes shows that the use of the CCOM6 schemes gives the highest numerical dissipation. This is expected since the CCOM6 scheme has the best spectral accuracy and provides the numerical dissipation closest to the true physical dissipation. To better illustrate the comparison of the dissipation property between a hybrid and full FD discretization, we look at 1D plot of numerical amplification factor as a function of wave propagation angle for different reduced wavenumber. This is presented in figures 3.21 to 3.23. The first thing that can be observed is that the numerical dissipation becomes the same as the physical dissipation for all wave propagation angle at low reduced wavenumber ($k\Delta = 0.3\pi$). This applies to all the spatial discretization scheme considered for the viscous term. At intermediate reduced wavenumber ($k\Delta = 0.6\pi$), the numerical dissipation of the CDS4/CDS4, CDS4/FS, DRP4/DRP4, DRP4/FS, CDS4_{opt}/CDS4_{opt} and CDS4_{opt}/FS cases show noticeable differences from the true physical dissipation. At large reduced wavenumber ($k\Delta = 0.9\pi$), the numerical dissipation of all the spatial schemes show noticeable differences from the true physical dissipation. A comparison of the different spatial schemes in figure 3.23 evidently proves that the CCOM6/CCOM6 and CCOM6/FS cases provide the closest numerical dissipation to the true physical dissipation (FS/FS case). As compared to the full FD discretization case, the numerical dissipation of the hybrid discretization cases tend to approach the true dissipation at large wave propagation angle. This can be seen clearly in figure 3.23.

3.4 Numerical experiments

3.4.1 Numerical setup

The analytical (exact and numerical) group velocity solutions determined through Fourier analysis will be verified in this section. Results from numerical experiments will be used to verify the results obtained from the analysis performed in sections 3.2 and 3.3. In these numerical experiments, the boundary conditions were kept periodic. A single frequency modulated Gaussian is used as the initial condition in order to localise the wave packets

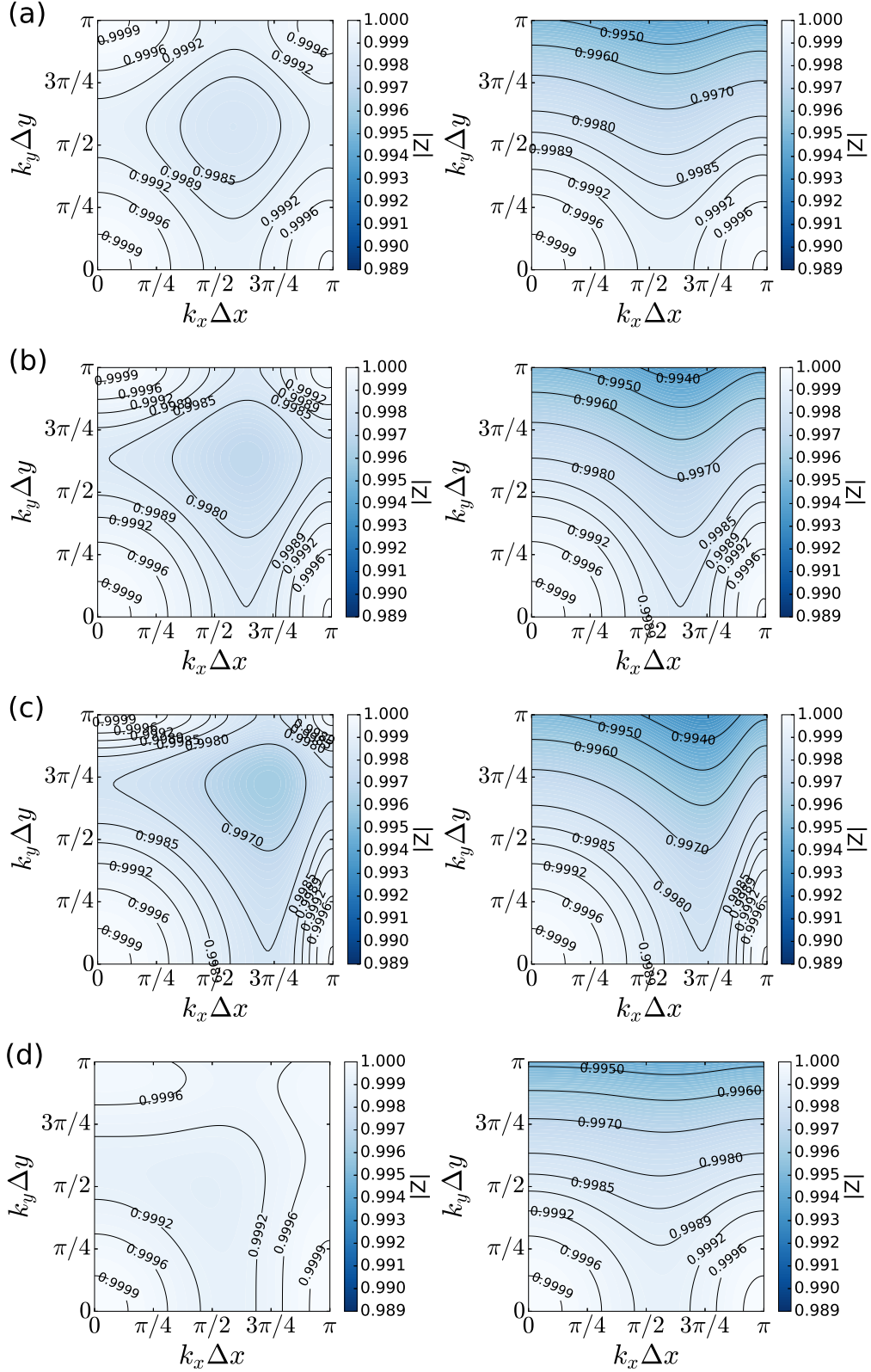


Figure 3.20: Comparison of numerical amplification factor, $|Z|$ between full FD (left figures) and hybrid FD/FS (right figures) spatial discretization for diffusion terms; (a) CDS4/CDS4 vs. CDS4/FS, (b) DRP4/DRP4 vs. DRP4/FS, (c) CCOM6/CCOM6 vs. CCOM6/FS and (d) CDS4_{opt}/CDS4_{opt} vs CDS4_{opt}/FS. $Re_a = 200$, $R_a = 0.1$ and RK4 temporal scheme. They represent cases 2a to 2d of table 3.2. All colour contour plots are ranged from 0.989 to 1.0. They represent solutions for ω_1^* .

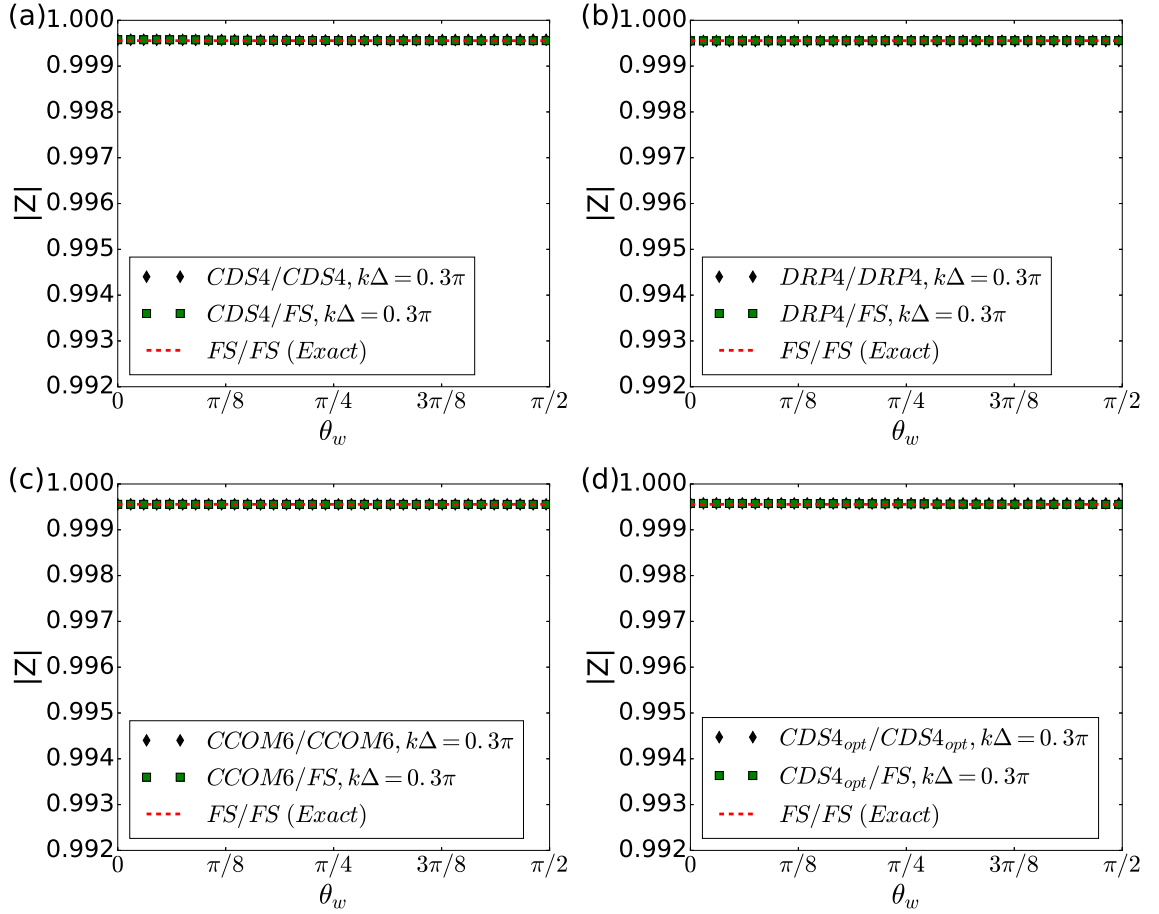


Figure 3.21: Comparison of numerical amplification factor, $|Z|$ between full FD and hybrid FD/FS spatial discretization for diffusion terms; (a) CDS4/CDS4 vs. CDS4/FS, (b) DRP4/DRP4 vs. DRP4/FS, (c) CCOM6/CCOM6 vs. CCOM6/FS and (d) CDS4_{opt}/CDS4_{opt} vs CDS4_{opt}/FS. FS/FS spatial scheme is used for convective terms. $Re_a = 200$, $R_a = 0.1$ and RK4 temporal scheme. $k\Delta = 0.3\pi$ where $k = \sqrt{k_x^2 + k_y^2}$. They represent cases 2a to 2d of table 3.2. They represent solutions for ω_1^* .

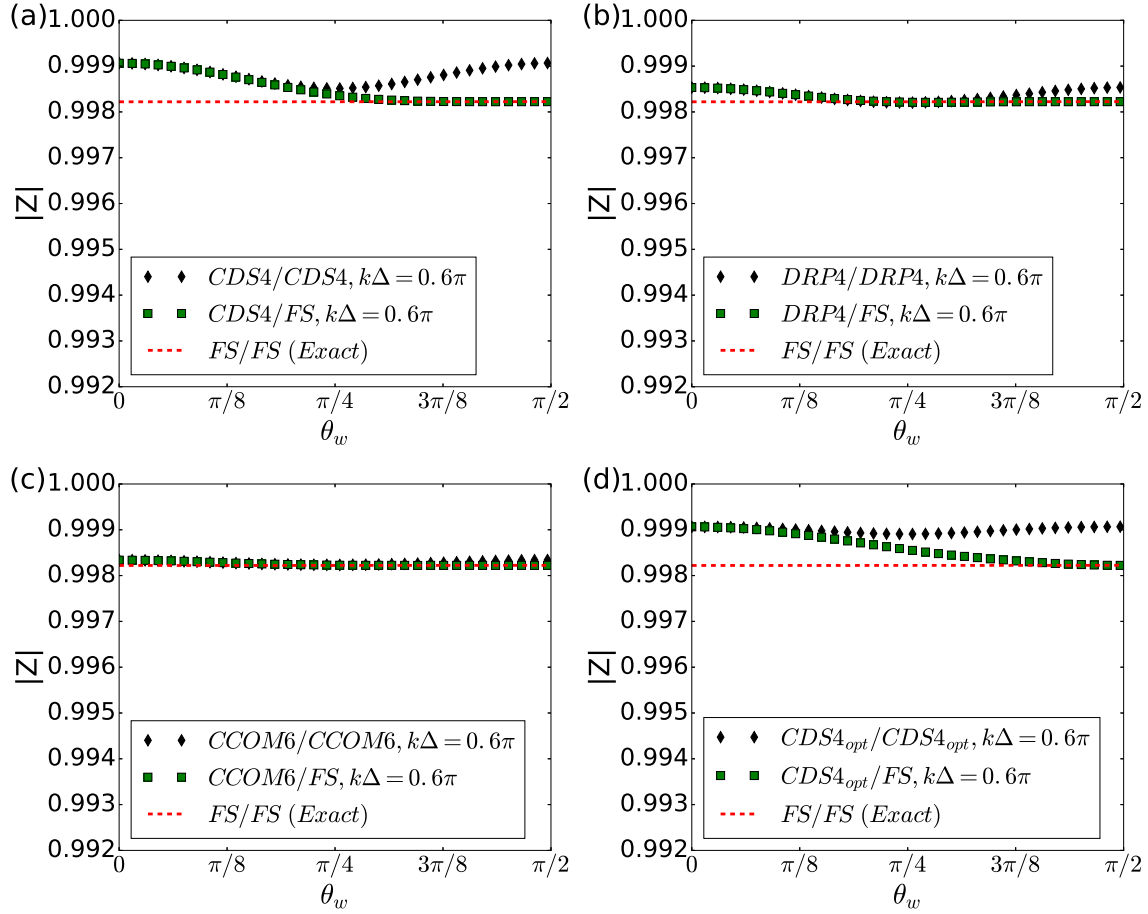


Figure 3.22: Comparison of numerical amplification factor, $|Z|$ between full FD and hybrid FD/FS spatial discretization for diffusion terms; (a) CDS4/CDS4 vs. CDS4/FS, (b) DRP4/DRP4 vs. DRP4/FS, (c) CCOM6/CCOM6 vs. CCOM6/FS and (d) CDS4_{opt}/CDS4_{opt} vs. CDS4_{opt}/FS. FS/FS spatial scheme is used for convective terms. $Re_a = 200$, $R_a = 0.1$ and RK4 temporal scheme. $k\Delta = 0.6\pi$ where $k = \sqrt{k_x^2 + k_y^2}$. They represent cases 2a to 2d of table 3.2. They represent solutions for ω_1^* .

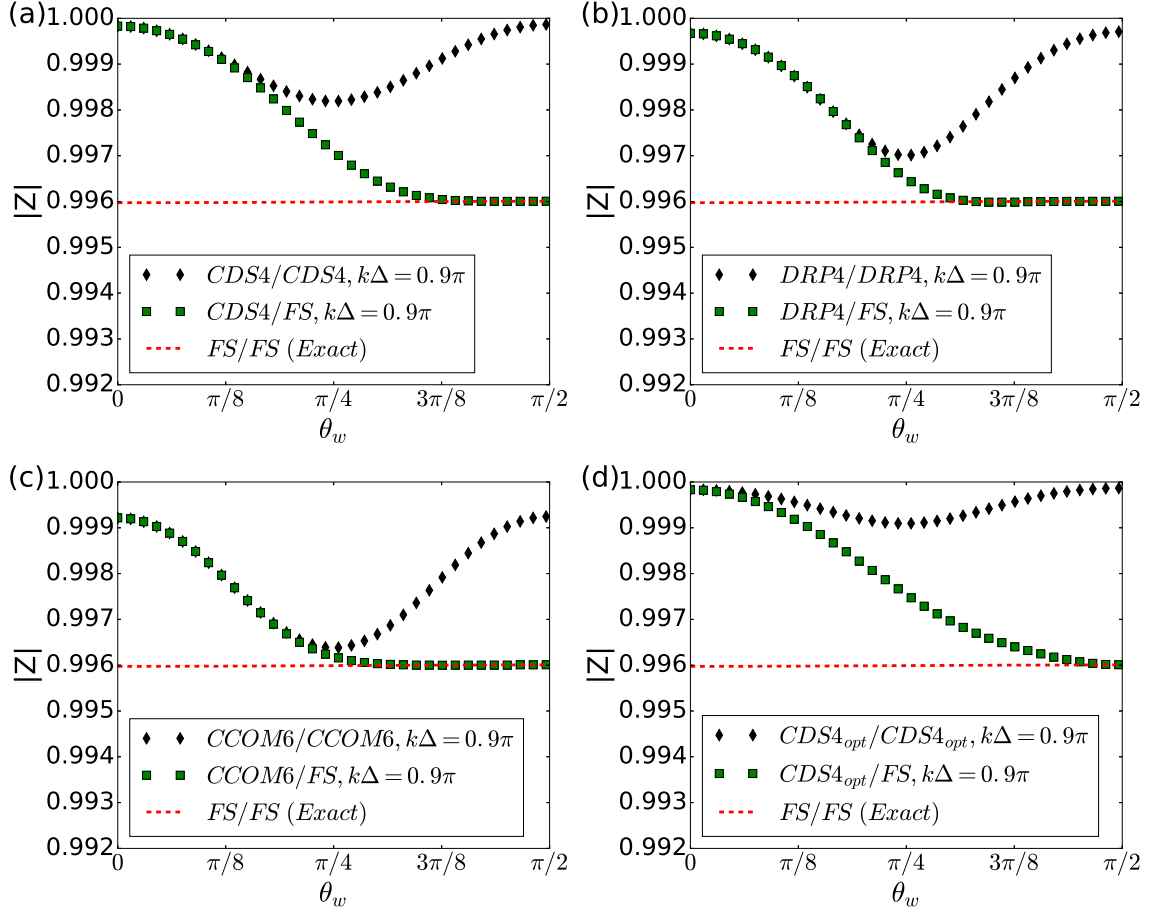


Figure 3.23: Comparison of numerical amplification factor, $|Z|$ between full FD and hybrid FD/FS spatial discretization for diffusion terms; (a) CDS4/CDS4 vs. CDS4/FS, (b) DRP4/DRP4 vs. DRP4/FS, (c) CCOM6/CCOM6 vs. CCOM6/FS and (d) CDS4_{opt}/CDS4_{opt} vs CDS4_{opt}/FS. FS/FS spatial scheme is used for convective terms. $Re_a = 200$, $R_a = 0.1$ and RK4 temporal scheme. $k\Delta = 0.9\pi$ where $k = \sqrt{k_x^2 + k_y^2}$. They represent cases 2a to 2d of table 3.2. They represent solutions for ω_1^* .

for easy comparison. A 2D uniform Cartesian grid (400 x 400) is used for most of the cases for grid converged solution. In the case of numerical solutions where the Fourier spectral spatial discretization method is used, a more refined grid of (600 x 600) was used for solutions with large reduced wavenumber initial conditions. The computational domain is either $[-8, 8] \times [-8, 8]$ or $[-12, 12] \times [-12, 12]$ depending on the comparison considered. The linearized compressible Navier-Stokes/Euler equations are solved numerically and compared with both physical and numerical group velocity solutions. For all numerical experiments, the single frequency modulated Gaussian initial condition was used. The single frequency modulated Gaussian initial condition is mathematically expressed as:

$$\phi(x, y, t = 0) = e^{-0.5(x^2 + y^2)} \sin(k_x x + k_y y), \quad (3.18)$$

where

$$k_x = k \cos(\theta_w) \quad k_y = k \sin(\theta_w). \quad (3.19)$$

θ_w represents the wave propagation angle (or alignment of the wave front with respect to the grid) which defines the wavenumber in both spatial directions. The variable ϕ represents either the perturbed pressure or density fields depending on the type of solution sought. For a pressure initial condition, the solution of the acoustic waves is obtained. x and y represent the grid coordinates in equation (3.18). For a given grid spacing, the specified wavenumber is adjusted to match the reduced wavenumber of the initial condition. Analytical solutions of $U_{grp,full}^*$, $V_{grp,full}^*$, $U_{grp,exact}$, $V_{grp,exact}$ and $|Z|$ can be extracted from the two dimensional wavenumber plot for each set of initial condition. This is illustrated in figure 3.24.

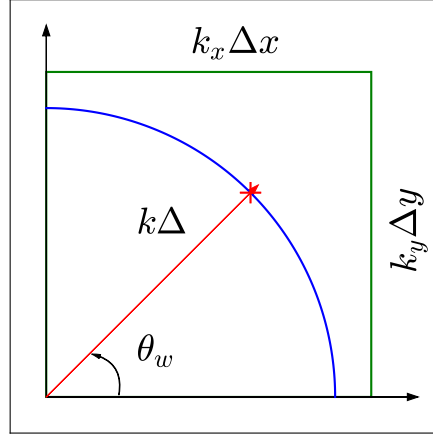


Figure 3.24: Extraction of group velocity/numerical amplification factor from 2D wavenumber plot for a given initial condition. Note $k = \sqrt{k_x^2 + k_y^2}$ and $\Delta = \Delta x = \Delta y$.

3.4.2 Numerical results

For verification purpose, the initial conditions used in this sub section are listed in table 3.3. A three dimensional visualization of the perturbed pressure variable is given in figures 3.25 and 3.26 for different time based on the initial conditions A1 and A3 in table 3.3. The numerical results were obtained using the CDS4/CDS4 spatial scheme and RK4 temporal scheme with the linearized Euler equations. The magnitude of the perturbed pressure variable is normalized such that the values are scaled from 0 to 1. The wave packets are initially positioned at center of the grid at $t = 0$. For a low reduced wavenumber initial condition (case A1), the wave packets travel in the correct direction and speed (figure 3.25). On the other hand, the wave packets travel in the opposite direction (figure 3.26) for a large reduced wavenumber initial condition (case A3). In figure 3.27, the effects of varying $k\Delta$ and θ_w were compared. The shaded patches represent the numerical solution of the CDS4/CDS4 scheme. The black arrows represent the correct solution obtained using Fourier spectral spatial discretization and the green arrows represent the analytical group velocity solution corresponding to the spatial discretization schemes used for the numerical solution. Each set of black arrows in figure 3.27a to 3.27d are calculated from the group velocities solution obtained from figures 3.1 corresponding to the initial conditions given in table 3.3.

Table 3.3: Initial conditions of reduced wavenumbers and wave propagation angles. Note $k = \sqrt{k_x^2 + k_y^2}$ and $\Delta = \Delta x = \Delta y$.

Case No.	$k\Delta$	θ_w [rad]	R_a
A1	$\pi/4$	$\pi/6$	0.1
A2	$\pi/2$	$\pi/6$	0.1
A3	$9\pi/10$	$\pi/6$	0.1
A4	$9\pi/10$	$\pi/4$	0.1

It can be seen that the numerical solution for the acoustic waves (shaded patches) matches the analytical group velocity solution (green arrows). The analytical group velocity solutions are obtained for specific values of k_x and k_y corresponding to the initial conditions. The product of the group velocities with the final time step gives the position of the wave packets. For low reduced wavenumber, the wave packets at $t_{max} = 3$ are located almost exactly at the same position as the reference solution predicted by the Fourier spectral spatial discretization (see figure 3.27a).

With increasing $k\Delta$, the wave packets at $t_{max} = 3$ are positioned further away from their exact solution (black arrows) as a result of the dispersive error. This is reflected in figures 3.27b to 3.27d. A change in θ_w also alters the values of k_x and k_y , which consequently change the final location of the wave packets. This is illustrated in a comparison between figures 3.27c and 3.27d where θ_w was changed from $\pi/6$ to $\pi/4$. Significant changes in the x and y position of the wave packets as predicted by the analytical group velocities (green arrow) were found. The error in group velocities leads to directional error in multidimensional space.

3.4.3 Numerical results - effect of varying spatial discretization schemes for the convection term

In this subsection, the case which uses the hybrid spectral/finite difference discretization will be compared to the cases using full Fourier spectral and full finite difference spatial discretization for the convective terms. Re_a will be taken as ∞ . In particular, we

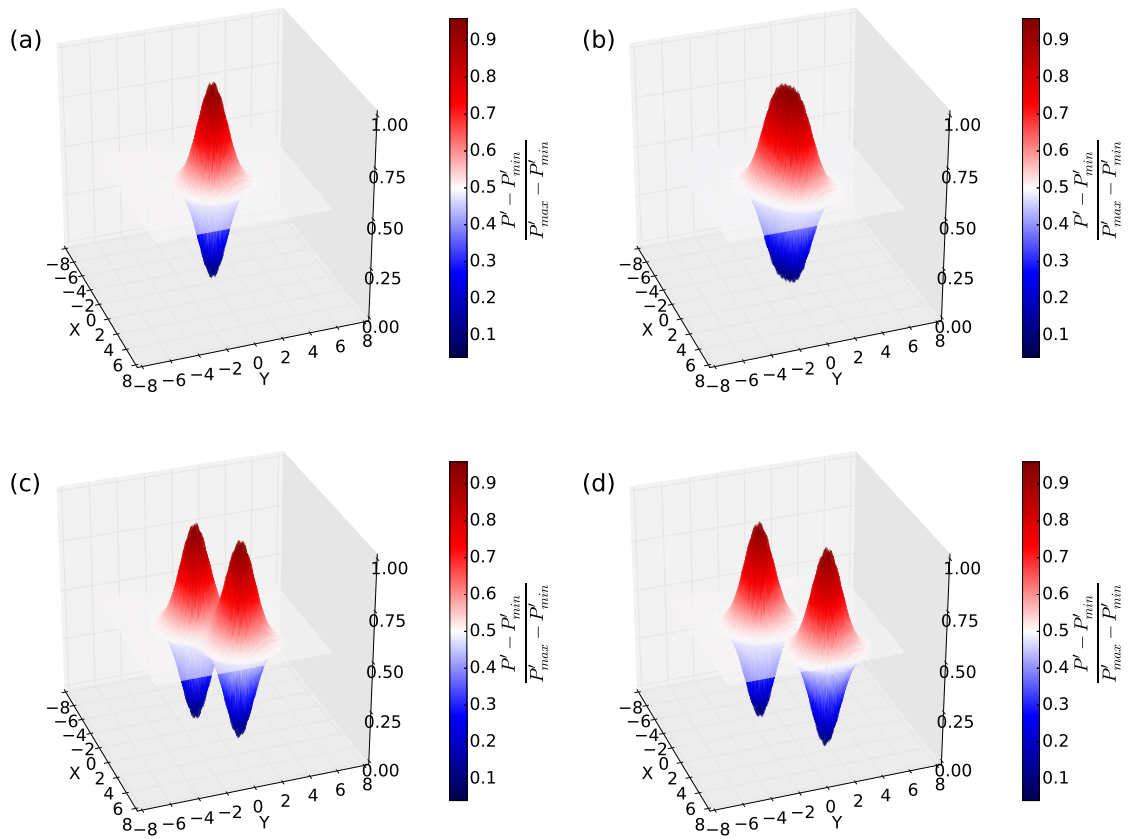


Figure 3.25: 3D Visualization of numerical solution of acoustic waves at different time interval; (a) $t = 0$, (b) $t = 1$, (c) $t = 2$, (d) $t = 3$. The numerical solution represent case A1 of table 3.3.

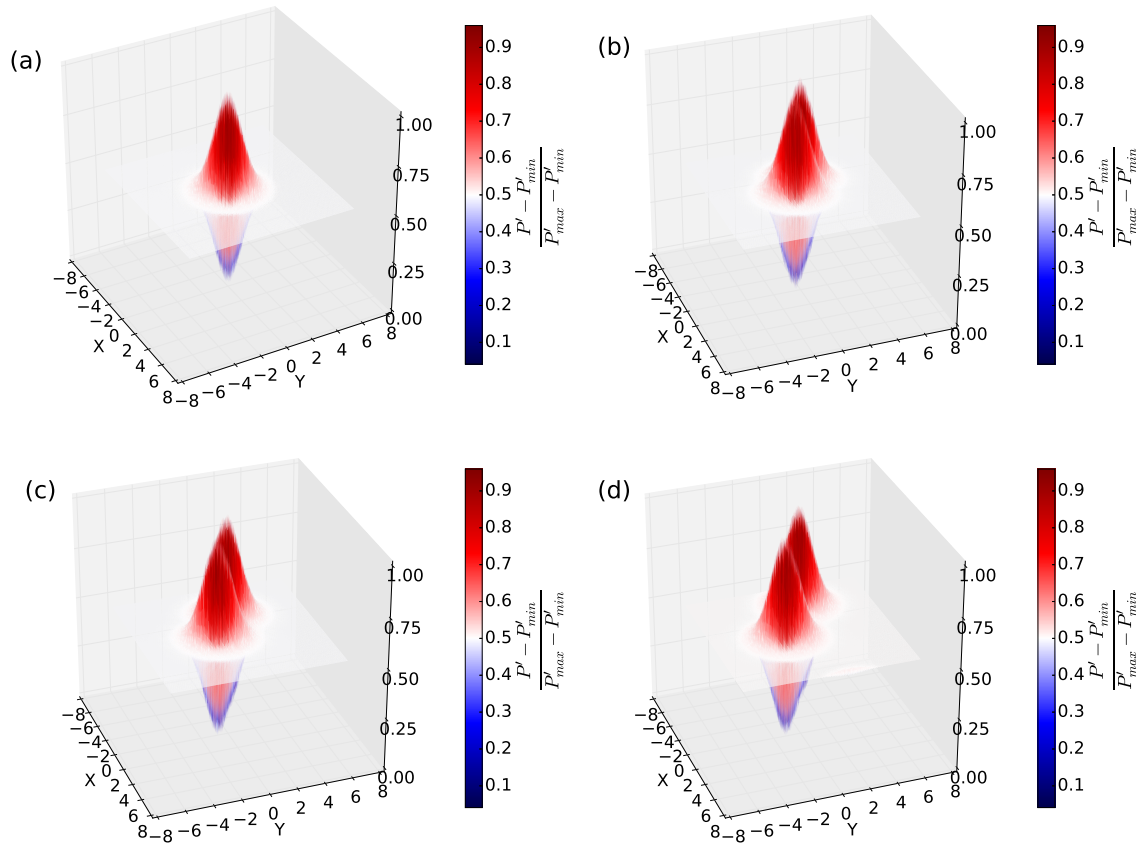


Figure 3.26: 3D Visualization of numerical solution of acoustic waves at different time interval; (a) $t = 0$, (b) $t = 1$, (c) $t = 2$, (d) $t = 3$. The numerical solution represent case A3 of table 3.3.

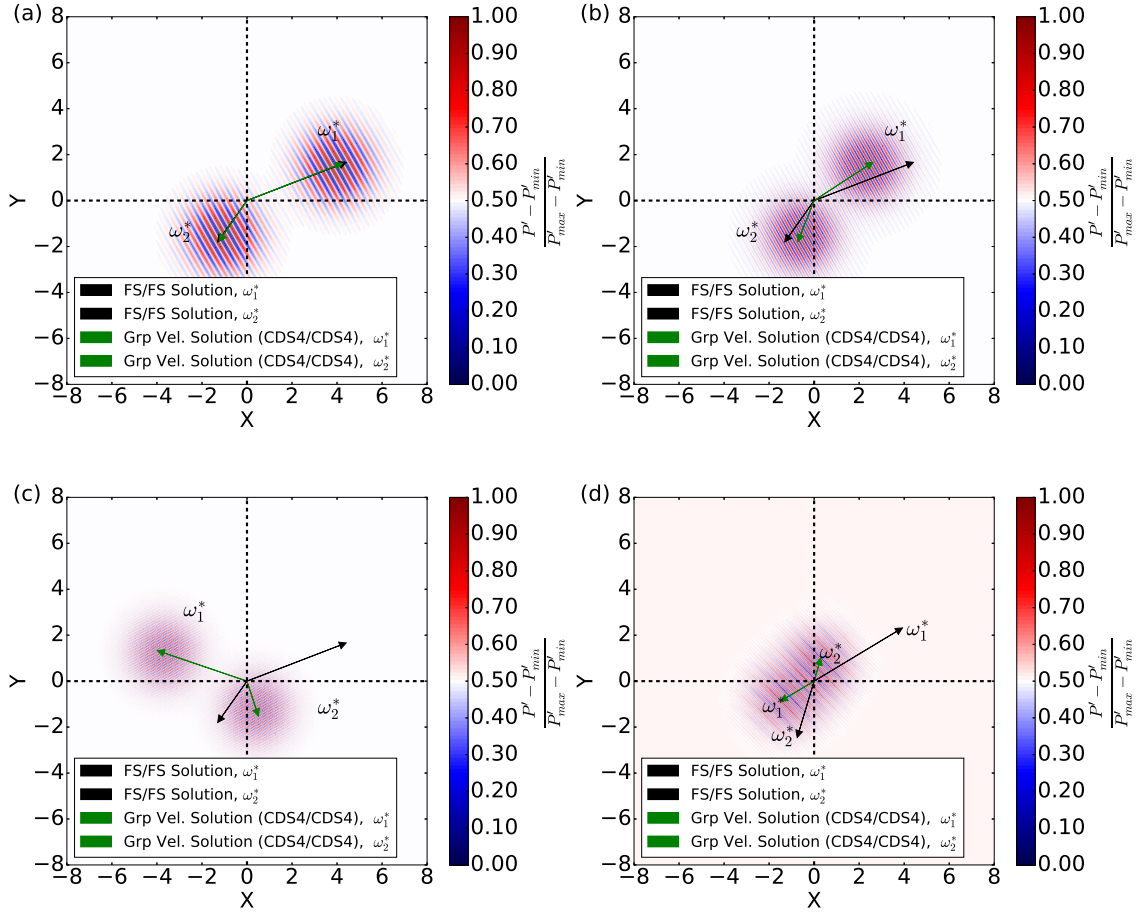


Figure 3.27: Comparison of physical group velocities (FS/FS) and numerical group velocities (CDS4/CDS4) of wave packets at $t_{max} = 3$ for different initial conditions. Numerical solutions are computed using RK4 temporal and CDS4/CDS4 spatial discretization in x and y , $M_x = 0.5$, $M_y = 0.0$, $R_a = 0.1$, $Re_a = \infty$. (a) Case A1, (b) Case A2, (c) Case A3, (d) Case A4. Wave packets are denoted as either ω_1^* or ω_2^* depending on the acoustic mode it represents. In figure (d), the wave packets of the different modes of the CDS4/CDS4 case are located in opposite y direction as compared to the FS/FS solution.

Table 3.4: Initial conditions of reduced wavenumbers and wave propagation angle. Note $k = \sqrt{k_x^2 + k_y^2}$ and $\Delta = \Delta x = \Delta y$.

Case No.	$k\Delta$	θ_w [rad]
B1	$9\pi/10$	$\pi/24$
B2	$9\pi/10$	$\pi/12$
B3	$9\pi/10$	$\pi/8$
B4	$9\pi/10$	$\pi/6$
B5	$9\pi/10$	$5\pi/24$
B6	$9\pi/10$	$\pi/4$

will consider two specific comparison of hybrid and full FD discretization; CDS4/CDS4 vs CDS4/FS and DRP4/DRP4 vs DRP4/FS. The aim is to illustrate the conditions for which the hybrid FD/FS case is either more or less accurate than the full FD case when compared to solutions based on the FS case numerically. The analytical group velocity results of the hybrid discretization cases shown here correspond to the results presented in figures 3.13a and 3.13c. The initial conditions used for these numerical experiments are listed in table 3.4. A large value of reduced wavenumber, $k\Delta = 0.9$ was chosen for these initial conditions in order to better reflect the dispersive error from the spatial discretization scheme. In figure 3.28, it can be seen that for low wave propagation angle ($\theta_w = \pi/24, \pi/12$), $V_{grp,full}^*$ of the CDS4/CDS4 and CDS4/FS cases have the same results. At intermediate wave propagation angle ($\theta_w = \pi/8, \pi/6$), $V_{grp,full}^*$ of the CDS4/CDS4 is closer to the exact result as compared to the CDS4/FS case. At large wave propagation angle ($\theta_w = 5\pi/24, \pi/4$), $V_{grp,full}^*$ of the CDS4/FS is closer to the exact result as compared to the CDS4/CDS4 case. A similar trend is observed for the comparison between the $V_{grp,full}^*$ of the DRP4/DRP4 and DRP4/FS cases in figure 3.29. For $\theta_w = \pi/24, \pi/12, \pi/8$, $V_{grp,full}^*$ of the DRP4/DRP4 and DRP4/FS cases have the same results. For $\theta_w = \pi/6$, $V_{grp,full}^*$ of the DRP4/DRP4 is closer to the exact result as compared to the DRP4/FS case. At large wave propagation angle ($\theta_w = 5\pi/24, \pi/4$), $V_{grp,full}^*$ of the DRP4/FS is closer to the exact result as compared to the DRP4/DRP4 case. It should be pointed out that the observation made here is only valid under the consideration of large reduced wavenumber.

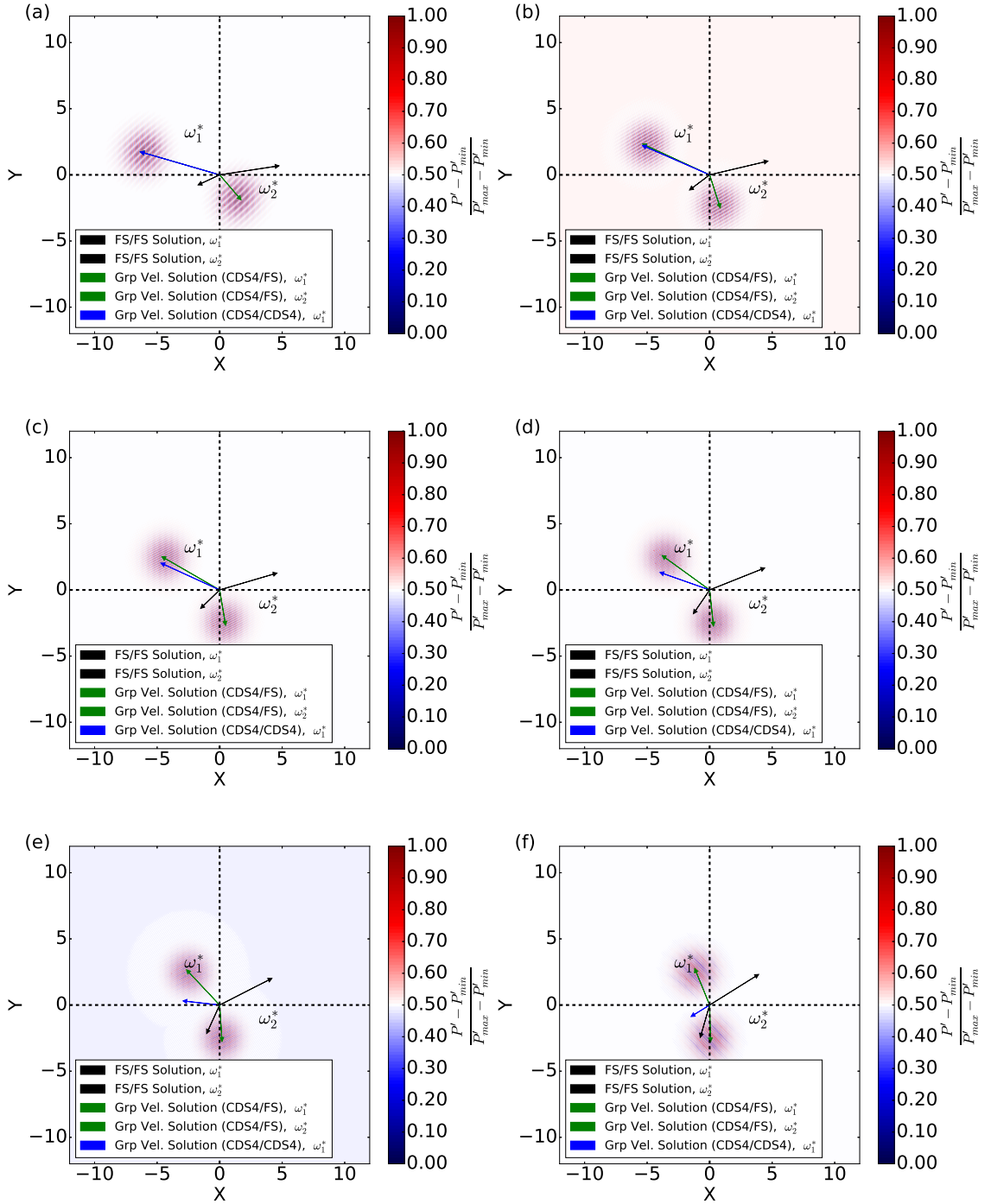


Figure 3.28: Comparison of physical group velocities (FS/FS) and numerical group velocities (CDS4/FS, CDS4/CDS4) of wave packets at $t_{max} = 3$ for different initial conditions. Numerical solutions are computed using RK4 temporal and CDS4/FS spatial discretization in x and y , $M_x = 0.5$, $M_y = 0.0$, $R_a = 0.1$, $Re_a = \infty$. (a) Case B1, (b) Case B2, (c) Case B3, (d) Case B4 (e) Case B5, (f) Case B6. Wave packets are denoted as either ω_1^* or ω_2^* depending on the acoustic mode it represents.

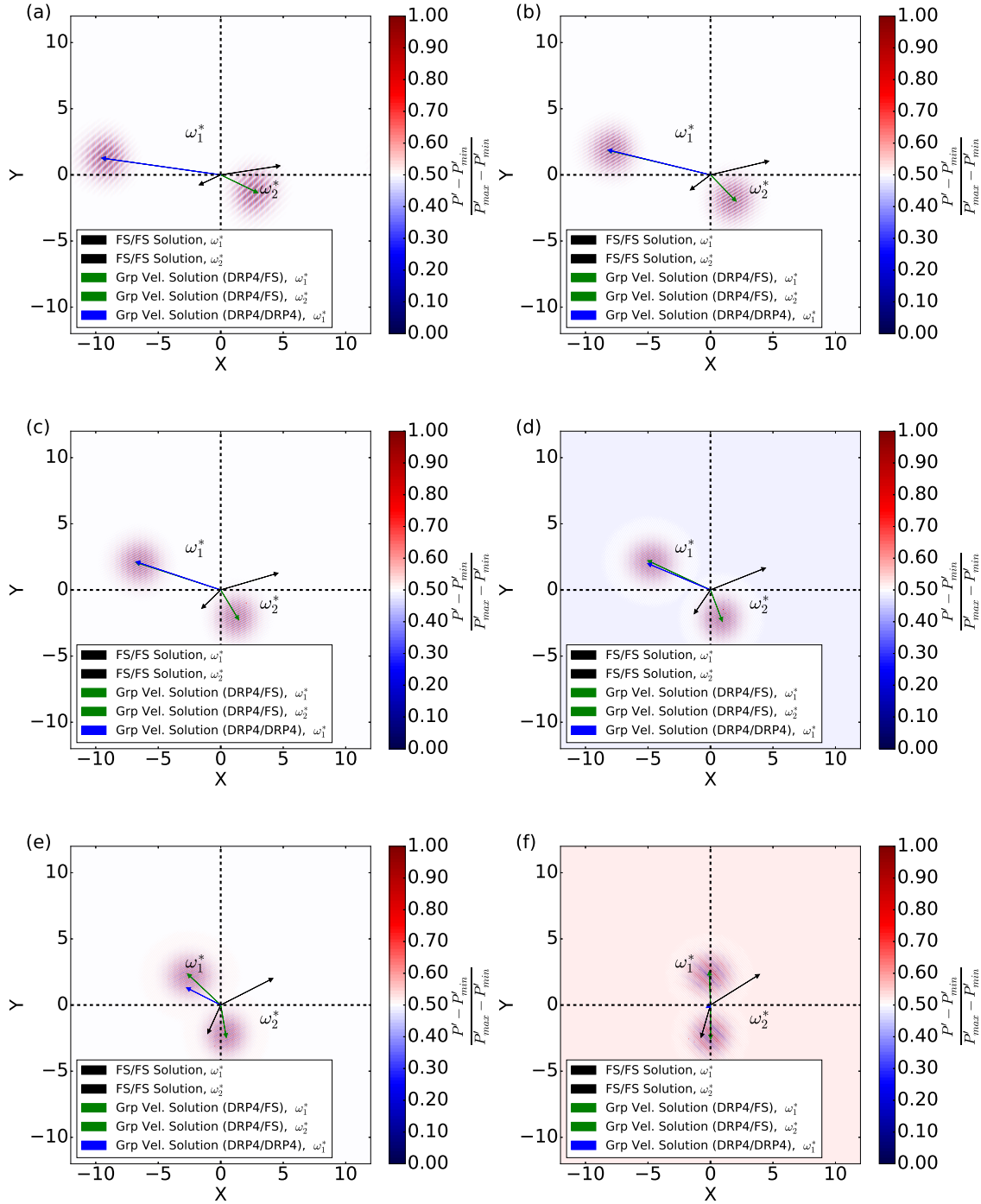


Figure 3.29: Comparison of physical group velocities (FS/FS) and numerical group velocities (DRP4/FS, DRP4/DRP4) of wave packets at $t_{max} = 3$ for different initial conditions. Numerical solutions are computed using RK4 temporal and DRP4/FS spatial discretization in x and y , $M_x = 0.5$, $M_y = 0.0$, $R_a = 0.1$, $Re_a = \infty$. (a) Case B1, (b) Case B2, (c) Case B3, (d) Case B4 (e) Case B5, (f) Case B6. Wave packets are denoted as either ω_1^* or ω_2^* depending on the acoustic mode it represents.

3.4.4 Numerical results - effect of varying spatial discretization schemes for the diffusion term

In this sub section, the effect of varying spatial discretization schemes for the diffusive term on the numerical amplification is investigated numerically. For sufficiently low CFL number, the use of central type schemes for the viscous term only causes numerical dissipation. In order to understand the effect of the viscous term on the amplitude of the numerical solution, different spatial discretization schemes were used for the viscous terms of the LCNSE. The evolution of the amplitude of the numerical solution was analysed. The numerical parameters and schemes used for this analysis is listed in table 3.5.

Table 3.5: Numerical parameters and schemes of different cases.

Case No.	Re_a	R_a	Convective scheme in (x/y)	Viscous scheme in (x/y)
C1	200	0.1	FS/FS	FS/FS
C2	200	0.1	FS/FS	CDS4/CDS4
C3	200	0.1	FS/FS	DRP4/DRP4
C4	200	0.1	FS/FS	CDS4/FS
C5	200	0.1	FS/FS	DRP4/FS

For the purpose of comparison, two different initial conditions are considered; $k\Delta = 0.9\pi, \theta_w = \pi/8$ and $k\Delta = 0.9\pi, \theta_w = \pi/4$. The aim is to compare the amplitude of the numerical solution for different wave propagation angle at high reduced wavenumber. The numerical results shown here correspond to the analytical results shown in figures 3.23a and 3.23b. For the case of $\theta_w = \pi/8$, the analytical results show that the case of the CDS4/CDS4 and CDS4/FS scheme have the same numerical dissipation while the case of the DRP4/DRP4 and DRP4/FS scheme have the same numerical dissipation as well. However, both the DRP4/DRP4 and DRP4/FS cases have a larger numerical dissipation than the case of the CDS4/CDS4 and CDS4/FS scheme. As before, the case with the FS/FS scheme have the most numerical dissipation. This same trend can be seen in figure 3.30a, where the maximum pressure fluctuation amplitude is plotted as a function of time for the different cases. For the case of $\theta_w = \pi/4$, the analytical results show that the case with the CDS4/CDS4 scheme have the least numerical dissipation. This is followed by the CDS4/FS, DRP4/DRP4, DRP4/FS and finally the FS/FS scheme. The case with the

FS/FS scheme have the most numerical dissipation. This same trend can be seen in figure 3.30b, where the maximum pressure fluctuation amplitude is plotted as a function of time for the different cases. The analytical and numerical results illustrated here confirms the finding that the numerical dissipation is a function of both the reduced wavenumber and wave propagation angle.

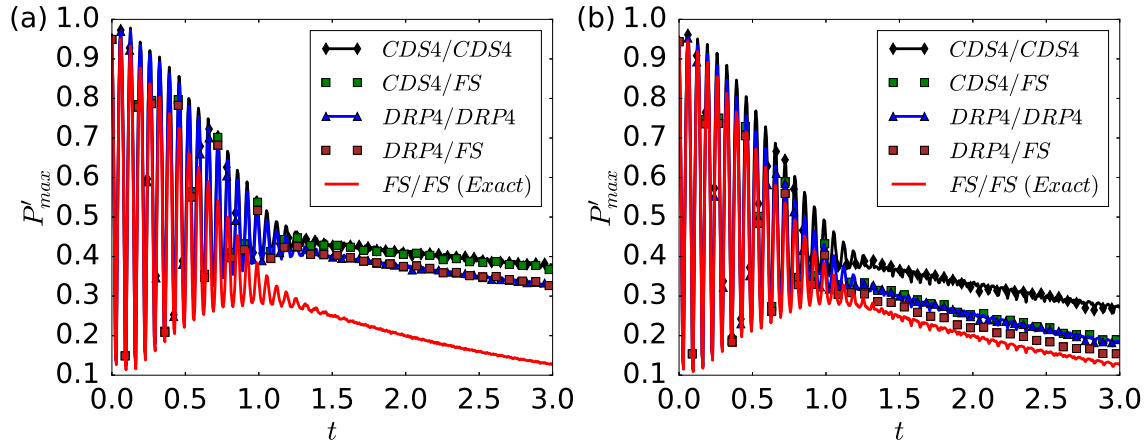


Figure 3.30: Comparison of P'_{max} as a function of time for different spatial discretization schemes used on the viscous term, (a) $k\Delta = 0.9\pi$ and $\theta_w = \pi/8$, (b) $k\Delta = 0.9\pi$ and $\theta_w = \pi/4$. FS/FS scheme is used for the convective terms. $Re_a = 200$, $R_a = 0.1$ and RK4 temporal scheme.

3.5 Chapter summary

In this chapter, linear spectral analysis method is extended to the two dimensional linearized compressible Navier Stokes equation (LCNSE). In deriving the linearized compressible Navier Stokes equation, an isothermal assumption was used to allow for simplifications in the energy equation. In doing so, one could obtain analytical expressions for its dispersion relation. The dispersion relation of the LCNSE was then used to study the dispersion and dissipation property of the coupled numerical schemes under the effects of space and time discretization. The effect of varying spatial discretization, CFL number (R), temporal discretization and cell Reynolds number was studied. In particular, the effect of using hybrid discretization (FD/FS) for both the convection and diffusion term of the LCNSE was compared against full FD discretization. For the purpose of quan-

tifying the dispersion error between a full FD and hybrid scheme, $V_{grp,full}^*$ was used to understand the propagation of error from the FD scheme in the x spatial direction to the y spatial direction. For the CDS4, DRP4 and CCOM6 schemes, the comparison of $V_{grp,full}^*$ between the full FD and its hybrid discretization counterpart can be split into three distinct region. At low wave propagation angle, the full FD and hybrid discretization scheme share the same numerical group velocity. At intermediate wave propagation angle, a region exists for which $V_{grp,full}^*$ of the full FD discretization become closer to the FS/FS solution. At large wave propagation angle, $V_{grp,full}^*$ of the hybrid discretization cases become closer to the FS/FS solution. This is expected since the resolution of the scheme will become closer to that of the FS scheme as the wave propagation angle approaches the direction where the FS method is used. For the CDS4_{opt} scheme, it was found that the dispersion error of the full FD scheme is lesser than the hybrid scheme for $0 \leq \theta_w \leq \pi/8$. For large wave propagation angle, the dispersion error of the hybrid scheme is always lesser than the full FD scheme for all spatial schemes considered. For the dissipation error, the minimum error is found to be at a wave propagation angle of $\pi/4$. Spatial scheme with better spectral properties such as the CCOM6 have numerical dissipation closer to the actual physical dissipation across all wave propagation angle. As compared to its full FD scheme counterpart, all hybrid schemes have numerical dissipation either similar or closer to the actual physical dissipation across all wave propagation angle.

With respect to the relative merits of a FD/FS method versus a full FD method, it was found that the use of FD/FS method on the viscous term tend to give more accurate results as compared to full FD method. As for the convective term, there exists a range of wave propagation angle at high reduced wavenumber for which the FD/FS method is less accurate than the full FD method. However, it is noted that this is a rather narrow range of wave propagation angle. Hence, FD/FS method is said to be more accurate than full FD method in general. The only drawback is that the use of FS method in any particular spatial direction is limited to periodic boundary conditions and not suited for flows with sharp spatial gradient.

Chapter 4

Multidimensional analysis and development of shock-capturing finite-difference schemes

In this chapter, linear spectral analysis method is extended to non linear shock capturing finite difference schemes. Following the same procedure as in previous chapter, the non linear spectral analysis method is extended to multidimensional wavenumber space. The analysis framework is then used to perform a spectral optimization of a hybrid scheme based on the combination of the Minimum Dispersion and Controllable Dissipation (MDCD) scheme and the Targeted Essentially Non Oscillatory (TENO) scheme. Various numerical experiments were conducted to compare the performance of the new scheme with existing schemes.

4.1 Review of shock-capturing finite-difference schemes

In this section, a series of commonly used shock capturing finite difference method will be discussed. Within the context of shock capturing finite difference method, several approaches exist; namely Total Variation Diminishing (TVD), Essentially Non Oscillatory (ENO), Weighted Essentially Non Oscillatory (WENO) as well as the recently introduced Targeted Essentially Non Oscillatory (TENO) schemes. TVD schemes are essentially a combination of upwind schemes with non-linear flux limiter. It degenerates to first order and produces excessive numerical dissipation near critical points. Due to its excessive dissipation, it may not accurately capture the shape of the shock front [Fu et al., 2016]. ENO schemes use an adaptive selection of stencils, such that the smoothest stencils is selected for the evaluation of numerical flux. Such a method produces lesser dissipation than TVD schemes. WENO schemes uses a weighted combination of sub stencils,

in which each set of stencil represents a linear upwind scheme. Weightings applied on each set of stencils are calculated based on a set of smoothness indicators, from which the linear schemes are recovered in the smooth region of the flow and the ENO property is utilised in the presence of discontinuity. The idea of TENO is to employ a cut off parameter from which the set of stencil located within the vicinity of a discontinuity is completely removed during the evaluation of the numerical flux. This follows the concept of the ENO scheme. The key advantage of the TENO approach lies in the minimization of the numerical dissipation from the background linear scheme while retaining the robust shock capturing property of the WENO scheme. Other key differences with respect to the WENO schemes lies in the modified parameters used within its smoothness measure so as to achieve better scale separation between the resolved and unresolved scale [Fu et al., 2016]. The formulation of the WENO and TENO schemes are described in the subsections below.

4.1.1 Key concepts of WENO scheme

In order to describe the WENO scheme, a general hyperbolic conservation law in 1D is considered. The one dimensional conservation law can be described as follows

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0. \quad (4.1)$$

$u(x, t)$ is the conservative variable and $f(u)$ is the flux function. By considering a uniformly discretized space, equation (4.1) can be written in a semi-discrete form using a conservative finite difference scheme:

$$\frac{\partial u_i}{\partial t} \approx - \frac{\hat{f}_{i+1/2} - \hat{f}_{i-1/2}}{\Delta x}. \quad (4.2)$$

In order to introduce the correct upwinding, the numerical flux at the cell interface is generally split into two parts as follow; $\hat{f}_{i+1/2} = \hat{f}_{i+1/2}^+ + \hat{f}_{i+1/2}^-$. In this chapter, the flux vector splitting approach of Lax-Friedreich [Jiang and Shu, 1996] is used. In the literature, the positive and negative flux components are sometimes referred as the left and right interface of the nodal point i and they are denoted with the superscript L and

R respectively. Equation (4.2) can be re-written as

$$\frac{\partial u_i}{\partial t} \approx - \left(\frac{\hat{f}_{i+1/2}^+ + \hat{f}_{i+1/2}^-}{\Delta x} - \frac{\hat{f}_{i-1/2}^+ + \hat{f}_{i-1/2}^-}{\Delta x} \right). \quad (4.3)$$

For the sake of brevity, only the positive part of the split numerical flux is described below. The stencils of the negative split numerical flux can be obtained through symmetry at the cell interface, $x_{i+1/2}$. The flux at the cell interface is interpolated with discrete f_i of the surrounding nodal values using a convex combination of r candidate-stencil fluxes. Mathematically, the numerical flux, $\hat{f}_{i+1/2}$ can be expressed as

$$\hat{f}_{i+1/2} = \sum_{k=0}^{r-1} \omega_k \hat{f}_{k,i+1/2} \quad (4.4)$$

The non linear weights in equation (4.4) are defined as

$$\omega_k = \frac{\alpha_k}{\sum_i \alpha_i}, \quad \alpha_k = \frac{c_k}{(\epsilon + \beta_k)^p} \quad (4.5)$$

ϵ represents a small number to avoid division by zero. For illustration purpose, the fifth order WENO scheme of [Jiang and Shu, 1996] will be presented. r is equal to 3 for the WENO5-JS scheme. ϵ is set to 1.0e-6 and p is set to 2.0. The linear weights are given by $c_0 = 0.1$, $c_1 = 0.6$, $c_2 = 0.3$. The sub schemes to be used in equation (4.4) are given as follows:

$$\begin{aligned} \hat{f}_{0,i+1/2} &= \frac{1}{3}f_{i-2} - \frac{7}{6}f_{i-1} + \frac{11}{6}f_i \\ \hat{f}_{1,i+1/2} &= -\frac{1}{6}f_{i-1} + \frac{5}{6}f_i + \frac{1}{3}f_{i+1} \\ \hat{f}_{2,i+1/2} &= \frac{1}{3}f_i + \frac{5}{6}f_{i+1} - \frac{1}{6}f_{i+2}. \end{aligned} \quad (4.6)$$

The local smoothness indicator, β_k determines the weighting contribution of each sub schemes towards the flux reconstruction at the cell interface. It is defined as:

$$\beta_k = \sum_{j=1}^2 \Delta x^{2j-1} \int_{x_{i-1/2}}^{x_{i+1/2}} \left(\frac{d^j}{dx^j} \hat{f}_k(x) \right)^2 dx \quad (4.7)$$

according to [Jiang and Shu, 1996]. Explicit expressions for the WENO5-JS scheme in terms of the cell averaged quantities, f_i are given by:

$$\begin{aligned}\beta_0 &= \frac{13}{12}(f_{i-2} - 2f_{i-1} + f_i)^2 + \frac{1}{4}(f_{i-2} - 4f_{i-1} + 3f_i)^2, \\ \beta_1 &= \frac{13}{12}(f_{i-1} - 2f_i + f_{i+1})^2 + \frac{1}{4}(f_{i-1} - f_{i+1})^2, \\ \beta_2 &= \frac{13}{12}(f_i - 2f_{i+1} + f_{i+2})^2 + \frac{1}{4}(3f_i - 4f_{i+1} + f_{i+2})^2.\end{aligned}\tag{4.8}$$

Details of the third and 7th order WENO-JS scheme can be found in [Liu et al., 1994, Jiang and Shu, 1996].

4.1.2 Key concepts of TENO scheme

In this chapter, the TENO5 and TENO6 scheme described in [Fu, 2018, Fu et al., 2018] is used for the analysis. As previously described, the key differences between the TENO and WENO type schemes lies in the use of a cut off parameter to remove a linear sub scheme if it crosses a discontinuity. The other major difference between the WENO and TENO scheme lies in the sub stencils used in the flux reconstruction. While the sub schemes used within the WENO scheme has the same stencil width, the sub stencils within the TENO schemes are constructed with incremental width. For example, the 7th order WENO is compose of four 4 point stencils while the 7th order TENO is compose of three 3 point stencils and two 4 point stencils. In the case of having two closely located discontinuity at both end of the main scheme's stencil width, the TENO scheme is able to guarantee the ENO property since there exist one centrally located sub scheme which can avoid crossing with discontinuities located at either end of the main scheme stencil width. As for the WENO scheme, the sub stencils are arranged spatially from the most upwind biased location to the most downwind biased location. This ensures that all WENO sub schemes crosses with the discontinuities located at either end of the main scheme stencil width. This is illustrated in figure 4.1. In this chapter, only the TENO5 scheme is presented for completeness. Further details of the TENO6 scheme can be found in [Fu, 2018, Fu et al., 2018]. The numerical flux of the TENO scheme can be expressed as

$$\hat{f}_{i+1/2} = \sum_{k=0}^{r-1} \omega_k \hat{f}_{k,i+1/2}. \quad (4.9)$$

The weighting of the TENO scheme is defined as

$$\omega_k = \frac{\alpha_k}{\sum_i \alpha_i}, \quad \alpha_k = c_k \delta_k, \quad (4.10)$$

where δ_k represents a sharp cut off function and is defined as

$$\delta_k = \begin{cases} 0, & \text{if } \chi_k < C_T. \\ 1, & \text{otherwise.} \end{cases} \quad (4.11)$$

C_T is taken to be 10^{-6} . The normalised smoothness indicator, χ_k is defined as

$$\chi_k = \frac{\gamma_k}{\sum_k \gamma_k}, \quad (4.12)$$

where

$$\gamma_k = \left(1.0 + \frac{\tau_k}{\beta_k + \epsilon} \right)^6. \quad (4.13)$$

β_k is given as

$$\begin{aligned} \beta_0 &= \frac{1}{4}(f_{i-1} - f_{i+1})^2 + \frac{13}{12}(f_{i-1} - 2f_i + f_{i+1})^2, \\ \beta_1 &= \frac{1}{4}(f_{i+2} - 4f_{i+1} + 3f_i)^2 + \frac{13}{12}(f_{i+2} - 2f_{i+1} + f_i)^2, \\ \beta_2 &= \frac{1}{4}(3f_i - 4f_{i-1} + f_{i-2})^2 + \frac{13}{12}(f_i - 2f_{i-1} + f_{i-2})^2. \end{aligned} \quad (4.14)$$

For the TENO5 scheme, the sixth order τ_5 is given as

$$\begin{aligned}
 \tau_5 = & \frac{1}{5040} [5788f_{i-2}^2 + f_{i-2}(-45681f_{i-1} + 64843f_i - 38947f_{i+1} + 8209f_{i+2}) \\
 & + f_{i-1}(93483f_{i-1} - 275836f_i + 173498f_{i+1} - 38947f_{i+2}) \\
 & + f_i(210993f_i - 275836f_{i+1} + 64843f_{i+2}) \\
 & + f_{i+1}(93483f_{i+1} - 45681f_{i+2}) + 5788f_{i+2}^2]
 \end{aligned} \tag{4.15}$$

The sub schemes to be used in equation (4.9) are given

$$\begin{aligned}
 \hat{f}_{0,i+1/2} &= -\frac{1}{6}f_{i-1} + \frac{5}{6}f_i + \frac{2}{6}f_{i+1} \\
 \hat{f}_{1,i+1/2} &= \frac{2}{6}f_i + \frac{5}{6}f_{i+1} - \frac{1}{6}f_{i+2} \\
 \hat{f}_{2,i+1/2} &= \frac{2}{6}f_{i-2} - \frac{7}{6}f_{i-1} + \frac{11}{6}f_i.
 \end{aligned} \tag{4.16}$$

For the TENO5 scheme, $c_{0,1,2} = [0.5065006634, 0.3699651429, 0.1235341937]$. The key advantage of the TENO scheme lies in its much reduced numerical dissipation at high reduced wavenumber as compared to the WENO scheme. It offers marginal improvement in terms of its dispersion property as compared to the WENO scheme of the same stencil width. This is primarily because of the cut off parameter which removes the background linear scheme if the smoothness indicator is below a specified value.

4.2 1D non linear spectral analysis

Unlike a linear scheme, the modified wavenumber of a non linear scheme cannot be easily derived analytically and therefore a numerical approach was introduced to deduce the spectral properties of the numerical scheme. One of the first non linear spectral analysis approach was the ADR method introduced by [Pirrozzoli, 2006]. The essential idea of ADR is based on the ratio of the spectra solution at time, τ of the primary Fourier mode with respect to its initial complex amplitude of Fourier mode. For a single mode initial condition, the solution spectra at time τ obtained through the use of a shock capturing finite difference scheme contains multiple Fourier modes instead of a single mode as in the

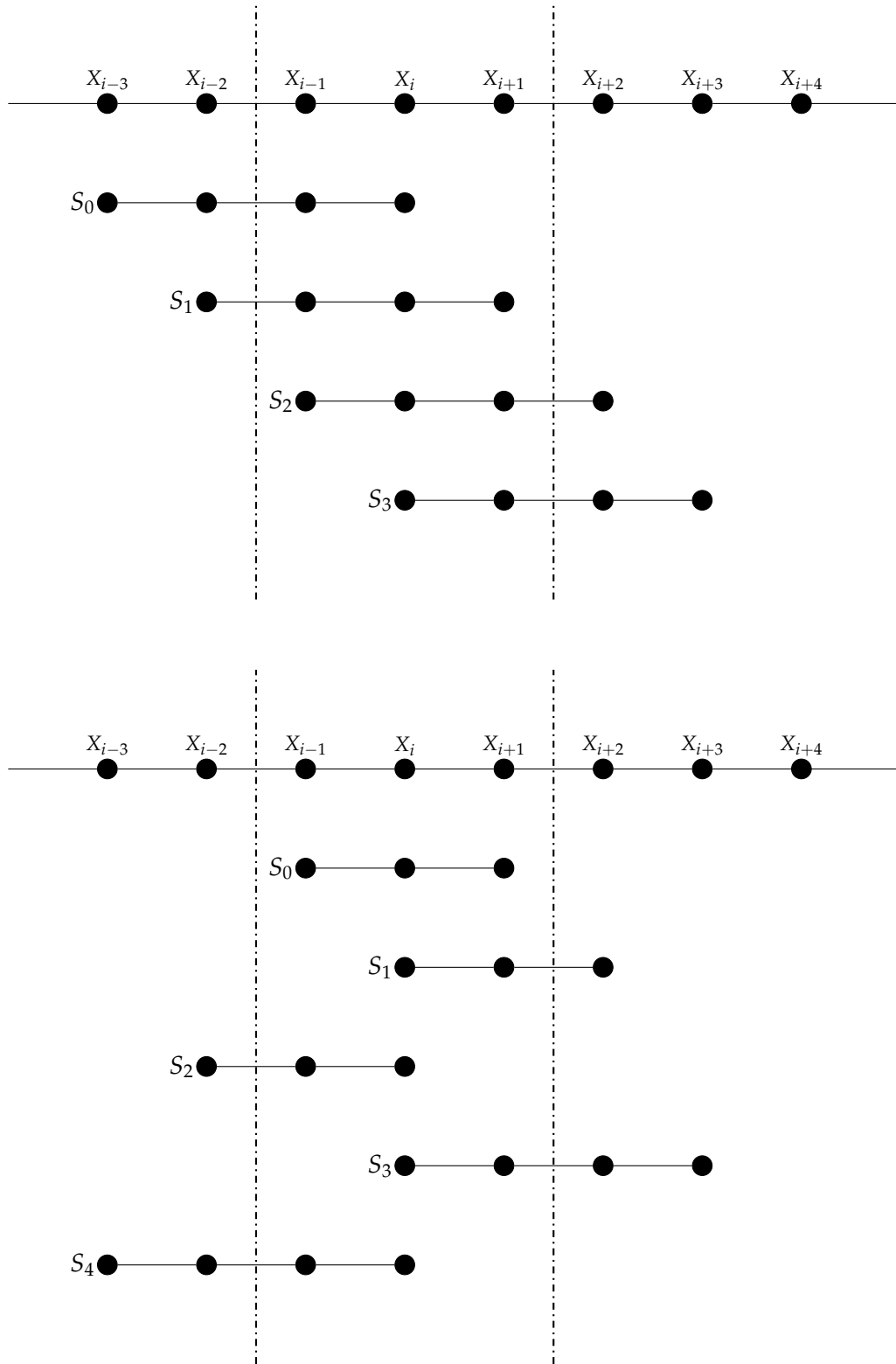


Figure 4.1: Sketch of sub stencils of schemes with closely located shock waves. Dashed lines represent two shock discontinuities. Classical 7th order WENO scheme (Top) and 7th order TENO scheme (Bottom). S_k represent the stencils of the sub schemes. Adapted from [Fu et al., 2017].

case of a linear scheme. Furthermore, the different Fourier modes may interact at later time stages which affect the evolution of each Fourier mode. The framework of the ADR method may be further simplified by neglecting the temporal discretization effect in the case of a very small time step and performing a Fourier analysis of the semi-discretized system instead [Pirroli, 2006]. A numerical flux, F_j at node j can be written in terms of its spatial derivative as

$$F(x_j) = \Delta x f'(x_j) = F(f_{j-p}, \dots, f_{j+q}). \quad (4.17)$$

In the context of a non linear scheme, the flux function must contain the harmonic modes in addition to the fundamental mode, $e^{ik_0 x_j}$, that is

$$F(x_j) = \hat{F}_{k_0} e^{ik_0 x_j} + \sum_{k=k_1}^{k_{max}} \hat{F}_k e^{ik x_j} \quad (4.18)$$

$\hat{F}_{k_0, 1, 2, \dots}$ is the complex amplitude of the Fourier modes. This is in contrast to linear schemes, for which the flux function contains only the fundamental mode. Similar to the ADR approach, a quasi linear analysis accounts for only the leading order Fourier modes of the non linear effects embodied within a shock capturing scheme. Therefore, only the primary mode is considered for further analysis. The complex amplitude of the leading order Fourier mode, $\hat{F}_{k_0}$ can thus be obtained through a Discrete Fourier Transform (DFT),

$$\hat{F}_{k_0} = \frac{1}{N} \sum_{j=0}^{N-1} F_j e^{-ik_0 x_j}. \quad (4.19)$$

F_j is the flux obtained numerically through the non linear differentiation given in equation (4.17). The real part of the modified wavenumber relates to the dispersion property and the imaginary part relates to the dissipation property. Using an initial condition, $f_j = e^{ik_0 x_j}$, which is a sinusoidal function with wavenumber k_0 and only the leading order Fourier mode in equation (4.18), the numerical flux can be expressed as follows:

$$F(x_j) = \hat{F}_{k_0} e^{ik_0 x_j} = \Delta x f'_j = ik_0^* \Delta x e^{ik_0 x_j}. \quad (4.20)$$

Using equation (4.20), the modified wavenumber of the non linear scheme can thus be expressed in terms of the leading order complex Fourier amplitude. The real and imaginary part of the modified wavenumber corresponds to the dispersion and dissipation property of the numerical scheme.

$$\Re(k_0^* \Delta x) = \Re(-i\hat{F}_{k_0}), \quad \Im(k_0^* \Delta x) = \Im(-i\hat{F}_{k_0}). \quad (4.21)$$

The leading order complex Fourier mode is obtained through equation (4.19). In order to obtain the dispersion or dissipation curve along the entire wavenumber spectrum, the wavenumber of the initial condition is varied for the entire spectrum so as to produce a list of fundamental complex Fourier modes. This method is general in the sense that it is applicable for both linear and non linear schemes. In the case of a linear scheme, the flux function computed from the numerical differentiation contains only the fundamental mode and therefore the calculation of the modified wavenumber is exact. As for the non linear scheme, the modified wavenumber is only an approximation since the harmonic modes are neglected during the calculation procedure. The dispersion and dissipation property of a range of WENO and TENO schemes are presented in figure 4.2. It can be seen that the TENO schemes have better dispersion property than the WENO schemes in general. Besides, the TENO schemes have lower numerical dissipation up to intermediate reduced wavenumber as compared to the WENO schemes. It should be noted that the spectral properties of the TENO scheme varies according to the specified value of C_T [Fu et al., 2017].

Since the harmonic modes are neglected during the calculation of the modified wavenumber for a non linear FD schemes, this place a stringent bound on the range of applicability of the quasi-linear theory. For the purpose of demonstrating its applicability, numerical results of the linear advection equation based on the WENO5 scheme are compared against theoretically predicted time evolution of (initially) isolated Fourier modes. A range of Fourier modes are considered; $k_x \Delta x = \frac{\pi}{8}, \frac{2\pi}{8}, \frac{3\pi}{8}, \frac{4\pi}{8}$. It should be noted that this analysis technique is applicable to all non linear schemes and the results shown below would draw the same conclusion irrespective of the non linear scheme considered. The analytical solution is given by

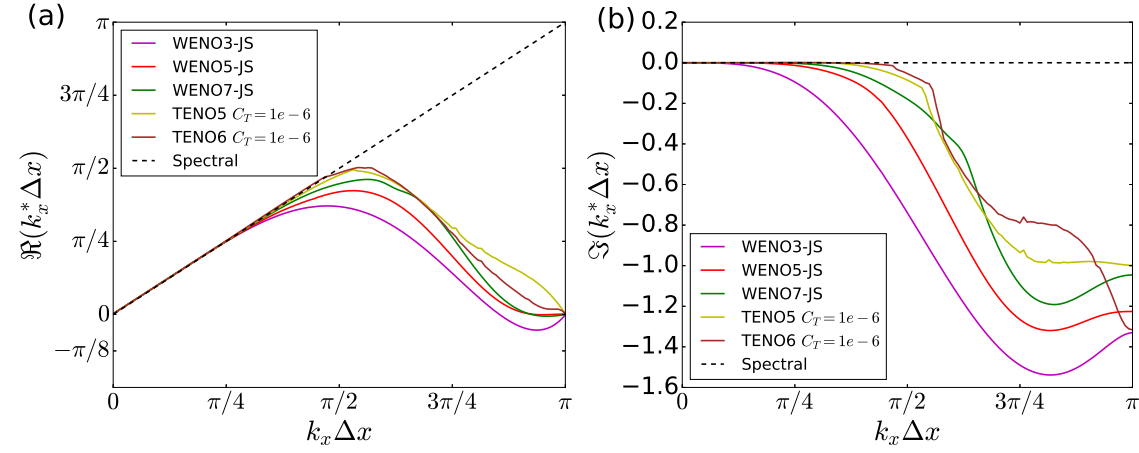


Figure 4.2: Comparison of (a) dispersion, $\Re(k_x^* \Delta x)$ and (b) dissipation, $\Im(k_x^* \Delta x)$ property of different FD schemes. The label WENOX-JS refers to the X^{th} order WENO scheme proposed by [Jiang and Shu, 1996].

$$\left| \frac{\hat{\phi}(k_x, t)}{\hat{\phi}(k_x, 0)} \right| = e^{(\bar{u}t/\Delta x)\Im(k_x^* \Delta x)}, \quad (4.22)$$

where $\bar{u}$ is the physical phase speed. For the purpose of comparison with the numerical results, the time step for the numerical simulation is chosen to be sufficiently small such that the error from the temporal discretization is negligible. This is critical since the analytical solution given in equation (4.22) only accounts for the spatial discretization error. It can be seen in figure 4.3 that quasi-linear analysis provides quantitatively correct prediction for the amplitude of the modes up to a time period where higher order effects related to the onset of spurious modes become important. This time period is shorter for marginally resolved waves. Similar results comparing analytical and numerical solution can be found in [Pirrozzoli, 2006]. It should be noted that the decay of the amplitude is slower for marginally resolved wave at later time periods primarily because of the transfer of energy to the harmonic modes which is not accounted for during the calculation of $k_x^* \Delta x$.

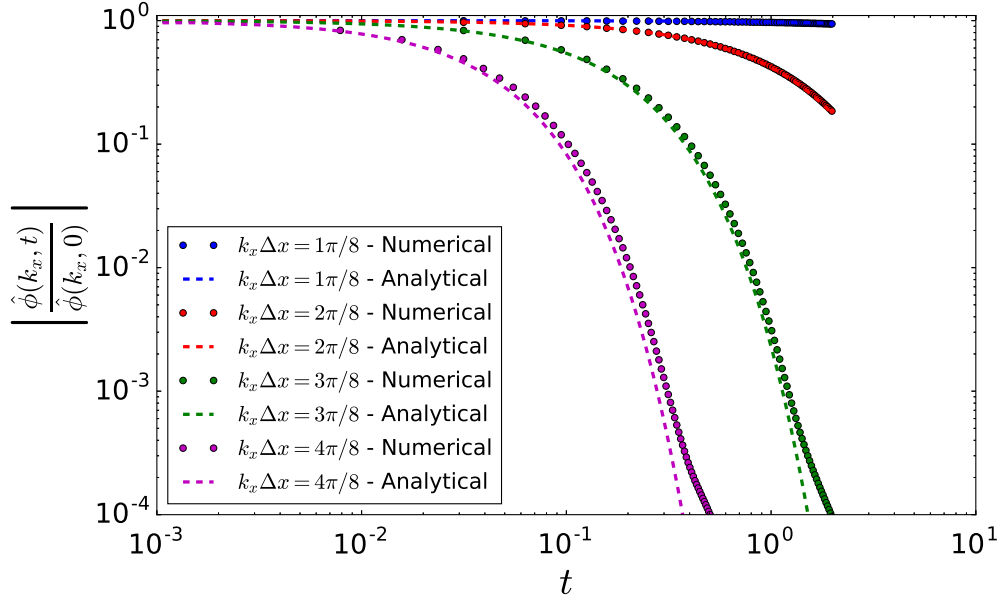


Figure 4.3: Time evolution of isolated Fourier modes amplitude. Dotted line represents analytical solution. Symbols represent numerical solution for different Fourier modes.

4.3 2D non linear spectral analysis

One dimensional non linear spectral analysis was used to determine the modified wavenumber relation of the non linear schemes in the previous section. In order to assess the accuracy of the numerical schemes in multidimensional space, the semi-discretized numerical dispersion relation of the two dimensional Linearised Euler equations (LEE) belonging to one of the acoustic modes are used [Tan et al., 2018]. $\bar{u}$, $\bar{v}$ and a are taken to be 1. The additional acoustic term accounts for the coupling effect of the numerical scheme in multi-dimensional space [Tan et al., 2018]. The semi-discretized dispersion relation of the two-dimensional LEE is given by

$$\omega_{semi}^* = \underbrace{\bar{u}k_x^* + \bar{v}k_y^*}_{advection} + a \underbrace{\sqrt{(k_x^*)^2 + (k_y^*)^2}}_{acoustic}. \quad (4.23)$$

Considering that $\Delta_x = \Delta_y = \Delta$, the semi-discretized dispersion relation is written as

$$\omega_{semi}^* \Delta = \bar{u}k_x^* \Delta + \bar{v}k_y^* \Delta + a \sqrt{(k_x^* \Delta)^2 + (k_y^* \Delta)^2}. \quad (4.24)$$

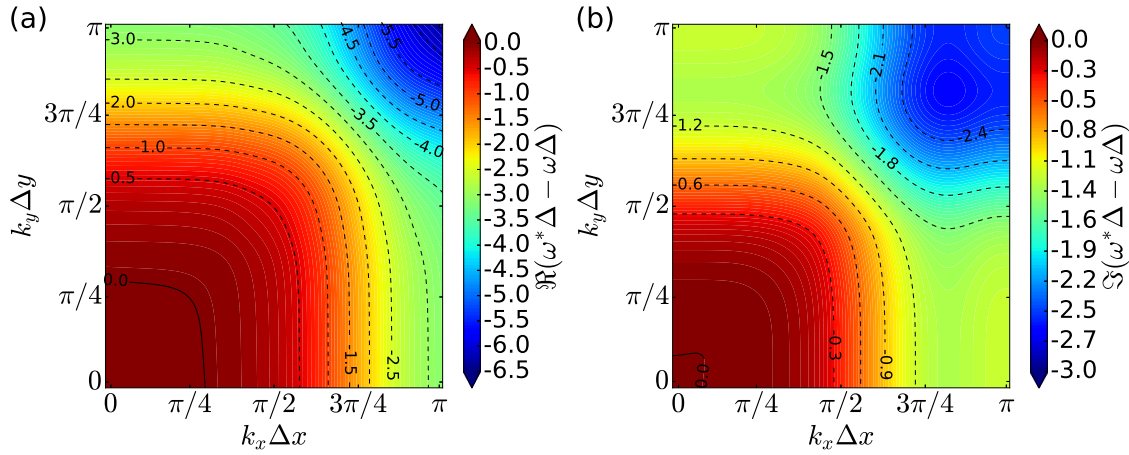


Figure 4.4: Measure of phase (a) and amplitude (b) error of WENO5-JS scheme in 2D wavenumber space based on the dispersion relation of the advection equation

A novel way to analyse the non linear schemes in multi dimensional wave space is to use the semi-discretized dispersion relation of the two dimensional advection and linearized Euler equations. The phase and amplitude error of the numerical scheme can be quantified using the real and imaginary component of the difference between the semi-discretized and physical dispersion relation, $(\omega_{semi}^* \Delta - \omega \Delta)$. The dispersion and dissipation property of the WENO5-JS, TENO5, TENO6 schemes based on the dispersion relation of the advection equation are plotted in figures 4.4, 4.5 and 4.6. The dispersion and dissipation property of the WENO5-JS, TENO5, TENO6 schemes based on the dispersion relation of the LEE are plotted in figures 4.7, 4.8 and 4.9. The key difference between the use of the advection and linearised Euler dispersion relation lies in the magnitude of $(\omega_{semi}^* \Delta - \omega \Delta)$ especially at intermediate and high reduced wavenumber. This suggests that the acoustic effect is more critical at intermediate and high reduced wavenumbers. Similar to the 1D non linear spectral analysis, the TENO schemes have lower phase and amplitude error at low and intermediate reduced wavenumber (in both spatial directions) as compared to the WENO schemes.

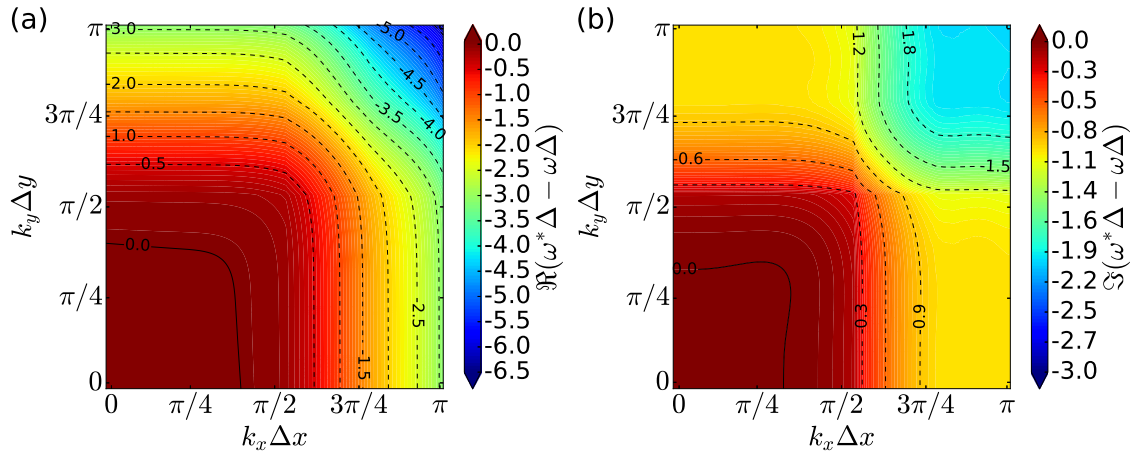


Figure 4.5: Measure of phase (a) and amplitude (b) error of TENO5 scheme in 2D wavenumber space based on the dispersion relation of the advection equation

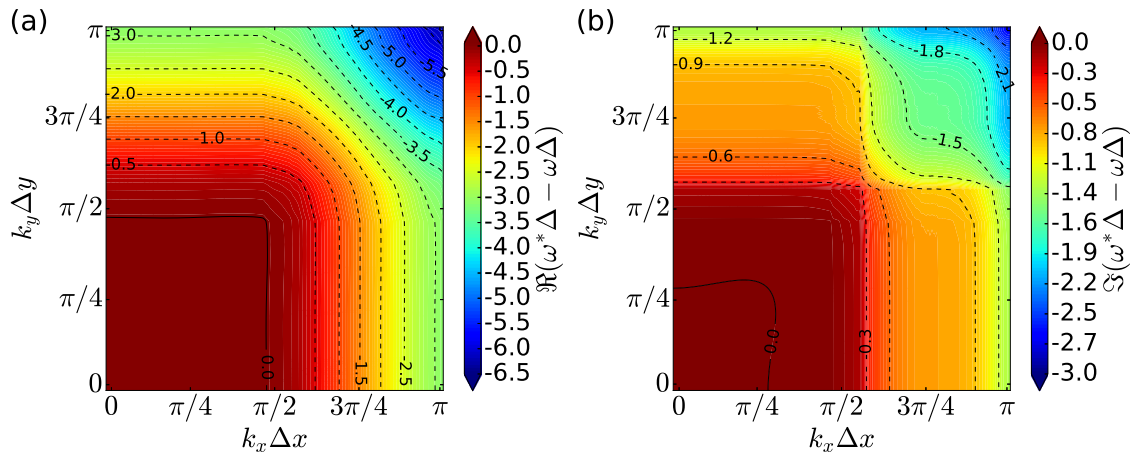


Figure 4.6: Measure of phase (a) and amplitude (b) error of TENO6 scheme in 2D wavenumber space based on the dispersion relation of the advection equation

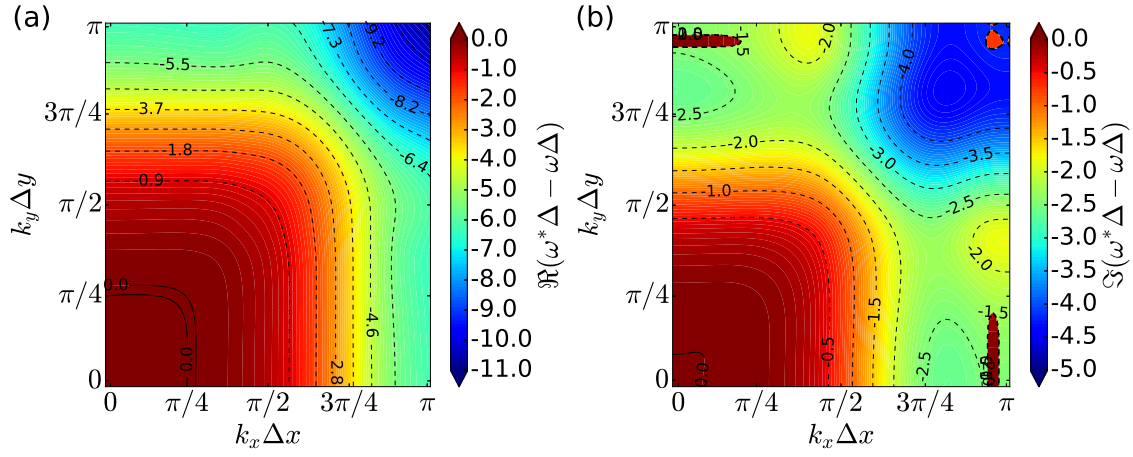


Figure 4.7: Measure of phase (a) and amplitude (b) error of WENO5-JS scheme in 2D wavenumber space based on the dispersion relation of the LEE

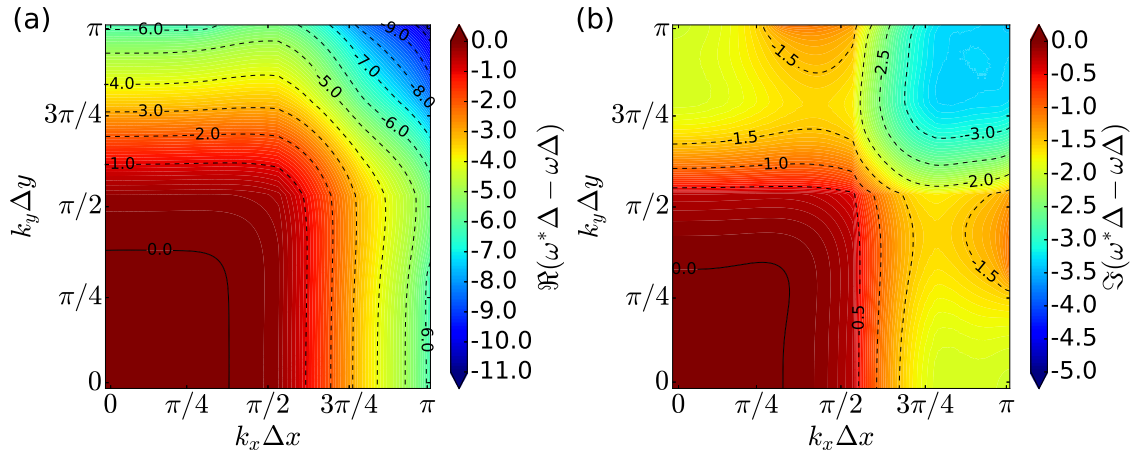


Figure 4.8: Measure of phase (a) and amplitude (b) error of TENO5 scheme in 2D wavenumber space based on the dispersion relation of the LEE

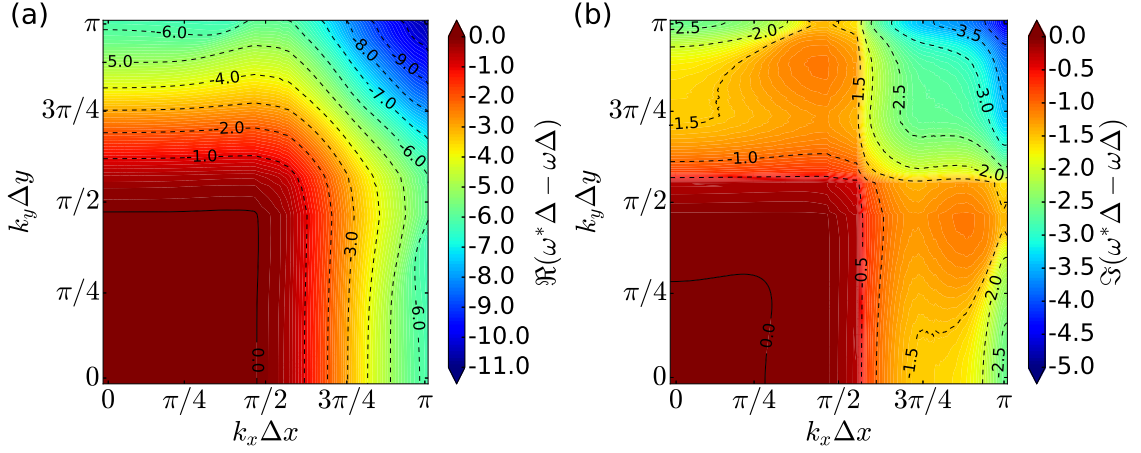


Figure 4.9: Measure of phase (a) and amplitude (b) error of TENO6 scheme in 2D wavenumber space based on the dispersion relation of the LEE

4.4 Formulation of MDCD-TENO and spectral optimization

In this part, we present a novel framework for which the numerical scheme can be optimized in multidimensional wavenumber space based on the dispersion relation of the two-dimensional convection or LEE. The basic idea is to optimize the weighting contribution of the linear part of the nonlinear scheme based on either the dispersion relation of the two-dimensional convection equation or LEE. The dissipation and dispersion error of the background linear scheme is the main source of dissipation and dispersion error in a non linear shock capturing scheme. Based on the work of [Sun et al., 2011], a novel approach was developed to separately optimise the dissipation and dispersion properties of linear finite difference schemes based on two independent parameters; γ_{disp} and γ_{diss} . These schemes are known as the minimal dispersion and controllable dissipation (MDCD) schemes. In this work, the TENO scheme is split into a linear and nonlinear part from which the weighting associated with the linear part of the TENO scheme can be expressed in terms of the two free parameters of the MDCD schemes. Expressing the linear scheme in terms of the weighting parameters allows for the specific tailoring of the dispersion and dissipation property of the numerical scheme. The only drawback of such an approach is that the schemes are optimized for their dissipation and dispersion properties at the expense of their formal order of accuracy. Different from the work of [Sun et al.,

2011], the cost function used in this optimization is the minimization of the integrated sum of dispersive error, E_{disp} in two-dimensional wavenumber space. Since the dispersion and dissipation property of the numerical scheme can be separately optimized, the cost function only considers the dispersion error. The dispersion error for every reduced wavenumber combination is multiplied by an exponential term, $e^{\beta(2\pi-k_x\Delta x-k_y\Delta y)}$ so as to ensure a larger weighting for error closer to the lower wavenumber range. β is a parameter which controls the magnitude of the weighting. The objective function is given as

$$E_{disp} = \frac{1}{e^{2\beta\pi}} \int_{r_1\pi}^{r_2\pi} \int_{r_1\pi}^{r_2\pi} |\Re(\omega_{scheme}^* \Delta - \omega \Delta)| e^{\beta(2\pi-k_x\Delta x-k_y\Delta y)} dk_x \Delta x dk_y \Delta y. \quad (4.25)$$

It should be noted that $\Delta = \Delta x = \Delta y$. r_1 and r_2 are set to 0.1 and 0.8 respectively. They represent the considered wavenumber range for which the error is integrated for the optimization process. The free parameters to be optimized in this context is the values of γ_{disp} and γ_{diss} used in the weighting of the of the sub schemes of the TENO6 scheme. The remaining parameters are kept the same as the original TENO6 scheme. By weighting the integrated error more in the low wavenumber range, the error in the low wavenumber range can be reduced more effectively through the optimization procedure.

4.4.1 The MD-CD-TENO scheme

The semi-discrete finite difference scheme in conservative form can be written as:

$$\frac{\partial f}{\partial x} = \frac{\hat{f}_{i+1/2} - \hat{f}_{i-1/2}}{\Delta x} \quad (4.26)$$

where $\hat{f}_{i+1/2}$ is the numerical flux. The numerical flux of the TENO scheme can be rewritten in terms of a combination of a linear and nonlinear part:

$$\hat{f}_{i+1/2} = \underbrace{\sum_{k=0}^r C_k^r \hat{f}_{k,i+1/2}^r}_{linear} + \underbrace{\sum_{k=0}^r (\omega_k - C_k^r) \hat{f}_{k,i+1/2}^r}_{nonlinear} \quad (4.27)$$

where

$$\begin{aligned}
 \hat{f}_{0,i+1/2}^3 &= -\frac{1}{6}f_{i-1} + \frac{5}{6}f_i + \frac{2}{6}f_{i+1} \\
 \hat{f}_{1,i+1/2}^3 &= \frac{2}{6}f_i + \frac{5}{6}f_{i+1} - \frac{1}{6}f_{i+2} \\
 \hat{f}_{2,i+1/2}^3 &= \frac{2}{6}f_{i-2} - \frac{7}{6}f_{i-1} + \frac{11}{6}f_i \\
 \hat{f}_{3,i+1/2}^3 &= \frac{3}{12}f_i + \frac{13}{12}f_{i+1} - \frac{5}{12}f_{i+2} + \frac{1}{12}f_{i+3}.
 \end{aligned} \tag{4.28}$$

The linear part mainly affects the formal order of accuracy while the nonlinear part is responsible for capturing the discontinuities. For the nonlinear part, ω_k is the weighting related to the relative smoothness of f on each set of candidate stencils. It is defined similarly as the original TENO scheme given in equations (4.10) to (4.13). For the linear part, C_k^r is the optimal weight which can be written in terms of the free parameters. The optimal weights are derived by comparing the expanded form of the linear part of equation (4.27) to the form of the minimized dispersion and controllable dissipation (MD CD) schemes given in equation (4.29). The general form of the MD CD schemes is given as [Sun et al., 2011]:

$$f'(x) = f'_C + \alpha f'_L + \beta f'_R, \tag{4.29}$$

where

$$\begin{aligned}
 f'_C &= \frac{1}{\Delta x} \sum_{m=-r+1}^{r-1} a_m f_m \\
 f'_L &= \frac{1}{\Delta x} \sum_{m=-r}^{r-1} (-1)^{r-m-1} \binom{2r-1}{r-m-1} f_m \\
 f'_R &= \frac{1}{\Delta x} \sum_{m=-r+1}^{r-1} (-1)^{r-m} \binom{2r-1}{r-m} f_m.
 \end{aligned} \tag{4.30}$$

The binomial coefficient $\binom{n}{k}$ is defined by $\binom{n}{k} = \frac{n!}{k!(n-k)!}$. $\gamma_{disp} = \alpha + \beta$ and $\gamma_{dissp} = \alpha - \beta$ are two independent parameters which can be used to separately optimize the dispersion

and dissipation property of the scheme separately. For the case of $r = 3$, the expanded form of the $(2r - 2)^{th}$ order MDCCD scheme is given as [Sun et al., 2011]

$$f'(x) = \frac{1}{\Delta x} \left[\begin{aligned} &(-\frac{1}{2}\gamma_{disp} - \frac{1}{2}\gamma_{diss})f_{i-3} + (2\gamma_{disp} + 3\gamma_{diss} + \frac{1}{12})f_{i-2} \\ &+ (-\frac{5}{2}\gamma_{disp} - \frac{15}{2}\gamma_{diss} - \frac{2}{3})f_{i-1} + 10\gamma_{disp}f_i + (\frac{5}{2}\gamma_{disp} - \frac{15}{2}\gamma_{diss} + \frac{2}{3})f_{i+1} \\ &+ (-2\gamma_{disp} + 3\gamma_{diss} - \frac{1}{12})f_{i+2} + (\frac{1}{2}\gamma_{disp} - \frac{1}{2}\gamma_{diss})f_{i+3} \end{aligned} \right]. \quad (4.31)$$

The resulting optimal weights, C_k^r are shown in table 4.1.

C_0	C_1	C_2	C_3
$\frac{1}{2} - \frac{3}{2}\gamma_{disp} + \frac{9}{2}\gamma_{diss}$	$\frac{1}{2} - 6\gamma_{disp}$	$\frac{3}{2}(\gamma_{disp} + \gamma_{diss})$	$6\gamma_{disp} - 6\gamma_{diss}$

Table 4.1: Optimal weights C_k for MDCCD-TENO6 scheme, $r = 3$

The key advantage of this framework is that this allow for specific tailoring of the dispersion or dissipation of the nonlinear scheme based on the absolute value of $|\gamma_{disp}|$ and $|\gamma_{diss}|$ respectively.

4.4.2 The hybrid scheme

Since the computation of the nonlinear term of the MDCCD-TENO6 scheme is very time consuming and that the nonlinear mechanism of the shock capturing scheme may deteriorate the spectral properties of the scheme even in the smooth region, a hybrid scheme which combines the MDCCD-TENO6 scheme with its linear counterpart is proposed. The reason for the use of the fourth order MDCCD scheme lies in the fact that the stencil width of the linear MDCCD scheme is the same as that of the TENO6 scheme. The hybridization strategy of the numerical flux is inherently based on the smoothness indicator of the TENO6 scheme. The numerical flux of the hybrid scheme is expressed as

$$\hat{f}_{i+1/2}^{Hybrid} = \sigma_{i+1/2}\hat{f}_{i+1/2}^{MDCCD} + (1 - \sigma_{i+1/2})\hat{f}_{i+1/2}^{MDCCD-TENO6}, \quad (4.32)$$

where $\sigma_{i+1/2}$ is the blending factor. $\hat{f}_{i+1/2}^{MDCCD}$ and $\hat{f}_{i+1/2}^{MDCCD-TENO6}$ are the numerical fluxes

of the MDCD scheme and the MDCD-TENO6 scheme. The numerical flux of the MDCD scheme is given by the linear part of equation (4.27) and the optimal weighting is provided in table 4.1. The blending factor is given by

$$\sigma_{i+1/2} = \min(1, \frac{r_{i+1/2}}{r_c}), \quad (4.33)$$

where r_c is a threshold parameter used to control the contribution of the linear scheme to the overall spectral property. r_c is set to 0.06 based on numerical experiments and the optimal spectral properties desired. A lower value of r_c would imply that a higher percentage of the numerical flux would be computed by the linear MDCD scheme. However, setting too low value of r_c would lead to a loss of shock capturing properties. $r_{i+1/2}$ is the blending function computed from the smoothness indicator, β_k of the TENO scheme;

$$r_{i+1/2} = \min(\frac{|\beta_k|}{\sum_{k=0}^3 |\beta_k|}) \quad k = 0, 1, 2, 3. \quad (4.34)$$

The algorithm works as follows:

$$f_{i+1/2}^{Hybrid} = \begin{cases} f_{i+1/2}^{MDCD} & \text{since } \sigma_{i+1/2} = 1, & \text{if } |\beta_{k,max} - \beta_{k,min}| < \Delta x^n, \\ \sigma_{i+1/2} \hat{f}_{i+1/2}^{MDCD} + (1 - \sigma_{i+1/2}) \hat{f}_{i+1/2}^{MDCD-TENO6}, & \text{else.} \end{cases} \quad (4.35)$$

n is set to 4 and 8 for one dimensional and multi-dimensional problems respectively. In equation (4.35), $\sigma_{i+1/2}$ is taken to be 1 if $|\beta_{k,max} - \beta_{k,min}|$ is less than Δx^n .

4.4.3 Spectral properties of the hybrid scheme

In this subsection, the spectral properties of the hybrid scheme with respect to the original TENO6 scheme will be analysed in both 1D and 2D wavenumber space. The proposed hybrid scheme will be denoted as the HYB-MDCD-TENO6 here-after. Since the dispersion and dissipation properties of the numerical scheme can be tailored separately, the value of γ_{disp} will first be optimized for its dispersion properties. In figure 4.10, the integrated error, E_{disp} is plotted as a function of γ_{disp} for different β values considered. The

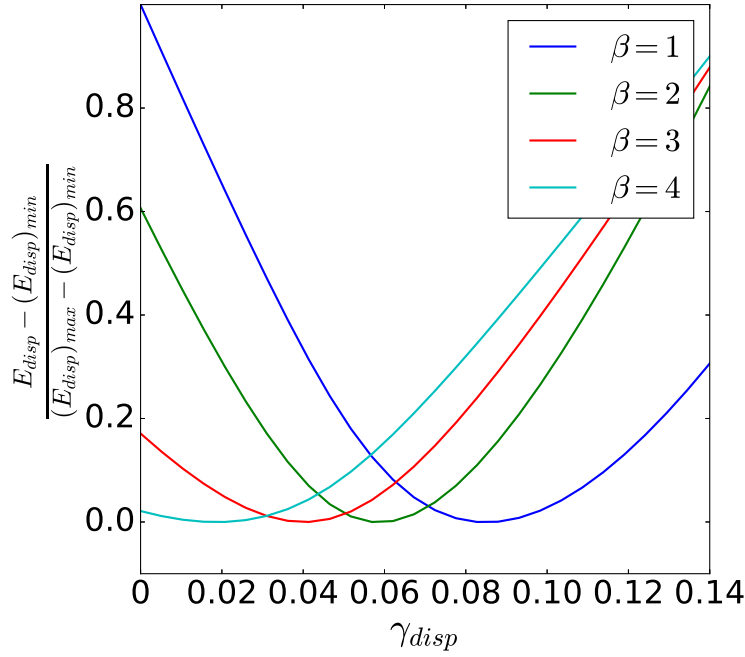


Figure 4.10: Comparison of normalized integrated dispersion error, $\frac{E_{disp} - (E_{disp})_{min}}{(E_{disp})_{max} - (E_{disp})_{min}}$ as a function of γ_{disp} for different β values

optimal value of γ_{disp} for each value of β considered is shown in table 4.2.

β	1	2	3	4
γ_{disp}	0.0827	0.0568	0.0413	0.0207

Table 4.2: Optimized values of γ_{disp} for different values of β

Using the framework of the MDCD scheme ensures that both the dispersion and dissipation property can be separately controlled through γ_{disp} and γ_{diss} respectively. For stability reason, the dissipation should be non negative for all wavenumber. It can be seen in figure 4.11 that an optimal γ_{disp} value of 0.0568 gives the best dispersion property for the hybrid scheme. Setting a lower than optimal value (e.g. $\gamma_{disp} = 0.0413$) would lead to a poorer dispersion properties than desired. On the other hand, setting a higher than optimal value (e.g. $\gamma_{disp} = 0.0827$) would lead to overshoot of the dispersion property beyond the exact solution. This can lead to spurious wave travelling at faster speed than the exact solution. In principle, the dissipation must be as small as possible but sufficiently large to ensure the stability of the simulation and the damping of the spurious

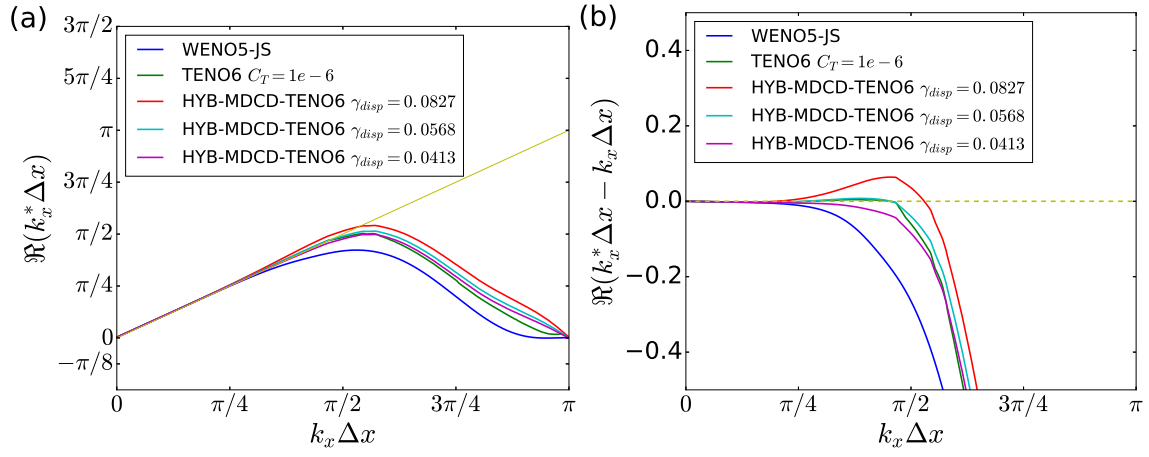


Figure 4.11: Comparison of (a) dispersion, $\Re(k_x^* \Delta x)$ property and (b) phase error, $\Re(k_x^* \Delta x - k_x \Delta x)$ of hybrid and baseline schemes

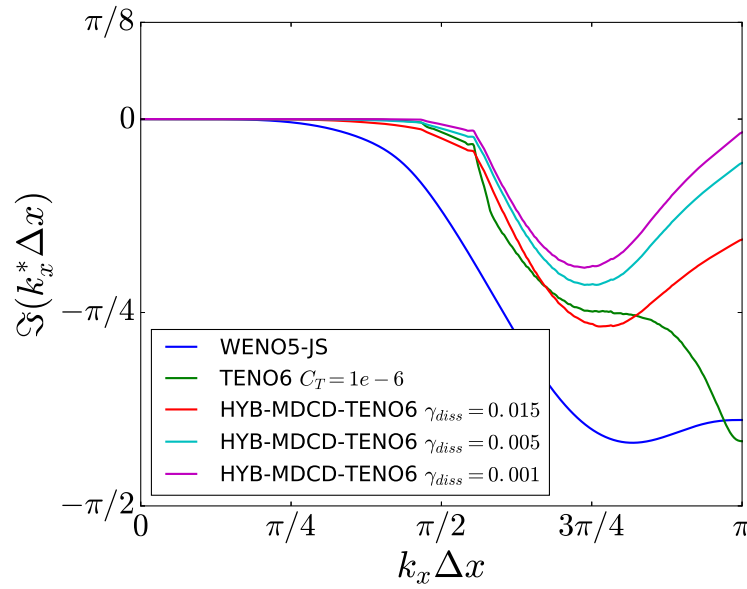


Figure 4.12: Comparison of dissipation, $\Im(k_1^* \Delta x)$ property of hybrid schemes with different values of γ_{diss}

numerical oscillation. Consequently, the optimal value of dissipation is problem dependent. A proper way to decide on the optimal value of γ_{diss} is to begin with a low value of 0.001 and then increasing it gradually if the numerical solution exhibits spurious oscillation near discontinuity. An advantage of using the MDCD scheme is that this allows for the flexibility in adjusting the dissipation without affecting the dispersion property. In the instance that there is no numerical stability issues or spurious numerical oscillation, the dissipation of the hybrid scheme can be significantly reduced by choosing a very small $|\gamma_{diss}|$. The flexibility in adjusting the dissipation makes it possible to develop a robust code for the simulation of problems with discontinuities. In principle, γ_{diss} can be chosen in an adaptive way. For the purpose of comparison, the value of γ_{diss} will be set to 0.001, 0.005 and 0.015. The dissipation property of the hybrid scheme under different values of γ_{diss} is shown in figure 4.12. It can be seen that choosing a larger value of γ_{diss} would lead to more numerical dissipation at intermediate wavenumber. In the remaining part of the chapter, γ_{diss} is set to 0.001 for all simulation test cases. In two-dimensional wavenumber space, the phase and amplitude error of the hybrid scheme is illustrated in figures 4.13 and 4.14. It can be seen that the hybrid scheme has the least phase error, although the result of the TENO6 scheme is very similar. As for the amplitude error, it can be seen that the hybrid scheme has the least amplitude error among the different schemes.

Other than optimizing the scheme based on the advection equation, the hybrid scheme can also be optimized based on the dispersion relation of the LEE. Using the dispersion relation of the two dimensional LEE leads to a different set of optimized values for γ_{disp} . The results are shown in table 4.3. A comparison of the dispersion error in two dimensional wavenumber space of the hybrid schemes with different values of γ_{disp} as compared to the baseline WENO5-JS and TENO6 scheme is shown in figure 4.15.

β	1	1.5	2	2.5	3
γ_{disp}	0.0879	0.0724	0.062	0.0517	0.0465

Table 4.3: Optimized values of γ_{disp} for different values of β

In figures 4.15a and 4.15b, it can be seen that using a higher than optimal value of γ_{disp} will lead to larger error in the low wavenumber range where the error should be almost

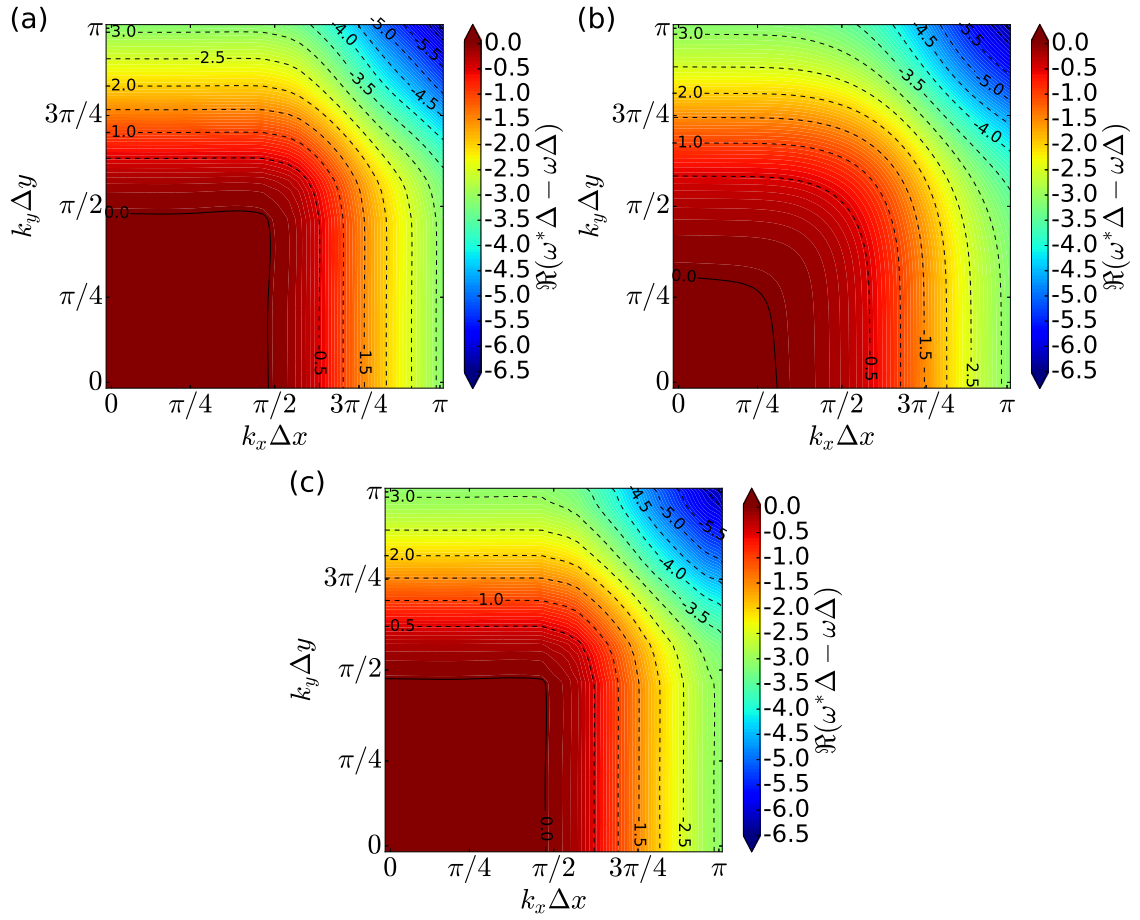


Figure 4.13: Comparison of phase error of (a) hybrid scheme ($\gamma_{disp} = 0.0568$) with baseline (b) WENO5-JS and (c) TENO6 $C_T = 1e-6$ schemes in two dimensional wavenumber space based on the dispersion relation of the two dimensional advection equation

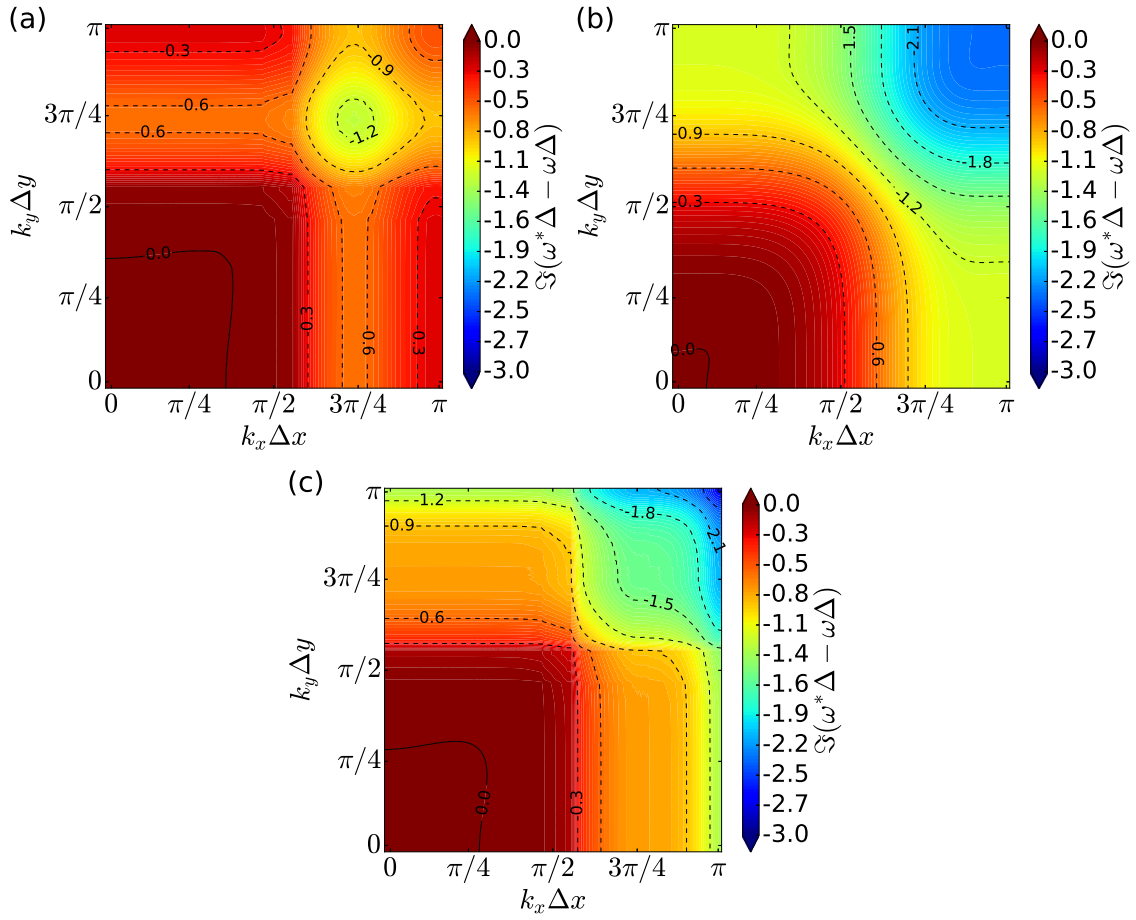


Figure 4.14: Comparison of amplitude error of (a) hybrid scheme ($\gamma_{diss} = 0.001$) with baseline (b) WENO5-JS and (c) TENO6 $C_T = 1e-6$ schemes in two-dimensional wavenumber space based on the dispersion relation of the two dimensional advection equation

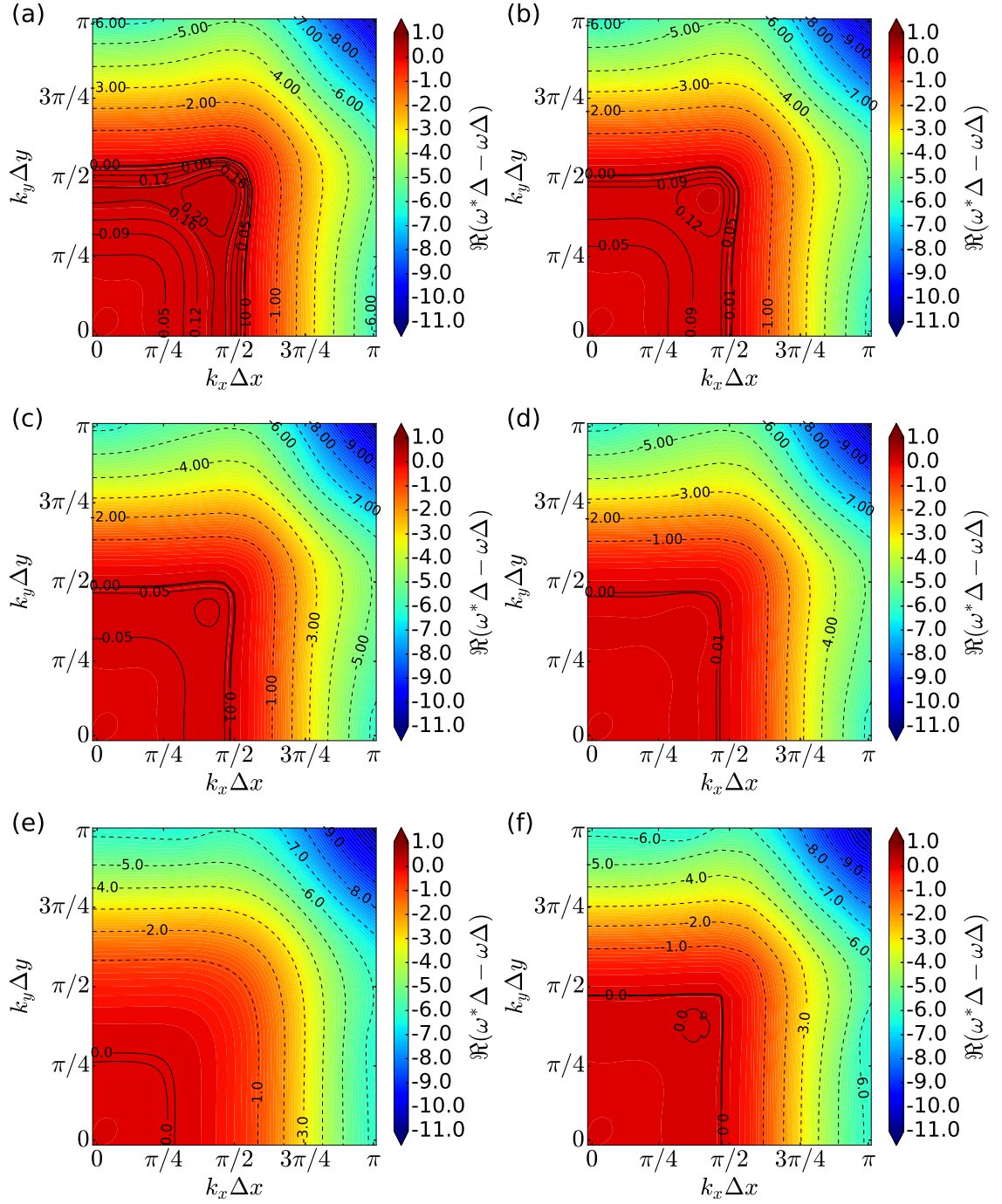


Figure 4.15: Comparison of dispersion error of (a) hybrid scheme ($\gamma_{disp} = 0.0879$), (b) hybrid scheme ($\gamma_{disp} = 0.0724$), (c) hybrid scheme ($\gamma_{disp} = 0.062$), (d) hybrid scheme ($\gamma_{disp} = 0.0517$), (e) WENO5-JS and (f) TENO6 $C_T = 1e-6$ schemes in two dimensional wavenumber space based on the dispersion relation of the two-dimensional LEE

zero. On the other hand, a comparison of figures 4.15c and 4.15d shows that using a lower than optimal value of γ_{disp} leads to greater error in the high wavenumber range instead. An optimal value of γ_{disp} is found to be about 0.062. This is shown in figure 4.15c. In the following section, the results of the hybrid schemes optimized based on the convection and linearized Euler equations will be compared with the baseline schemes.

4.5 Characteristic wise reconstruction and code parallelization

In the following sections, the WENO5, WENO7, TENO5, TENO6 and HYB-MDCD-TENO6 schemes are applied to solve the compressible Euler and Navier-Stokes equations. In order to avoid any numerical oscillation when dealing with flows having discontinuities, local characteristic decomposition method is used. This involves the projection of the numerical flux vector onto the characteristic space.

4.5.1 Characteristic wise reconstruction

For the sake of brevity, the procedure is illustrated here using the one-dimensional Euler equations of gas dynamics. In conservative form, the equation can be written as

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} = \mathbf{0}, \quad (4.36)$$

where

$$\mathbf{U} = \begin{bmatrix} \rho \\ \rho u \\ e \end{bmatrix}, \quad \mathbf{F} = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ u(e + p) \end{bmatrix}. \quad (4.37)$$

where ρ is the density, u is the velocity and $e = \frac{p}{\gamma-1} + \frac{1}{2}\rho u^2$ is the total energy. γ is set to 1.4. $c = \sqrt{\gamma p / \rho}$. The inviscid fluxes are computed by considering the local characteristic flux decomposition. This procedure involves the following steps [Sun et al., 2011]:

1. At each fixed $x_{i+1/2}$, the average state $\mathbf{U}_{i+1/2}$ is computed by the Roe average [Roe, 1981].

2. The left eigenvector matrix, $\mathbf{L}_{i+1/2}$ and right eigenvector matrix, $\mathbf{R}_{i+1/2}$ are evaluated at the average state. Eigenvalues $\lambda_{i+1/2}$ of the Jacobian matrix, $\frac{\partial \mathbf{F}}{\partial \mathbf{U}}$ are computed at the averaged states.
3. For each candidate stencils, the local characteristic decomposition of the fluxes are computed by $\mathbf{W}_m = \mathbf{L}_{i+1/2} \mathbf{F}_m$, $m \in [i - r + 1, i + r]$. r is chosen as either 2 or 3 depending on the scheme considered.
4. The numerical characteristic flux is split using the Lax-Friedreich splitting method [Jiang and Shu, 1996, He et al., 2015, Peng et al., 2019] as follows: $\mathbf{W}_m^\pm = \frac{1}{2}(\mathbf{L}_{i+1/2} \mathbf{F}_m \pm \alpha(\mathbf{L}_{i+1/2} \mathbf{U}_m))$, where $\alpha = \max_{i+1/2}(|u_{i+1/2}| + c_{i+1/2})$, corresponds to the maximum eigenvalue of the Jacobian matrix. For the sake of simplicity and robustness [He et al., 2015, Jiang and Shu, 1996, Peng et al., 2019], the maximum eigenvalue is used for all components of the numerical flux. The maximum eigenvalue used corresponds to the maximum eigenvalue across all grid points.
5. In the case of the WENO/TENO scheme, flux function reconstruction is performed as follows;
 $\hat{\mathbf{W}}_{i+1/2}^\pm = \sum_{k=0}^n \omega_k^\pm \mathbf{W}_{k,i+1/2}^\pm$, $n = 2, 3$ depending on the scheme. $\omega_k^\pm$ is the weighting of the TENO/WENO scheme computed according to the characteristic variables on each stencil.
 In the case of the HYB-MDCD-TENO6 scheme, $\hat{\mathbf{W}}_{i+1/2}^\pm = \sigma_{i+1/2} \hat{\mathbf{W}}_{i+1/2}^{\pm, \text{MDCD}} + (1 - \sigma_{i+1/2}) \hat{\mathbf{W}}_{i+1/2}^{\pm, \text{MDCD-TENO6}}$. It should be noted that $\sigma_{i+1/2}$ is a vector and it varies for each flux component.
6. After the WENO/TENO or HYB-MDCD-TENO6 reconstruction of the projected variables, the obtained values are then projected back to the physical space by projecting onto the right eigenvectors of the cell interface: $\hat{\mathbf{F}}_{i+1/2}^\pm = \mathbf{R}_{i+1/2} \hat{\mathbf{W}}_{i+1/2}^\pm$

In step 1, Roe averaged primitive variables are computed as [Roe, 1981]:

$$\bar{u} = \frac{\sqrt{\rho_i} u_i + \sqrt{\rho_{i+1}} u_{i+1}}{\sqrt{\rho_i} + \sqrt{\rho_{i+1}}}, \quad (4.38)$$

$$\bar{h} = \frac{\sqrt{\rho_i}h_i + \sqrt{\rho_{i+1}}h_{i+1}}{\sqrt{\rho_i} + \sqrt{\rho_{i+1}}}, \quad (4.39)$$

$$\bar{c} = \sqrt{(\gamma - 1)(\bar{h} - \frac{1}{2}\bar{u}^2)}, \quad (4.40)$$

$$h = \frac{p}{(\gamma - 1)\rho} + \frac{1}{2}u^2 + \frac{p}{\rho}. \quad (4.41)$$

In step 2, the eigenvalue matrix is given as:

$$\Lambda = \begin{bmatrix} u - c & & \\ & u & \\ & & u + c \end{bmatrix}. \quad (4.42)$$

In step 3, the left and right eigenvector matrix are given as:

$$\mathbf{L}_{i+1/2} = \begin{bmatrix} \mathbf{l}_0 \\ \mathbf{l}_1 \\ \mathbf{l}_2 \end{bmatrix} = \begin{bmatrix} \frac{\gamma-1}{4} \frac{\bar{u}^2}{\bar{c}^2} + \frac{1}{2} \frac{\bar{u}}{\bar{c}} & -\frac{\gamma-1}{2} \frac{\bar{u}}{\bar{c}^2} - \frac{1}{2} \frac{1}{\bar{c}} & \frac{\gamma-1}{2} \frac{1}{\bar{c}^2} \\ 1 - \frac{\gamma-1}{2} \frac{\bar{u}^2}{\bar{c}^2} & \frac{\gamma-1}{2} \frac{\bar{u}}{\bar{c}^2} & -\frac{\gamma-1}{2} \frac{1}{\bar{c}^2} \\ \frac{\gamma-1}{4} \frac{\bar{u}^2}{\bar{c}^2} - \frac{1}{2} \frac{\bar{u}}{\bar{c}} & -\frac{\gamma-1}{2} \frac{\bar{u}}{\bar{c}^2} + \frac{1}{2} \frac{1}{\bar{c}} & \frac{\gamma-1}{2} \frac{1}{\bar{c}^2} \end{bmatrix}, \quad (4.43)$$

$$\mathbf{R}_{i+1/2} = \begin{bmatrix} \mathbf{r}_0 & \mathbf{r}_1 & \mathbf{r}_2 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 \\ \bar{u} - \bar{c} & \bar{u} & \bar{u} + \bar{c} \\ \frac{\bar{u}^2}{2} + \frac{\bar{c}}{\gamma-1} - \bar{u}\bar{c} & \frac{\bar{u}^2}{2} & \frac{\bar{u}^2}{2} + \frac{\bar{c}}{\gamma-1} + \bar{u}\bar{c} \end{bmatrix}. \quad (4.44)$$

The characteristic wise reconstruction technique can be extended to the multidimensional Euler equations. In this case, this involves the right eigenvector, left eigenvector and eigenvalue of the Jacobians, $\frac{\partial \mathbf{F}}{\partial \mathbf{U}}$, $\frac{\partial \mathbf{G}}{\partial \mathbf{U}}$ and $\frac{\partial \mathbf{H}}{\partial \mathbf{U}}$. This is provided in appendix A.1 and A.2 for 2D and 3D respectively. For the discretization of the viscous term of the Navier-Stokes equation, standard 4th order central or one sided differencing schemes are used. For second order derivatives, the first order differentiation is applied two times for cross derivative terms. For non-crossed second order derivatives, second order derivatives formulas are used directly. For nodal points close to the boundary of each processor domain, one sided differencing formula is used when computing the second order derivatives. This is

necessary in order to keep the number of ghost points fixed on each side of the processor domain.

4.5.2 Code parallelization

When characteristic wise reconstruction methods are used in multi-dimensional space, this can lead to considerable slowdown in computational performance. In order to speed up the computation of the solver, parallelization technique is employed. In this sub section, we describe the technique used to parallelize the code. The computational code was developed in C++ and uses the in-built MPI and OPENMP library to perform domain decomposition. Hybrid MPI-OMP technique is used to maximise performance. MPI is used to decompose the domain into multiple processors domain and OPENMP is used on each processor domain. For each processor domain, the total number of ghost points used in each spatial direction is decided based on the stencil width of the scheme used for the spatial discretization. The domain decomposition process of a 2D domain is illustrated in figure 4.16. The other key aspect of code parallelization is to ensure communication between the ghost points of each processor domain and the interior points of adjacent processor domain. For a 2D domain decomposition, this would require up to $4n$ send and receive commands, where n represents the number of ghost points on each side of the processor domain. For a 3D domain decomposition, this would require up to $6n$ send and receive commands. For this purpose, the MPI_Sendrecv command was used. In order to define the physical boundary, the grid points located at the edge of the physical domain needs to be identified. This is usually identified by using a global indexing method to identify the nodal points (interface and ghost points) related to the physical boundary. Ghost point based boundary method is then used to impose the physical boundary condition.

4.6 Numerical experiments

In this section, numerical results for different canonical cases based on the one dimensional advection as well as the one, two and three dimensional Euler/Navier Stokes

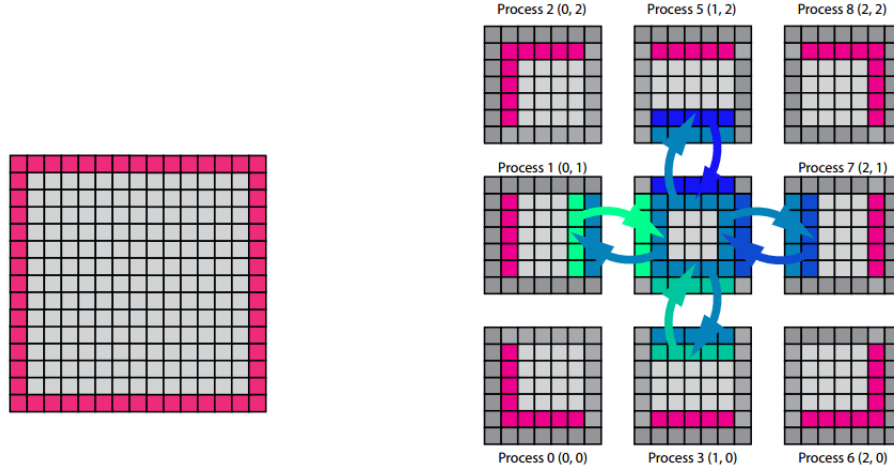


Figure 4.16: Illustration of 2D domain decomposition and information communication between processors. Adapted from [Moore, 2016].

equations are discussed.

4.6.1 1D Advection

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0 \quad (4.45)$$

The initial condition of this problem [Peng and Shen, 2015] is given as follows:

$$u_0(x) = \begin{cases} \frac{1}{6}(G(x, \beta, z - \delta) + G(x, \beta, z + \delta) + 4G(x, \beta, z)), & -0.8 \leq x \leq -0.6, \\ 1, & -0.4 \leq x \leq -0.2, \\ 1 - |10(x - 0.1)|, & 0 \leq x \leq 0.2, \\ \frac{1}{6}(F(x, \alpha, \alpha - \delta) + F(x, \alpha, \alpha + \delta) + 4F(x, \alpha, a)), & 0.4 \leq x \leq 0.6, \\ 0, & \text{otherwise} \end{cases} \quad (4.46)$$

where

$$G(x, \beta, z) = e^{-\beta(x-z)^2}, F(x, \alpha, a) = \sqrt{\max(1 - \alpha^2(x-a)^2, 0)}$$

$$a = 0.5, \quad z = -0.7, \quad \delta = 0.005, \quad \alpha = 10, \quad \beta = \log 2/36\delta^2$$

It composed of a smooth combination of Gaussian, a square wave, a sharp triangle wave and a half ellipse. The exact solution of equation (4.45) at time t with the initial condition $u_0(x)$ is given by $u(x, t) = u_0(x - t)$. The computational domain is taken to be $[-1, 1]$. Periodic boundary condition is applied at both ends. The results at $t=2$ with 200 points are shown in figure 4.17a. Detailed plots of the square wave and Gaussian are presented in figures 4.17b and 4.17c. It can be seen that the results of the hybrid scheme are almost similar to the baseline TENO6 scheme for the same grid resolution. Also, it can be seen that both the TENO5 and TENO6 schemes generally give better results than the baseline WENO5-JS and WENO7-JS scheme. Similar results highlighting the superiority of the TENO scheme with respect to the WENO scheme can be found in [Fu et al., 2016].

4.6.2 1D Euler

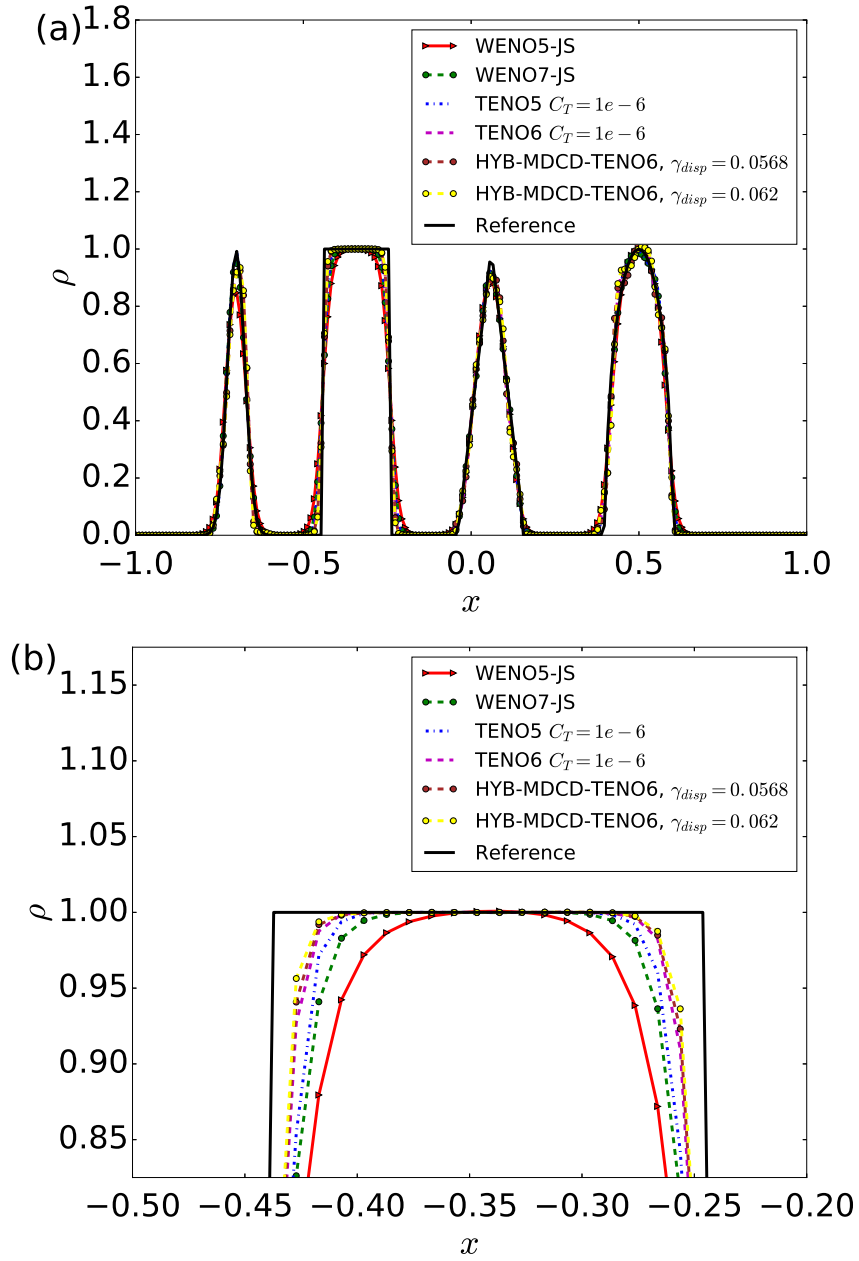
The one dimensional Euler equations are given in equations (4.36) and (4.37). Three typical examples are considered as given in sub sections below.

1D Euler - Sod

The initial condition of the Sod problem is given by:

$$(\rho, u, p) = \begin{cases} (1.0, 0, 1.0), & \text{if } x \leq 0, \\ (0.125, 0, 0.1), & x > 0. \end{cases} \quad (4.47)$$

The solutions are compared at $t = 0.14$. For the purpose of comparison, a uniform grid of 200 points are used. The reference result is computed using the WENO5-JS scheme with a fine grid of 2000 points. For the purpose of numerical verification, the reference result is compared against exact solution of the shock tube problem. The procedure for calculating the exact solution and its comparison with the reference numerical solution are shown in



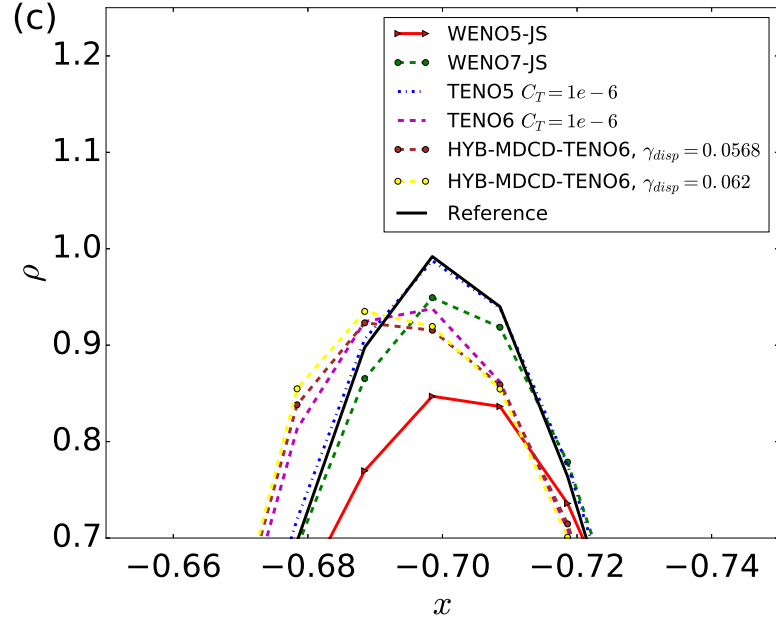


Figure 4.17: (a) Solution of the linear advection equation for different schemes with initial condition given in equation (4.46) at $t=2$, (b) Detailed plot of the square wave. (c) Detailed plot of the Gaussian.

appendix A.3. The computational domain is taken to be $[-0.5, 0.5]$. Dirichlet boundary conditions are imposed on both ends of the boundaries. The results are plotted in figure 4.18. It can be seen that the results of the hybrid scheme are closer to the reference results as compared to the baseline TENO6 scheme. Also, it can be seen that the both the TENO5 and TENO6 give better results than the baseline WENO5-JS and WENO7-JS scheme. As previously mentioned, the blending factor is a measure of the usage of the linear MDCD scheme. It can be clearly seen that σ remain 1.0 when the flow region is smooth and become less than 1.0 when the flow display a sharp change in gradient. By utilizing the linear MDCD scheme in the smooth region of the flow, better spectral properties of the spatial discretization scheme can be achieved.

1D Euler - Lax

The initial condition of the Lax problem [Peng et al., 2019] is given by:

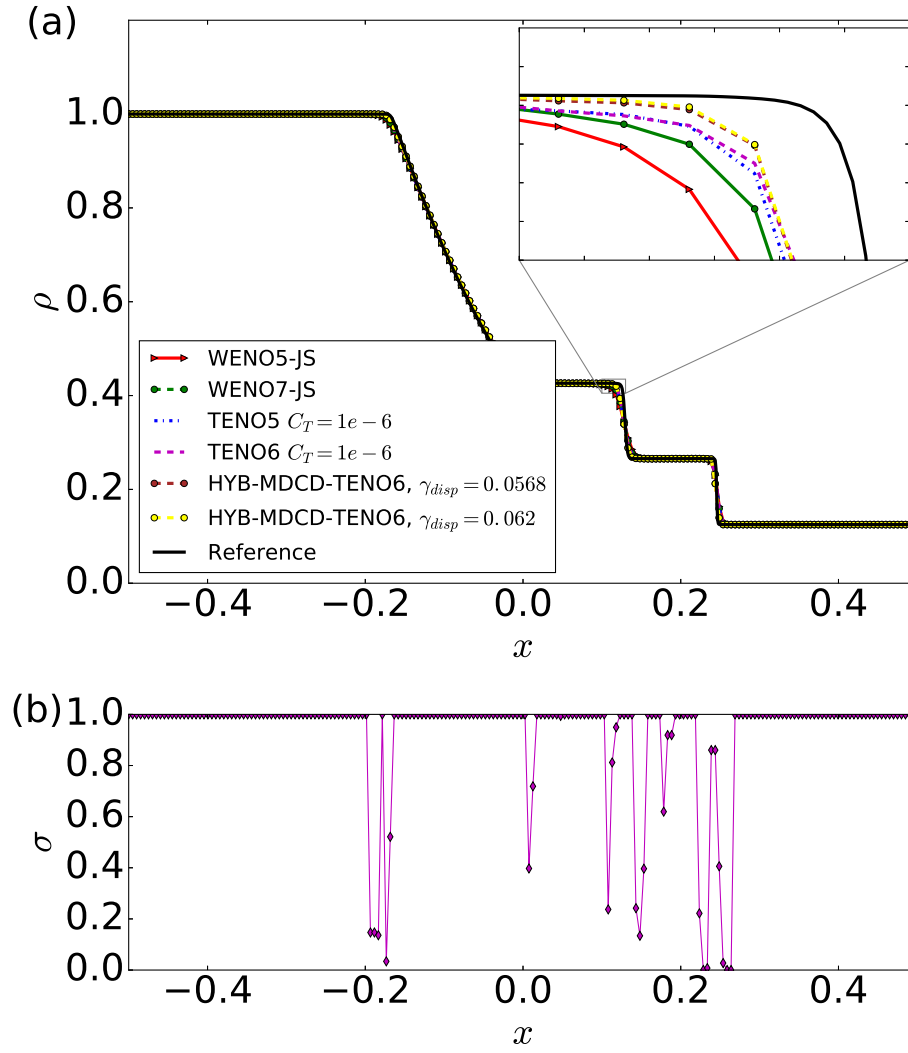


Figure 4.18: (a) Comparison of density profile at $t = 0.14$ for Sod problem, (b) Plot of blending factor, $\sigma(x, t)$ of first flux component at $t = 0.14$ for HYB-MDCD-TENO6, $\gamma_{disp} = 0.0568$ scheme.

$$(\rho, u, p) = \begin{cases} (0.445, 0.698, 3.528), & \text{if } x \leq 0, \\ (0.5, 0, 0.571), & x > 0. \end{cases} \quad (4.48)$$

The solutions are compared at $t = 0.13$. For the purpose of comparison, a uniform grid of 200 points are used. The reference result is computed using the WENO5-JS scheme with a fine grid of 2000 points. The computational domain is taken to be $[-0.5, 0.5]$. Dirichlet boundary conditions are imposed on both ends of the boundaries. The results are plotted in figure 4.19. It can be seen that the results of the hybrid scheme are closer to the reference results as compared to the baseline TENO6 scheme. Also, it can be seen that the both the TENO5 and TENO6 schemes give better results than the baseline WENO5-JS and WENO7-JS scheme. For the plot of the blending factor, it can be clearly seen that σ remain 1.0 when the flow region is smooth and become less than 1.0 when the flow display a sharp change in gradient.

1D Euler - Shu-Osher

This test problem represents an interaction between a Mach 3 shockwave and a sine entropy wave which generates a flow field with both small scale structures and discontinuities. The initial condition of the Lax problem [Peng et al., 2019] is given by:

$$(\rho, u, p) = \begin{cases} (0.445, 0.698, 3.528), & \text{if } x < -4, \\ (1.0 + \frac{1}{5} \sin(5x), 0, 1.0), & x \geq -4. \end{cases} \quad (4.49)$$

The solutions are compared at $t = 1.8$. For the purpose of comparison, a uniform grid of 200 points are used. The reference result is computed using the WENO5-JS scheme with a fine grid of 2000 points. The computational domain is taken to be $[-5.0, 5.0]$. Dirichlet boundary conditions are imposed on both ends of the boundaries. This test measures the ability of the numerical scheme to resolve the waves with short wavelength. The results are plotted in figure 4.20. It can be seen that the results of the hybrid scheme are very similar to the reference results as compared to the baseline TENO6 scheme. Also, it can be seen that the both the TENO5 and TENO6 schemes give better results than the

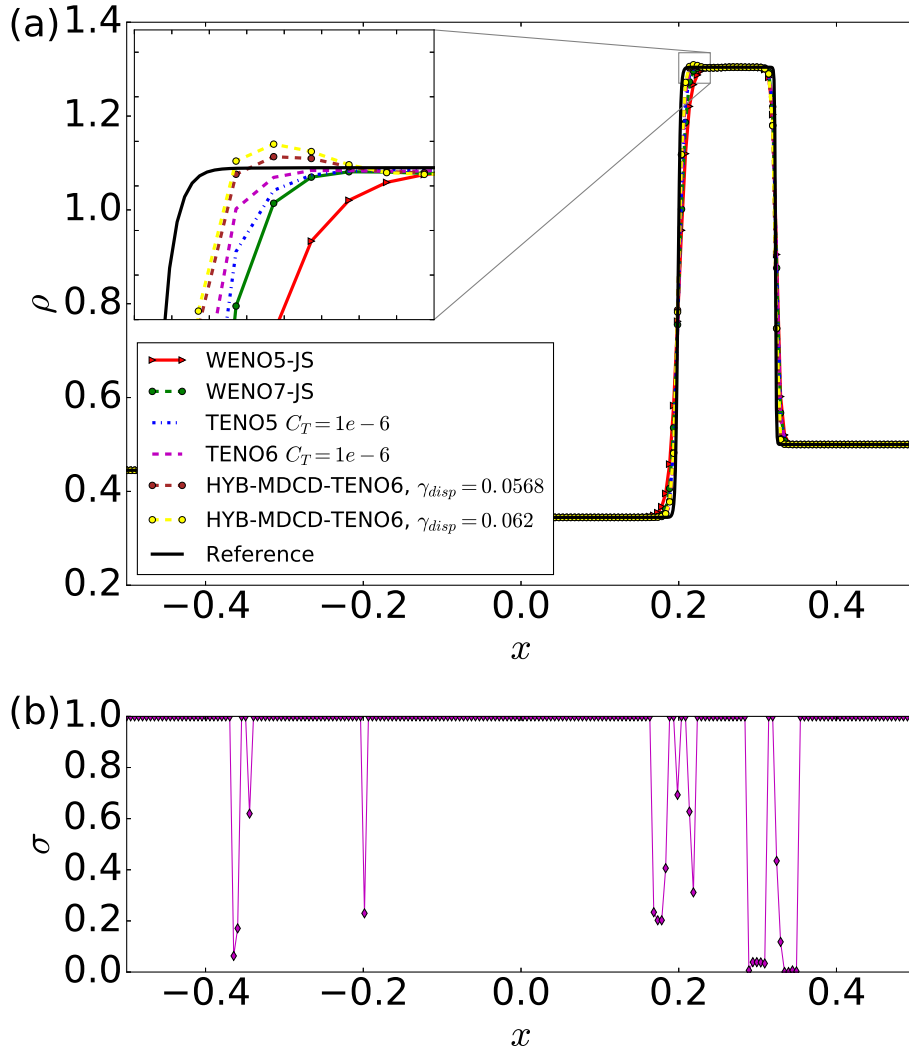


Figure 4.19: (a) Comparison of density profile at $t = 0.13$ for Lax problem, (b) Plot of blending factor, $\sigma(x, t)$ of first flux component at $t = 0.13$ for HYB-MDCD-TENO6, $\gamma_{disp} = 0.0568$ scheme.

baseline WENO5-JS and WENO7-JS scheme. As for the plot of the blending factor, it can be clearly seen that σ remain 1.0 when the flow region is smooth and become less than 1.0 when the flow display a sharp change in gradient.

4.6.3 2D Euler

The two dimensional Euler equations for ideal gas are given by:

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} + \frac{\partial \mathbf{G}}{\partial y} = \mathbf{0} \quad (4.50)$$

where the vectors $\mathbf{U}$, $\mathbf{F}$, $\mathbf{G}$ are expressed as:

$$\mathbf{U} = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ e \end{bmatrix} \quad \mathbf{F} = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ eu + pu \end{bmatrix} \quad \mathbf{G} = \begin{bmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ ev + pv \end{bmatrix} \quad (4.51)$$

In this section, two problems are tested. The first test is the double Mach reflection and the second test is the shock vortex interaction problem. Numerical results of the different schemes are compared with the original WENO5-JS scheme under a coarse grid. A fine grid case based on the WENO5-JS scheme with uniform grid in x and y is used for reference comparison.

2D Euler - Double Mach Reflection

The double Mach reflection test is a close representation of planar shock reflection in the air from a wedge. Instead of orientating the geometry to create an angled surface, the shock is orientated at an angle and the wall is kept parallel to the bottom domain. For this case, only the two dimensional Euler equation is considered. It is a widely used benchmark to test the ability of the numerical scheme to capture shock and resolve the small scale structures. For the present simulation, the computational domain is taken to be $[0,4] \times [0,1]$. From $x \geq \frac{1}{6}$, the lower boundary is set to be a reflecting free slip wall. At the initial state, a right moving Mach 10 shock is placed at $x = \frac{1}{6}$ with an incidence angle

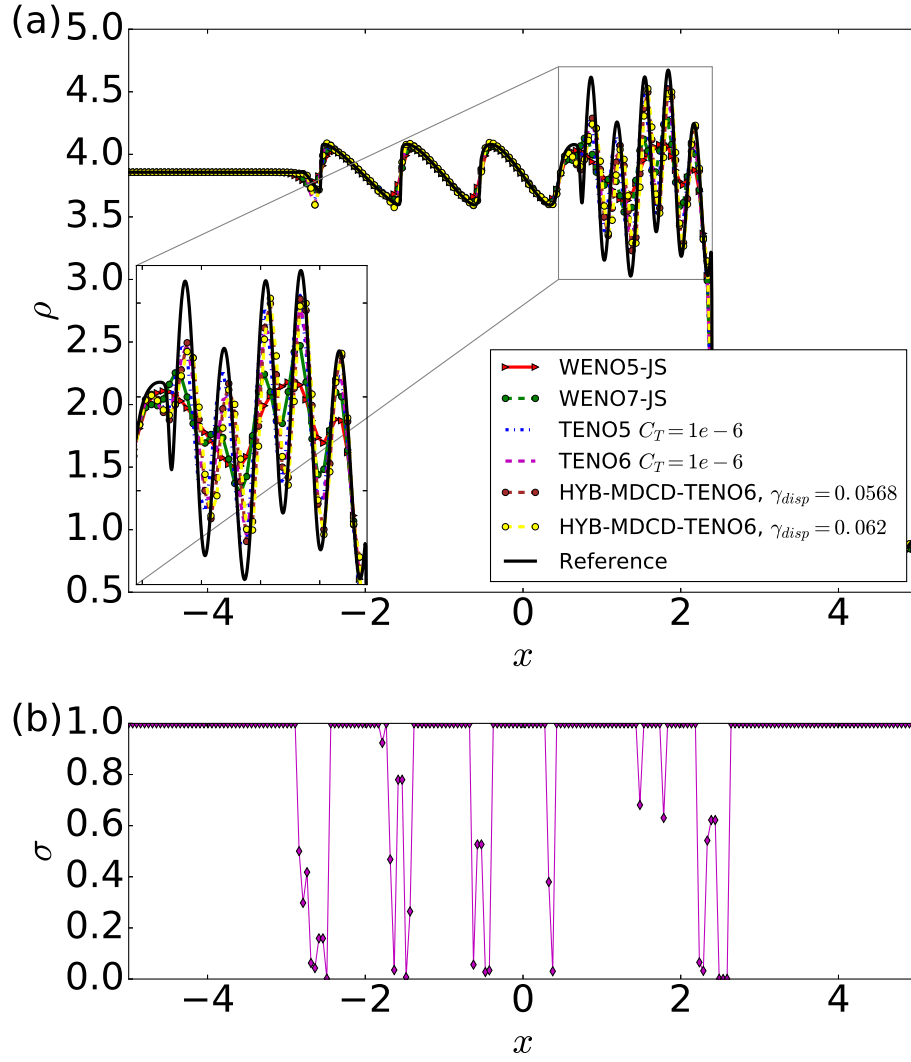


Figure 4.20: (a) Comparison of density profile at $t = 1.8$ for Shu-Osher problem, (b) Plot of blending factor, $\sigma(x, t)$ of first flux component at $t = 1.8$ for HYB-MDCD-TENO6, $\gamma_{disp} = 0.0568$ scheme.

of 60° to the x -axis. For the top boundary, the fluid variables are defined to exactly follow the evolution of the Mach 10 shock wave. Mathematically the top boundary is defined as:

$$(\rho, u, v, p) = \begin{cases} (8.0, 8.25 \sin(60), -8.25 \cos(60), 116.5), & \text{if } x < (\frac{1}{6} + (1.0 + 10t / \sin(60))), \\ (1.4, 0, 0, 1), & \text{otherwise.} \end{cases} \quad (4.52)$$

Inflow conditions are imposed fixed values based on the pre-shock condition while the outflow values at the ghost points are linearly extrapolated from the interior points. The initial condition is:

$$(\rho, u, v, p) = \begin{cases} (8.0, 8.25 \sin(60), -8.25 \cos(60), 116.5), & \text{if } x < (\frac{1}{6} + \frac{y}{\tan(60)}), \\ (1.4, 0, 0, 1), & \text{otherwise.} \end{cases} \quad (4.53)$$

The results are compared at $t = 0.2$ and they are illustrated in figure 4.21. As the shock propagates from left to right, a self similar shock structure with two triple points evolve. At the primary triple point, the incident shock, reflected shock and Mach stem intersects. A secondary triple points is formed from the intersection of the reflected shock, bowed Mach stem and a secondary reflected shock [Kemmm, 2016]. A primary slip line emanates from both triple points. It can be seen that the cases using the TENO5 and TENO6 scheme are able to produce finer scale structure along the primary slip line (curled flow structure) as compared to the baseline WENO5-JS scheme. As compared to the fine grid WENO5-JS case, both the TENO5 and TENO6 cases are able to produce either similar or finer scale structures despite using a coarser grid. The hybrid schemes are able to produce even finer scale structures at the primary slip line as compared to the baseline TENO6 scheme. A plot of the blending factor in the x and y direction for the hybrid scheme is shown in figure 4.22. It can be seen that at region where there is sharp change in the gradient of the flow, the blending factor approaches zero. At region where the gradient of the flow is smooth, the blending factor approaches one. At region of intermediate gradient, the

blending factor lies between zero and one.

2D Euler - Shock Vortex Interaction

This problem describes the interaction of a stationary shock and a vortex. Details of the initial and boundary conditions were obtained from [Peng et al., 2019]. The computational domain is set to $[0,2] \times [0,1]$. A Mach 1.1 shock is positioned at $x = 0.5$ and normal to the x -axis. Its left and right states are given as

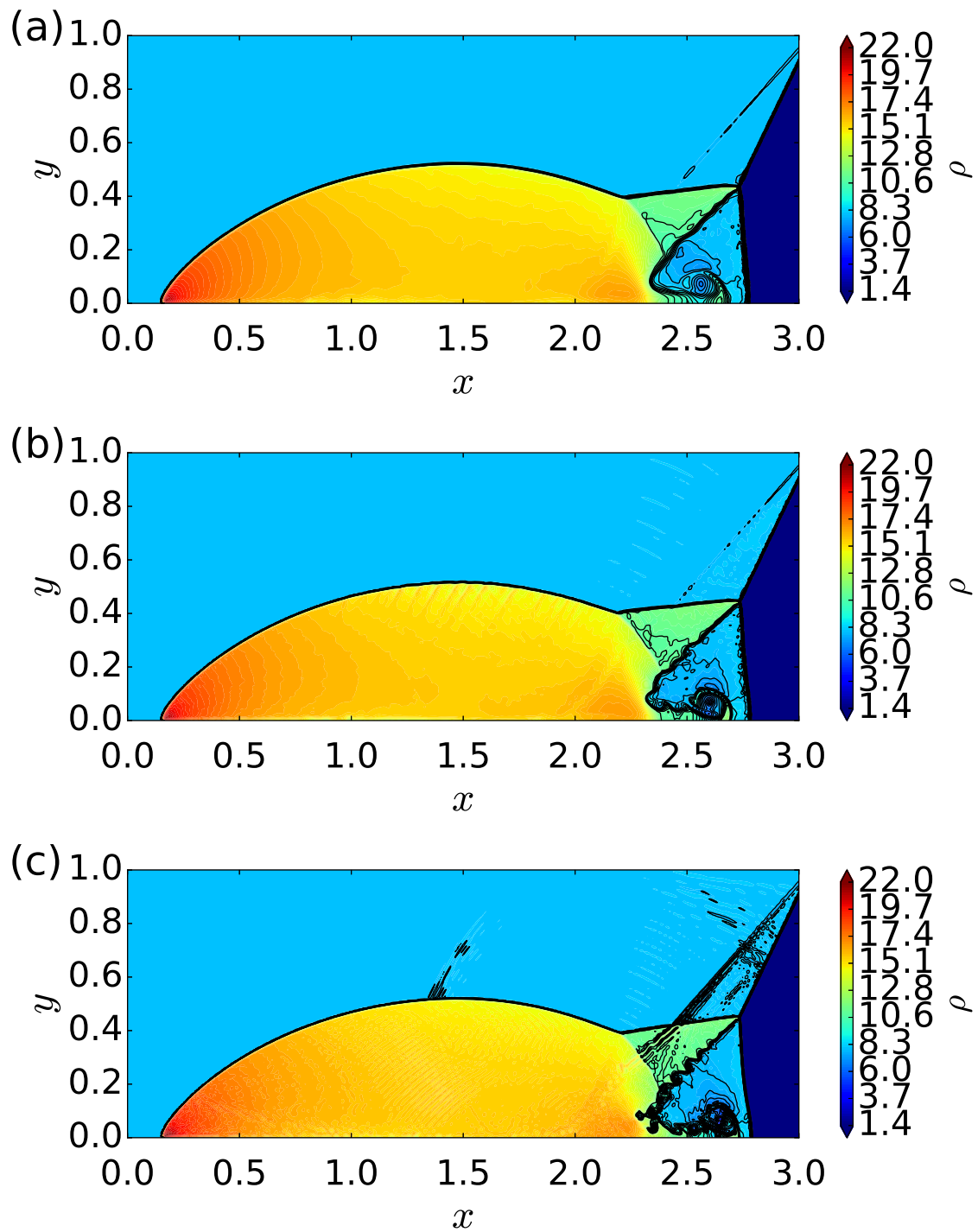
$$(\rho, u, v, p) = \begin{cases} (1.0, 1.1\sqrt{\gamma}, 0, 1), & \text{if } x < 0.5, \\ (1.1691, 1.1133, 0, 1.245), & \text{otherwise.} \end{cases} \quad (4.54)$$

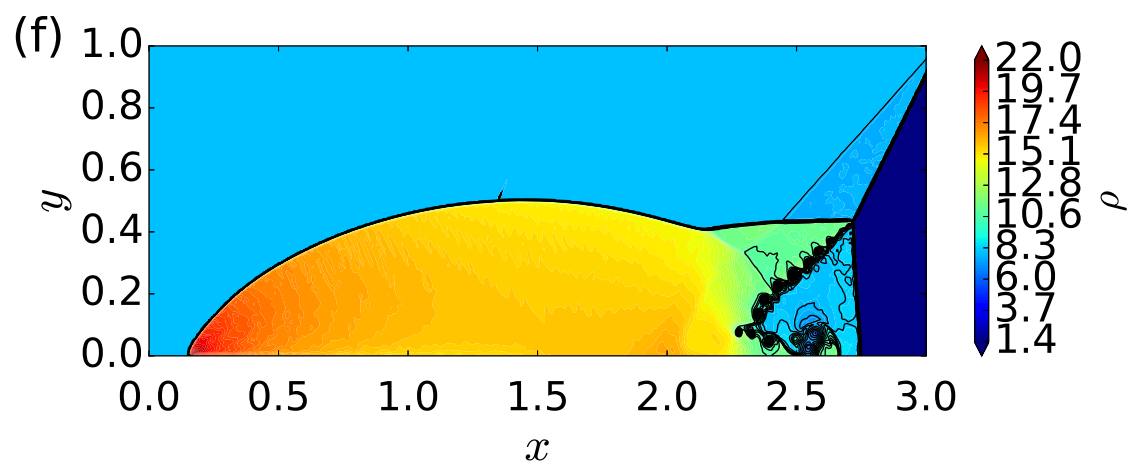
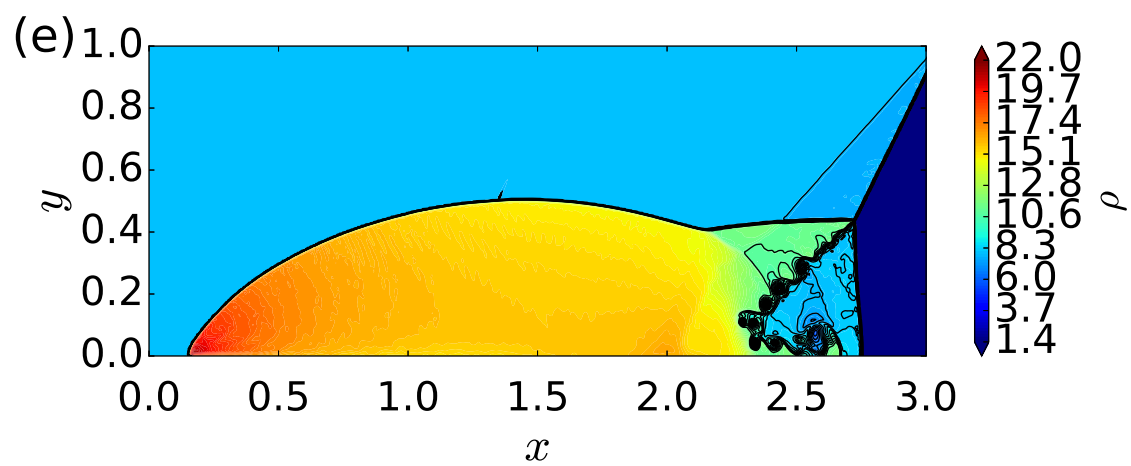
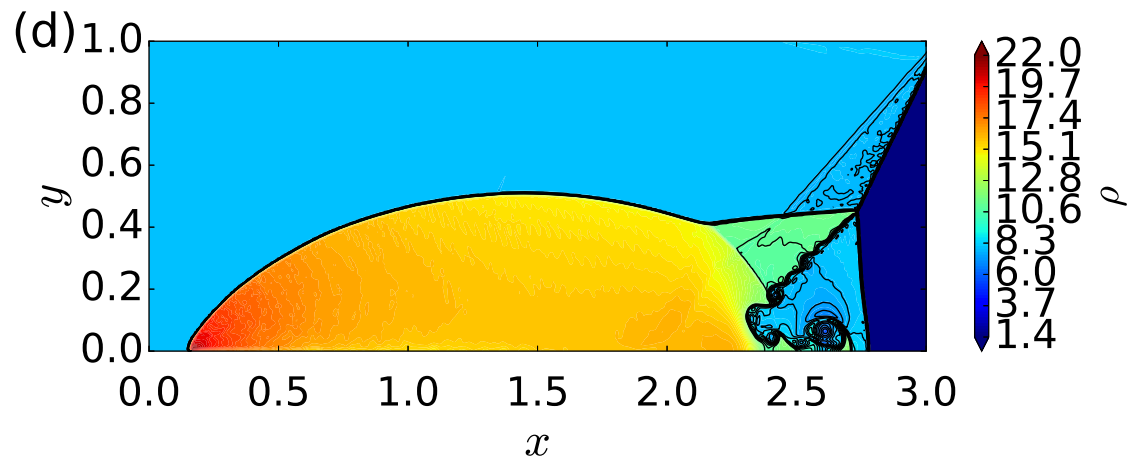
A small vortex is superposed on the left state region and its center is located at $(x_c, y_c) = (0.25, 0.5)$. The initial condition to the left of the normal shock is given by:

$$\begin{aligned} \rho &= (1 - (\gamma - 1)) \frac{\epsilon^2}{4\alpha\gamma} e^{2\alpha(1-r^2)} \frac{1}{r^{\gamma-1}}, \\ u &= 1.1\sqrt{\gamma} + \epsilon\tau e^{\alpha(1-r^2)} \frac{(y - y_c)}{r}, \\ v &= -\epsilon\tau e^{\alpha(1-r^2)} \frac{(x - x_c)}{r}, \\ p &= \rho^\gamma, \end{aligned} \quad (4.55)$$

where $\tau = r/r_c$ and $r = \sqrt{(x - x_c)^2 + (y - y_c)^2}$. $\epsilon = 0.3$ is a measure of the strength of the vortex. $\alpha = 0.204$ controls the decay rate of the vortex and $r_c = 0.05$ is the critical radius at which the vortex has the maximum strength. A grid of $(N_x, N_y) = (250, 100)$ is used. The reference results is computed on a refined grid of $(N_x, N_y) = (1000, 400)$. Both inflow and outflow values at the ghost points are linearly extrapolated from the interior points. Top and bottom boundary conditions are imposed symmetry boundary condition.

The results are compared at $t = 0.6$ and they are illustrated in figure 4.23. Density distribution of different results at $y=0.5$ are illustrated in figure 4.24. It can be seen that the different spatial discretization methods give very similar results although the TENO5,





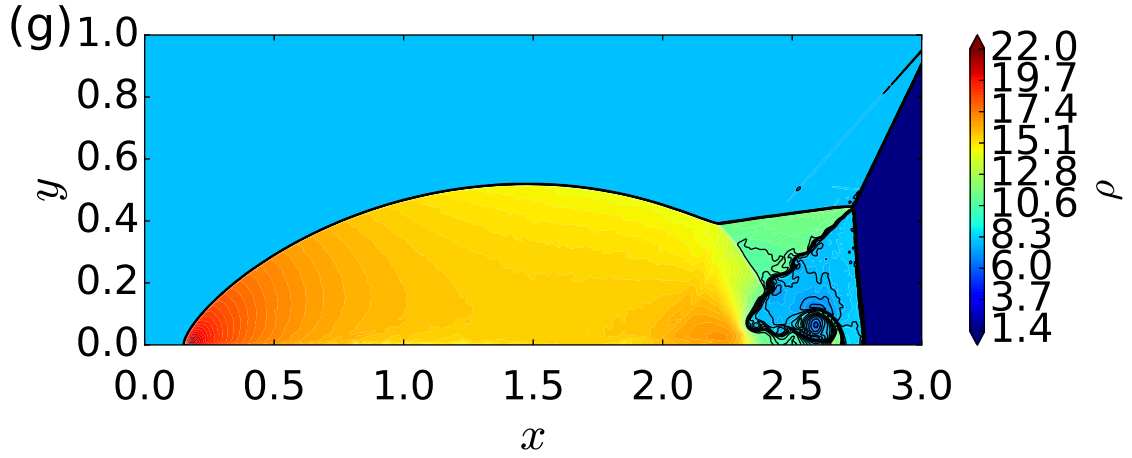


Figure 4.21: Comparison of density contour at $t = 0.2$ for double Mach reflection problem. (a) WENO5-JS $\Delta x = \Delta y = \frac{1}{240}$, (b) WENO7-JS $\Delta x = \Delta y = \frac{1}{240}$, (c) TENO5, $C_T = 1e - 6$ $\Delta x = \Delta y = \frac{1}{240}$, (d) TENO6, $C_T = 1e - 6$ $\Delta x = \Delta y = \frac{1}{240}$, (e) HYB-MDCD-TENO6 $\gamma_{disp} = 0.0568$ $\Delta x = \Delta y = \frac{1}{240}$, (f) HYB-MDCD-TENO6 $\gamma_{disp} = 0.062$ $\Delta x = \Delta y = \frac{1}{240}$, (g) WENO5-JS $\Delta x = \Delta y = \frac{1}{480}$. Solid lines for ρ ranges from 1.4 to 11 with 25 equally separated levels.

TENO6 and HYB-MDCD-TENO6 schemes has slightly more numerical noise at region close to the normal shock. It can be seen that all methods capture the shock and vortex well. It can be seen that the HYB-MDCD-TENO6 schemes are able to achieve sharper normal shock profile and lower vortex core density as compared to the baseline TENO6 schemes. This is because of the lower numerical dissipation. Also, it can be seen that both the TENO5 and TENO6 cases give better results than the WENO5-JS and WENO7-JS cases at these regions. A plot of the blending factor in the x and y direction for the hybrid scheme is shown in figure 4.25.

It can be clearly seen that the blending factor approaches zero at location where the normal shock and bow shock is present. At region where the vortex core is present, the blending factor remain at values close to 1 where most of the linear scheme is being utilized in the computation of the numerical flux. There exist region where the blending factor can become lesser than 1.0 despite being a 'smooth' region of the flow. This is because of the presence of numerical oscillation propagating from the discontinuous region of the flow.

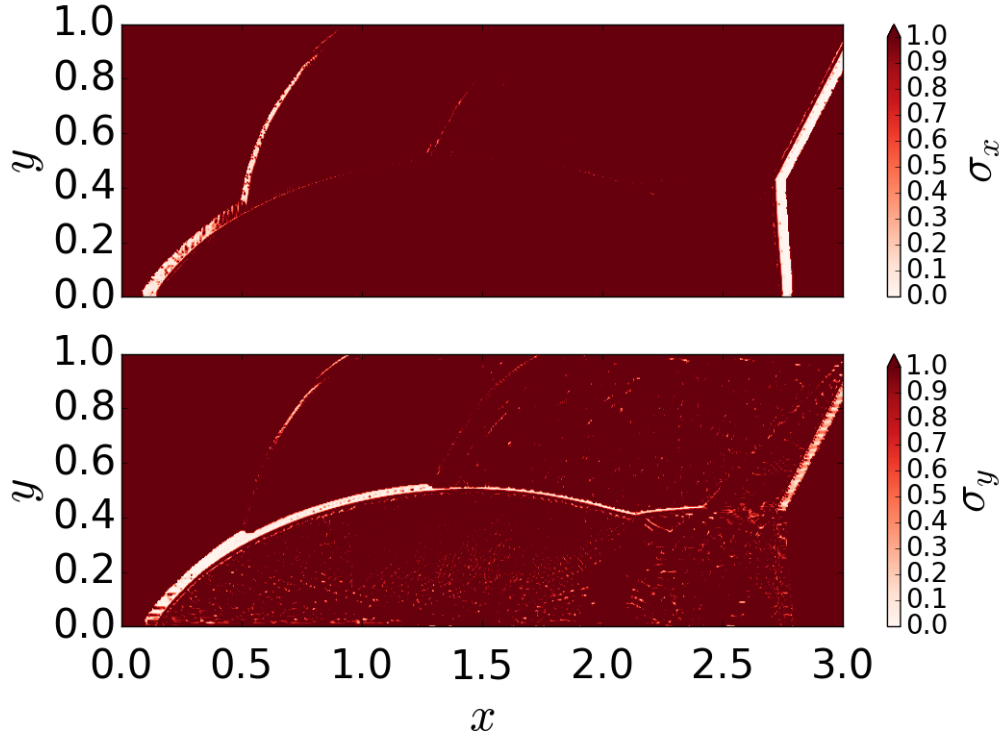
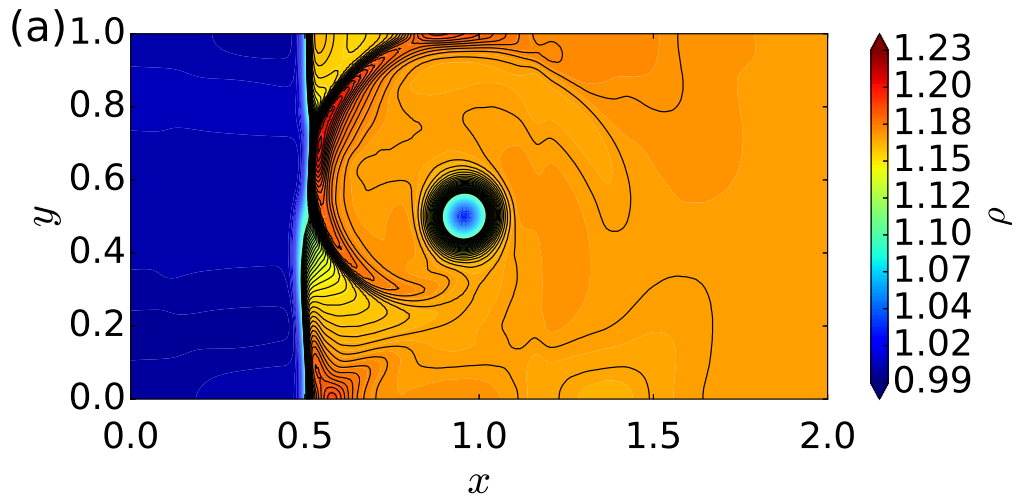
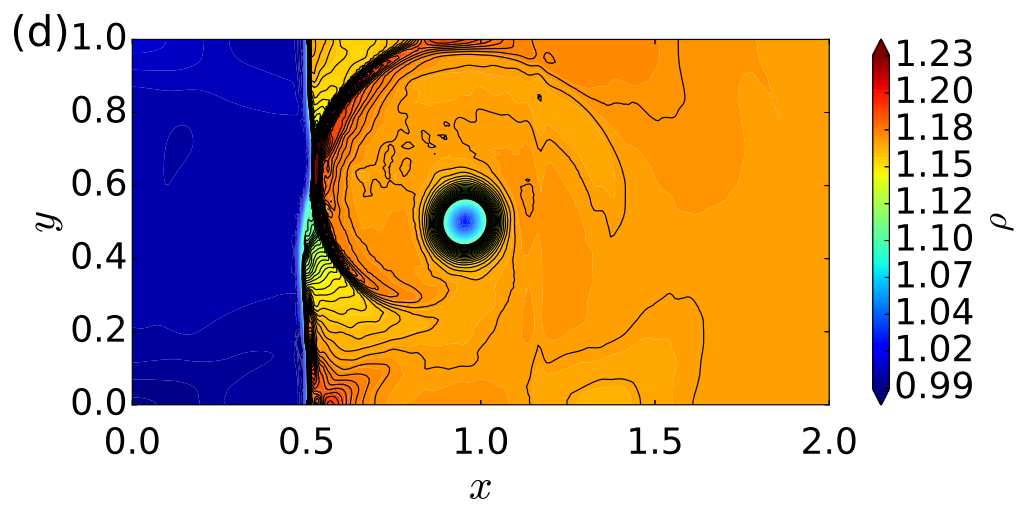
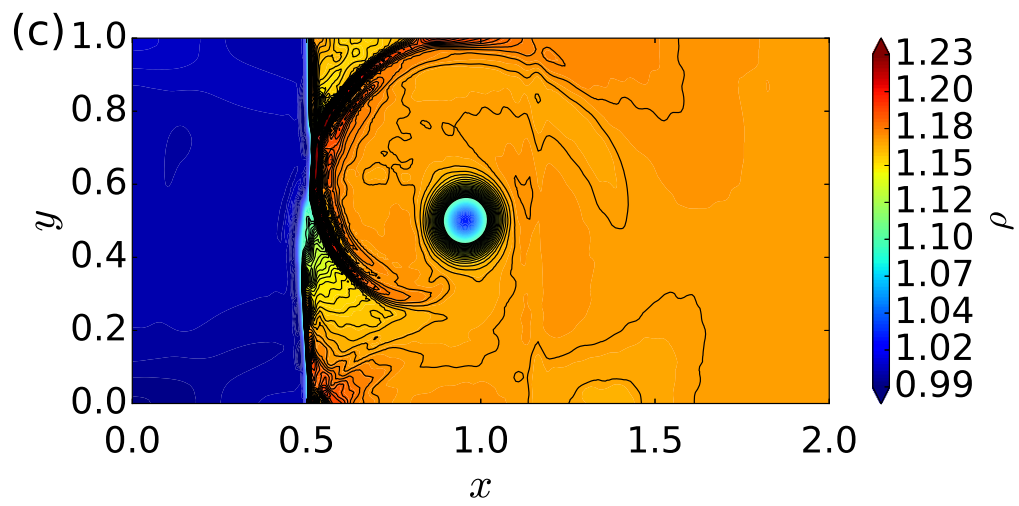
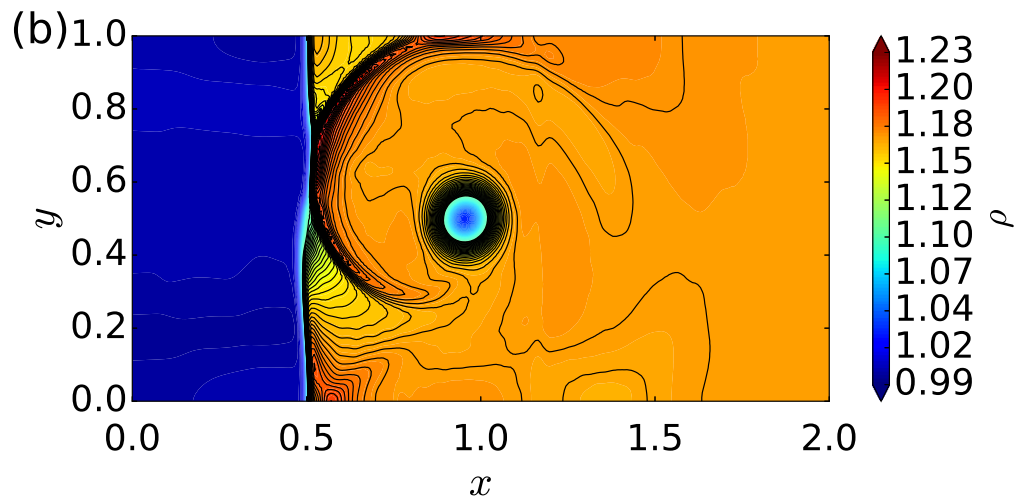


Figure 4.22: Plot of the blending factor, $\sigma_x(x, y, t)$ and $\sigma_y(x, y, t)$ of the first flux components in each spatial direction at $t = 0.2$ for HYB-MDCD-TENO6, $\gamma_{disp} = 0.0568$ scheme. n is taken to be 8.





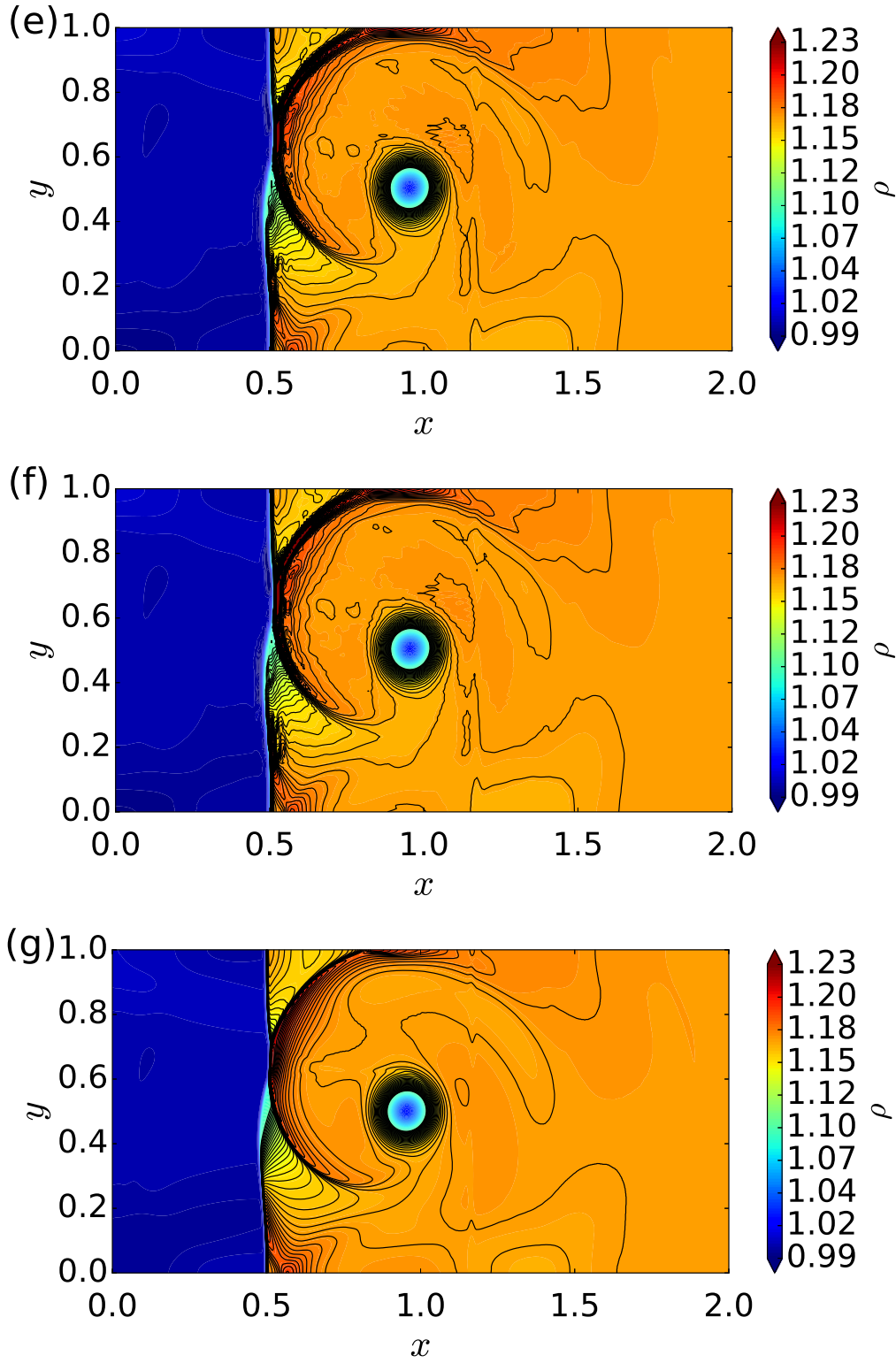


Figure 4.23: Comparison of density contour at $t = 0.6$ for shock vortex interaction problem. (a) WENO5-JS, (b) WENO7-JS, (c) TENO5, $C_T = 1e - 6$, (d) TENO6, $C_T = 1e - 6$, (e) HYB-MDCD-TENO6 $\gamma_{disp} = 0.0568$, (f) HYB-MDCD-TENO6 $\gamma_{disp} = 0.062$, (g) WENO5-JS fine grid. Solid lines for ρ ranges from 1.1 to 1.22 with 45 equally separated levels.

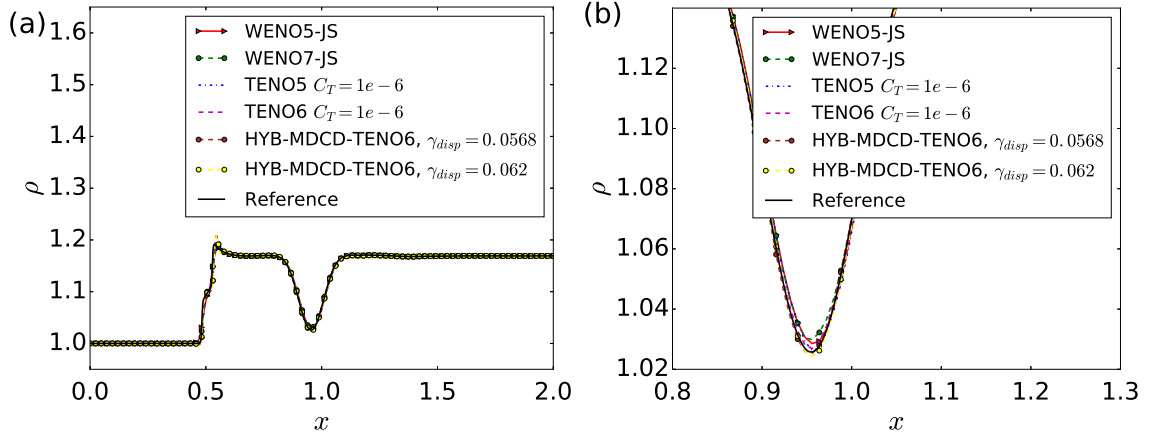


Figure 4.24: Plot of density distribution at $y = 0.5$ for the different schemes at $t = 0.6$.

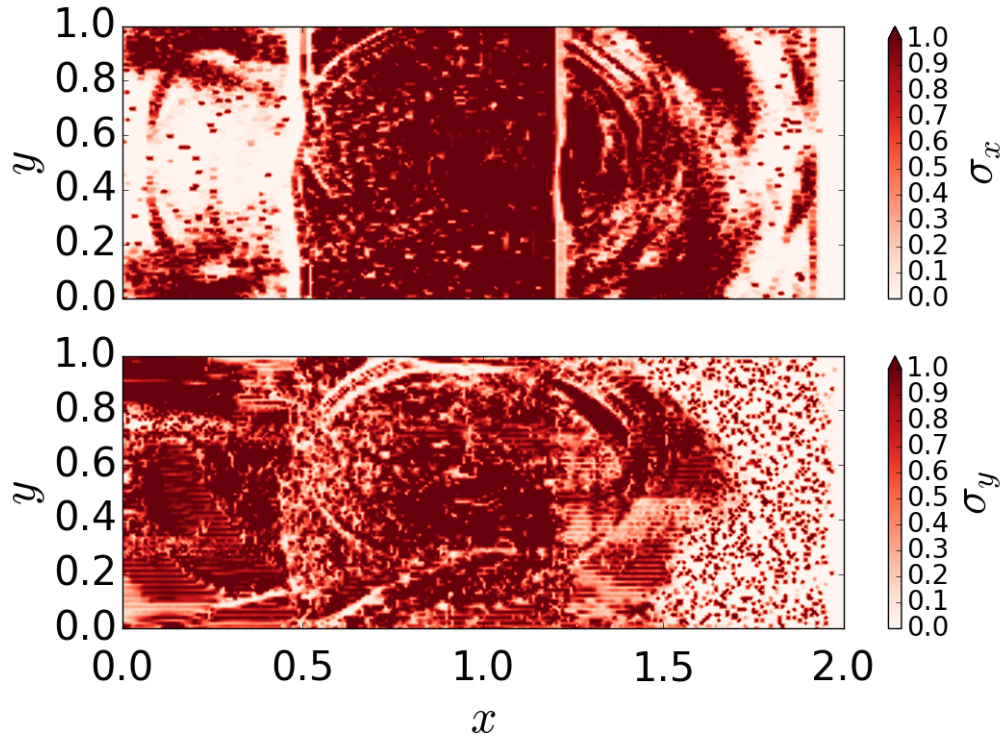


Figure 4.25: Plot of the blending factor, $\sigma_x(x, y, t)$ and $\sigma_y(x, y, t)$ of the first flux components in each spatial direction at $t = 0.6$ for HYB-MDCD-TENO6, $\gamma_{disp} = 0.0568$ scheme.

4.6.4 2D Navier-Stokes

The governing equation of the non dimensional form of the two dimensional compressible Navier-Stokes equations for idea gas are given by:

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} + \frac{\partial \mathbf{G}}{\partial y} = \frac{1}{Re} \frac{\partial \mathbf{F}^v}{\partial x} + \frac{1}{Re} \frac{\partial \mathbf{G}^v}{\partial y} \quad (4.56)$$

where the vectors $\mathbf{U}$, $\mathbf{F}$, $\mathbf{G}$, $\mathbf{F}^v$ and $\mathbf{G}^v$ are expressed as:

$$\mathbf{U} = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ e \end{bmatrix} \quad \mathbf{F} = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ eu + pu \end{bmatrix} \quad \mathbf{G} = \begin{bmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ ev + pv \end{bmatrix} \quad (4.57)$$

$$\mathbf{F}^v = \begin{bmatrix} 0 \\ \tau_{xx} \\ \tau_{xy} \\ u\tau_{xx} + v\tau_{xy} + q_x \end{bmatrix} \quad \mathbf{G}^v = \begin{bmatrix} 0 \\ \tau_{yx} \\ \tau_{yy} \\ u\tau_{yx} + v\tau_{yy} + q_y \end{bmatrix}.$$

The viscous stress tensor and heat flux are given by:

$$\tau_{xx} = \mu \left(\frac{4}{3} \frac{\partial u}{\partial x} - \frac{2}{3} \frac{\partial v}{\partial y} \right), \quad \tau_{yy} = \mu \left(\frac{4}{3} \frac{\partial v}{\partial y} - \frac{2}{3} \frac{\partial u}{\partial x} \right), \quad \tau_{xy} = \tau_{yx} = \mu \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right), \quad (4.58)$$

$$q_x = \mu \frac{1}{(\gamma - 1)M^2 Pr} \frac{\partial T}{\partial x}, \quad q_y = \mu \frac{1}{(\gamma - 1)M^2 Pr} \frac{\partial T}{\partial y}. \quad (4.59)$$

Other derived quantities can be calculated from the vector $\mathbf{U}$ as follows:

$$p = (e - \frac{1}{2}\rho(u^2 + v^2))(\gamma - 1), \quad T = \frac{\gamma M^2 p}{\rho}. \quad (4.60)$$

The viscosity is computed based on Sutherland's law:

$$\mu = T^{1.5} \frac{1.0 + T_{ref}}{T + T_{ref}}, \quad (4.61)$$

where $T_{ref} = \frac{110.4}{T_\infty}$. T_∞ is defined as the dimensional free stream temperature. In this subsection, one problem is tested. The test problem concerns the impingement of a shock wave onto a spatially evolving mixing layer.

2D Navier-Stokes - Shock Shear Layer

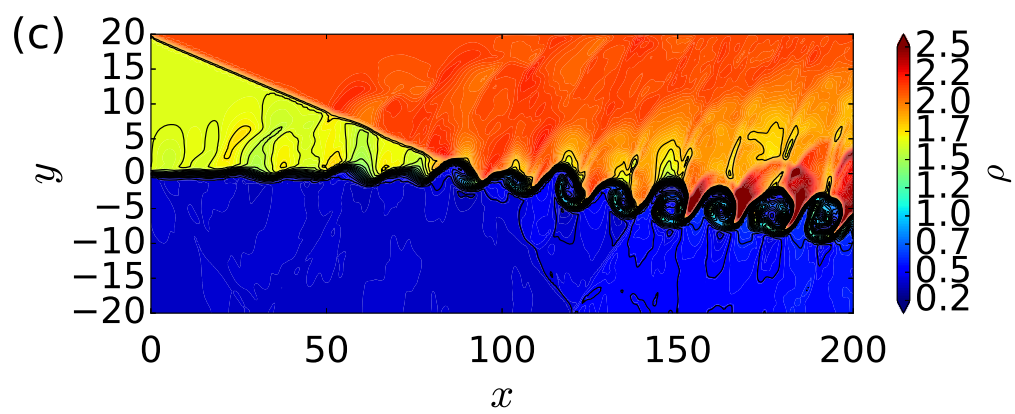
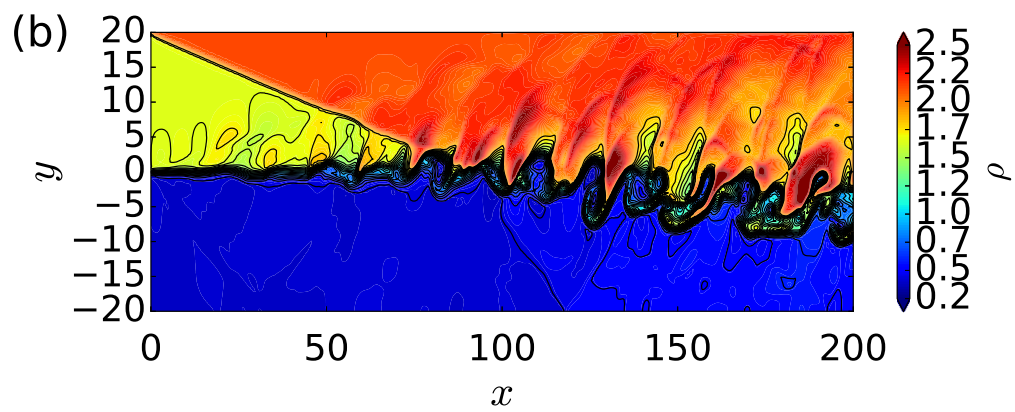
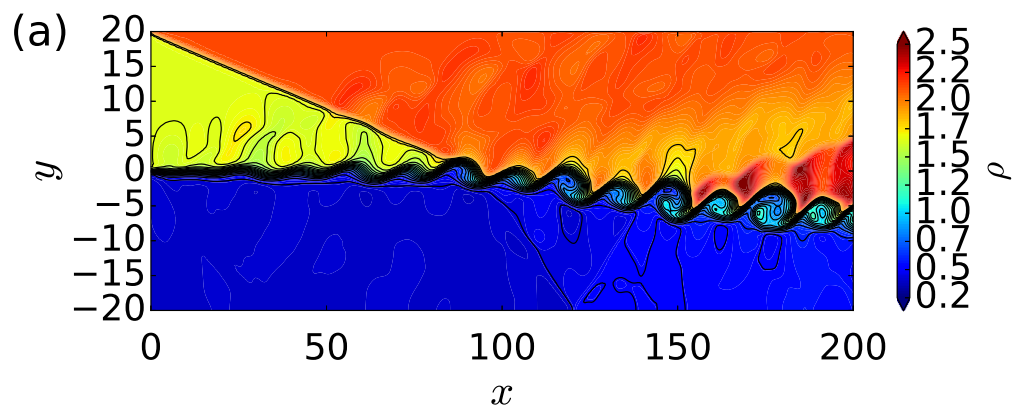
The impingement of a shock wave onto a spatially evolving mixing layer is designed to test the resolution of a scheme when shock waves interact with vortices. In this setup, fluctuation is imposed onto the vertical component of the velocity at the inlet so as to perturb the mixing layer. For this case, the two dimensional Navier Stokes equations are solved. As the shear layer evolves spatially, an oblique shock from the top boundary travels through the mixing layer, reflects from the free slip wall at the lower boundary and passes through the mixing layer again. It is noted that a free slip instead of a no slip wall is used at the bottom boundary in order to avoid any boundary layer formation, which may complicate the reflection of the oblique shock. For the present simulation, the computational domain is taken to be $[0,200] \times [-20,20]$. The inlet condition is given as $u = 2.5 + 0.5 \tanh(2y)$. The initial condition is given as [Peng and Shen, 2015, Peng et al., 2019]:

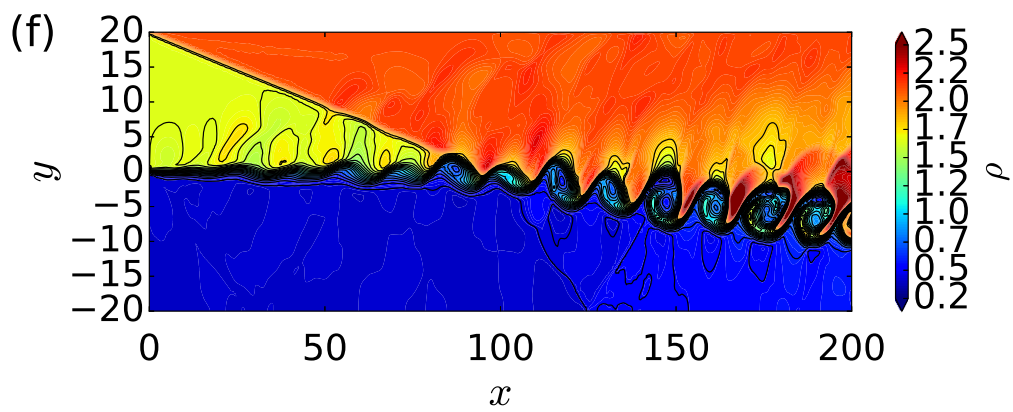
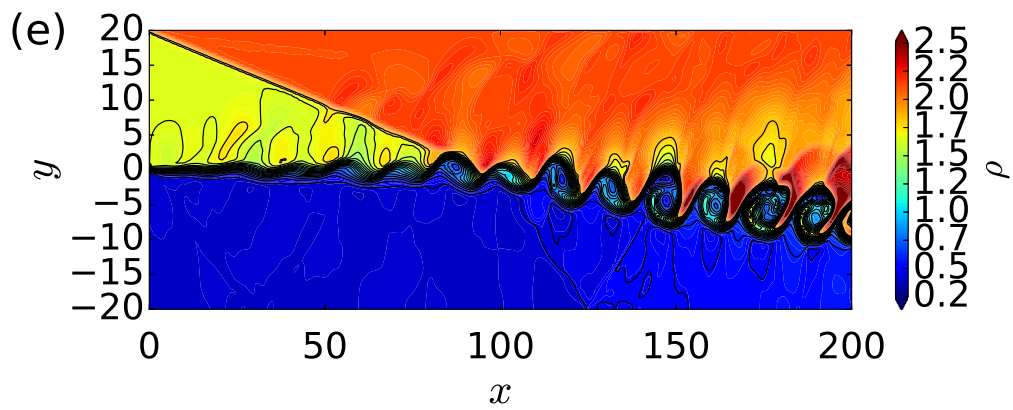
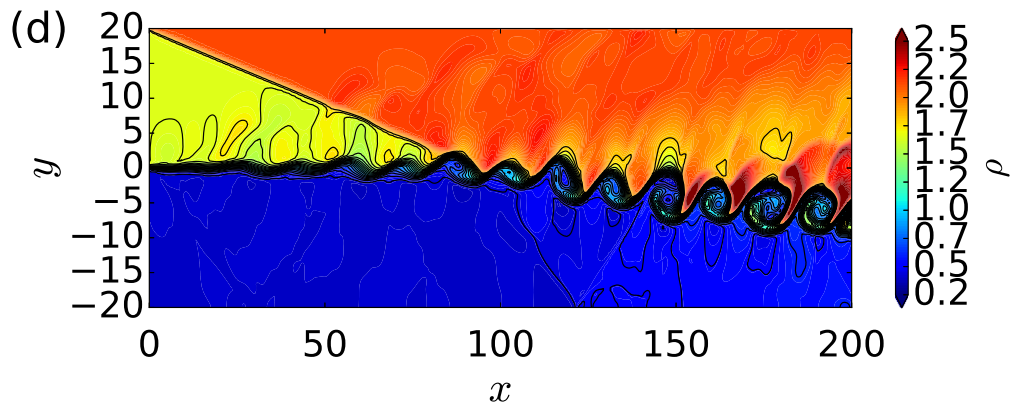
$$(\rho, u, v, p) = \begin{cases} (0.3626, 2.0, 0.0, 0.3327), & \text{if } y < 0, \\ (1.6374, 3.0, 0.0, 0.3327), & \text{otherwise.} \end{cases} \quad (4.62)$$

Post shock condition $(\rho, u, v, p) = (2.1101, 2.9709, -0.1367, 0.4754)$ is imposed at the top boundary and a free slip wall is imposed at the bottom boundary. The freestream Mach number and Reynolds number is 0.6 and 500 respectively. The Prandtl number is set to 0.72 and the freestream temperature is set to 300K. The vertical fluctuations imposed at the inlet are given by:

$$\begin{aligned}
 v' &= \sum_{k=1}^2 a_k \cos(2\pi kt/T + \phi_k) \exp(-y^2/b) \\
 b &= 10 \quad a_1 = a_2 = 0.05 \quad \phi_1 = 0 \quad \phi_2 = \pi/2 \\
 T &= \frac{\lambda}{u_c} \quad \lambda = 30 \quad u_c = 2.68
 \end{aligned} \tag{4.63}$$

An equally spaced grid of $(N_x, N_y) = (500, 100)$ is used. The reference result is calculated on a refined grid of $(N_x, N_y) = (2000, 400)$. Density contours are shown in figure 4.26 at $t = 120$. In figure 4.26, it can be observed that the WENO5-JS, TENO5, TENO6 and HYB-MDCD-TENO6 cases obtain similar results which is very comparable to the reference result. However, it should be noted that the self similar structure of the downstream vortices of the reference case showcases smaller scale structure close to its vortex core. As compared to the baseline TENO6 case, the HYB-MDCD-TENO6 cases showcase presence of smaller scale structure within its downstream vortex core from $X \gtrsim 160$ onward. A plot of the blending factors, σ_x and σ_y of the first flux component in each spatial directions is shown in figure 4.27. The 'white line' region where the blending factor is close to zero corresponds to the location of the impinging oblique shock interacting with the mixing layer.





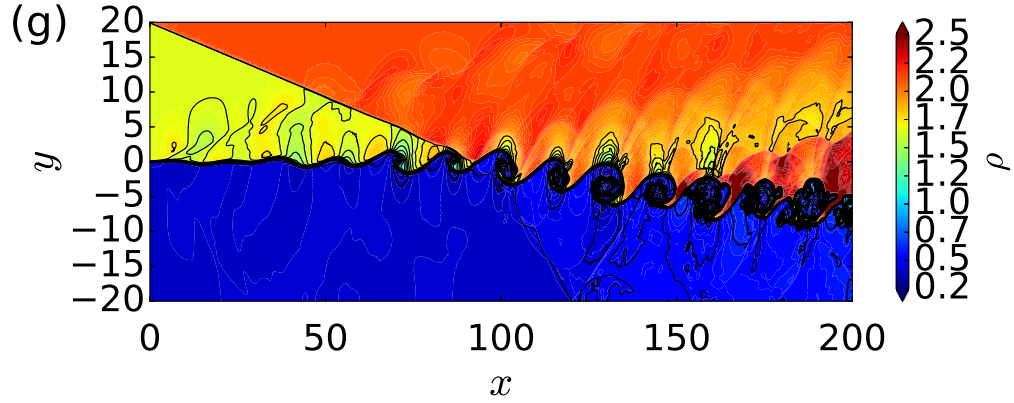


Figure 4.26: Comparison of density contour at $t = 120$ for shock shear layer problem. (a) WENO5-JS, (b) WENO7-JS, (c) TENO5, $C_T = 1e - 6$, (d) TENO6, $C_T = 1e - 6$, (e) HYB-MDCD-TENO6 $\gamma_{disp} = 0.0568$, (f) HYB-MDCD-TENO6 $\gamma_{disp} = 0.062$, (g) WENO5-JS fine grid. Solid lines for ρ ranges from 0.228 to 1.8 with 20 equally separated levels.

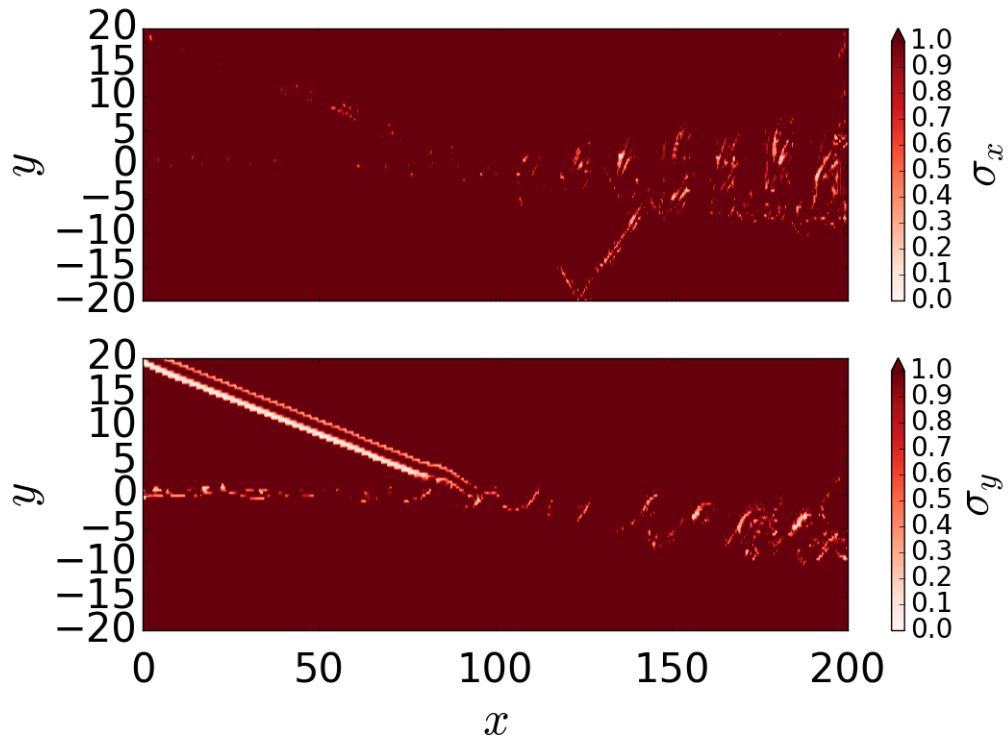


Figure 4.27: Plot of the blending factor, $\sigma_x(x, y, t)$ and $\sigma_y(x, y, t)$ of the first flux components in each spatial direction at $t = 120$ for HYB-MDCD-TENO6, $\gamma_{disp} = 0.0568$ scheme.

4.6.5 3D Euler/Navier Stokes

In this section, the governing equation of the three dimensional compressible Navier Stokes equations in generalized coordinate system will be presented. The computational code was written based on generalized coordinate system for which a transformation system is used to transform the variables from the physical grid to the computational grid and vice versa. For problems involving the Euler equation, the viscous terms are not taken into account. In the case of a non-moving grid, the Jacobian matrix remain unchange for all time steps and the transformation matrix need not consider the time derivative terms. The conservative variables, $\mathbf{U}'$ are marched in time in the computational domain. The transformation metric and Jacobian are computed once during the pre-run step and used again when writing out the data to transform back to physical space.

$$\frac{\partial \mathbf{U}'}{\partial t} + \frac{\partial \mathbf{F}'}{\partial \xi} + \frac{\partial \mathbf{G}'}{\partial \eta} + \frac{\partial \mathbf{H}'}{\partial \zeta} = \frac{1}{Re} \frac{\partial \mathbf{F}_v'}{\partial \xi} + \frac{1}{Re} \frac{\partial \mathbf{G}_v'}{\partial \eta} + \frac{1}{Re} \frac{\partial \mathbf{H}_v'}{\partial \zeta} \quad (4.64)$$

$$\begin{aligned} \mathbf{U}' &= \mathbf{U}/|\mathbf{J}| \\ \mathbf{F}' &= (\zeta_x \mathbf{F} + \zeta_y \mathbf{G} + \zeta_z \mathbf{H})/|\mathbf{J}| \\ \mathbf{G}' &= (\eta_x \mathbf{F} + \eta_y \mathbf{G} + \eta_z \mathbf{H})/|\mathbf{J}| \\ \mathbf{H}' &= (\zeta_x \mathbf{F} + \zeta_y \mathbf{G} + \zeta_z \mathbf{H})/|\mathbf{J}| \\ \mathbf{F}_v' &= (\zeta_x \mathbf{F}_v + \zeta_y \mathbf{G}_v + \zeta_z \mathbf{H}_v)/|\mathbf{J}| \\ \mathbf{G}_v' &= (\eta_x \mathbf{F}_v + \eta_y \mathbf{G}_v + \eta_z \mathbf{H}_v)/|\mathbf{J}| \\ \mathbf{H}_v' &= (\zeta_x \mathbf{F}_v + \zeta_y \mathbf{G}_v + \zeta_z \mathbf{H}_v)/|\mathbf{J}| \end{aligned} \quad (4.65)$$

where the vectors $\mathbf{U}$, $\mathbf{F}$, $\mathbf{G}$, $\mathbf{H}$, $\mathbf{F}_v$, $\mathbf{G}_v$ and $\mathbf{H}_v$ are expressed as:

$$\begin{aligned}
\mathbf{U} &= \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ \rho E \end{bmatrix} & \mathbf{F} &= \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ \rho uw \\ \rho Eu + pu \end{bmatrix} & \mathbf{G} &= \begin{bmatrix} \rho v \\ \rho vu \\ \rho v^2 + p \\ \rho vw \\ \rho Ev + pv \end{bmatrix} & \mathbf{H} &= \begin{bmatrix} \rho w \\ \rho wu \\ \rho wv \\ \rho w^2 + p \\ \rho Ew + pw \end{bmatrix} \\
\mathbf{F}_v &= \begin{bmatrix} 0 \\ \tau_{xx} \\ \tau_{yx} \\ \tau_{zx} \\ u\tau_{xx} + v\tau_{xy} + w\tau_{xz} + q_x \end{bmatrix} & \mathbf{G}_v &= \begin{bmatrix} 0 \\ \tau_{yx} \\ \tau_{yy} \\ \tau_{yz} \\ u\tau_{yx} + v\tau_{yy} + w\tau_{yz} + q_y \end{bmatrix}, & & & (4.66) \\
\mathbf{H}_v &= \begin{bmatrix} 0 \\ \tau_{zx} \\ \tau_{zy} \\ \tau_{zz} \\ u\tau_{zx} + v\tau_{zy} + w\tau_{zz} + q_z \end{bmatrix}.
\end{aligned}$$

The viscous stress tensor and heat flux vector are given by:

$$\begin{aligned}
\tau_{xx} &= \mu \left(\frac{4}{3} \frac{\partial u}{\partial x} - \frac{2}{3} \left(\frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) \right) & \tau_{yy} &= \mu \left(\frac{4}{3} \frac{\partial v}{\partial y} - \frac{2}{3} \left(\frac{\partial u}{\partial x} + \frac{\partial w}{\partial z} \right) \right) \\
\tau_{zz} &= \mu \left(\frac{4}{3} \frac{\partial w}{\partial z} - \frac{2}{3} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) \right) & \tau_{xy} = \tau_{yx} &= \mu \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \\
\tau_{yz} = \tau_{zy} &= \mu \left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right) & \tau_{xz} = \tau_{zx} &= \mu \left(\frac{\partial w}{\partial x} + \frac{\partial u}{\partial z} \right)
\end{aligned} \tag{4.67}$$

$$q_j = \frac{\mu}{(\gamma - 1)M_\infty^2 Pr} \frac{\partial T}{\partial x_j}, \quad j = 1, 2, 3 \tag{4.68}$$

The Jacobian matrix is given by

$$\mathbf{J} = \begin{bmatrix} \tilde{\zeta}_x & \tilde{\zeta}_y & \tilde{\zeta}_z \\ \eta_x & \eta_y & \eta_z \\ \zeta_x & \zeta_y & \zeta_z \end{bmatrix}. \quad (4.69)$$

In order to determine the Jacobian matrix, the following relation should be noted:

$$\underbrace{\begin{bmatrix} d\tilde{\zeta} \\ d\eta \\ d\zeta \end{bmatrix}}_A = \underbrace{\begin{bmatrix} \tilde{\zeta}_x & \tilde{\zeta}_y & \tilde{\zeta}_z \\ \eta_x & \eta_y & \eta_z \\ \zeta_x & \zeta_y & \zeta_z \end{bmatrix}}_B \underbrace{\begin{bmatrix} dx \\ dy \\ dz \end{bmatrix}}_C, \quad (4.70)$$

$$\underbrace{\begin{bmatrix} dx \\ dy \\ dz \end{bmatrix}}_C = \underbrace{\begin{bmatrix} x_{\tilde{\zeta}} & x_{\eta} & x_{\zeta} \\ y_{\tilde{\zeta}} & y_{\eta} & y_{\zeta} \\ z_{\tilde{\zeta}} & z_{\eta} & z_{\zeta} \end{bmatrix}}_D \underbrace{\begin{bmatrix} d\tilde{\zeta} \\ d\eta \\ d\zeta \end{bmatrix}}_A. \quad (4.71)$$

Since $[A] = [B][C]$ and $[A] = [D]^{-1}[C]$, therefore $[B] = [D]^{-1}$:

$$\mathbf{J} = \underbrace{\begin{bmatrix} \tilde{\zeta}_x & \tilde{\zeta}_y & \tilde{\zeta}_z \\ \eta_x & \eta_y & \eta_z \\ \zeta_x & \zeta_y & \zeta_z \end{bmatrix}}_B = \underbrace{\begin{bmatrix} x_{\tilde{\zeta}} & x_{\eta} & x_{\zeta} \\ y_{\tilde{\zeta}} & y_{\eta} & y_{\zeta} \\ z_{\tilde{\zeta}} & z_{\eta} & z_{\zeta} \end{bmatrix}}_{D^{-1}}^{-1} \quad (4.72)$$

Solving this analytically leads to the following relation for the transformation metric

$$\begin{aligned}
\tilde{\xi}_x &= (y_\eta z_\zeta - y_\zeta z_\eta) |\mathbf{J}| \\
\tilde{\xi}_y &= (z_\eta x_\zeta - z_\zeta x_\eta) |\mathbf{J}| \\
\tilde{\xi}_z &= (x_\eta y_\zeta - x_\zeta y_\eta) |\mathbf{J}| \\
\eta_x &= (y_\zeta z_\xi - y_\xi z_\zeta) |\mathbf{J}| \\
\eta_y &= (z_\zeta x_\xi - z_\xi x_\zeta) |\mathbf{J}| \\
\eta_z &= (x_\zeta y_\xi - x_\xi y_\zeta) |\mathbf{J}| \\
\zeta_x &= (y_\xi z_\eta - y_\eta z_\xi) |\mathbf{J}| \\
\zeta_y &= (z_\xi x_\eta - z_\eta x_\xi) |\mathbf{J}| \\
\zeta_z &= (x_\xi y_\eta - x_\eta y_\xi) |\mathbf{J}|
\end{aligned} \tag{4.73}$$

It should be noted that the transformation metric, shown in equation (4.73) does not take into account the time derivative term. As such, geometric conservation law (GCL) [Thomas and Lombard, 1979] need not be enforced since the source term used for enforcing GCL [Shen et al., 2009] only exists if the time derivative term of the grid metric is considered. The basic idea is to set $(d\tilde{\xi}, d\eta, d\zeta) = (1, 1, 1)$ and then compute the terms within $[D]^{-1}$ numerically using conventional finite difference schemes. This implies that the computational domain is set to a uniform grid spacing of 1.0 in all spatial directions. For the points located close to the boundary, the transformation metric are computed using one sided differencing scheme. Finally, the Jacobian and transformation metrics are used within the governing equation of the Navier Stokes equation at each time step. In practice, it is not necessary to use WENO/TENO scheme for the calculation of the grid metric since it is not subjected to a sharp gradient phenomenon. The lost in accuracy is limited since the transformation is only done during the pre and post processing step of the computation for a non moving grid. An important point to note concerns the computation of the viscous term of the Navier Stokes. The viscous terms are expressed in terms of the coordinates of the physical domain but it is being computed in terms of the coordinates of the computational domain during run time. Therefore, a transformation is required to transform the velocity and temperature derivatives to the physical domain

during the calculation procedure. Mathematically, the first order velocity and temperature derivatives in physical domain are computed using chain rule:

$$\begin{aligned}
 \frac{\partial \phi}{\partial x} &= \frac{\partial \xi}{\partial x} \frac{\partial \phi}{\partial \xi} + \frac{\partial \eta}{\partial x} \frac{\partial \phi}{\partial \eta} + \frac{\partial \zeta}{\partial x} \frac{\partial \phi}{\partial \zeta} \\
 \frac{\partial \phi}{\partial y} &= \frac{\partial \xi}{\partial y} \frac{\partial \phi}{\partial \xi} + \frac{\partial \eta}{\partial y} \frac{\partial \phi}{\partial \eta} + \frac{\partial \zeta}{\partial y} \frac{\partial \phi}{\partial \zeta} \\
 \frac{\partial \phi}{\partial z} &= \frac{\partial \xi}{\partial z} \frac{\partial \phi}{\partial \xi} + \frac{\partial \eta}{\partial z} \frac{\partial \phi}{\partial \eta} + \frac{\partial \zeta}{\partial z} \frac{\partial \phi}{\partial \zeta}
 \end{aligned} \tag{4.74}$$

where ϕ can represent the velocity components or the temperature variable. For the purpose of halo exchange between processors, MPI subarray data type is used to create a 2D plane data for information exchange. For the purpose of computing global average quantities, the MPI_Reduce function is used to sum up all the local sum of each processor domain. For the following 3D example, the characteristic wise reconstruction method is not used since there is no strong shock. For the convective term, numerical flux is split before flux reconstruction is performed. To improve the numerical stability of the solver, the 7 point filter based on [Bogey and Bailly, 2004] is applied in all spatial directions with a filter strength of 0.3. It should be noted that the filter is applied separately in each spatial direction. The filter applied is a low pass filter that selectively adds dissipation to damp the high wavenumber/unresolved structures that lead to numerical instabilities as well as the grid to grid oscillation incurred from the coordinate transformation [Bogey and Bailly, 2004].

3D Euler - Taylor Green Vortex

The inviscid Taylor Green vortex is a test case used to assess the built in dissipation of the numerical method. This is quantitatively assessed through the total kinetic energy and enstrophy. The computational domain is $[0, 2\pi] \times [0, 2\pi] \times [0, 2\pi]$ with periodic boundary conditions imposed on all sides. The total kinetic energy and enstrophy are defined as

$$E_k(t) = \frac{1}{(2\pi)^3} \int_0^{2\pi} \int_0^{2\pi} \int_0^{2\pi} \frac{\rho_i u_i u_i}{2} dx dy dz, \quad \Omega(t) = \frac{1}{(2\pi)^3} \int_0^{2\pi} \int_0^{2\pi} \int_0^{2\pi} \frac{\omega_i \omega_i}{2} dx dy dz \quad (4.75)$$

where ω_i stands for the vorticity component. The initial condition is given as [Brachet et al., 1983, Fu et al., 2017]:

$$\begin{aligned} u(x, y, z, 0) &= \sin(x) \cos(y) \cos(z) \\ v(x, y, z, 0) &= -\cos(x) \sin(y) \cos(z) \\ w(x, y, z, 0) &= 0 \\ \rho(x, y, z, 0) &= 1.0 \\ p(x, y, z, 0) &= 100 + \frac{1}{16} [(\cos(2x) + \cos(2y))(2 + \cos(2z)) - 2] \end{aligned} \quad (4.76)$$

The pressure is defined such that to limit the Mach number to be less than 0.1. A uniform grid of 64^3 and 128^3 are considered. The simulation is run up to $t = 10$. For the purpose of illustration, a visualization of the isosurfaces of u as time evolves is shown in figure 4.28. A comparison of the total kinetic energy and the enstrophy for the different spatial discretization schemes are presented in figures 4.29 and 4.30 for a grid size of 64^3 and 128^3 respectively. For the decay of the total kinetic energy, it can be clearly seen that the HYB-MDCD-TENO6 cases offer the smallest decay among the different spatial discretization schemes. It is an indication that the hybrid scheme is less dissipative for non linear simulations with broadband length-scales. Also, it can be seen that both the TENO5 and TENO6 schemes are less dissipative than the baseline WENO5-JS and WENO7-JS schemes. A larger value of enstrophy implies the presence of more vortical structures in the flow. The resolved vortical structures (isosurfaces of Q criterion) from different schemes are illustrated in figure 4.31. It can be seen that the present HYB-MDCD-TENO6 scheme is essentially able to capture more small scale flow structure than the baseline WENO5-JS, WENO7-JS, TENO5 and TENO6 schemes.

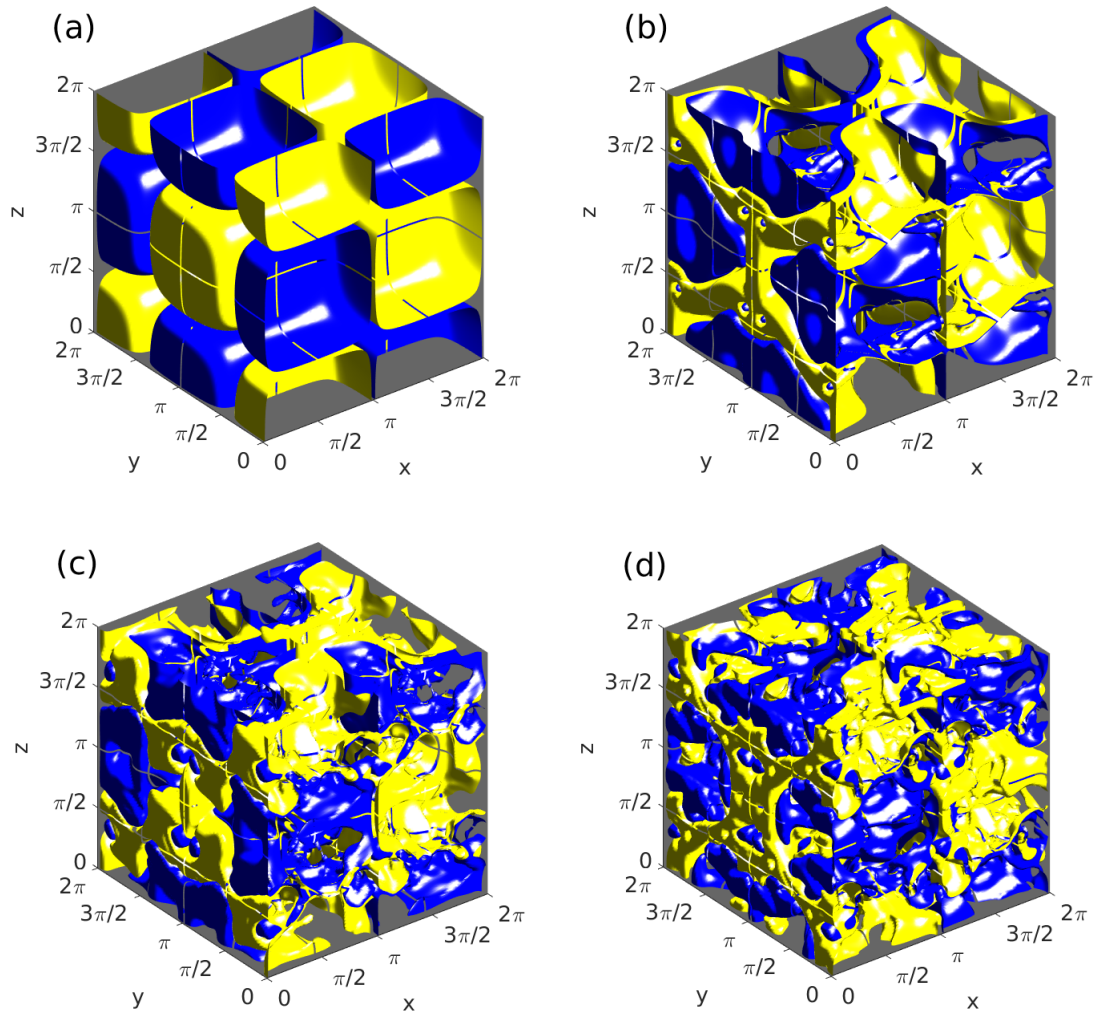


Figure 4.28: (a) Iso-surface of u at $t = 0$, (b) Iso-surface of u at $t \approx 5$, (c) Iso-surface of u at $t \approx 8$, (d) Iso-surface of u at $t = 10$, Isosurface value of -0.05 and 0.05 are used respectively. Grid size of 128^3 , WENO5-JS scheme for the convective terms.

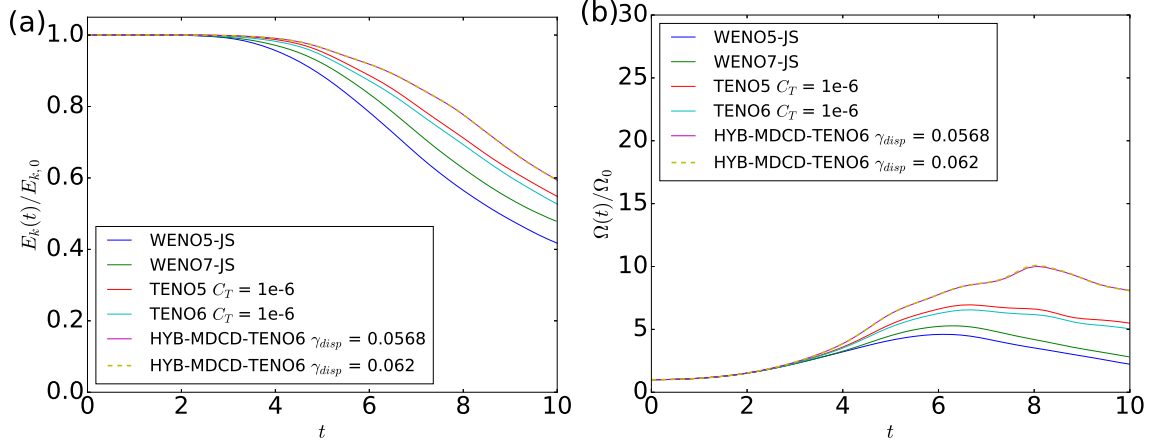


Figure 4.29: (a) Evolution of normalized total kinetic energy, $E_k(t)/E_k(0)$ (b) entrosphy, $\Omega(t)/\Omega(0)$ for different spatial discretization schemes. The grid size is 64^3 .

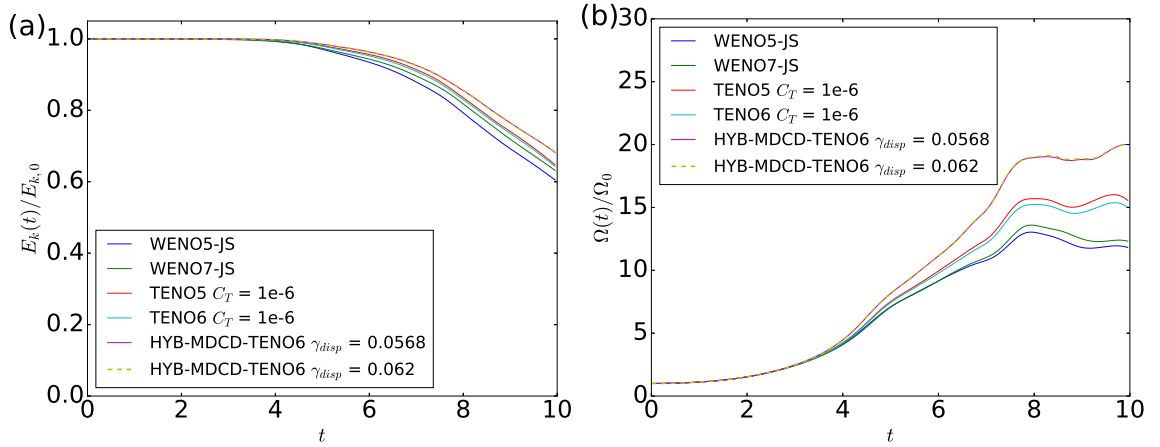


Figure 4.30: (a) Evolution of normalized total kinetic energy, $E_k(t)/E_k(0)$ (b) entrosphy, $\Omega(t)/\Omega(0)$ for different spatial discretization schemes. The grid size is 128^3 .

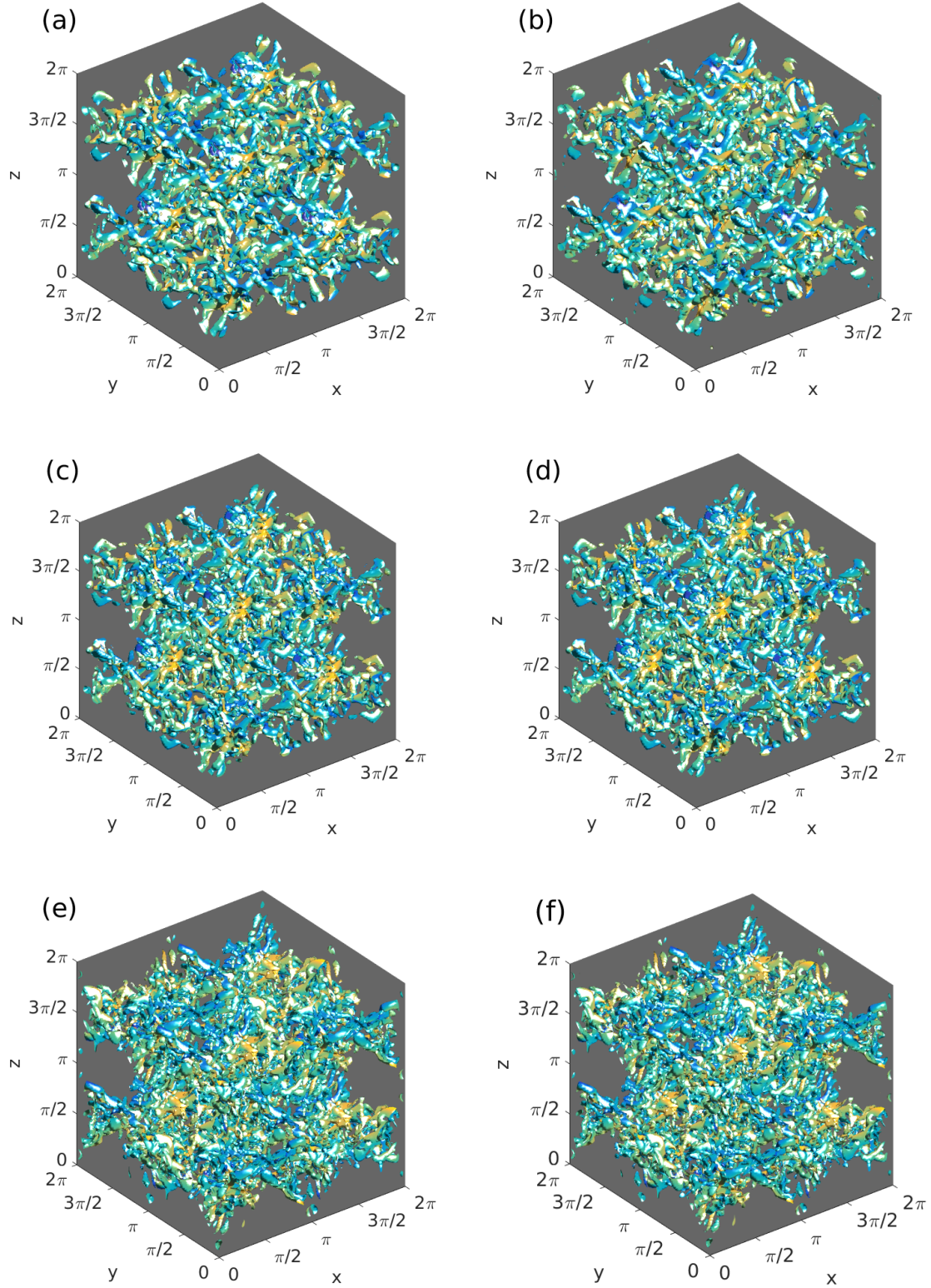


Figure 4.31: Comparison of Isosurface of Q criterion at $t = 10$, (a) WENO5-JS, (b) WENO7-JS, (c) TENO5, $C_T = 1e - 6$, (d) TENO6, $C_T = 1e - 6$, (e) HYB-MDCD-TENO6 $\gamma_{disp} = 0.0568$, (f) HYB-MDCD-TENO6 $\gamma_{disp} = 0.062$. Isosurface value of 0.005 is used respectively. Grid size of 128^3 . Isosurfaces are coloured with the u velocity component.

4.7 Chapter summary

In this chapter, multidimensional spectral analysis of non linear shock capturing scheme was presented. A semi-discrete analysis was considered since Von Neumann analysis is limited to the analysis of linear schemes. It is shown that quasi-linear analysis provides quantitatively correct prediction for the amplitude of the modes up to a time period where higher order effects related to the onset of spurious modes become important. This is primarily because the contribution of the harmonic modes (as a result of the non linear differentiation) are neglected during the calculation of the modified wavenumber of the spatial scheme. These harmonic modes are not present in the case of a linear scheme.

Using the semi-discretized dispersion relation of the two dimensional advection and linearized Euler equations, the dispersion and dissipation property of the non linear scheme in two dimensional wavespace can be quantified. In order to optimize the spectral properties of the non linear scheme while preserving the shock capturing capabilities of the baseline TENO6 scheme, the TENO6 scheme was split into a linear and non linear counterpart. The coefficients of the linear part of the scheme are then expressed in terms of two free parameters (γ_{disp} and γ_{diss}) based on the approach of the MD CD scheme. This allows for the separate control or optimization of the dispersion and dissipation properties of the numerical scheme. A further consideration was taken into account to hybridize the MD CD scheme with the MD CD-TENO scheme such that a fully linear scheme is utilized for flux reconstruction in the smooth region of the flow and a hybrid scheme is utilized for flux reconstruction at non smooth region of the flow. This approach is achieved by using the absolute difference of the maximum and minimum smoothness indicator of the TENO scheme for a given stencil to discern if the flow is sufficiently smooth to use a fully linear scheme for flux reconstruction. In the non smooth region of the flow, an indicator based on the ratio of the minimum smoothness indicator is used to determine the maximum allowable contribution of the linear scheme towards flux reconstruction.

Based on the multidimensional spectral analysis considered, values of $\gamma_{disp} = 0.0568$ and $\gamma_{diss} = 0.062$ are determined based on the dispersion relation of the two dimensional ad-

vection and linearized Euler equation respectively. A value of $\gamma_{diss} = 0.001$ was selected to ensure that the numerical dissipation remain very close to zero but still negative for all reduced wavenumber considered. The prescribed values of γ_{disp} are considered universal since they were optimized for the exact dispersion relation. As for the prescribed values of γ_{diss} , a minimum value of 0.001 should be used although it can be increased gradually for problems involving very strong shock. Through a series of numerical experiments, it was found that the numerical results of the HYB-MDCD-TENO6 schemes optimized based on either the dispersion relation of the advection or the Linearized Euler equation give very similar results in terms of resolution characteristic. Although, it should be mentioned that the scheme optimized based on the linearized Euler equation tend to give slightly better results in some of the numerical experiments. In all cases, it was found that the HYB-MDCD-TENO6 scheme provides better resolution than existing baseline TENO and WENO-JS schemes for the same grid size considered.

From an engineering perspective, the non linear hybrid scheme that was developed in this chapter is especially suited for the study of flow involving both broadband length scale and shock phenomenon. This can be found in real-life examples such as the flow over a supercritical airfoil, hypersonic flow over the nose cone of a spacecraft, flow within the nozzle of a rocket, etc. Such flows are usually characterized by the interaction of the boundary layer and a shock. In some cases where the shock is sufficiently strong, it induces separation downstream due to the adverse pressure gradient.

Chapter 5

Conclusions

In this chapter, a summary of the key results of the previous chapters as well as recommendations for future research is presented.

5.1 Summary of Contributions

For the full discretization analysis of the 1D advection equation, a comparison of explicit and implicit temporal discretization scheme was made at an intermediate value of $R = 1.5$. Although the implicit Crank Nicolson is unconditionally stable across all wavenumber, the use of intermediate CFL number give rise to a much larger dispersion error at intermediate and large wavenumber as compared to the RK4 and RK3 scheme. When the governing equation is changed from the 1D advection to the 1D Linearized Euler equation, the dispersion relation composed of three different modes; one entropy and two acoustic modes. A comparison of the numerical amplification factor, group and phase velocities of the three different modes show that the dispersion relation belonging to the largest eigenvalue ($\omega = \bar{u} + a$) provides the limiting criteria for the stability limit as well as the onset of dispersion error. When the linear spectral analysis method is extended to the two dimensional wavespace, the dispersion and dissipation properties of the coupled schemes become a function of both the reduced wavenumber and the wave propagation angle. In the case of the two dimensional advection equation, group velocities of spatial discretization schemes for which the modified wavenumber is only a function of the wavenumber in one spatial direction (CDS4, DRP4, CCOM6) display variation in only one spatial direction when the CFL number is low.

When the two dimensional linear spectral analysis method is extended to the two dimensional linearized Compressible Navier Stokes equations (LCNSE), viscous and acoustic effects are taken into account in addition to the convection effects. The addition of the acoustic term to the dispersion relation leads to a coupling of the resolution characteristic such that the group velocities in either spatial direction become a function of the wavenumber in both spatial directions. Viscous effects are related to the cell Reynolds number, Re_a . As Re_a reduces, viscous effects become more dominant. In particular, the effect of using hybrid discretization (FD/FS) for both the convection and diffusion term of the LCNSE was compared against full FD discretization. For the purpose of quantifying the dispersion error between a full FD and hybrid scheme, $V_{grp,full}^*$ was used to understand the propagation of error from the FD scheme in the x spatial direction to the y spatial direction. In order to clearly see the propagation of dispersion error from one spatial direction to another, $k\Delta$ is set to 0.9π . For the CDS4, DRP4 and CCOM6 schemes, the comparison of $V_{grp,full}^*$ between the full FD and its hybrid discretization counterpart can be split into three distinct region. At low wave propagation angle, the full FD and hybrid discretization scheme share the same numerical group velocity. At intermediate wave propagation angle, a region exists for which the numerical group velocity of the full FD discretization become closer to the FS/FS solution. At large wave propagation angle, the numerical group velocity of the hybrid discretization cases become closer to the FS/FS solution. This is expected since the resolution of the scheme become closer to that of the FS scheme as the wave propagation angle approaches the direction where the FS method is used. For the CDS4_{opt} scheme, it was found that the dispersion error of the full FD scheme is lesser than the hybrid scheme for $0 \leq \theta_w \leq \pi/8$. For large wave propagation angle, the dispersion error of the hybrid scheme is always lesser than the full FD scheme for all spatial schemes considered. For the dissipation error, the minimum error is found to be at a wave propagation angle of $\pi/4$. Spatial scheme with better spectral properties such as the CCOM6 have numerical dissipation closer to the actual physical dissipation across all wave propagation angle. As compared to its full FD scheme counterpart, all hybrid FD/FS schemes have numerical dissipation either similar or closer to

the actual physical dissipation across all wave propagation angle.

The two dimensional spectral analysis method was extended to non linear finite difference schemes based on a quasi-linear assumption. In this assumption, the contribution of the harmonic modes (as a result of the non linear differentiation) are neglected during the calculation of the modified wavenumber of the spatial scheme. As such, quasi-linear analysis provides quantitatively correct prediction for the amplitude of the modes up to a time period where higher order effects related to the onset of spurious modes become important. Using the semi-discretized dispersion relation of the two dimensional advection and linearized Euler equations, the dispersion and dissipation property of the non linear scheme in two dimensional wavespace can be quantified based on $\Re(\omega^*\Delta - \omega\Delta)$ and $\Im(\omega^*\Delta - \omega\Delta)$ respectively. The baseline TENO6 scheme was split into a linear and non linear counterpart. The coefficients of the linear part of the scheme are then expressed in terms of two free parameters (γ_{disp} and γ_{diss}) based on the approach of the MDCD scheme. This allows for the separate control or optimization of the dispersion and dissipation properties of the numerical scheme. A further consideration was taken into account to hybridize the MDCD scheme with the MDCD-TENO6 scheme such that the linear MDCD scheme is utilized for flux reconstruction in the smooth region of the flow and the HYB-MDCD-TENO6 scheme is used at the non smooth region of the flow. Based on the multidimensional spectral analysis considered, values of $\gamma_{disp} = 0.0568$ and $\gamma_{diss} = 0.062$ are proposed based on the dispersion relation of the two dimensional advection and linearized Euler equation respectively. A value of $\gamma_{diss} = 0.001$ was selected to ensure that the numerical dissipation remain very close to zero but still negative for all wavenumber considered. Through a series of numerical experiments, it was found that the hybrid scheme optimized based on the linearized Euler equation tend to give slightly better results than the one optimized based on the advection equation in some of the numerical experiments. In all cases, it was found that the HYB-MDCD-TENO6 scheme provides better resolution than existing baseline TENO and WENO-JS schemes for the same grid size considered.

From an engineering perspective, the analysis framework developed in this research can be used to quantify the localized spectral error (under both spatial and temporal discretization) in the context of an adaptive mesh refinement method. It would then provide a universal indicator (irrespective of flow properties) on the amount of mesh refinement required at specific regions of the computational domain.

5.2 Future Research

For the purpose of future research, it is recommended to extend the methodology to finite volume or finite element method as described in [Sengupta et al., 2012]. For finite volume method, the discretization of the one dimensional convection equation is given as:

$$\int \left(\left[\frac{\partial u}{\partial t} \right] \Delta x + c(u_{j+1/2}^+ - u_{j-1/2}^+) \right) = 0 \quad (5.1)$$

This approach is based on the flux vector splitting method. The superscript represents the right moving quantities, indicating the balance of incoming and outgoing fluxes through the cell interface. Different representation of the flux quantity can be used, as given in [Leonard, 1979]. For finite element method, the basic idea is to approximate $u(x, t)$ by a finite series:

$$u(x, t) = \sum_{j=1}^N u_j(t) \psi_j(x). \quad (5.2)$$

where $\psi_j(x)$ is the basis function. By substituting equation 5.2 into the one dimensional convection equation and then multiplying the resulting equation by $\psi_i(x)$ and integrating over the whole domain, the resulting discrete equation of the interior nodes based on the Galerkin approximation with linear basis function is given by [Sengupta et al., 2012]:

$$\frac{1}{6} \left(\frac{\partial u_{i+1}}{\partial t} + 4 \frac{\partial u_i}{\partial t} + \frac{\partial u_{i-1}}{\partial t} \right) + \frac{c}{2\Delta x} (u_{i+1} - u_{i-1}) = 0. \quad (5.3)$$

From this equation, one can obtain both the semi-discretized and fully discretized dispersion relation, from which the numerical amplification factor as well as the group and phase velocities of the coupled scheme can be derived. Interested readers can refer to

[[Sengupta, 2004](#)] for more details.

Secondly, it is recommended to modify the methodology to the use of global matrix spectral analysis method to account for non periodic problems as reported in [[Sengupta and Bhole, 2014](#)], $u' = \frac{1}{\Delta x}[C]u$. However, due to the way the $[C]$ matrix is constructed, such method is restricted to linear type schemes. Thirdly, it is recommended to extend the methodology to the case of non uniform grid, as reported in [[Babucke and Kloker, 2009](#)]. The basic idea is to take into account the metric coefficient for which a specific grid stretching has to be defined. Therefore, the analysis will only be valid for the specific type of mesh considered. Interested readers can refer to [[Babucke and Kloker, 2009](#)] for more details. Finally, it is recommended to investigate the use of the newly developed hybrid shock capturing scheme on more realistic three dimensional shock turbulence interaction problems.

Appendix A

Appendix

A.1 Eigenvector and Eigenvalues of 2D Euler

The right (R), left (L) eigenvectors and eigenvalues (λ) of the two dimensional Euler equation are given below [Rohde, 2012]. They are used for transforming the numerical flux to and from the characteristic space.

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} + \frac{\partial G(U)}{\partial y} = 0 \quad (\text{A.1})$$

The following quantities are defined as follows; $q = \frac{u^2+v^2}{2}$, $a = \sqrt{\frac{\gamma p}{\rho}}$, $h = \frac{a^2}{\gamma-1} + q$.

$$J_f = \frac{\partial F(U)}{\partial U} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ (\gamma-1)q - u^2 & (3-\gamma)u & (1-\gamma)v & \gamma-1 \\ -uv & v & u & 0 \\ (\gamma-1)qu - hu & h - (\gamma-1)u^2 & (1-\gamma)uv & \gamma u \end{pmatrix} \quad (\text{A.2})$$

$$R_f = \begin{pmatrix} 1 & 1 & 1 & 0 \\ u-a & u & u+a & 0 \\ v & v & v & -1 \\ h-au & q & h+au & -v \end{pmatrix} \quad (\text{A.3})$$

$$L_f = R_f^{-1} = \begin{pmatrix} \frac{(\gamma-1)q+au}{2a^2} & \frac{(1-\gamma)u-a}{2a^2} & \frac{(1-\gamma)v}{2a^2} & \frac{(\gamma-1)}{2a^2} \\ \frac{a^2-(\gamma-1)q}{a^2} & \frac{(\gamma-1)u}{a^2} & \frac{(\gamma-1)v}{a^2} & \frac{(1-\gamma)}{a^2} \\ \frac{(\gamma-1)q-au}{2a^2} & \frac{(1-\gamma)u+a}{2a^2} & \frac{(1-\gamma)v}{2a^2} & \frac{(\gamma-1)}{2a^2} \\ v & 0 & -1 & 0 \end{pmatrix} \quad (\text{A.4})$$

$$\lambda_f = \begin{pmatrix} u-a & 0 & 0 & 0 \\ 0 & u & 0 & 0 \\ 0 & 0 & u+a & 0 \\ 0 & 0 & 0 & u \end{pmatrix} \quad (\text{A.5})$$

$$J_g = \frac{\partial G(U)}{\partial U} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ -uv & v & u & 0 \\ (\gamma-1)q-v^2 & (1-\gamma)u & (3-\gamma)v & \gamma-1 \\ (\gamma-1)qv-hv & (1-\gamma)uv & h-(\gamma-1)v^2 & \gamma v \end{pmatrix} \quad (\text{A.6})$$

$$R_g = \begin{pmatrix} 1 & 1 & 1 & 0 \\ u & u & u & 1 \\ v-a & v & v+a & 0 \\ h-av & q & h+av & u \end{pmatrix} \quad (\text{A.7})$$

$$L_g = R_g^{-1} = \begin{pmatrix} \frac{(\gamma-1)q+av}{2a^2} & \frac{(1-\gamma)u}{2a^2} & \frac{(1-\gamma)v-a}{2a^2} & \frac{(\gamma-1)}{2a^2} \\ \frac{a^2-(\gamma-1)q}{a^2} & \frac{(\gamma-1)u}{a^2} & \frac{(\gamma-1)v}{a^2} & \frac{(1-\gamma)}{a^2} \\ \frac{(\gamma-1)q-av}{2a^2} & \frac{(1-\gamma)u}{2a^2} & \frac{(1-\gamma)v+a}{2a^2} & \frac{(\gamma-1)}{2a^2} \\ -u & 1 & 0 & 0 \end{pmatrix} \quad (\text{A.8})$$

$$\lambda_g = \begin{pmatrix} v-a & 0 & 0 & 0 \\ 0 & v & 0 & 0 \\ 0 & 0 & v+a & 0 \\ 0 & 0 & 0 & v \end{pmatrix} \quad (\text{A.9})$$

A.2 Eigenvector and Eigenvalues of 3D Euler

The right (R), left (L) eigenvectors and eigenvalues (λ) of the three dimensional Euler equation are given below [Rohde, 2012]. They are used for transforming the numerical flux to and from the characteristic space.

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} + \frac{\partial G(U)}{\partial y} + \frac{\partial H(U)}{\partial z} = 0 \quad (\text{A.10})$$

The following quantities are defined as follows; $q = \frac{u^2+v^2+w^2}{2}$, $a = \sqrt{\frac{\gamma p}{\rho}}$, $h = \frac{a^2}{\gamma-1} + q$.

$$J_f = \frac{\partial F(U)}{\partial U} = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ (\gamma-1)q - u^2 & u - (\gamma-2)u & (1-\gamma)v & (1-\gamma)w & \gamma-1 \\ -uv & v & u & 0 & 0 \\ -uw & w & 0 & u & 0 \\ (\gamma-1)qu - hu & h - (\gamma-1)u^2 & (1-\gamma)uv & (1-\gamma)uw & \gamma u \end{pmatrix} \quad (\text{A.11})$$

$$R_f = \begin{pmatrix} 1 & 1 & 1 & 0 & 0 \\ u-a & u & u+a & 0 & 0 \\ v & v & v & -1 & 0 \\ w & w & w & 0 & 1 \\ h-au & q & h+au & -v & w \end{pmatrix} \quad (\text{A.12})$$

$$L_f = R_f^{-1} = \begin{pmatrix} \frac{(\gamma-1)q+au}{2a^2} & \frac{(1-\gamma)u-a}{2a^2} & \frac{(1-\gamma)v}{2a^2} & \frac{(1-\gamma)w}{2a^2} & \frac{(\gamma-1)}{2a^2} \\ \frac{a^2-(\gamma-1)q}{a^2} & \frac{(\gamma-1)u}{a^2} & \frac{(\gamma-1)v}{a^2} & \frac{(\gamma-1)w}{a^2} & \frac{(1-\gamma)}{a^2} \\ \frac{(\gamma-1)q-au}{2a^2} & \frac{(1-\gamma)u+a}{2a^2} & \frac{(1-\gamma)v}{2a^2} & \frac{(1-\gamma)w}{2a^2} & \frac{(\gamma-1)}{2a^2} \\ v & 0 & -1 & 0 & 0 \\ -w & 0 & 0 & 1 & 0 \end{pmatrix} \quad (\text{A.13})$$

$$\lambda_f = \begin{pmatrix} u-a & 0 & 0 & 0 & 0 \\ 0 & u & 0 & 0 & 0 \\ 0 & 0 & u+a & 0 & 0 \\ 0 & 0 & 0 & u & 0 \\ 0 & 0 & 0 & 0 & u \end{pmatrix} \quad (\text{A.14})$$

$$J_g = \frac{\partial G(U)}{\partial U} = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 \\ -uv & v & u & 0 & 0 \\ (\gamma-1)q-v^2 & (1-\gamma)u & v-(\gamma-2)v & (1-\gamma)w & \gamma-1 \\ -vw & 0 & w & v & 0 \\ (\gamma-1)qv-hv & (1-\gamma)uv & h-(\gamma-1)v^2 & (1-\gamma)vw & \gamma v \end{pmatrix} \quad (\text{A.15})$$

$$R_g = \begin{pmatrix} 1 & 1 & 1 & 0 & 0 \\ u & u & u & 1 & 0 \\ v-a & v & v+a & 0 & 0 \\ w & w & w & 0 & -1 \\ h-av & q & h+av & u & -w \end{pmatrix} \quad (\text{A.16})$$

$$L_g = R_g^{-1} = \begin{pmatrix} \frac{(\gamma-1)q+av}{2a^2} & \frac{(1-\gamma)u}{2a^2} & \frac{(1-\gamma)v-a}{2a^2} & \frac{(1-\gamma)w}{2a^2} & \frac{(\gamma-1)}{2a^2} \\ \frac{a^2-(\gamma-1)q}{a^2} & \frac{(\gamma-1)u}{a^2} & \frac{(\gamma-1)v}{a^2} & \frac{(\gamma-1)w}{a^2} & \frac{(1-\gamma)}{a^2} \\ \frac{(\gamma-1)q-av}{2a^2} & \frac{(1-\gamma)u}{2a^2} & \frac{(1-\gamma)v+a}{2a^2} & \frac{(1-\gamma)w}{2a^2} & \frac{(\gamma-1)}{2a^2} \\ -u & 1 & 0 & 0 & 0 \\ w & 0 & 0 & -1 & 0 \end{pmatrix} \quad (\text{A.17})$$

$$\lambda_g = \begin{pmatrix} v-a & 0 & 0 & 0 & 0 \\ 0 & v & 0 & 0 & 0 \\ 0 & 0 & v+a & 0 & 0 \\ 0 & 0 & 0 & v & 0 \\ 0 & 0 & 0 & 0 & v \end{pmatrix} \quad (\text{A.18})$$

$$J_h = \frac{\partial H(U)}{\partial U} = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 \\ -uw & w & 0 & u & 0 \\ -vw & 0 & w & v & 0 \\ (\gamma-1)q-w^2 & (1-\gamma)u & (1-\gamma)v & w-(\gamma-2)w & \gamma-1 \\ (\gamma-1)qw-hw & (1-\gamma)uw & (1-\gamma)vw & h-(\gamma-1)w^2 & \gamma w \end{pmatrix} \quad (\text{A.19})$$

$$R_h = \begin{pmatrix} 1 & 1 & 1 & 0 & 0 \\ u & u & u & -1 & 0 \\ v & v & v & 0 & 1 \\ w-a & w & w+a & 0 & 0 \\ h-aw & q & h+aw & -u & v \end{pmatrix} \quad (\text{A.20})$$

$$L_h = R_h^{-1} = \begin{pmatrix} \frac{(\gamma-1)q+aw}{2a^2} & \frac{(1-\gamma)u}{2a^2} & \frac{(1-\gamma)v}{2a^2} & \frac{(1-\gamma)w-a}{2a^2} & \frac{(\gamma-1)}{2a^2} \\ \frac{a^2-(\gamma-1)q}{a^2} & \frac{(\gamma-1)u}{a^2} & \frac{(\gamma-1)v}{a^2} & \frac{(\gamma-1)w}{a^2} & \frac{(1-\gamma)}{a^2} \\ \frac{(\gamma-1)q-aw}{2a^2} & \frac{(1-\gamma)u}{2a^2} & \frac{(1-\gamma)v}{2a^2} & \frac{(1-\gamma)w+a}{2a^2} & \frac{(\gamma-1)}{2a^2} \\ u & -1 & 0 & 0 & 0 \\ -v & 0 & 1 & 0 & 0 \end{pmatrix} \quad (\text{A.21})$$

$$\lambda_h = \begin{pmatrix} w-a & 0 & 0 & 0 & 0 \\ 0 & w & 0 & 0 & 0 \\ 0 & 0 & w+a & 0 & 0 \\ 0 & 0 & 0 & w & 0 \\ 0 & 0 & 0 & 0 & w \end{pmatrix} \quad (\text{A.22})$$

A.3 Exact Solution of the 1D Euler - Shock Tube

In this section, the procedure for determining the exact solution of the 1D Euler - Shock Tube problem is outlined. For the purpose of numerical verification, the reference numerical solution of the WENO5-JS, $N_x = 2000$ is compared against the exact solution. The solution is separated into four uniform region, with constant parameters (pressure, density and velocity); the left (L) and right (R) regions which are imposed from the initial condition and two intermediate regions, denoted by subscript (1) and (2). The shock and contact discontinuity propagate with constant velocities. The expansion wave extends through the new zone (Expansion) and its flow parameter vary continuously. It is noted that the shock wave and contact discontinuity propagate to the right while the expansion fan propagate to the left.

The following initial conditions are provided; $\rho_R, p_R, u_R = 0, a_R = \sqrt{\frac{\gamma p_R}{\rho_R}}, \rho_L, p_L, u_L = 0, a_L = \sqrt{\frac{\gamma p_L}{\rho_L}}$.

Step 1: Compute the compatibility equation to determine M_s , the Mach number of the shock defined in physical units.

$$M_s - \frac{1}{M_s} = a_L \frac{\gamma + 1}{\gamma - 1} \left(1 - \left[\frac{p_R}{p_L} \left(\frac{2\gamma}{\gamma + 1} M_s^2 - \frac{\gamma - 1}{\gamma + 1} \right) \right]^{\frac{\gamma - 1}{2\gamma}} \right) \quad (\text{A.23})$$

Since M_s appears on both side of the equation, an iterative method such as newton raphson can be used to determine the roots of the equation.

Step 2: The discontinuous jump between region (1) and (R) is described by the Rankine-Hugoniot relations. From this, ρ_1, p_1 and u_1 can be determined:

$$\begin{aligned}
\frac{p_1}{p_R} &= \frac{2\gamma}{\gamma+1} M_s^2 - \frac{\gamma-1}{\gamma+1} \\
\frac{\rho_R}{\rho_1} &= \frac{2}{\gamma+1} \frac{1}{M_s^2} + \frac{\gamma-1}{\gamma+1} \\
u_1 &= \frac{2}{\gamma+1} \left(M_s - \frac{1}{M_s} \right)
\end{aligned} \tag{A.24}$$

Step 3: Since the contact discontinuity is only a discontinuity of the density function and the pressure and velocity remain continuous. u_2 and p_2 are calculated using:

$$u_2 = u_1 \quad p_2 = p_1 \tag{A.25}$$

ρ_2 is calculated by considering the expressions for the invariants and taking into account that $u_L = 0$. ρ_2 and a_2 can be calculated from the following relations:

$$\frac{\rho_2}{\rho_L} = \left(\frac{p_2}{p_L} \right)^{1/\gamma} \quad u_2 = \frac{2}{\gamma-1} (a_L - a_2) \tag{A.26}$$

Step 4: To complete the exact solution, the extend of each region (x_1, x_2, x_3, x_4) for a given time value, t should be determined (see figure A.1).

$$\begin{aligned}
x_1 &= x_0 - a_L t, \quad x_2 = x_0 + (u_2 - a_2) t, \\
x_3 &= x_0 + u_2 t, \quad x_4 = x_0 + M_s t.
\end{aligned} \tag{A.27}$$

Step 5: The exact solution inside the expansion fan ($x_1 \leq x \leq x_2$) is calculated considering the characteristics relations and an isentropic flow condition:

$$\begin{aligned}
u_{exp} &= \frac{2}{\gamma-1} \left(a_L + \frac{x - x_0}{t} \right), \quad a_{exp} = a_L - (\gamma-1) \frac{u_{exp}}{2}, \\
p_{exp} &= p_L \left(\frac{a_{exp}}{a_L} \right)^{\frac{2\gamma}{\gamma-1}}, \quad \rho_{exp} = \frac{\gamma p_{exp}}{a_{exp}^2}
\end{aligned} \tag{A.28}$$

For the initial condition given in chapter 4 for the 1D shock tube problem:

$$(\rho, u, p) = \begin{cases} (1.0, 0, 1.0), & \text{if } x \leq 0, \\ (0.125, 0, 0.1), & x > 0. \end{cases} \quad (\text{A.29})$$

The following exact solution is obtained and compared with the reference numerical solution at $t = 0.14$ in figure A.1.

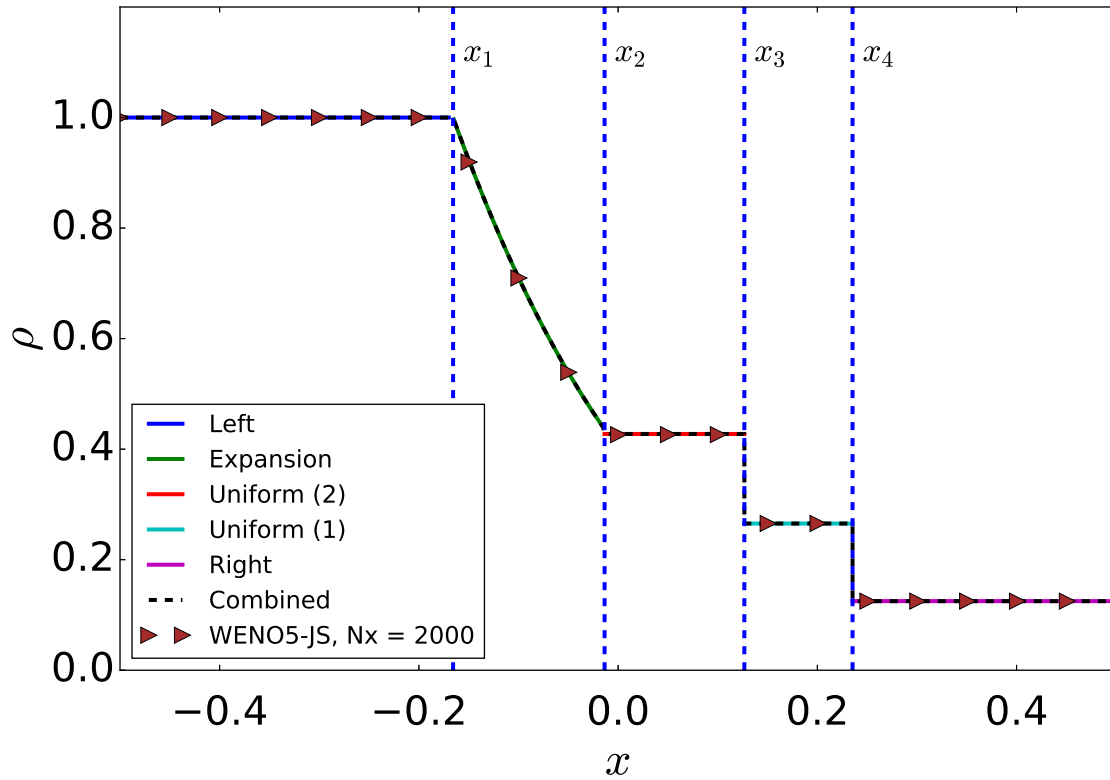


Figure A.1: (a) Comparison of density profile between reference numerical solution and exact solution at $t = 0.14$

It can be seen that the reference numerical result and the exact solution matches.

A.4 Details of Boundary Conditions

The details of the ghost point boundary method used in Chapter 3 and 4 are described in this section. In particular, periodic, dirichlet, outflow, symmetry slip wall and non-slip wall boundary conditions are described. To keep the discussion simple, the procedure for determining the values at the ghost points are described within the context of a serial code in one dimensional space. By using this method, the same scheme can be used throughout the entire computational domain, even at the boundary. Hence, no boundary scheme is needed.

A.4.1 Periodic Boundary Condition

Grid index ranges from 0 to $N-1$ (index notation of Python and C programming language). For illustration sake, we will use 3 ghost points on each end of the boundary. Mathematically, the values at the ghost points can be specified as follows:

$$\phi_{-1,-2,-3} = \phi_{N-1,N-2,N-3}, \quad \phi_{N,N+1,N+2} = \phi_{0,1,2} \quad (\text{A.30})$$

A.4.2 Dirichlet Boundary Condition

Dirichlet boundary condition is presented for just one side of the boundary. $\phi_{\text{specified value}}$ can represent any variable and is a value provided by the simulation problem.

$$\phi_{-1,-2,-3} = \phi_{\text{specified value}} \quad (\text{A.31})$$

A.4.3 Outflow Boundary Condition

In some test cases, the ghost point values at the outflow boundary are constructed using a linear extrapolation technique.

$$\tilde{\phi}(X - X_i) = a(X - X_i) + b, \quad (\text{A.32})$$

where X_i is centered at the boundary point. Coefficients a and b are then determined using the ϕ_i and ϕ_{i-1} values at X_i and X_{i-1} respectively. For $X = X_i$:

$$\tilde{\phi}(0) = b = \phi_i \quad (\text{A.33})$$

For $X = X_{i-1}$:

$$\begin{aligned} \tilde{\phi}(-\Delta x) &= -a\Delta x + \phi_i = \phi_{i-1} \\ a &= \frac{\phi_i - \phi_{i-1}}{\Delta x} \end{aligned} \quad (\text{A.34})$$

This results in the following formula for $X = X_{i+1,i+2,i+3}$:

$$\begin{aligned} \tilde{\phi}(\Delta x) &= \frac{\phi_i - \phi_{i-1}}{\Delta x} \Delta x + \phi_i \\ \tilde{\phi}(2\Delta x) &= \frac{\phi_i - \phi_{i-1}}{\Delta x} 2\Delta x + \phi_i \\ \tilde{\phi}(3\Delta x) &= \frac{\phi_i - \phi_{i-1}}{\Delta x} 3\Delta x + \phi_i \end{aligned} \quad (\text{A.35})$$

A.4.4 Symmetry Boundary Condition

The mathematical condition for symmetry is achieved by assuming a zero gradient boundary condition (no flux entering or leaving the domain). The ghost point values are set according to the way as described below. For the velocity vector (u , v and w), only the component perpendicular to the boundary plane are set equal but opposite values to enforce the zero gradient condition. The remaining velocity components as well as the pressure (p), total energy (e), temperature (T) and density (ρ) are set to be equal to the values reflected across the boundary interface. For illustration sake, a 2D domain and one end of the boundary will be considered. For a vertical boundary plane, the ghost point values are set as follows:

$$u_{-1,-2,-3} = -u_{1,2,3} \quad \phi_{-1,-2,-3} = \phi_{1,2,3}, \quad \phi \in [v, p, e, \rho, T] \quad (\text{A.36})$$

For a horizontal boundary plane, the ghost point values are set as follows:

$$v_{-1,-2,-3} = -v_{1,2,3} \quad \phi_{-1,-2,-3} = \phi_{1,2,3}, \quad \phi \in [u, p, e, \rho, T] \quad (\text{A.37})$$

A.4.5 Slip Wall Boundary Condition

For a slip wall boundary, it is assumed that the tangential velocity components are non-zero at the boundary interface and the perpendicular velocity component at the boundary interface is set to zero. Also, a zero gradient condition is imposed on the ghost points to prevent any flux from entering or leaving the interface. For illustration sake, a 2D domain is considered. For a horizontal free slip wall, the ghost point values are set as follows:

$$\begin{aligned} v_{-1,-2,-3} &= -v_{1,2,3} \quad \phi_{-1,-2,-3} = \phi_{1,2,3}, \quad \phi \in [u, p] \\ v_0 &= v_{wall} = 0. \end{aligned} \quad (\text{A.38})$$

In this approach, the pressure gradient is taken to be zero across the interface. Density and pressure are non-zero at the wall. Depending on the temperature boundary condition, the density is determined from the approach outlined in subsection A.4.7. Total energy, e can then be computed from the equation of state.

A.4.6 Non-Slip Wall Boundary Condition

For a non slip wall boundary, the, it is assumed that the all velocity components are zero at the boundary interface. Also, a zero gradient condition is imposed on the ghost points to prevent any flux from entering or leaving the interface. For illustration sake, a 2D domain is considered. For a horizontal non-slip wall, the ghost point values are set as follows:

$$\begin{aligned} v_{-1,-2,-3} &= -v_{1,2,3} \quad \phi_{-1,-2,-3} = \phi_{1,2,3}, \quad \phi \in [u, p] \\ u_0 &= u_{wall} = 0, \quad v_0 = v_{wall} = 0. \end{aligned} \quad (\text{A.39})$$

In this approach, the pressure gradient is taken to be zero across the interface. Density and pressure are non-zero at the wall. Depending on the temperature boundary condition, the density is determined from the approach outlined in subsection A.4.7. Total energy, e can then be computed from the equation of state.

A.4.7 Adiabatic or Isothermal Wall Boundary Condition

The temperature variable at the wall is specified based on whether a isothermal or adiabatic wall is considered. In the case of an adiabatic wall, the temperature gradient across the interface is set to zero. The temperatures at the wall are calculated according to the governing equations, from the evolving pressure and density. The ghost point values for an adiabatic horizontal wall are set as follows:

$$\begin{aligned} T_{-1,-2,-3} &= T_{1,2,3}, & P_{-1,-2,-3} &= P_{1,2,3}, \\ v_{-1,-2,-3} &= -v_{1,2,3}, & u_{-1,-2,-3} &= u_{1,2,3}, \\ \rho &= \frac{\gamma M^2 P}{T}, & e &= \frac{P}{(\gamma - 1)} + \frac{1}{2} \rho (u^2 + v^2). \end{aligned} \quad (\text{A.40})$$

For an isothermal wall, the temperature values at the wall are specified and the values at the ghost points are linearly extrapolated from interior points.

$$T_0 = T_{wall} = T_{\text{specified value}}, \quad T_{-1,-2,-3} = \frac{T_1 - T_0}{\Delta x} (n \Delta x) + T_0, \quad n = -1, -2, -3. \quad (\text{A.41})$$

The ghost point values of the remaining primitive variables are calculated as follows:

$$\begin{aligned} v_{-1,-2,-3} &= -v_{1,2,3}, & u_{-1,-2,-3} &= u_{1,2,3}, \\ \rho &= \frac{\gamma M^2 P}{T}, & e &= \frac{P}{(\gamma - 1)} + \frac{1}{2} \rho (u^2 + v^2). \end{aligned} \quad (\text{A.42})$$

Bibliography

- [Abarbanel and Gottlieb, 1981] Abarbanel, S. and Gottlieb, D. (1981). Optimal Time Splitting for Two- and Three Dimensional Navier-Stokes Equations with Mixed Derivatives. *Journal of Computational Physics*, 41:1–33.
- [Adam, 1977] Adam, Y. (1977). Highly accurate compact implicit methods and boundary conditions. *Journal of Computational Physics*, 24:10–22.
- [Adams and Shariff, 1996] Adams, N. A. and Shariff, K. (1996). A High-Resolution Hybrid Compact-ENO Scheme for Shock-Turbulence Interaction Problems. *Journal of Computational Physics*, 127:27–51.
- [Ames, 1977] Ames, W. F. (1977). *Numerical Methods for Partial Differential Equations*. Academic Press, 2 edition.
- [Babucke and Kloker, 2009] Babucke, A. and Kloker, M. (2009). Accuracy Analysis of Finite Difference Methods on Non-Uniform Grids. Technical Report 1, University of Stuttgart, Institute for Aerodynamics and Gasdynamics, Pfaffenwaldring 21, 70550 Stuttgart.
- [Bhumkar et al., 2014] Bhumkar, Y. G., Sheu, T. W. H., and Sengupta, T. K. (2014). A dispersion relation preserving optimized upwind compact difference scheme for high accuracy flow simulations. *Journal of Computational Physics*, 278:378–399.
- [Bodart et al., 2009] Bodart, J., Cazalbou, J.-B., and Laurent, J. (2009). Large scale simulation of turbulence using a hybrid spectral/finite difference solver. pages 1–5, Moffet Field, USA. 21st International Conference on Parallel Computational Fluid Dynamics.

- [Bogey and Bailly, 2004] Bogey, C. and Bailly, C. (2004). A family of low dispersive and low dissipative explicit schemes for flow and noise computations. *Journal of Computational Physics*, 194:194–214.
- [Brachet et al., 1983] Brachet, M. E., Meiron, D. I., Orszag, S. A., Nickel, B. G., Morf, R. H., and Frisch, U. (1983). Small-scale structure of the TaylorGreen vortex. *Journal of Fluid Mechanics*, 130:411–452.
- [Canuto et al., 2006] Canuto, C., Hussaini, M. Y., Quarteroni, A., and Zang, T. A. J. (2006). *Spectral Methods, Fundamentals in Single Domain*. Springer, Berlin, Heidelberg, 1 edition.
- [Costa and Don, 2007] Costa, B. and Don, W. S. (2007). High order Hybrid central WENO finite difference scheme for conservation laws. *Journal of Computational and Applied Mathematics*, 204:209–218.
- [De and Eswaran, 2006] De, A. K. and Eswaran, V. (2006). Analysis of a new high resolution upwind compact scheme. *Journal of Computational Physics*, 218:398–416.
- [Fan, 2016] Fan, P. (2016). The standard upwind compact difference schemes for incompressible flow simulations. *Journal of Computational Physics*, 322:74–112.
- [Fauconnier and Dick, 2013] Fauconnier, D. and Dick, E. (2013). Spectral analysis of non-linear finite difference discretizations. *Journal of Computational and Applied Mathematics*, 246:113–121.
- [Ferziger and Peric, 2002] Ferziger, J. H. and Peric, M. (2002). *Computational Methods for Fluid Dynamics*. Springer Nature Switzerland AG., 3 edition.
- [Fornberg, 1988] Fornberg, B. (1988). Generation of finite difference formulas on arbitrarily spaced grids. *Mathematics of Computation*, 51:699–706.
- [Fu, 2018] Fu, L. (2018). A Hybrid Method with TENO Based Discontinuity Indicator for Hyperbolic Conservation Law. *Communications in Computational Physics*, 26:973–1007.

- [Fu et al., 2018] Fu, L., Hu, X. Y., , and Adams, N. A. (2018). Improved Five and Six Point Targeted Essentially Nonoscillatory Schemes with Adaptive Dissipation. *AIAA Journal*, 57(3).
- [Fu et al., 2016] Fu, L., Hu, X. Y., and Adams, N. A. (2016). A family of high-order targeted ENO schemes for compressible-fluid simulations. *Journal of Computational Physics*, 305:333–359.
- [Fu et al., 2017] Fu, L., Hu, X. Y., and Adams, N. A. (2017). Targeted ENO schemes with tailored resolution property for hyperbolic conservation laws. *Journal of Computational Physics*, 349:97–121.
- [Harten, 1983] Harten, A. (1983). High resolution schemes for hyperbolic conservation laws. *Journal of Computational Physics*, 49:357–393.
- [Harten et al., 1987] Harten, A., Engquist, B., Osher, S., and Chakravarthy, S. R. (1987). Uniformly high order accurate essentially non-oscillatory schemes, III. *Journal of Computational Physics*, 71:231–303.
- [He et al., 2015] He, Z. W., Zhang, Y. S., Li, X. l., Li, L., and Tian, B. (2015). Preventing numerical oscillations in the flux-split based finite difference method for compressible flows with discontinuities. *Journal of Computational Physics*, 300:269–287.
- [Hirsh, 1975] Hirsh, R. S. (1975). Higher order accurate difference solutions of fluid mechanics problems by a compact differencing technique. *Journal of Computational Physics*, 19:90–109.
- [Jiang and Shu, 1996] Jiang, G. S. and Shu, C. W. (1996). Efficient Implementation of Weighted ENO Schemes. *Journal of Computational Physics*, 126:202–228.
- [Kemm, 2016] Kemm, F. (2016). On the proper setup of the double Mach reflection as a test case for the resolution of gas dynamics codes. *Computers and Fluids*, 132:72–75.
- [Kim and Lee, 1996] Kim, J. W. and Lee, D. J. (1996). Optimized compact finite difference schemes with maximum resolution. *AIAA Journal*, 34:887–893.

- [Kopal, 1961] Kopal, Z. (1961). *Numerical analysis, with emphasis on the application of numerical techniques to problems of infinitesimal calculus in single variable*. Springer US, 2 edition.
- [Lele, 1992] Lele, S. K. (1992). Compact Finite Difference Schemes with Spectral like Resolution. *Journal of Computational Physics*, 103:16–42.
- [Leonard, 1979] Leonard, B. P. (1979). A stable and accurate convective modelling procedure based on quadratic upstream interpolation. *Computer Methods in Applied Mechanics and Engineering*, 19:59–98.
- [Li et al., 2012] Li, X. L., Leng, Y., and He, Z. W. (2012). Optimized sixth-order monotonicity-preserving scheme. In *Seventh International Conference on Computational Fluid Dynamics (ICCFD7)*. International Conference on Computational Fluid Dynamics, International Conference on Computational Fluid Dynamics.
- [Li, 1997] Li, Y. (1997). Wavenumber-extended high order upwind biased finite difference schemes for convective scalar transport. *Journal of Computational Physics*, 133:235–255.
- [Liu et al., 1994] Liu, X. D., Osher, S., and Chan, T. (1994). Weighted Essentially Non-oscillatory Schemes. *Journal of Computational Physics*, 115:200–212.
- [Marie et al., 2009] Marie, S., Ricot, D., and Sagaut, P. (2009). Comparison between lattice Boltzmann method and Navier Stokes high order schemes for computational aeroacoustics. *Journal of Computational Physics*, 228:1056–1070.
- [Moin, 2001] Moin, P. (2001). *Fundamentals of Engineering Numerical Analysis*. Cambridge University Press.
- [Moore, 2016] Moore, S. (2016). Applied numerical methods. Lecture Notes for High Performance Computing.
- [Orszag, 1969] Orszag, S. (1969). Numerical Methods for the Simulation of Turbulence. *AIP Physics of Fluid*, 12:2–250.

- [Peng and Shen, 2015] Peng, J. and Shen, Y. (2015). Improvement of weighted compact scheme with multi-step strategy for supersonic compressible flow. *Computers and Fluids*, 115:243–255.
- [Peng et al., 2019] Peng, J., Zhai, C. L., Ni, G., Yong, H., and Shen, Y. (2019). An adaptive characteristic-wise reconstruction WENO-Z scheme for gas dynamic euler equations. *Computers and Fluids*, 179:34–51.
- [Pirrozzoli, 2002] Pirrozzoli, S. (2002). Conservative Hybrid Compact-WENO Schemes for Shock-Turbulence Interaction. *Journal of Computational Physics*, 178:81–117.
- [Pirrozzoli, 2006] Pirrozzoli, S. (2006). On spectral properties of shock-capturing schemes. *Journal of Computational Physics*, 219:489–497.
- [Pirrozzoli, 2007] Pirrozzoli, S. (2007). Performance analysis and optimization of finite-difference schemes for wave propagation problems. *Journal of Computational Physics*, 222:809–831.
- [Rai and Moin, 1991] Rai, M. M. R. and Moin, P. (1991). Direct simulations of turbulent flow using finite-difference schemes. *Journal of Computational Physics*, 96:15–53.
- [Roe, 1981] Roe, P. L. (1981). Approximate Riemann solvers, parameter vectors, and difference schemes. *Journal of Computational Physics*, 43:357–372.
- [Rohde, 2012] Rohde, A. (2012). Eigenvalues and eigenvectors of the Euler equations in general geometries. *AIAA*. 2001-2609.
- [Sengupta, 2004] Sengupta, T. K. (2004). *Fundamentals of Computational Fluid Dynamics*. Universities Press, 1 edition.
- [Sengupta, 2013] Sengupta, T. K. (2013). *High Accuracy Computing Methods, Fluid Flows and Wave Phenomena*. Cambridge University Press.
- [Sengupta and Bhole, 2014] Sengupta, T. K. and Bhole, A. (2014). Error dynamics of diffusion equation: Effects of numerical diffusion and dispersive diffusion. *Journal of Computational Physics*, 266:240–251.

- [Sengupta et al., 2012] Sengupta, T. K., Bhumkar, Y. G., Rajpoot, M. K., Suman, V. K., and Saurabh, S. (2012). Spurious waves in discrete computation of wave phenomena and flow problems. *Applied Mathematics and Computation*, 218:9035–9065.
- [Sengupta and Dipankar, 2004] Sengupta, T. K. and Dipankar, A. (2004). A Comparative Study of Time Advancement Methods for Solving Navier Stokes Equations. *Journal of Scientific Computing*, 21:225–250.
- [Sengupta et al., 2007] Sengupta, T. K., Dipankar, A., and Sagaut, P. (2007). Error dynamics: Beyond von Neumann analysis. *Journal of Computational Physics*, 226:1211–1218.
- [Sengupta et al., 2003] Sengupta, T. K., Ganeriwal, G., and S., D. (2003). Analysis of central and upwind compact schemes. *Journal of Computational Physics*, 230:688–694.
- [Sengupta et al., 2011a] Sengupta, T. K., Rajpoot, M. K., and Bhumkar, Y. G. (2011a). Space-time discretizing optimal DRP schemes for flow and wave propagation problems. *Computer and Fluids*, 47:144–154.
- [Sengupta et al., 2011b] Sengupta, T. K., Rajpoot, M. K., Saurabh, S., and Vijay, V. V. S. N. (2011b). Analysis of anisotropy of numerical wave solutions by high accuracy finite difference methods. *Journal of Computational Physics*, 230:27–60.
- [Sengupta et al., 2006] Sengupta, T. K., Sircar, S. K., and Dipankar, A. (2006). High Accuracy Schemes for DNS and Acoustics. *Journal of Scientific Computing*, 26:151–193.
- [Sescu, 2008] Sescu, A. (2008). Multidimensional optimization of finite difference schemes for Computational Aeroacoustics. *Journal of Computational Physics*, 227:4563–4588.
- [Shen and Yang, 2007] Shen, Y. and Yang, G. (2007). Hybrid finite compactWENO schemes for shock calculation. *International Journal for Numerical methods in Fluids*, 53:531–560.
- [Shen et al., 2009] Shen, Y., Zha, G., and Chen, X. (2009). High order conservative differencing for viscous terms and the application to vortex-induced vibration flows. *Journal of Computational Physics*, 228:8283–8300.

- [Stegeman et al., 2012] Stegeman, P. C., Young, M. E., Soria, J., and Ooi, A. (2012). Analysis of the anisotropy of group velocities error due to spatial finite difference schemes from the solution of the 2D linear Euler equations. *International Journal For Numerical Methods in Fluids*, 71:805–829.
- [Suman et al., 2017] Suman, V. K., Sengupta, T. K., Prasad, C. J. D., Mohan, K. S., and Sanwalia, D. (2017). Spectral analysis of finite difference schemes for convection diffusion equation. *Computers and Fluids*, 150:95–114.
- [Sun et al., 2011] Sun, Z. S., Ren, Y. S., Larricq, C., Zhang, S. Y., and Yang, Y. C. (2011). A class of finite difference schemes with low dispersion and controllable dissipation for DNS of compressible turbulence. *Journal of Computational Physics*, 230:4616–4635.
- [Tam and Webb, 1993] Tam, C. K. W. and Webb, J. C. (1993). Dispersion Relation Preserving Finite Difference Schemes for Computational Acoustics. *Journal of Computational Physics*, 107:262–281.
- [Tan et al., 2018] Tan, R., Ooi, A., and Sandberg, R. (2018). Numerical Anisotropy of the 2D Linearised Euler Equations under Spatial and Temporal Discretization for a Hybrid Spectral/Finite Difference Method. *21st Australasian Fluid Mechanics Conference*.
- [Thomas and Lombard, 1979] Thomas, P. D. and Lombard, C. K. (1979). Geometric Conservation Law and Its Application to Flow Computations on Moving Grids. *AIAA Journal*, 17:1030–1037.
- [Trefethen, 1982] Trefethen, L. (1982). Group Velocities in Finite Differences Schemes. *Society of Industrial Applied Mathematics (SIAM) Review*, 24:113–136.
- [Vichnevetsky and Bowles, 1982] Vichnevetsky, R. and Bowles, J. (1982). *Fourier Analysis of Numerical Approximations of Hyperbolic Equations*. SIAM, Society for Industrial and Applied Mathematics.
- [You et al., 2006] You, D., Mittal, R., Wang, M., and Parviz, M. (2006). Analysis of stability and accuracy of finite-difference schemes on a skewed mesh. *Journal of Computational Physics*, 213:184–204.

- [Zhong, 1998] Zhong, X. (1998). High-order finite difference schemes for numerical simulation of hypersonic boundary-layer transition. *Journal of Computational Physics*, 144:662–709.
- [Zingg, 2006] Zingg, D. W. (2006). Comparison of High-Accuracy Finite-Difference Methods for Linear Wave Propagation. *SIAM Journal on Scientific Computing*, 22:476–502.