Spurious waves in discrete computation of wave phenomena and flow problems

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Abstract

In the present work, we focus on spurious propagating disturbances (q-waves). To establish the existence of q-waves in computations, we compare properties of different numerical methods drawn from finite difference, finite volume and finite element methods. Existence and properties of q-waves are demonstrated with propagation of wave-packets following one-dimensional (1D) convection equation; skewed wave propagation and by solution of linearized rotating shallow water wave equation (LRSWE). Specific numerical experiments are performed with parameters that convert a wave-packet into a q-wave. We also show the case where q-waves are created additionally to physical disturbances those propagate downstream. Formation of q-waves are shown in the case of a discrete shielded vortex in the uniform flow and incompressible transitional flow past an aerofoil by solving the Navier–Stokes equation. In performing this exercise, we establish critical wavenumber range beyond which q-waves are created. Relevance of this information for DNS and LES is discussed. We have further discussed the case of spurious caustics in discrete computing.

1. Introduction

Simultaneous creation of physical and spurious waves in specific computations has been known as reported in Vichnevetsky & Bowles [1], Poinset & Veynante [2], Baum & Levine [3], Baum et al. [4] and the other references contained therein. The physical waves (acoustic, vortical and entropic waves [5]) which arise naturally have been termed as p-waves, while non-physical waves which arise due to numerical methods are termed as the q-waves [1,2]. Spurious numerical waves have been identified as parasite waves by Trefethen [6], who conjectured that this is due to numerical group velocity and traced it to earlier work in [7]. In Trefethen [6], no quantitative measure was provided but the author suggested that the parasite waves occur for wavenumbers very close to the Nyquist limit. Vichnevetsky and co-authors in [1,7] have reported semi-discrete analysis for CD₂ scheme and Galerkin finite element methods for 1D convection equation to explain q-waves qualitatively. In contrast, authors in [2] have identified auxiliary conditions for creating q-waves. In the present work, existence of q-waves is related to the numerical group velocity.

The 1D convection equation has been used extensively [1,8,9] to explain properties of spatial discretization. We note that in [1,2,7], analysis of this equation was performed for a semi-discrete system, i.e., no effects of time discretization were included in the analysis. The shortcoming of ignoring time discretization in the analysis, was rectified in [6,8,10].

With the correct numerical dispersion relation [11], roles of phase and dispersion errors are highlighted in [12] for signal propagation questioning the basis of von Neumann error analysis for linear dynamical system, based on the assumption of...
identical governing equation for signal and error. This counter-intuitive observation is a consequence of correct numerical dispersion relation which also explains the genesis of q-waves.

For the analysis of space–time discretization schemes, model 1D convection equation is used, given as,

\[
\frac{\partial u}{\partial t} + c \frac{\partial u}{\partial x} = 0, \quad c > 0
\]  

(1)

As a mathematical equation, Eq. (1) convects the initial solution to the right at the group velocity (which is equal to the phase speed c, at all times due to non-dispersive nature of Eq. (1)).

Space–time dependence of Eq. (1) is explained by the Fourier–Laplace representation of the unknown by,

\[
u(x, t) = \int \hat{u} e^{i(k x - \omega t)} dk d\omega,
\]

which in turn provides the exact dispersion relation as, \(\omega = kc\). In analysing Eq. (1), early works treated spatial and time discretization independently and used the numerical dispersion relation as,

\[
\omega_{eq} = keq c
\]

(2)

where \(\omega_{eq}\) and \(keq\) are the equivalent circular frequency and wavenumber in obtaining first derivative numerically with respect to \(t\) and \(x\). This uses the assumption that the numerical and the physical phase speeds are same. Use of Eq. (2) can be noted in [6], as in Eq. (1.9), where second order central differencing was used for spatial derivative and Crank-Nicolson, second and fourth order leap-frog schemes were used for temporal discretization.

Analyses in [11,12] obtained the correct dispersion relation by expressing the unknown \(u\) using a hybrid representation via the bi-lateral Laplace transform at the \(j\)th node as, \(u(x, t) = \int U(k, t) e^{i k x} dk\).

Using this hybrid representation, exact spatial derivative is given by, \(\frac{\partial u}{\partial x}\) exact = \(\int ik U(k, t) \ e^{ikx} dk\). In contrast, any discrete method represents the same spatial derivative \(u'_j\) (denoted by a prime) by,

\[
[u'_j]_{\text{numerical}} = \int ik_{eq} U(k, t) \ e^{ikx} dk
\]

(3)

In discrete computations, difference of \(k_{eq}\) with \(k\) acts as a source of error. Many researchers have tried to increase the accuracy of numerical schemes by minimizing the departure of \(k_{eq}\) from \(k\), adopting appropriate error norms - as in [11,13–16]. Even in this approach, efforts have been directed in either solving periodic problems [16] or just simply evaluating the property of interior nodes of non-periodic problems [13,15]. However, a global matrix spectral analysis is used for non-periodic problems. Even in this approach, efforts have been directed in either solving periodic problems or just simply evaluating the property of interior nodes of non-periodic problems.

Comparison of Eqs. (3) and (4) yields,

\[
[i k_{eq}]_j = \frac{1}{h} \sum_{l=1}^{N} C_{jl} e^{i(k_{l} - k) h}
\]

(5)

In computations, \(C_{jl}\)'s are real, while \(|k_{eq}|\) is in general complex, with real part representing the numerical phase and imaginary part is the numerical dissipation added by the choice of a method via the entries of the \([C]\)- matrix.

One of the consequences of using Eq. (2) as the numerical dispersion relation gives rise to incorrect numerical group velocity as,

\[
\frac{d\omega_{eq}}{dk} = \frac{dk_{eq}}{dk}
\]

(6)

The numerical dispersion relation is re-evaluated [11,12] by starting from the discretized equation as indicated next. Main important properties of different numerical methods are obtained by using the hybrid spectral representation of unknown in Eq. (1), which gives

\[
\int \left[ \frac{\partial U}{\partial t} + \frac{c}{h} \sum_{l=1}^{N} UC_{jl} e^{i(k_{l} - k) h} \right] e^{ikx} dk = 0
\]

(7)

The implicit condition of Eq. (7) is reinterpreted as,

\[
\frac{dU}{U} = \left[ \frac{1}{h} \sum_{l=1}^{N} C_{jl} e^{i(k_{l} - k) h} \right]
\]

(8)
where the first factor within the square bracket on the right hand side is the well-known CFL number ($N_c$). Since the right hand side of Eq. (8) is node-dependent, the left hand side is also written in terms of the nodal amplification factor ($G_j = U_j(t, \tau^{(n+1)})/U_j(t, \tau^{(n)}))$.

In general, $G_j$ is seen to be a complex quantity and implies that the numerical scheme amplifies or attenuates the Fourier–Laplace transform $U(k, t)$ and also introduces a phase shift. For the four-stage Runge–Kutta time integration scheme, $G_j$ is obtained [11,12] as,

$$G_j = 1 - A_1 + \frac{A_2^2}{2} + \frac{A_3^2}{6} + \frac{A_4^2}{24}$$  \tag{9}$$

where $A_i = N_c \sum_{j=1}^{N_c} C_{ij} e^{i(\xi_j-x_k)}$. It is shown in [11,12] that all discretization methods introduce phase error which can be quantified. If the initial condition for Eq. (1) is given by $u(x_j, t=0) = u_j^0 = \int A_0(k) e^{i\omega t} dk$, then the general solution at any arbitrary later time can be written as,

$$u_j^n = \int A_0(k) |[G_j]|^n e^{i(k\Delta x - n\beta)} dk$$  \tag{10}$$

where $|G_j| = (G_j')^2 + (G_j'')^2$ and $\tan(\beta) = -\frac{n\omega}{cN}$, indicates the phase shift per time step, with $G_j'$ and $G_j''$ as the real and imaginary parts of $G_j$. From Eq. (10), $n\beta = kcNt$, where $c_0$ is the numerical wavenumber dependent phase speed, distinct from $c$. All discrete solution methods are dispersive, in contrast to the non-dispersive nature of Eq. (1) which was noted in [6]. The numerical phase speed is given by, $c_N = \frac{c_0}{c_{Nc}}$.

Numerical dispersion relation is correctly obtained as $\omega_{BE} = c_N k$, instead of its analytic counterpart: $\omega = c k$ and this helped in obtaining the scaled numerical phase speed and group velocity at the $j$th discrete node for the solution of Eq. (1) as [12],

$$\left[ \frac{c_N}{c} \right]_{ij} = \frac{\beta_j}{\omega \Delta t}; \quad \left[ \frac{\omega_{GN}}{c} \right]_{ij} = \frac{1}{hN_c} \frac{d\beta_j}{dk}$$  \tag{11}$$

It is readily apparent that any discrete computing method can be investigated by using Eqs. (9) and (11) in $(N_c, k\Delta)$-plane, with these two as the natural independent variables for the analysis. This can be used for non-periodic problems with properties obtained at all the nodes. Characteristics of some well-known finite difference methods have been reported in [11] for various explicit and implicit discretizing techniques. Global spectral matrix stability analysis shows that many compact schemes suffer from numerical instability near the inflow of the computational domain.

Here, we show that $q$-waves are solely due to extreme forms of dispersion error for different numerical methods. At times, physical disturbances can propagate upstream as in bypass transition [17,18] and this should be distinguished from $q$-waves. Thus, for DNS of bypass transitional flows, one would like to capture the $p$-waves associated with bypass transition, while avoiding the $q$-waves which arise solely due to poor numerical properties at high wavenumbers. In the next section, we quantify the parameter combinations for which $q$-waves are generated in different numerical methods.

2. Prediction of parameter ranges in creating spurious numerical waves

For discrete methods, closeness between physical and numerical dispersion relation can be realized only for limited ranges of space and time steps. In [10], compact schemes were characterized for the full-domain by a spectral analysis, with numerical group velocity used to measure dispersion error. For the four-stage Runge–Kutta time integration scheme, $G_j$ is obtained [11,12] as,

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For compact schemes, the [C]- matrix is given by $[A]^{-1} [B]$. Having obtained the [C]- matrix, it is easy to obtain the amplification factor $G_j$, for general time integration schemes. For RK4 method one can obtain $G_j$ from Eq. (9). This approach is used for obtaining $G_j$ for the explicit spatial scheme (CD4) (for which $[C] = [B]$) and the optimized upwind compact scheme (OUCS3) [10] for spatial discretization with RK4 time integration scheme.

For any function $f$, first order spatial derivatives are represented in OUCS3 scheme for the interior nodes by [10],

$$p_{j,j-1} f_{j-1} + p_{j,2} f_{j} = \frac{1}{\Delta} \sum_{k=-2}^{2} q_{k} f_{j+k}; \quad 3 \leq j \leq N-2$$  \tag{13}$$

where \( p_{j,1} = D = \frac{\alpha}{2} \), \( q_{\pm 2} = \pm \frac{5}{6} + \frac{\xi}{60} \), \( q_{\pm 1} = \pm \frac{5}{9} + \frac{\xi}{60} \) and \( q_0 = -\frac{11}{720} \) with \( D = 0.3793894912 \), \( E = 1.57557379 \), \( F = 0.18205192 \). Here $\xi$ is the upwind parameter and $\xi = 0$ implies central scheme. One can use the boundary closure schemes given in [10] for $j = 1, 2, N-1$ and $N$.

For finite volume scheme, we investigate the QUICK scheme [19] for Eq. (1) using flux vector splitting of the convection term giving,
\[
\int \frac{\partial u}{\partial t} \Delta x + c \left( u_{j+1/2}^+ - u_{j-1/2}^- \right) = 0
\]  \hspace{1cm} (14)

In the above, RK4 time integration is used for the jth cell and the superscript for the second set of terms indicate right moving quantities, showing the balance of incoming and outgoing fluxes through the cell interfaces. One of the representative flux quantity is given by [8],

\[
u_{j+1/2}^- = u_{j-1}^+ + \frac{1}{4} \left[ (1 - \kappa)(u_{j-1} - u_{j-2}) + (1 + \kappa)(u_j - u_{j-1}) \right] \hspace{1cm} (15)
\]

where \( \kappa = 1/2 \) for the QUICK scheme. Other flux term, \( \nu_{j+1/2}^+ \) can be similarly obtained [19]. These expressions help one obtain the \( [C] \)- matrix in Eqs. (4) and (5) which in turn yields \( G_j \). A similar analysis of compact scheme-based flux vector splitting finite volume methods is given in [20].

For finite element methods, we analyse the streamwise upwind Petrov–Galerkin (SUPG) method described in [21]. Among the finite element formulations, Galerkin methods belong to the class of solutions for PDEs where the solution residue is minimized giving rise to the weak formulation of problems. In this approach, the dependent variable \( u(x,t) \), for a one-dimensional space–time dependent problem is expressed in an expansion of the form,

\[
u(x,t) = \sum_{i=1}^{N} \phi_i(x) \ u_i(t) \hspace{1cm} (16)
\]

where \( \phi_1, \ldots, \phi_N \) are the basis functions and are chosen as low-order polynomials localized about an element. Galerkin methods have been used in diverse applications, including meteorology, oceanography and other problems which require tracking wave phenomena [22]. It is shown in [8,22] that the dispersion property of Galerkin method using linear basis functions (G1FEM) is far superior even when one uses Euler time integration. It has been specifically noted that in weak formulations, space–time discretization is considered together which gives rise to the better dispersion relation preserving (DRP) properties.

However, it has been noted in Strang and Fix [23] that Galerkin methods do not work for hyperbolic problems due to their non-dissipative nature. This has been further identified in terms of \( G \) in [8,22] due to unstable nature of the discretization at the boundary element of the inflow in G1FEM, for Eq. (1). Similarly, expression for the amplification factor in solving 1D convection equation by quadratic basis functions (G2FEM) is given in [22].

One method of removing problems of Galerkin FEM is to make the discrete equation dissipative. Dendy [24] and Wahlbin [25] have proposed dissipative Galerkin procedures. The procedure of [24] was furthermore adopted by Raymond & Garder [26] and an optimal procedure advocated in following an approximate form of phase error proposed in [27] for 1D convection equation. Brooks & Hughes [28] have adopted the methodology in [24,26], in their Petrov–Galerkin formulation and called it “Streamline Upwind/ Petrov–Galerkin (SUPG)” method. In [26], the authors also refer to “ghost” or q-waves following the work in [29]. This was projected as due to recombination of noise reflected from the boundary. A complete analysis of the above mentioned q-waves is provided here for SUPG formulation.

The discretized form of Eq. (1) for G1FEM is given in [8,22] by using the Galerkin approximation with linear basis functions. One obtains, for a uniformly spaced grid, the discrete equation as,

\[
h \left( \frac{du_{j+1}}{dt} + 4 \frac{du_j}{dt} + \frac{du_{j-1}}{dt} \right) + c \left( u_{j+1} - u_{j-1} \right) = 0 \hspace{1cm} (17)
\]

for any interior node, \( j \). For the boundary nodes \( j = 1, N \) one obtains,

\[
j = 1: h \left( \frac{2 du_1}{dt} + \frac{du_2}{dt} \right) + c(u_2 - u_1) = 0 \hspace{1cm} (18)
\]

\[
j = N: h \left( \frac{2 du_N}{dt} + \frac{du_{N-1}}{dt} \right) + c(u_N - u_{N-1}) = 0 \hspace{1cm} (19)
\]

Three aspects are evident from the above discrete equations for the Galerkin approximation with linear basis functions: (i) the non-dissipative nature of the discrete equation for the interior nodes with the symmetric stencil; (ii) instability at the node \( j = 1 \) due to the non-physical one-sided nature of the stencil, with information propagating from the interior to the boundary, which is contrary to the physical description given by Eq. (1) and (iii) overly dissipative nature at \( j = N \) [8].

Using the hybrid Fourier–Laplace representation of \( u \) in Eqs. (17)–(19), one can obtain the effectiveness of the derivative discretization \( k_{eq}^{(i)} \) for G1FEM as [22],

\[
j = 1 : k_{eq}^{(1)} = \frac{3}{h} \left( \frac{e^{kh} - 1}{e^{kh} + 2} \right) \hspace{1cm} (20)
\]

\[
2 \leq j \leq N - 1 : k_{eq}^{(1)} = \frac{3 \sin kh}{h(2 + \cos kh)} \hspace{1cm} (21)
\]
If one adopts Euler time stepping for the discretized equations for G2FEM in Eqs. (26)–(30), one obtains the numerical amplification factor for G1FEM is given as [22],

\[
j = 1 : G^{(1)} = 1 - 3Nc \left( \frac{e^{ikh} - 1}{e^{ikh} + 2} \right)
\]

If one adopts Euler time stepping for discretized Eqs. (17)–(19), the numerical amplification factor for G1FEM is given as [22],

\[
j = 1 : G^{(1)} = 1 - 3Nc \left( \frac{\sin kh}{2 + \cos kh} \right)
\]

If instead of using linear basis functions, one adopts quadratic Lagrange basis functions (G2FEM) for a uniformly spaced grid, then the discrete equations of Eq. (1) are as given in [22],

\[
j = 1 : \left( 18 \frac{du_1}{dt} + 9 \frac{du_2}{dt} - 2 \frac{du_3}{dt} \right) + \frac{5c}{h} (-6u_1 + 7u_2 - u_3) = 0
\]

\[
j = 2 : \left( 9 \frac{du_1}{dt} + 50 \frac{du_2}{dt} + 8 \frac{du_3}{dt} - 2 \frac{du_4}{dt} \right) + \frac{5c}{h} (-7u_1 + 8u_3 - u_4) = 0
\]

\[
j = N-1 : \left( 9 \frac{du_{N-1}}{dt} + 50 \frac{du_{N-2}}{dt} + 8 \frac{du_{N-3}}{dt} - 2 \frac{du_{N-4}}{dt} \right) + \frac{5c}{h} (7u_{N-1} - 8u_{N-3} + u_{N-5}) = 0
\]

Using hybrid Fourier–Laplace transform of the unknown u in Eqs. (26)–(30), one obtain the effectiveness of the derivative discretization \(k^{(2)}_{\text{eq}}\) for G2FEM as [22],

\[
j = 1 : k^{(2)}_{\text{eq}} = \frac{5}{ih} \left( -6 + 7e^{ikh} - e^{2ikh} \right)
\]

\[
j = 2 : k^{(2)}_{\text{eq}} = \frac{5}{ih} \left( -7e^{-ikh} + 8e^{ikh} - e^{2ikh} \right)
\]

\[
j = N - 1 : k^{(2)}_{\text{eq}} = \frac{5}{ih} \left( \frac{5 \sin kh(4 - \cos kh)}{12 + 4 \cos kh - \cos 2kh} \right)
\]

If one adopts Euler time stepping for the discretized equations for G2FEM in Eqs. (26) to (30), one obtains the numerical amplification factor for G2FEM as [22],

\[
j = 1 : G^{(2)} = 1 - 5Nc \left( \frac{6 + 7e^{ikh} - e^{2ikh}}{18 + 9e^{ikh} - 2e^{2ikh}} \right)
\]

\[
j = 2 : G^{(2)} = 1 - 5Nc \left( \frac{-7e^{-ikh} + 8e^{ikh} - e^{2ikh}}{9e^{-ikh} + 50 + 8e^{ikh} - 2e^{2ikh}} \right)
\]

\[
j = N - 1 : G^{(2)} = 1 - 5Nc \left( \frac{\sin kh(4 - \cos kh)}{12 + 4 \cos kh - \cos 2kh} \right)
\]
It has been shown in [22] that G1FEM suffers from numerical instability at \( j = 1 \) and G2FEM suffers the same for \( j = 1 \) and 2. Also, it is shown that there is overstability at \( j = N \) for G1FEM and at \( j = (N - 1) \) and \( N \) for G2FEM.

To apply the Galerkin method for wave propagation problems, the numerical instability occurring at the boundaries and near boundaries must be cured by introducing dissipation everywhere [24,25]. The dissipation constant was obtained optimally for solving wave problems by Raymond & Gardner [26]. In [21,26], the discrete equation at the interior nodes (\( 2 < j < (N - 1) \)) is given for the 1D convection equation as,

\[
\frac{h}{6} \left[ \frac{1}{2} \frac{\partial}{\partial t} u_{j-1} + 4 \frac{\partial}{\partial t} u_j + \frac{1}{2} \frac{\partial}{\partial t} u_{j+1} + c \left( u_{j+1} - u_{j-1} \right) = \beta c \left( u_{j+1} - 2u_j + u_{j-1} \right) \right]
\]

where \( \beta \) is the streamwise diffusion parameter. The optimal value of \( \beta \) is taken as \( 1/\sqrt{15} \), based on the work in [26]. In this reference, the analytical solution of Eq. (41) was taken from [27] in arriving at the optimal \( \beta \). However, the analytical solution was derived on the basis of a semi-discrete analysis considering no error in time discretization. Hence, this optimal value should not be treated as universal and will depend on time discretization method. We will simply provide analysis for SUPG method with \( \beta \) of [26]. The right hand side of Eq. (41) represents the lowest order dissipation term. The \( k_{eq}^{SUPG} \) of the SUPG method for Eq. (41) can be obtained as [22],

\[
k_{eq}^{SUPG} = \frac{6}{h} \left[ \sinh k - 2\beta(1 - \cos k) \right] \left[ 1 + 2\beta \sin^2 k \right] - 6N_c \left[ 4 + 2\cos k \sinh k + 2\beta^2(1 - \cos k) \sinh k \right] \left[ 4(2 + \cos k)^2 + \beta^2 \sin^2 k \right]
\]

Adopting Euler time stepping for Eq. (41), the numerical amplification factor for the SUPG method can be obtained as,

\[
G_{SUPG}^{n+1} = \left[ \frac{4(1 - \cos k)(2 + \cos k) - \sin^2 k}{4(2 + \cos k)^2 + \beta^2 \sin^2 k} \right] - 6N_c \left[ 4 + 2\cos k \sinh k + 2\beta^2(1 - \cos k) \sinh k \right] \left[ 4(2 + \cos k)^2 + \beta^2 \sin^2 k \right]
\]

In Figs. 1a and 1b, we show the numerical amplification factor \( G_0(N_c, k) \) and the non-dimensional group velocity \( V_g/N_c \), respectively, for the methods: (a) \( RK_4-\text{OUCS3} \); (b) \( RK_4-CD_2 \) and (c) \( RK_4-\text{QUICK} \) obtained using Eqs. (9) and (11). For Euler-SUPG method, contours of \( G_0(N_c, k) \) are obtained from Eq. (43) while the \( V_g/N_c \) contours are evaluated using Eq. (41). In these figures, properties of these methods are shown for an interior node. It has been established [12] that any numerical method for DNS must be neutrally stable, as evident from Eq. (45). From the contour plots in Fig. 1a, one notes only a narrow range of \( N_c \), available for which the OUCS3 and \( CD_2 \) schemes have neutral stability for full range of \( k \), marked by hatched lines. In comparison, neither QUICK nor SUPG scheme has neutrally stable region.

The main interest here is to compare the dispersion property of these methods in terms of \( V_g/N_c \) and identify reasons for which \( q \)-waves are created in solving Eq. (1). The \( V_g/N_c \) contours shown in Fig. 1b, indicate that all these methods produce dispersion error, except near the origin. The contour plots show a continuous line along which \( V_g \) is zero. For \( CD_2 \) and OUCS3 spatial schemes, this is a \( k = 0 \) line constant parallel to \( N_c \)-axis, while for the other two methods, these lines are curved. From Eq. (11), condition of zero group velocity corresponds to \( h \tan^{-1} \left( \frac{\tan \theta}{\tan \phi} \right) = 0 \), which gives the condition \( G_{eq}^{SUPG} = G_{eq}^{QUICK} \). For \( RK_4 \) time integration and central spatial schemes, this condition further simplifies to \( \tan \phi = \frac{A_1}{A_2 - iA_3} \). This explains why the zero group velocity condition is not a function of \( N_c \) for central schemes, while for QUICK and SUPG methods, this line is a strong function of \( N_c \), as shown in Fig. 1b. For the solution of Eq. (1), if \( V_g/N_c \) is negative, the numerical waves would propagate upstream, despite the physical requirement of downstream movement. Such unphysical upstream propagating components are called the \( q \)-waves. Thus, in solving Eq. (1) by \( RK_4-CD_2 \) method, \( q \)-waves are created for \( kh > \pi/2 \) and for \( RK_4-\text{OUCS3} \) method, \( q \)-waves are created for \( kh > 2.391 \), for any time step. We denote this limiting value as \( (kh)_{cr} \) of the method in Table 1. It is noted that \( (kh)_{cr} \) for the OUCS3 method is significantly higher in comparison to the other three methods. The maximum and minimum values of the numerical group velocities are lowest for \( CD_2 \) method followed by OUCS3 method. In comparison, QUICK and SUPG methods have significantly higher magnitude of maximum and minimum group velocity, due to large numerical dissipation.

The maximum upstream propagation speed for the \( RK_4-CD_2 \) method is found here as \( -2.502c \), as compared to \( V_{g0} = -c \) reported in [1,2]. In the same way, \( RK_4-\text{OUCS3} \) method displays \( q \)-waves with maximum upstream propagation speed of \( -2.1c \) which is many times larger than the value provided in Table 9.5 in [2] for fourth and sixth order compact schemes. While \( V_{g0} < 0 \) is the necessary parameter for \( q \)-waves, observation of \( q \)-waves also depends upon the real and imaginary part of the implicit filter associated with the numerical method. It is easy to see that excessive filtering and/ or damping removes \( q \)-waves. In Table 1, we have noted these two parameters at \( (kh)_{cr} \) for the four methods compared here. This clearly shows that the appearance of \( q \)-waves is more likely for the OUCS3 method as compared to the other methods, due to its lower filtering and less added dissipation. Note that for \( CD_2 \) method, \( q \)-waves will appear for \( kh > \pi/2 \), where the low-pass property of the method will filter the signal that is 38\% at each time step, and in contrast for OUCS3 method at \( (kh)_{cr} = 2.391 \), the
corresponding filtering is equal to only 7%, and there is an additional attenuation due to low numerical dissipation. It is seen that at $kh = 2.4$, the CD$_2$ method filters the signal (while spatially discretizing) by more than 70%. In comparison to these two methods, QUICK and SUPG add excessive numerical dissipation that also prevents $q$-waves at the cost of numerical accuracy.
For the SUPG method, $q$-waves are created for very small values of $N_c$ and very high values of $kh$. However, at these high values of $kh$, SUPG method introduces a very large quantum of numerical dissipation.

Fig. 1b. Normalized numerical group velocity ($V_{gN}/c$) contours in $(N_c, kh)$-plane for the solution of the Eq. (1) where space and time discretization schemes are as indicated in the respective frames. Note the $q$-wave region is shown by the hatched region.
2.1. Effect of initial condition on the spurious numerical solution

Further elaboration on the role of $q$-waves is noted by solving Eq. (1) for the propagation of a wave-packet, whose central wavenumber is chosen in a manner to highlight the properties in Fig. 1a and 1b. Here, propagation of a wave-packet which is given by the following initial condition is considered,

$$u(x, t)|_{t=0} = e^{-\pi(x-x_0)^2} \cos[k_0(x-x_0)]$$

(44)

where $x_0$ is the center of the wave-packet at $t = 0$, whose central wavenumber is given by $k_0$.

While solving Eq. (1), situations can arise where $p$-waves are accompanied by $q$-waves. This is explored in the cases depicted in Fig. 2 for wave-packets characterized by different values of $\alpha$. Equation (1) is solved again for different wave-packets using $RK_4$-CD$_2$ method whose initial conditions are shown in Fig. 2(a), which propagate in a domain, $0 \leq x \leq 20$ discretized with 1024 equi-spaced points. The wave-packet (with $k_0 h = 0.5$) is centered at $x_0 = 8$ at $t = 0$ in all the cases and move to the right with $c = 0.1$. Calculated results are obtained using time step corresponding to $N_t = 0.1$. Different values of $\alpha$ determine the width of the packet in the physical plane and their spectra are displayed in Fig. 2(b) at $t = 0$. In Fig. 2(c) and (d), computed solutions are shown at $t = 20$ and 60, respectively. For higher values of $\alpha$, band-width of the packet increases progressively, as seen from Fig. 2(b) for the Fourier transform of the initial condition. It is clearly evident that the grid used is inadequate in representing the initial condition for $\alpha = 2000$ from the non-zero value of the Fourier transform at $kh = \pi$. We have noted from Fig. 1b that $q$-waves are present for $kh > \pi/2$ and thus, the presence of $q$-waves for $\alpha = 100$ is investigated in the inset of Fig. 2(b). We note that there are components of the initial condition those spill over $kh = \pi/2$ and are responsible for $q$-waves. It is seen from Fig. 1b that $|V_{\text{ph}}|$ for the $RK_4$-CD$_2$ method increases with $kh$. For a lower $\alpha$ case, created $q$-waves, propagate upstream at slower speed as compared to higher $\alpha$ cases due to this reason. However, the reason that the spectral contents of $p$- and $q$-waves do not change with time can be explained with the help of results in [12], where the error dynamics of Eq. (1) is analyzed. The numerical error $e$ for Eq. (1) is governed by [12],

$$\frac{\partial e}{\partial t} + c \frac{\partial e}{\partial x} = -c \left[1 - \frac{C_k}{C_p} \frac{\partial N}{\partial x} \right] \int \left[ i k |A_0||G|^1/M \, e^{ik(x-ct)} \right] dk - \int \frac{L||G||}{3t} |A_0||G|^1/M \, e^{ik(x-ct)} \right] dk$$

(45)

The reason that $q$-waves are created is strictly related to spectral content of the initial condition. For wave-packets, integrals in Eq. (45) can be represented by corresponding integrands evaluated at $k_0 h$. For higher $\alpha$, the initial condition also represents a higher value of $\alpha$ which explains higher values of excited $kh$ through the first term on the right hand side of Eq. (45). The higher wavenumber error components with $kh > \pi/2$ for higher $\alpha$ are responsible for the faster moving $q$-waves. This explains the extent and amplitude of $q$-waves shown for the different cases in Fig. 2(c) and (d). For the chosen values of $k_0 h$ and $N_t$, for the cases depicted in Fig. 2, $RK_4$-CD$_2$ method has $|G| = 1$ and $V_{\text{ph}}/c = 0.87318$. Thus, the actual signal travels at a slower speed as compared to the exact solution, while the $q$-waves travel at speeds depending upon $V_{\text{ph}}$ of the error components created. Both the $p$- and the $q$-waves have $|G| = 1$ (as indicated in Fig. 1a) and thus the third term on the right hand side of Eq. (45) does not contribute at all to the error. It is noted that the other two terms on the right hand side of Eq. (45) provide dispersion effects. Thus, the variations of solution during $t = 20$ and 60 are simply due to dispersion error and $p$- and $q$-waves amplitude decrease as a consequence of Parseval’s formula that relates the original and its transform in expressing the energy spectrum of a signal.

It would be particularly problematic in DNS, as $q$-waves are persistent for the choice of numerical parameters in DNS requiring $|G| = 1$. In such a situation, created $q$-waves would not attenuate. Other parts of $q$-waves would attenuate for which $|G| < 1$. Persistent $q$-waves can be eliminated by filtering, which will only remove high $kh$ components responsible for the $q$-waves. It is presumed that the grid would be chosen in such a manner that the physical signals are distinguished from the $q$-waves in $k$-space and the latter can be filtered alone, without affecting the former.

Another aspect of dispersion error is related to the Gibbs’ phenomena which occurs due to sharp discontinuity in the solution and causes spurious oscillations [12,30]. This is caused by the first term on the right hand side of Eq. (45). If the solution has a discontinuity, then it acts as a forcing term for the numerical phase error. Such spurious oscillations can trigger numerical instability. This problem of spurious oscillation near discontinuity can be reduced by using DRP methods or by using a proper filter [31].

2.2. Effect of grid on spurious numerical solution

Spurious generation of flow structures due to inadequate grid resolution has been studied in [32]. Spurious wave propagation in regular grids for hyperbolic equations is well covered in the literature [1,6,33,34]. Reflection at the boundaries can

<table>
<thead>
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<th>Table 1</th>
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<td><strong>Comparison of resolution properties and q-wave limits of the different numerical schemes.</strong></td>
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<tr>
<td>Discretization scheme</td>
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<tr>
<td>CD$_2$</td>
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<td>OUCS3</td>
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<td>QUICK</td>
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<td>SUPG</td>
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Fig. 2. Comparison of propagation of the wave-packets with different values of $\alpha$ obtained by RK4-CD2 method using $N_p=0.1$ and $k_0 h=0.5$. (a) Initial conditions of the wave-packets with indicated values of $\alpha$; (b) Fourier transform of the initial conditions in (a); (c) and (d) Solution of Eq.(1) at the indicated times.
be controlled using non-reflecting boundary conditions as suggested in [35]. Early studies with irregular grids can be found in [36,37]. The anisotropic wave propagation is studied in [38] when structured grids are used with different aspect ratios for high accuracy compact schemes. It is shown that the grid aspect ratio must match the propagation direction, otherwise $q$-waves are created. Wave propagation in non-uniform grid was also studied in [39], while mesh refinement study was attempted in [40]. In [39], relations are derived which apply to propagation and internal reflection of spurious solution. Addition of artificial dissipation or use of an absorbing modified upwind boundary stencil is suggested for avoiding spurious waves in [40]. A single step change in the grid size of a piecewise uniform mesh was shown to create scattering in [41].

The choice of number of points per wave also plays an important role in creation and propagation of $q$-waves. For the cases of Fig. 2, we have used 1024 points to resolve packets of different $\alpha$ and noted that the initial condition for $\alpha = 2000$ is not resolved in the chosen grid. In Fig. 3, we have considered two cases of wave-packets with $k_0 h = 0.1$ and 3.0, respectively - whose propagation following Eq. (1) is studied using 1024 and 8192 points for a value of $\alpha = 30000$ and calculations are performed with step size corresponding to $N_c = 0.1$, using $RK_4$-$CD_2$ method. Center of the wave-packet is located at $x_0 = 7.9961$ as shown in Fig. 3(a) and (b) as initial condition. We note that the properties of numerical methods remain invariant if the non-dimensional parameters $kh$ and $N_c$ are held same. Although, the wave-packet is characterized by the central wavenumber $k_0 h$, the actual band-width of the waves are different for different number of points, i.e., $k_0$ for 1024 and 8192 points are entirely different and their physical plane portraits are also different. Due to the difference of band-widths around $k_0 h = 0.1$ for $N = 1024$ and 8192 in Fig. 1b, excited $kh$ is larger for $N = 1024$, as compared to 8192 points. A part of $kh$ for $N = 1024$ is in the hatched region of Fig. 1b for $RK_4$-$CD_2$ case, while for $N = 8192$, a smaller fraction of $kh$ is in the hatched region causing lesser $q$-waves. The $q$-waves with wavenumbers closer to $\pi/2$ move slower and remain close to the p-waves and the wavenumbers close to $\pi$ move faster and are seen farther to the left. For $k_0 h = 3.0$, results are also shown using the same two grids. Results with $N = 1024$ points are the same for $k_0 h = 0.1$ and 3.0 - as in both the cases the initial conditions are not resolved and incorrect. The plot of the signal at $t = 0$ shows it as a delta function for any value of $kh$ chosen in the coarser grid. However, for 8192 points, the initial condition for $k_0 h = 3.0$ is more correctly represented. As this case has $kh > (kh)_c$, the actual signal (corresponding to $k_0 h = 3$) moves in the upstream direction and additional $q$-waves are created by the side-band, whose wavenumbers lie between $k_h = \pi/2$ and $\pi$. Since these later waves are relatively slow, they are seen to trail behind the left-moving wave-front corresponding to $k_0 h = 3$. In [42], spurious modes are classified as spectral pollution and non-spectral pollution and it is noted that the latter can be partially avoided by mesh refinement, while the former persists even when the mesh is refined as shown here in Fig. 3. For the case with $N = 8192$ for $k_0 h = 0.1$ the signal moves in the correct direction, with some $q$-waves. However for the case of $k_0 h = 3.0$, the main signal propagated in the wrong direction.

This case is counter-intuitive because the equivalent delta function case with 1024 points (with all $kh$ excited) propagates in the correct direction at the correct speed, while the wave-packet (described by 1024 points) travel in the wrong direction and this happens despite increasing the number of points! This is due to the fact that with $N = 1024$, $k_0 h = 3.0$ and $k_0 h = 0.1$ have identical initial spectrum, which for $k_0 h = 0.1$ should propagate downstream. Thus, increasing the number of points alone is not adequate, one must pay close attention to the basic numerical properties of the space-time discretization techniques, in fixing the number of grid points.

2.3. Grid resolution of a wave-packet using different methods

Here, we consider a packet with $k_0 = 50$ following Eq. (1), using $CD_2$ and OUCS3 [10] spatial discretization schemes with $RK_4$ time integration method. The wave-packet with $\alpha = 30000$ is shown in Fig. 4(a) that propagates with group velocity (and phase speed) of 0.1 and Eq. (1) is solved using $N_c = 0.1$ in a domain of length 10, with 4096 uniformly distributed points. The signal is characterized by $k_0 h = 0.1221$ and has numerical propagation speed close to the exact value. The Fourier transform of the initial signal (as shown in top right frame of Fig. 4) shows the signal to be band-limited up to $kh = 2$ (approx.). Due to this, $RK_4$-$CD_2$ method shows propagation speed of $V_{gn} = 0.987559c$ while $RK_4$-OUCS3 method has even more accurate propagation speed of $V_{gn} = 0.999867c$. This is reflected in the displayed computed solutions at $t = 10$ and 20 in Fig. 4. One can note that the solution obtained by $RK_4$-OUCS3 method has almost negligible $q$-waves. Whenever $q$-waves are present, their energy come from the signal and the fact that the amplitude remains very close to one also indicates the near-absence of $q$-waves for this case. In contrast, for $RK_4$-$CD_2$ method there is a range of $kh$ from $\pi/2$ to $\pi$ which create significant $q$-waves, even when a large number of points are used. We have noted that this is a non-dissipative central scheme with $|G| = 1$ for the chosen numerical parameters and the attenuation of signal amplitude is a consequence of Parseval’s formula that indicates the energy of the p-waves is siphooned off to the $q$-waves. This example highlights the need of high accuracy DRP schemes to obtain an accurate numerical solution.

3. Analysis of numerical methods for one-dimensional skewed wave propagation

In this section, we consider propagation of wave in two-dimensions by considering a skewed wave with the convection velocity $w$ in the direction of $s$. Wave propagates making an angle $\theta$ with respect to the $x$-axis, such that $x = s \cos \theta$ and $y = s \sin \theta$. For the oblique propagation one can write the governing equation as,
Fig. 3. shows the initial condition of a wave-packet for $k_0h = 0.10$ with $N = 1024$ and 8192 grids. Fig. 4(b) shows the initial condition of a wave-packet for $k_0h = 3.00$ with $N = 1024$ and 8192 grids. In Fig. 4(c) and (e) propagation of wave-packet is shown with $N = 8192$ grid points for $k_0h = 0.10$ and $k_0h = 3.00$, respectively. In Fig. 4(d), propagation of a wave-packet is shown with $N = 1024$ points for the cases $k_0h = 0.10$ and $k_0h = 3.00$. Both cases in Fig. 4(d) are identical due to lack of resolution for $N = 1024$ grid.
Fig. 4. Effect of different methods on the propagation of a packet with \( \alpha = 30000 \), \( k_0 = 50 \), \( N_c = 0 \). Using 4096 points for the solution of Eq. (1) by RK4-CD2 and RK4-OUCS3 methods. (a) The initial condition and its Fourier transform are shown; (b) Solution of Eq. (1) using RK4-OUCS3 method at different times and (c) Solution of Eq. (1) using RK4-CD2 method at the same time instants.
\[
\frac{\partial f}{\partial t} + u \frac{\partial f}{\partial x} + v \frac{\partial f}{\partial y} = 0
\]  
(46)

where, \( u = w \cos \theta \), \( v = w \sin \theta \). It has been shown in [12] that many discrete schemes are not very efficient in supporting non-dissipative and non-dispersive analytical properties. Computed solutions display dispersion as numerical group velocity different from the physical group velocity. The numerical approximation of the first derivatives, in terms of the values \( f_j \) can be once again written as [38],

\[
\left\{ \frac{\partial f}{\partial x} \right\} = \frac{1}{\Delta x} \mathcal{C}(f); \quad \left\{ \frac{\partial f}{\partial y} \right\} = \frac{1}{\Delta y} \mathcal{C}(f),
\]

where \([\mathcal{C}]\) and \([\mathcal{C}]\) are not necessarily banded.

### 3.1. Analysis of full discretization

For multi-dimensional wave propagation problems one must consider full discretization, taking into account the effects of temporal discretization [12]. If we use Eq. (46) as the model equation, then a numerical scheme for space–time dependent problems can be assessed by using the ratio of numerical group velocity to exact phase speed as the quantifier for the DRP property for 2D problem, as well.

The physical dispersion relation for Eq. (46) is given by,

\[
\omega = uk_x + vk_y
\]

(47)

while the dispersion relation for the numerical approximation of Eq. (46) is given by,

\[
\omega_N = uw k_x + vn k_y
\]

(48)

where \( w \) and \( v \) are numerical phase speeds with \( k_x \) and \( k_y \) are wavenumber components in \( x \)- and \( y \)-directions, respectively. Consideration of temporal discretization along with spatial discretization gives the dispersion relation as, \( \omega_N = c_N |k| \), with \( \omega_N \) as the numerical circular frequency and \( c_N \) as the numerical phase speed. The numerical phase speed in the \( x \)- and \( y \)-directions are given by,

\[
c_{Nx} = \frac{\omega_N}{k_x}; \quad c_{Ny} = \frac{\omega_N}{k_y}
\]

(49)

The \( x \)- and \( y \)-components of numerical group velocity are given by,

\[
V_{gNx} = \frac{\partial \omega_N}{\partial k_x}; \quad V_{gNy} = \frac{\partial \omega_N}{\partial k_y}
\]

(50)

Results in Fig. 4, have indicated that RK4-OUCS3 discretization method provides excellent results with neutral stability and very low phase and dispersion error, for low CFL numbers and is used here. The governing Eq. (46) is rewritten as,

\[
\frac{\partial f}{\partial t} + L(f) = 0
\]

(51)

where \( L(f) = u \frac{\partial \omega}{\partial x} + v \frac{\partial \omega}{\partial y} \) and \( L(f) \) can be obtained as [38],

\[
\Delta t L(f) = \int_{-k_m}^{k_m} \int_{-k_n}^{k_n} F(k_x, k_y, t) \left\{ Nc_x \tilde{A}_x + Nc_y \tilde{A}_y \right\} e^{i(k_x x + k_y y)} \, dk_x \, dk_y
\]

(52)

where, \( k_m = \frac{\Delta x}{\lambda} \) and \( k_n = \frac{\Delta y}{\lambda} \) with

\[
\tilde{A}_x = \sum_{n=1}^{Nc_x} \tilde{C}_{mn} p_m; \quad \tilde{A}_y = \sum_{n=1}^{Nc_y} \tilde{C}_{mn} p_m; \quad Nc_x = \frac{\Delta t}{\Delta x}; \quad Nc_y = \frac{\Delta t}{\Delta y}
\]

(53)

\( Nc_x \) and \( Nc_y \) represent the CFL numbers in \( x \)- and \( y \)-directions, respectively. Grid spacings \( \Delta x \), \( \Delta y \) are related by the grid aspect ratio, \( \lambda = \frac{\Delta y}{\Delta x} \). Therefore,

\[
Nc_y = Nc_x \left( \frac{\tan \beta}{\lambda} \right)
\]

(54)

If the wave propagation direction (\( \theta \)) and grid aspect ratio (\( \lambda \)) are fixed, then one can only fix one of the CFL number. Let \( \tilde{A} = \left( Nc_x \tilde{A}_x + Nc_y \tilde{A}_y \right), \) where \( \tilde{A} \) is a complex number with real \((\tilde{A})\) and imaginary parts \((\tilde{A})\) given by,
The numerical amplification factor $G$ is defined as $G(k_x, k_y) = \frac{F(k_x, k_y, \tau_{n+1})}{F(k_x, k_y, \tau_n)}$ and is related to $A$ as given in Eq. (9). The magnitude of $G$ is $|G| = \sqrt{\left| (G)_{\text{real}} \right|^2 + \left| (G)_{\text{imag}} \right|^2}$, where $(G)_{\text{real}}$ and $(G)_{\text{imag}}$ represent real and imaginary parts of $G$, respectively.

Consider the Fourier–Laplace spectral representation of the numerical solution of Eq. (46) as,

$$f^n = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} F_0 e^{i(k_x x + k_y y - \omega_0 t_n)} \, dk_x \, dk_y$$

where $f^n$ is the function value at the $n$th time level, $t_n$ and $F_0(k_x, k_y)$ is the spectrum of the initial condition.

Numerical solution at the $n$th time level can also be given in terms of initial amplitude and the numerical amplification factor by,

$$f^n_{\text{tr}} = \int_{-k_{\text{max}}}^{k_{\text{max}}} \int_{-k_{\text{max}}}^{k_{\text{max}}} F_0 G^n e^{i(k_x x + k_y y)} \, dk_x \, dk_y$$

Comparing Eqs. (56) and (58), one gets the numerical phase speeds in $x$- and $y$-directions as,

$$\frac{c_{n_x}}{u} = \frac{\beta_{n_x}}{N_{cx} k_x \Delta x} ; \quad \frac{c_{n_y}}{v} = \frac{\beta_{n_y}}{N_{cy} k_y \Delta y}$$

The $x$- and $y$-components of normalized numerical group velocities are similarly obtained as,

$$\frac{V_{g_{nx}}}{u} = \frac{1}{u \Delta t} \frac{\partial \beta_{n_x}}{\partial k_x} ; \quad \frac{V_{g_{ny}}}{v} = \frac{1}{v \Delta t} \frac{\partial \beta_{n_y}}{\partial k_y}$$

Contour plots of the numerical amplification factor and the normalized group velocity in the $x$ and $y$-directions are shown in Fig. 5 for $RK_4$-OUCS3 scheme. These plots quantify the region over which DRP property of the chosen numerical schemes is maintained. Basic numerical properties can be analyzed for different directions of propagation ($\theta$) and grid aspect ratio ($\lambda$). In Fig. 5, we have shown these properties for $\lambda = 1$ and $\theta = 60^\circ$ in the left column and for $\lambda = \tan \theta$ in the right column. One notices that for the latter grid aspect ratio, the CFL numbers in $x$ and $y$-directions become identical which makes the numerical properties $\theta$-independent. Results for $\theta = 30^\circ$ have been provided in [38] and the present results complement those in that reference. Here, the $q$-waves occur for significantly higher values of wavenumbers. The hatched area in $(V_{g_{nx}}/u)$ and $(V_{g_{ny}}/v)$ contours shown in Fig. 5 corresponds to $q$-waves.

### 3.2. Skewed wave propagation at $\theta = 60^\circ$

An example of skewed wave propagation is shown in Fig. 6 by solving Eq. (46) using $RK_4$-OUCS3 scheme with the initial condition given by,

$$f_0(x_1, y_m) = e^{-160(k_0 x_1)^2} e^{i(k_0 y_m)}$$

Here, we have considered the case in which the wave propagates along $\theta = 60^\circ$, a domain $[0, 5] \times [0, 5]$ is chosen with 1001 points in $x$-direction for all the reported cases. The number of points in $y$-direction along with the length of the domain are fixed by the grid aspect ratio $\lambda$ and hence the direction of propagation $\theta$. The wavenumber of the wave-packet is fixed as $k_0 = 10$ and thus, we have 125 points per wave (ppw), approximately. The problem is solved for the aspect ratio of $\lambda = 1$ and is shown in Fig. 6.

In this skewed wave propagation problem, initially the wave is aligned along the $s$-direction although the solution is computed as a 2D problem. The wave has zero thickness across the $s$-direction and behaves like a delta ($\delta$) function in the direction normal to $s$. Thus, all the wavenumbers would be excited in a direction normal to $s$ with equal amplitude which makes this a challenging problem to be solved numerically. The sharp discontinuity present in the initial and subsequent numerical solutions would cause spurious dispersion due to the Gibb’s phenomenon [30]. This will be readily evident when one tries to resolve this wave and study it’s propagation by evaluating the derivatives numerically in the Cartesian $(x, y)$-plane. Here the wave propagation direction is in the increasing $x$- and $y$-directions, which is considered as positive $s$-direction. Higher wavenumber components would propagate upstream due to the properties shown in Fig. 5 and such spurious disturbances traveling along negative $s$-direction are noted in Fig. 6.
4. Linearized rotating shallow water equation (LRSWE)

We have discussed the generation of $q$-waves for the nondispersive one-dimensional and skewed wave propagation problems so far. To demonstrate $q$-waves for dispersive multi-dimensional systems, we consider solution of the LRSWE \[62\]. This represents a dispersive system governed by the following equations for the unknowns $u$ and $v$ (the Cartesian components of velocity of disturbance waves) and the elevation $g_1$ of the waves forming over shallow water of mean depth $H$,

\[
\begin{align*}
\frac{\partial v}{\partial t} + f u + g \frac{\partial g_1}{\partial y} &= 0 \\
\frac{\partial u}{\partial t} - f v + g \frac{\partial g_1}{\partial x} &= 0 \\
\frac{\partial g_1}{\partial t} + H \left( \frac{\partial u}{\partial x} \frac{\partial v}{\partial y} \right) &= 0
\end{align*}
\] (62) (63) (64)

Here, $f$ and $g$ are the coriolis parameter and gravitational acceleration, respectively. Equations \(62\) - \(64\) represent a coupled system of first order partial differential equations, which can also be written as a single equation.

\[\lambda = 1, \theta = 60^\circ \quad \lambda = \tan \theta \]

\[\begin{array}{cc}
(a) & \min: 0.99968; \max: 1 \\
(b) & \min: -5.7721; \max: 1.0139 \\
(c) & \min: -5.7721; \max: 1.0138
\end{array}
\]

\[\begin{array}{cc}
(a) & \min: 0.9999; \max: 1 \\
(b) & \min: -5.7721; \max: 1.0139 \\
(c) & \min: -5.7721; \max: 1.0138
\end{array}
\]

\[\begin{array}{cc}
(a) & \min: 0.9968; \max: 1 \\
(b) & \min: -5.7721; \max: 1.0139 \\
(c) & \min: -5.7721; \max: 1.0138
\end{array}
\]

\[\begin{array}{cc}
(a) & \min: 0.9999; \max: 1 \\
(b) & \min: -5.7721; \max: 1.0139 \\
(c) & \min: -5.7721; \max: 1.0138
\end{array}
\]

\[\begin{array}{cc}
(a) & \min: 0.9999; \max: 1 \\
(b) & \min: -5.7721; \max: 1.0139 \\
(c) & \min: -5.7721; \max: 1.0138
\end{array}
\]

**Fig. 5.** Contours of (a) $|G|$; (b) $(V_{gN}/u)$ and (c) $(V_{gN}/v)$ using RK$_4$-OUCS3 scheme for the case of grid aspect ratio $\lambda = 1$ and wave propagation angle $\theta = 60^\circ$ (as shown in the left column) and for the case of $\lambda = \tan \theta$ (as shown in the right column). Note the $q$-wave region is shown by the hatched region.
Fig. 6. Skewed 1D wave propagation along $\theta = 60^\circ$ shown at indicated times. $q$-waves are identified as the disturbances traveling along negative $x$- and negative $y$-directions. Various physical and computational parameters used are propagation angle: $\theta = 60^\circ$, grid aspect ratio: $\lambda = 1$, computational domain: $[0:5]$, central wavenumber of packet: $k_0 = 10$, number of points in x-direction: $N_x = 1001$, points per wave (ppw): 125, phase speed: $c = 0.1$, $(\text{CFL})_x = N_c x = 0.1$ and $(\text{CFL})_y = N_c y = 0.1732$. 
The geostrophic mode has zero group velocity and phase speed, while the inertia gravity modes [43].

4.1. Analysis of numerical methods for LRSWE

To solve LRSWE numerically, it is noted that Eq. (65) has third order time derivative and involves higher order spatial derivatives, while Eqs. (62)–(64) involve only first order derivatives in space and time. Thus, we have solved the set of first order equations, as in [38]. The geostrophic mode has zero group velocity and phase speed, while the inertia gravity modes have exact estimates for $x$- and $y$-components of normalized group velocity as given in [38, 43, 44].

\[
\frac{(V_{gx})_{2,3}}{c} = \frac{\pm k_x c}{\sqrt{f^2 + c^2 k_y^2}}; \quad \frac{(V_{gy})_{2,3}}{c} = \frac{\pm k_y c}{\sqrt{f^2 + c^2 k_x^2}}
\]

(67)

The exact estimates for the phase speeds in $x$- and $y$-directions are similarly given as,

\[
\frac{(c_{nx})_{2,3}}{c} = \frac{\pm \sqrt{f^2 + c^2 k_y^2}}{k_x c}; \quad \frac{(c_{ny})_{2,3}}{c} = \frac{\pm \sqrt{f^2 + c^2 k_x^2}}{k_y c}
\]

(68)

Here, numerical group velocity and phase speed for RK4-UCS3 are presented next. Corresponding modal amplification factors are obtained from Eqs. (62)–(64) as,

\[
G_1 = 1; \quad G_2 = G_r - i G_i \quad \text{and} \quad G_3 = G_r + i G_i
\]

(69)

where

\[
G_r = 1 - \frac{1}{2} \gamma^2 + \frac{1}{24} \gamma^4; \quad G_i = \gamma - \frac{1}{6} \gamma^3; \quad \gamma = a^2 + b^2 + p^2
\]

with

\[
a = 2N_\alpha \left( \frac{q_x \sin(2k_x \Delta x) + q_y \sin(k_x \Delta x)}{1 + 2p_r \cos(k_x \Delta x)} \right); \quad b = 2N_\gamma \left( \frac{q_x \sin(2k_y \Delta y) + q_y \sin(k_y \Delta y)}{1 + 2p_r \cos(k_y \Delta y)} \right)
\]

and $p = f \Delta t$. The numerical dispersion relations using Eq. (69) are given by,

\[
(\omega_n)_{1,2,3} = \frac{1}{\Delta t} \tan^{-1} \left( \frac{G_r}{G_i} \right)
\]

(70)

For inertia gravity modes the $x$- and $y$-components of normalized numerical group velocity are given by [38],

\[
\frac{(V_{gxn})_{2,3}}{c} = \frac{\pm d_x \frac{d}{d^2} a \frac{d \phi}{\gamma d(k_x \Delta x)}}{d^2 \gamma d(k_x \Delta x)}; \quad \frac{(V_{gyn})_{2,3}}{c} = \frac{\pm d_x \frac{d}{d^2} b \frac{d \psi}{\gamma d(k_y \Delta y)}}{d^2 \gamma d(k_y \Delta y)}
\]

(71)

where

\[
\phi = 2 \left( \frac{q_x \sin(2k_x \Delta x) + q_y \sin(k_x \Delta x)}{1 + 2p_r \cos(k_x \Delta x)} \right); \quad \psi = 2 \left( \frac{q_x \sin(2k_y \Delta y) + q_y \sin(k_y \Delta y)}{1 + 2p_r \cos(k_y \Delta y)} \right)
\]

\[
\xi_1 = \tan^{-1} \left( \frac{G_r}{G_i} \right)
\]

Normalised numerical phase speeds in $x$- and $y$-directions, respectively are given by,

\[
\frac{(c_{nx})_{2,3}}{c} = \pm \frac{-\xi_1}{N_{c_y k_x \Delta x}}; \quad \frac{(c_{ny})_{2,3}}{c} = \pm \frac{\xi_1}{N_{c_y k_y \Delta y}}
\]

(72)

These numerical properties are shown in Fig. 7 for grid aspect ratio, $\lambda = \frac{\Delta y}{\Delta x} = \tan \theta$ where $\theta = 45^\circ$ and $N_{c_x} = N_{c_y} = 0.2$.

The $|G|$ contours shown in top frame of Fig. 7, show neutrally stable region for a small range of $k_x \Delta x$ and $k_y \Delta y$ near the origin. The $q$-wave region is marked with the dashed horizontal and vertical lines in group velocity contours $(\frac{V_{gxn}}{V_{gyn}})$ and $(\frac{V_{gyn}}{V_{gxn}})$, respectively.
4.2. Genesis of q-waves for LRSWE

Presence of spurious solutions in the representation of inertia gravity waves is discussed in [45]. In [46] a second-order finite volume-finite element method is used to solve viscous and inviscid shallow water equations and used appropriate limiters to suppress spurious oscillations. All these spurious modes refer to high wavenumber oscillation obtained in a modal analysis, unlike the generation of additional modes due to space–time integration strategies studied in [8].

Presence of \(q\)-waves is shown here by considering propagation of a 2D wave-packet given by,

\[
\begin{align*}
  u(x, y, t = 0) &= 0 \\
  v(x, y, t = 0) &= 0 \\
  \eta_1(x, y, t = 0) &= e^{-\left[(x-x_0)^2/\Delta x^2 + (y-y_0)^2/\Delta y^2\right]} \sin(k_x x + k_y y)
\end{align*}
\]

in the domain of size \(0 \leq x, y \leq 120\). This initial wave-packet is purposely taken as stretched in one direction, so as to mimic similar effects seen for the skewed wave in Fig. 6. In [38], wave-packet propagation was studied using shallow water equation for which a Gaussian packet was used as the initial condition. A case is considered for \(\theta = 45^\circ\) and \(\lambda = \tan 45^\circ\). \(f\Delta t = 2 \times 10^{-7}\) and \(N_{c_\varepsilon} = 0.2\). Here, the hatched area represents the corresponding negative group velocity \(q\)-wave region.

\[\eta_1(x, y, t = 0) = e^{-\left[(x-x_0)^2/\Delta x^2 + (y-y_0)^2/\Delta y^2\right]} \sin(k_x x + k_y y)\]

The numerical properties corresponding to this aspect ratio case are shown in Fig. 7. Corresponding solutions are shown in Fig. 8, which shows significant dispersion of two wave-packets moving opposite to each other, as shown at \(t = 3\). We note that this packet is centered at \(k_0 h = 2.3365\), which is the exact limit \((k_0 h = 2.3365)\) of \(q\)-waves for RK\(_4\)-OUCS3 scheme. Thus,
there will be side-band wavenumbers around the central $k_0h$ of the wave-packet, which will create $q$-waves. Presence of $q$-waves can be observed from $t = 6$ onwards in Fig. 8. The gap between the separated wave-packets $A$ and $B$ fills up due to upstream propagating wave components which originate from both $A$ and $B$. Furthermore, higher wavenumber

![Fig. 8](image-url)

*Fig. 8.* Computed wave-packet at different instants using RK$_{4}$-OUCS3 method for $\theta = 45^\circ$ and grid aspect ratio $\lambda = \tan 45^\circ$. 
components generated from the packet $A$ move in negative $x$- and $y$-directions and similarly for the packet $B$, the $q$-waves move in positive $x$- and $y$-directions. These are shown by solid arrows in the frames at $t = 12$ and $t = 15$.

5. Presence of $q$-waves in Navier–Stokes simulation

So far, we have discussed about the computational aspects of $q$-wave generation in solving model equations for both non-dispersive and dispersive systems. Present investigation is aimed at ascertaining the numerical properties of solving Navier–Stokes equation. Primarily, the dispersion error and its extreme form in creating $q$-waves are investigated. We also note that in a flow with discontinuity in the interior, will cause $q$-waves emanating from the discontinuity. Such discontinuities have high wavenumber components for which the numerical group velocity components will indicate propagation opposite to physical direction. This phenomenon is independent of initial and boundary conditions. Thus, $q$-waves can occur for numerical simulation of physical flows as well, for the following reasons.

Firstly, the numerical method is capable of creating $q$-waves at high wavenumbers when relevant spectral components are created due to non-linearity and/or aliasing. For the examples studied here with Eq. (1), high wavenumber components must be present with the initial condition. Secondly, creation of $q$-waves is determined by the properties of the adopted numerical method, dictated by $V_{gN}$ contours for the appropriate governing transport equation. Thus, for the same governing equation and same grid, one method may demonstrate $q$-waves, while another method will not show the same. As many external fluid dynamical problems are convection-dominated, information obtained from Eq. (1) is relevant for many flow processes. If we consider nonlinear governing equation, then higher wavenumbers having $kh > (kh)_{cr}$ can be created by

![Fig. 9a. Top frame shows the schematic of a discrete shielded vortex in a uniform flow and the bottom frame shows vorticity distribution along $Y = 0$ line.](image-url)
the product terms, creating $q$-waves. Additionally, high wavenumbers can also be created from linear operators which require product term evaluation in the transformed plane [8] for the Laplacian operator.

Presence of $q$-waves in numerical simulation of non-dispersive as well as dispersive model equations has been shown in previous sections. Hence, we show $q$-waves in full Navier–Stokes simulation for two flow problems.

Fig. 9b. Numerical solutions for vorticity of the discrete shielded vortex in a uniform flow following Navier–Stokes equation at the indicated instants are shown in the left column and corresponding 2D FFT are shown in right column. For this case, we have chosen $Re = 5000$, $K = 50$ and $\beta = 100$. 
5.1. Simulation of a discrete vortex in a uniform flow

We have considered a domain $ABCD$ of size $\frac{1}{C_0}$ as shown in Fig. 9a. Initially, a discrete shielded vortex is centered at $(0.0019,0.0019)$, which is defined as,

Numerical solutions for vorticity of the discrete shielded vortex in a uniform flow following Navier–Stokes equation at the indicated instants are shown in the left column and corresponding 2D FFT are shown in right column. For this case, we have chosen $Re = 5000$, $K = 50$ and $\beta = 30000$.

5.1. Simulation of a discrete vortex in a uniform flow

We have considered a domain $ABCD$ of size $[-1, 1] \times [-1, 1]$ as shown in Fig. 9a. Initially, a discrete shielded vortex [47] is centered at $(0.0019,0.0019)$, which is defined as,
\[ \omega = K \left(1 - \beta r^2\right) e^{-\beta r^2} \]  

In the above equation, \( r \) is a distance from the center of the vortex and \( K \) is a peak value of vorticity at the center of the vortex. A discrete shielded vortex is shown in the top frame of Fig. 9a while the vorticity distribution along \( Y = 0 \) line is shown in the bottom frame. We have used a Cartesian grid with 512 equi-spaced points in each direction. The calculations follow the formulation and methodology of [8] and is briefly recounted here. The governing stream function and vorticity transport equations in \((x, y)\)-plane are solved in the transformed \((\xi, \eta)\)-plane by,

\[
\frac{\partial}{\partial \xi} \left[ h_1 \frac{\partial \psi}{\partial \xi} \right] + \frac{\partial}{\partial \eta} \left[ h_1 \frac{\partial \psi}{\partial \eta} \right] = -h_1 h_2 \omega \tag{74}
\]

\[
h_1 h_2 \frac{\partial \omega}{\partial t} + h_2 u \frac{\partial \omega}{\partial \xi} + h_1 v \frac{\partial \omega}{\partial \eta} = \frac{1}{Re} \left[ \frac{\partial}{\partial \xi} \left( h_1 \frac{\partial \omega}{\partial \xi} \right) + \frac{\partial}{\partial \eta} \left( h_1 \frac{\partial \omega}{\partial \eta} \right) \right] \tag{75}
\]

where \( h_1 \) and \( h_2 \) are the scale factors of the transformation given by, \( h_1 = \sqrt{x_1^2 + y_1^2} \) and \( h_2 = \sqrt{x_2^2 + y_2^2} \). For the used grid, \( h_1 = h_2 \). As shown in Fig. 9a, we have prescribed a uniform flow at the inflow boundary \( AB \). Convective boundary condition (the Sommerfeld boundary condition) is applied on the normal component of velocity, at the outflow boundaries \( BC, CD \) and \( DA \) for updating streamfunction and vorticity. The convective boundary condition is given by [48],

\[
\frac{\partial u_c}{\partial t} + u_c(x, y, t) \frac{\partial u_c}{\partial n} = 0 \tag{76}
\]

where \( u_c \) is the normal component of velocity and \( u_c(x, y, t) \) is the convection velocity at the outflow at time \( t \), which is obtained from the normal component of velocity at the previous time step, i.e., \( u_c(x, y, t) = u(x, y, t - \Delta t) \). For the spatial discretization of convective terms in Eq. (75), we have used OUCS3 scheme and dissipation terms are discretized using \( CD_2 \) scheme. Time integration is performed using \( RK_4 \) time integration method. For non-dimensionalization, we have used free-stream velocity \( U_\infty \) as a reference velocity scale and \( 1/K \) as the time scale. The length scale is fixed from these scales as, \( U_\infty /K \). This fixes our Reynolds number \( Re = \frac{U_\infty L}{\nu} \). For the present simulations, we have used \( Re = 5000 \) and a time step of \( \Delta t = 0.0001 \).

For the results shown in Fig. 9b, we have chosen \( \beta = 100 \) and \( K = 50 \). Navier–Stokes solutions at different instants are shown in the left column of Fig. 9b while the corresponding 2D FFT of vorticity are shown in the right column. Two-dimensional Fourier transform has been done by using a square patch of length two, with the vortex located at the center and then padding a uniform flow in a larger square of length 18 with the smaller patch placed at the center of the larger domain, thus constructed. As the Fourier transform is done using FFT, used algorithm assumes the flow to periodic over the domain. Padding a uniform flow in a larger square of length 18 with the smaller patch placed at the center of the larger domain, thus constructed. As the Fourier transform is done using FFT, used algorithm assumes the flow to periodic over the domain. Present exercise is used to study an isolated vortex and if FFT is performed over a smaller domain, then the implied periodic extensions in all directions would produce a picture which is not intended in the first place. Thus, the present padding procedure would significantly reduce this artifice of periodicity of FFT, apart from removing any aliasing accrued during the solution of VTE.

The top left frame shows initial condition. One notes the vortex convect to the right in subsequent time frames. The maximum and minimum values of vorticity in the domain are marked in each frame. Amount of added numerical dissipation can be reduced by grid refinement and computing at smaller time steps. In such a case the maximum and minimum values of vorticity will be more closer to the initial condition. Corresponding 2D FFT of vorticity in the complete domain shows large values of the Fourier amplitude localized near the origin. This shows that the simulation is well resolved and the high wavenumber components are highly attenuated.

To show the presence of \( q \)-waves, in the second case we have purposefully chosen higher value of \( \beta = 30000 \) so that the vorticity variation in the initial condition is very steep, as in Fig. 4. For this simulation, once again we have chosen \( K = 50 \) and \( Re = 5000 \). Solutions for this case, at different instants are shown in the left column of Fig. 9c and the corresponding 2D FFT of vorticity are shown in the right column. As discussed earlier, initial condition shown in top left frame shows a steep variation of vorticity with a small size shielded vortex. It’s corresponding 2D FFT has a broad spectrum as compared to the case shown in Fig. 9b. In subsequent time frames, presence of this broad spectrum results in right propagating vortex accompanied by left propagating \( q \)-waves. Thus, \( q \)-waves can be present in the Navier–Stokes simulation. Next, we discuss their effects on the simulation of the aerofoil.

### 5.2. Transitional flow past a NACA-0012 aerofoil

Here, we show \( q \)-waves while solving problems of CFD and specifically discuss their role on transitional flows. Present background disturbances at smaller scales than the critical wave lengths will create disturbances which travel upstream with respect to the local mean flow. This causes evanescent unsteady separation, caused by spurious dispersion at high wavenumber. Such separation also alters local pressure gradient, thereby creating instabilities. The net effect of this numerical behaviour is similar to the unsteady separation bubbles shown experimentally and theoretically, on the no-slip walls in [18] during bypass transition. Such bubbles will propagate downstream or upstream, depending upon the group velocity of the response field. However, in a moving frame of reference (with respect to local convection speed), this could be an upstream propagating disturbance, as discussed in [18] for bypass growth mechanism created by periodic train of vortices in the freestream.
As effects of $q$-waves are similar to what has been noted in bypass transition, computing bypass transition can be strongly affected by presence of $q$-waves. This is demonstrated with the solution of Navier–Stokes equation for flow past an aerofoil and means of removing the $q$-waves are also indicated.

**Fig. 10.** Streamfunction contours of flow field around NACA-0012 aerofoil, for $Re = 9 \times 10^6$ at $10^6$ AOA at the indicated time instants when the solution is filtered using (a) 2nd order filter with $\alpha_1 = 0.499$; (b) upwind filter with $\alpha_1 = 0.45, \eta_2 = 0.001$. Note the propagation of $q$-wave disturbance present in Fig. (a) are absent in Fig. (b).

As effects of $q$-waves are similar to what has been noted in bypass transition, computing bypass transition can be strongly affected by presence of $q$-waves. This is demonstrated with the solution of Navier–Stokes equation for flow past an aerofoil and means of removing the $q$-waves are also indicated.
Presented bypass transitional flow past NACA-0012 aerofoil at high Reynolds number of $Re = 9 \times 10^6$ is of computational interest only, as the flow at such a high Reynolds number would be turbulent and hence three-dimensional. At the same time, computing the flow in a 2D framework would display bypass transitional nature, if the flow is forced to be strictly two-dimensional. Such a flow would display wide-band spectrum at this very high Reynolds number. It is extremely likely that such a wide-band flow would display $q$-waves, which will significantly alter the 2D bypass transitional flow. Such a flow experiences varying pressure gradient, favorable one near the leading edge, followed by increasing adverse pressure gradient as the flow approaches trailing edge of the aerofoil. This flow experiencing physical instability is intended to be calculated without any models for transition and/ or turbulence.

We have generated an orthogonal grid having $(701 \times 251)$ points with the outer boundary placed at a distance of ten chord from the aerofoil surface [8]. The aerofoil is kept at ten degrees angle of attack. Governing stream function and vorticity transport equations are solved on a O-grid topology. Following initial and boundary conditions are used in solving the governing equations. On the aerofoil surface, following no-slip conditions are used,

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figures/figure10c}
\caption{FFT of the vorticity data for a constant $\eta$ line near the aerofoil surface is obtained at the indicated instants for the cases shown in Fig. 10(a) and (b).}
\end{figure}
\[ \psi = \text{constant}; \quad \frac{\partial \psi}{\partial \eta} = 0 \]  

(77)

These conditions also help fix the wall vorticity, which is required as the boundary condition for the vorticity transport equation, Eq. (75). In O-grid topology, one introduces a cut starting from the trailing edge of the aerofoil to the outer boundary. Periodic boundary conditions apply at the cut, which is introduced to make the computational domain simply-connected. For the stream function equation Eq. (74), at the outer boundary, Sommerfeld boundary condition is used on the wall-normal component of the velocity field. Resultant value of streamfunction is used to calculate the vorticity value at the outer boundary.

From the stream function equation the wall vorticity is calculated as,

\[ \omega_{\text{body}} = \left. \frac{1}{h^2} \right|_{\text{body}} \frac{\partial^2 \psi}{\partial \eta^2} \]  

(78)

Equation (74) is solved by Bi-CGSTAB method and Eq. (75) is solved using RK4-OUCS3 method, with dissipation term discretized using CD2 scheme. In order to attenuate high wavenumber components which can lead to numerical instability, vorticity values are filtered [49]. Problem of aliasing becomes important for this high Reynolds number flows. Aliasing in the solution by high accuracy methods can be cured by using multi-dimensional filters as in [50]. Performance of a filter is judged by its ability to leave smaller wavenumber components unaffected, while filtering the higher wavenumbers, which are known to create numerical instabilities and aliasing problems.

Computed flow fields around the aerofoil at indicated times are shown in Fig. 10(a), with the help of streamline contours. Only selective contours are shown to indicate the presence of \( q \)-waves. As the flow evolves, a separation bubble near the trailing edge of the aerofoil, identified as the \( q \)-wave in the frames is seen to move upstream. As it moves upstream, the separation bubble becomes bigger in length. To band-limit high wavenumbers, a filtering operation on computed vorticity is performed in the following manner. A second order filter [31] with a filtering coefficient of \( \alpha_1 = 0.499 \) is applied for all the points in azimuthal direction and for the first forty lines in wall-normal direction from the aerofoil surface. Additionally, an extra order composite filter [31] with \( \alpha_1 = 0.49 \) is applied in the complete domain in the wall-normal direction. Application of these symmetric stencil filters does not change the dispersion relation - it only attenuates high wavenumber components. Even though these high wavenumber components are attenuated, they continue to propagate upstream. This is the reason for the formation of \( q \)-waves in the present case.

We have recomputed the same case using an upwind filter [49] with a filtering coefficient, \( \alpha_1 = 0.45 \) and a upwind parameter, \( \eta_2 = 0.001 \). Corresponding results are shown in Fig. 10(b), at the same times shown in Fig. 10(a). It is seen that there are no discrete upstream traveling separation bubbles in this case on the top surface. Instead, we note downstream moving \( p \)-waves in this case. These \( p \)-waves are due to the bypass event described in [18]. Here, we have severe adverse pressure gradient near the trailing edge of the top surface of the aerofoil. The prevalent adverse pressure gradient makes the flow very sensitive to even trace amounts of background numerical disturbances, which trigger bypass transition as described in [18].

To avoid ambiguities in identifying computed vortical structures as either physical or numerical, one can study the spectrum of the flow field. We have computed the Fourier transform of the vorticity field at the same times for which the streamline contours are shown in Figs. 10(a) and (b). FFT is obtained for a set of points along a constant \( \eta \)-line, close to the aerofoil.

Fig. 11. Normalized numerical group velocity \( (V_{\text{NC}}/c) \) contours in \((N_c, \kh)\)-plane for the solution of the Eq. (1) using RK4-OUCS3 scheme for the cases: (i) without the filter and (ii) with the upwind filter [49]. Note that for the upwind filter case, there is a small range of \( N_c \) in which \( q \)-wave region is absent.
For this periodic grid line, the Fourier transforms are obtained in the transformed plane and are shown in Fig. 10(c). It can be seen from Fig. 10(c) that the upwind filter, reduces low wavenumber components lesser as compared to the second order filter with chosen filter parameters. However, it attenuates high wavenumber components more. In addition to this, use of upwind filter with chosen filter parameters removes $q$-waves. This is observed in Fig. 11, from the $V_{MN}/c$ contours for the solution of Eq. (1) using RK$_4$-OUCS3 method without and with the upwind filter [49]. One can notice that unlike the case without filter, for upwind filter $V_{MN}/c = 0$ contour turns away from the $kh$-axis for smaller values of $N_c$. This is a maximum allowable range of $N_c$ in which computations will not create $q$-waves.

6. Formation of spurious caustics in discrete computing

Up till now, we have focused our complete attention on $q$-waves. Next, we further add a discussion on spurious caustics noted specifically due to the numerical dispersion. A caustic is viewed as a boundary between a region with a complicated wave pattern, due to interference between two groups of waves, and a neighboring region including no waves [51]. Authors in [52], have

![Diagram](image)

Fig. 12. Contours of $\partial V_{MN}/\partial kh$ in $(N_c, kh)$-plane for the solution of the Eq. (1) where space and time discretization schemes are as indicated in the respective frames. Here we have specifically shown the zero contours corresponding to spurious caustics condition in [52].
defined caustic as focusing of different rays in a single location. They have further shown a linear dispersive mechanism which results in sudden local error burst while solving polychromatic solutions and referred this as spurious caustics.

Fig. 13. Solutions at the indicated instants of Eq. (1) using RK-OUCS3 scheme are shown for the initial condition given in the top left frame. Initial condition consists of prescription of two wave packets centered at \( x_1 = 1.0 \) and \( x_2 = 1.50 \). The central wavenumbers of the respective packets are \( k_1 h = 1.47741 \) and \( k_2 h = 0.6032 \). Computations are performed with \( N_c = 0.10 \).

defined caustic as focusing of different rays in a single location. They have further shown a linear dispersive mechanism which results in sudden local error burst while solving polychromatic solutions and referred this as spurious caustics.
phenomenon. Existence of spurious caustics was shown for some finite difference schemes for a particular value of $N_c$ and the equivalent condition for caustic is given by

$$\frac{\partial V_{GN}}{\partial k} = 0$$

(79)

The wavenumber corresponding to Eq. (79), is defined as a critical wavenumber $k_c$ at which a polychromatic solution can show a large amplification due to superposition. This results in the existence of a region of high energy followed by a region with very low fluctuation level [52]. In the present case, we have considered the case of CD2 and OUCS3 spatial discretization schemes with RK4 time integration method for the solution of 1D convection equation. In Fig. 12, we have shown the $\{\frac{\partial V_{GN}}{\partial k} = 0\}$ contour in the $(N_c, kh)$-plane for these two combinations of space–time discretization schemes. In the top and the bottom frames of Fig. 12, we have marked wavenumbers with fixed value of $N_c$ for which Eq. (79) is satisfied. For the case of RK4 – CD2 scheme we have chosen two wavenumbers for $N_c = 2.4$, marked by A and B in Fig. 12(a). Similarly, for the case of RK4 – OUCS3 scheme, we have chosen two wavenumbers for $N_c = 0.1$, marked by C and D in Fig. 12(b). To numerically investigate the existence of spurious caustics, we have chosen the initial condition with two wave-packets centered at $x_1$ and $x_2$ respectively, given as

$$u(x, t = 0) = e^{-32(x-x_1)^2} \cos[k_1(x - x_1)] + e^{-32(x-x_2)^2} \cos[k_2(x - x_2)]$$

(80)

Since the values of $|G|$ for A and B are 0.5977 and 0.8633 respectively, far lower than the required neutral stability, solution is heavily damped. Caustics phenomenon will not be seen due to the overstability. Thus, we have considered RK4 – OUCS3 scheme to investigate numerically existence of spurious caustics for the selected wavenumbers corresponding to C and D in Fig. 12(b) for which we have $|G| = 1$ identically. For these wavenumbers, values of $V_{GN}/c$ at C and D are 1.0139 and 0.9984, respectively. Thus, in a numerical exercise, wave-packet corresponding to C will propagate faster than the packet for D. This has been taken into consideration while choosing $x_1$ and $x_2$.

For the central wavenumbers at C and D, $k_1 h = 1.4774$ and $k_2 h = 0.6032$, respectively for $N_c = 0.1$. These wave-packets are centered at $x_1 = 1.0$ and $x_2 = 1.50$. We have chosen a domain of size $0 \leq x \leq 75$ with 10001 equi-spaced points. In Fig. 13, numerical results of Eq. (1) are shown for indicated time instants. The left top frame shows the initial condition given by Eq. (80). As time advances, the packets start superimposing each other resulting in wave-packet interaction via linear superposition, as shown in later frames. Due to superimposition of these two wave-packets, resultant amplitude increases in the intermediate frames before coming apart again at $t = 60000$. As the wave-packets cross over, the resultant amplitude again drops to unity. Presence of caustic(s) would have focused these two packets during interaction stage with resultant amplitude greater than two.

7. Conclusions

In the present work, we quantitatively explain how spurious upstream propagating waves (or $q$-waves) are created in discrete computations. The genesis was shown by Trefethen [6] with numerical group velocity for only second order central difference scheme used along with three time integration schemes, similar analysis was also presented earlier in Vichnevetsky & Bowles [1] and later by Poinset & Veynante [2], for few classical numerical methods. Here, we provide a comprehensive overview of the phenomenon of creation of $q$-waves as universal to all discrete computations. This has been based on a global spectral analysis tool for general discretization methods in [10]. We focus mainly upon high accuracy finite difference methods. Resultant properties shown are novel and help one quantify the onset of $q$-waves, with the help of numerical group velocity contours in $(N_c, kh)$-plane. To establish the existence of $q$-waves in computations, we also compare properties of different generic numerical methods drawn from finite difference, finite volume and finite element methods. We have studied propagation of wave-packets using finite difference schemes for the case of (i) one-dimensional convection equation; (ii) skewed wave propagation and (iii) solution of LRSWE. These latter flow models highlight specifically the creation of $q$-waves, which have not been provided before.

Presence of $q$-waves for Navier–Stokes simulation is shown for the case of convecting discrete shielded vortex in a uniform flow. Existence and properties of $q$-waves are also demonstrated for a practical flow by considering incompressible transitional flow past an aerofoil by solving the Navier–Stokes equation. We discuss about possible existence of truly upstream propagating physical disturbances in bypass transition. Finally, we discuss about filters which can control $q$-waves and a specific case is demonstrated for high angle of attack aerodynamics with the help of a upwind filter in [49]. Finally, we have shown presence of spurious caustics in discrete computing for RK4 – OUCS3 scheme. Spurious caustics can be caused due to the superimposition of two wave-packets resulting in increase in amplitude of the solution beyond the sum of individual amplitudes. However, computed results show that the packets penetrate each other clearly.

References
