Implicit gradients based novel conservative numerical scheme for compressible flows

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Abstract

This paper introduces a novel approach to compute the numerical fluxes at the cell boundaries for a cell-centered conservative numerical scheme. Explicit gradients used in deriving the reconstruction polynomials are replaced by high-order gradients computed by compact finite differences, referred to as implicit gradients in this paper. The new approach has superior dispersion and dissipation properties in comparison to the compact reconstruction approach. A problem-independent shock capturing approach via Boundary Variation Diminishing (BVD) algorithm is used to suppress oscillations for the simulation of flows with shocks and material interfaces. Several numerical test cases are carried out to verify the proposed method’s capability using the implicit gradient method for compressible flows.

Keywords: Implicit gradients, Shock-capturing, BVD algorithm.

1. Introduction

Compressible flow simulations involving discontinuities, such as shock waves and material interfaces, and turbulence is a challenging task. The choice of numerical approaches significantly affects the simulation quality, and different target applications place different demands on the numerical scheme. For compressible flows, even for smooth initial data, the flow may develop sudden changes in pressure and density mathematically treated as discontinuities. These discontinuities will result in spurious oscillations (Gibbs phenomenon), which can be mitigated by introducing additional dissipation. Even for incompressible flows, numerical schemes can fail if there is discontinuous initial data \cite{1}. On the other hand, the numerical scheme should have low dispersion and low dissipation to capture the small scales in amplitude and phase accurately. This numerical dissipation needed to stabilize the discontinuities will significantly impact the fine scales of turbulence. These conflicting requirements pose a significant challenge in developing numerical schemes for simulating such flows \cite{2}. These requirements are similar to the Kobayashi-Maru test, a fictional no-win scenario \cite{3}. Unlike in the fictional world where Kirk cheats, researchers in the real world try to develop meaningful solutions as nature cannot be fooled.

This paper focuses on the low dispersion and dissipation part and proposes a novel algorithm based on implicit gradients for regular hexahedral (i.e., Cartesian) grids. It is demonstrated that such low dispersion and dissipation schemes can be constructed by linearly high-order schemes that achieve high-order accuracy for linear equations but second-order accurate at best for nonlinear equations. Specifically, we construct low dispersion and dissipation schemes based on a finite-volume scheme with the kappa solution reconstruction scheme of Van Leer \cite{4, 5} by making two key modifications: (1) replace cell-averaged solutions by point-valued solutions and (2) express the kappa scheme with first- and second-derivatives and replace them by those computed by implicit methods. The first modification is introduced to construct a high-order conservative finite-difference scheme, rather than a finite-volume scheme, so that high-order accuracy can be achieved (for linear equations) in multi-dimensions simply by applying a one-dimensional scheme in each coordinate direction. As pointed out in Refs.\cite{16, 17}, however, methods based on the finite-volume method with point-valued solutions (instead of cell-averaged solutions) can achieve third- or higher-order accuracy for linear equations but can only be second-order accurate for nonlinear equations. While high-order accuracy can be achieved for nonlinear equations by introducing high-order flux reconstruction \cite{16, 17, 18}, the linearly high-order schemes are obviously more computationally efficient since expensive flux reconstruction is not necessary. Moreover, it has been demonstrated that linearly high-order schemes significantly improve the resolution of complex three-dimensional turbulent-flow simulations at a little additional cost over conventional second-order finite-volume schemes widely used in practical unstructured-grid computational fluid dynamics codes, despite not being genuinely high-order accurate for such nonlinear problems \cite{10, 11, 12, 13, 14, 15}. This paper explores linearly high-order schemes combined with implicit gradients and demonstrates that these schemes can produce significantly accurate solutions for strongly nonlinear problems with shock waves. As we will show, the second modification of implicit gradients is
another important ingredient for developing lower dispersion and dissipation schemes. Extensions to genuinely high-order schemes are possible with flux reconstruction, but we would rather focus on the linearly high-order schemes here because of their surprisingly excellent performance.

The proposed method is conservative and based on an upwind flux computed with solutions reconstructed by the kappa scheme of Van Leer [1, 5]. This method is expected to be third-order accurate because the kappa scheme is a quadratic reconstruction scheme. However, contrary to expectations, it results in a fourth-order upwind finite-difference scheme (at least for linear equations) if combined with high-order accurate gradients on regular grids. Specifically, we will express the kappa scheme in terms of the first and second derivatives of the solution and then compute these derivatives by high-order gradient methods. In particular, conservative schemes with exceptionally low dispersion and dissipative errors can be obtained if the gradients are computed implicitly (globally coupled linear systems). Implicit gradient methods are not new: high-order compact schemes from Ref. [6] can be directly applied to compute the gradients on regular grids. However, in our schemes, implicit gradients are used not directly for approximating the flux divergence but for evaluating the derivatives in solution reconstruction schemes within a framework of conservative finite-volume-type schemes. It allows us to easily construct stable high-resolution shock-capturing schemes incorporating Riemann solvers and various monotonicity-preserving mechanisms in the solution reconstruction, which would not be simple to incorporate if the flux divergence is directly computed by implicit gradient methods as typical in the so-called compact schemes. In this paper, we will employ the fourth- and sixth-order compact finite difference schemes of Lele [6] as implicit gradient methods. Second derivatives are computed, in the same way, for a given set of gradient values as the gradients are computed for a given set of solution values. More specifically, we define the numerical solutions as point values at cell centers (not cell averages) and evaluate the numerical flux with solution values reconstructed at a face by a quadratic Legendre polynomial as in the unlimited kappa-scheme of Van Leer [4, 5] with first and second derivatives computed by implicit gradient methods [6]. For shock capturing, we will combine the proposed schemes with the BVD algorithm [7]. The proposed method has the following advantages:

(a) It generates fourth-order upwind finite-difference schemes with a quadratic reconstruction for linear equations, which typically leads to third-order accuracy at best.

(b) It generates practical low-dispersion/dissipation schemes that can be easily implemented for structured-grid codes.

(c) It has superior dissipation and dispersion properties as compared to the direct compact reconstruction approach of Ref. [8] (please see Remarks 3.2 and Section 3.1.4 and Equations (20) in the main text), and

(d) the implicit gradient approach combined with the shock-capturing approach via the Boundary Variation Diminishing (BVD) algorithm gives superior results of flows with shocks, material interfaces and small scale features than the approach presented in [9].

To the best of the authors’ knowledge, the combination of the kappa scheme and the implicit gradient methods has not been explored, and its superior dissipative property despite being only linearly high-order has not been revealed elsewhere. This paper provides a detailed account of the implicit gradient-based schemes and demonstrates their performance for an extensive series of inviscid-flow problems involving shock waves.

BVD algorithm was initially proposed by Sun et al. [7] which combines a non-polynomial reconstruction scheme, THINC (Tangent of Hyperbola for Interface Capturing), for discontinuous regions and an unlimited polynomial based reconstruction for the smooth regions of flows. The proposed methodology adaptively chooses the scheme with minimum Total Boundary Variation (TBV), reducing the numerical dissipation. Following their idea, Chamarthi and Frankel [9] have presented a new algorithm named HOCUS (High-Order Central Upwind Scheme), which combined the MP scheme and a linear-compact scheme using the BVD principle, which is used in the present approach. Our focus is on the novel linearly high-order method with implicit gradients and its demonstration for various nonlinear inviscid problems. Extensions to genuinely high-order accuracy, viscous-flow problems, and comparison with other high-order schemes are addressed in the future work.

The rest of the paper is organized as follows. Section 2 introduces the governing equations of the inviscid compressible flows. In Section 3 a brief description of the cell-centered conservative approach is presented and the novel reconstruction schemes are introduced along with the implementation details. Numerical results and discussion are presented in Section 4 and finally, in Section 5 we provide concluding remarks.

2. Governing equations

The governing equations of inviscid compressible flows are

\[ Q_t + F(U)_x + G(U)_y + H(U)_z = 0, \]  

(1)
where \( \mathbf{Q} \) is the conserved variable vector, \((\rho, \rho u, \rho v, \rho w, \rho E)^T\), in which \( \rho \), \( u \), \( v \), \( w \), and \( \rho E \) are the density, the three Cartesian velocity components and the total energy with relation \( E = e + \frac{1}{2}(u^2 + v^2 + w^2) \), where \( e \) is the internal energy per unit mass. The fluxes \( \mathbf{F} \), \( \mathbf{G} \), and \( \mathbf{H} \) are defined as follows:

\[
\mathbf{F} = \begin{pmatrix}
\rho u \\
\rho u^2 + p \\
\rho u v \\
\rho u w \\
u(\rho E + p)
\end{pmatrix}, \quad
\mathbf{G} = \begin{pmatrix}
\rho v \\
\rho u v + \rho p \\
\rho v^2 + p \\
\rho v w \\
v(\rho E + p)
\end{pmatrix}, \quad
\mathbf{H} = \begin{pmatrix}
\rho w \\
\rho u w + \rho p \\
\rho w^2 + p \\
\rho w v \\
w(\rho E + p)
\end{pmatrix}.
\]

The system of equations is closed with the ideal gas equation of state which relates the thermodynamic pressure \( p \) and the total energy:

\[
p = (\gamma - 1)(E - \rho \left(\frac{u^2 + v^2 + w^2}{2}\right)),
\]

where \( \gamma \) is the ratio of specific heats of the fluid (\( \gamma = 1.4 \) for air at standard conditions).

3. Numerical methods

The time evolution of the vector of cell-centered conservative variables \( \hat{\mathbf{Q}} \) is given by the following semi-discrete relation applied to a Cartesian cell \( I_{j,i,k} = [x_{j-1/2}, x_{j+1/2}] \times [y_{i-1/2}, y_{i+1/2}] \times [z_{k-1/2}, z_{k+1/2}] \), expressed as an ordinary differential equation:

\[
\frac{d}{dt} \hat{\mathbf{Q}}_{j,i,k} = \mathbf{Res}_{j,i,k},
\]

where \( \mathbf{Res}_{j,i,k} \) denotes the residual:

\[
\mathbf{Res}_{j,i,k} = \frac{1}{\Delta x} \left( \hat{\mathbf{F}}_{j-\frac{1}{2},i,k} - \hat{\mathbf{F}}_{j+\frac{1}{2},i,k} \right) + \frac{1}{\Delta y} \left( \hat{\mathbf{G}}_{j,i-\frac{1}{2},k} - \hat{\mathbf{G}}_{j,i+\frac{1}{2},k} \right) + \frac{1}{\Delta z} \left( \hat{\mathbf{H}}_{j,i,k-\frac{1}{2}} - \hat{\mathbf{H}}_{j,i,k+\frac{1}{2}} \right),
\]

and \( \hat{\mathbf{F}} \), \( \hat{\mathbf{G}} \), and \( \hat{\mathbf{H}} \), are regarded as numerical approximations of the convective fluxes in the \( x \)-, \( y \)-, and \( z \)-directions respectively, and \( \mathbf{Res}_{j,i,k} \) is the residual function. In the following subsections, we provide the details of the computation of convective fluxes, including the novel implicit gradient method (3.1), shock-capturing algorithm (3.2), and the details of Riemann solver (3.3). Note that we define the cell-centered numerical solution \( \hat{\mathbf{Q}} \) as a point-valued solution at the cell center, not a cell-averaged solution. It simplifies the introduction of implicit gradients, the implementations of boundary conditions and initial values, and most importantly, it leads to linearly high-order finite-difference schemes that preserves the design order of accuracy in multi-dimensions as in the above form without high-order flux quadrature as required in the finite-volume method with cell averages. Hence, the flux \( \hat{\mathbf{F}} \) is computed only at the center of a face in the \( x \)-direction, and similarly the fluxes \( \hat{\mathbf{G}} \) and \( \hat{\mathbf{H}} \) are computed only at the centers of faces in the \( y \)- and \( z \)-directions, respectively, as in a one-dimensional scheme.

3.1. Spatial discretization of fluxes

In this section, we present the spatial discretization of fluxes. As mentioned, we can consider only one-dimensional scenario as it can be easily extended to multi-dimensional (2D and 3D) problems as a finite-difference scheme via dimension by dimension approach. The governing equations (1) are discretized on a uniform grid with \( N \) cells on a spatial domain spanning \( x \in [x_n, x_b] \). The cell center locations are at \( x_j = x_n + (j - 1/2)\Delta x \), \( \forall j \in \{1, 2, \ldots, N\} \), where \( \Delta x = (x_b - x_n) / N \). The cell interfaces, indexed by half integer values, are at \( x_{j+\frac{1}{2}}, \forall j \in \{0, 1, 2, \ldots, N\} \). Let \( I_j = [x_{j-1/2}, x_{j+1/2}] \) be a control volume (a computational cell) of width \( \Delta x = x_{j+1/2} - x_{j-1/2} \).

3.1.1. Upwind flux (Riemann solver)

The numerical fluxes in the Equation (3), \( \hat{\mathbf{F}}_{j-\frac{1}{2}} \) and \( \hat{\mathbf{F}}_{j+\frac{1}{2}} \), are computed by a Riemann solver. There are several types of Riemann solvers in literature [19] [20] [21] [22] [23] [24] [25], and the canonical form of Riemann flux can be written as:

\[
\hat{\mathbf{F}}_{j+\frac{1}{2}}^{\text{Riemann}} = F_{j+\frac{1}{2}}(Q_j^L, Q_j^R),
\]

\[
F_{j+\frac{1}{2}}^{\text{Riemann}} = \frac{1}{2} \left[ F(Q_{j+\frac{1}{2}}^L) + F(Q_{j+\frac{1}{2}}^R) \right] - \frac{1}{2} |A_{j+\frac{1}{2}}| (Q_{j+\frac{1}{2}}^R - Q_{j+\frac{1}{2}}^L),
\]

where \( L \) and \( R \) are adjacent values of a reconstructed solution polynomial at a cell interface, as shown in Fig. 1 and \( |A_{j+\frac{1}{2}}| \) denotes the characteristic signal velocity evaluated at the cell interface in a hyperbolic equation or in the case of Euler equations, the inviscid Jacobian.
3.1.2 Solution reconstruction with the kappa scheme

The procedure of obtaining the values at the interface from cell center variables is called reconstruction or interpolation. It is obvious from the Equation (7), a core problem is how to reconstruct the left- and right-side values, $Q_{j+1/2}^L$ and $Q_{j+1/2}^R$, for cell boundaries, which can fundamentally influence the numerical solution. Representing these numerical approximations of $L$ and $R$ at cell interface as a piecewise constant is equivalent to first-order approximation, i.e.,

$$Q_{j+1/2}^L = \hat{Q}_j,$$
$$Q_{j+1/2}^R = \hat{Q}_{j+1}.$$  \hspace{1cm} (8)

Therefore, a linear approximation of the solution, shown in Fig. 1 is a second-order spatial approximation, while a quadratic representation on each cell leads to a third-order spatial approximation. By considering a general local representation, as explained in [4], the quadratic approximation can be expressed in terms of Legendre polynomials, valid for $x_{j-1/2} \leq x \leq x_{j+1/2}$:

$$Q(x) = \hat{Q}_j + Q_j'(x-x_j) + \frac{3Q_j''}{2}\kappa \left[(x-x_j)^2 - \frac{\Delta x^2}{12}\right],$$ \hspace{1cm} (9)

where $\hat{Q}_j$ is the cell-center value and $Q_j'$, $Q_j''$ are the estimations of the first and second derivatives within the cell $j$. The Equation (8) is the basis for the Monotonic Upstream-centered Scheme for Conservation Laws (MUSCL) scheme or popularly known as the kappa scheme of Van Leer [4, 5]. The WENO schemes are an extension of the MUSCL scheme to an arbitrary order of accuracy (see derivations in Ref. [26]). Note, however, that the kappa scheme is used here with the point-valued solutions stored at the cell center, $\hat{Q}_j$, whereas it is used with the cell-averaged solution in MUSCL. Such a scheme can still achieve third-order accuracy for linear equations with $\kappa = \frac{1}{3}$, but can only be second-order accurate for nonlinear equations [16, 17]. However, while it remains second-order accurate for nonlinear equations, it can achieve fourth-order accuracy for linear equations if the derivatives $Q_j'$ and $Q_j''$ are evaluated with high-order gradients. Fourth-order accuracy with a quadratic polynomial may be an unexpected result, and this is the main contribution of this work.

For the numerical approximations of the Riemann problem, we need the values at the cell interfaces only. By setting $x = x_j \pm \Delta x/2$ within a cell $j$ gives us the interface values:

$$Q_{j+1/2}^L = \hat{Q}_j + \frac{1}{2}Q_j' + \frac{\kappa}{4}Q_j''$$ \hspace{1cm} or \hspace{1cm} $Q_{j-1/2}^L = \hat{Q}_{j-1} + \frac{1}{2}Q_{j-1}' + \frac{\kappa}{4}Q_{j-1}''$, \hspace{1cm} (10)

$$Q_{j+1/2}^R = \hat{Q}_j - \frac{1}{2}Q_j' + \frac{\kappa}{4}Q_j''$$ \hspace{1cm} or \hspace{1cm} $Q_{j-1/2}^R = \hat{Q}_{j+1} - \frac{1}{2}Q_{j+1}' + \frac{\kappa}{4}Q_{j+1}''$.

In order to define these approximations completely, the derivatives $Q_j'$ and $Q_j''$ have to be estimated. Typically, these derivatives are computed explicit finite-difference formulas as we will show in the next section. Or they can be evaluated by implicit gradient methods, which is the main point of this paper, as we will discuss in a subsequent section.

Remark 3.1. Both conservative, $Q$, and primitive variables, $U$, can be used for the evaluation of the gradients in the implicit gradient approach explained above. For shock-capturing purposes (will be explained in Section 3.1.3), gradients of the primitive variables are used for reconstruction in this paper and the primitive variable...
vector is, $U = (\rho, u, v, p)^T$.

3.1.3. Second-order explicit gradients: Baseline scheme

First, we consider, for comparison, explicit gradient methods as in a typical MUSCL-type scheme. By using $\kappa = \frac{1}{2}$ and substituting the following explicit central differences for the derivatives in Equation (10),

$$Q'_j = \frac{\hat{Q}_{j+1} - \hat{Q}_{j-1}}{2\Delta x},$$
$$Q''_j = \frac{\hat{Q}_{j+1} - 2\hat{Q}_j + \hat{Q}_{j-1}}{\Delta x^2},$$

we obtain the following third order reconstruction formulas,

$$Q^L_{j+\frac{1}{2}} = \frac{1}{6} \left( -\hat{Q}_{j-1} + 5\hat{Q}_j + 2\hat{Q}_{j+1} \right),$$
$$Q^R_{j-\frac{1}{2}} = \frac{1}{6} \left( 2\hat{Q}_j - 5\hat{Q}_j + \hat{Q}_{j+1} \right).$$

These reconstruction schemes lead to a linearly third-order scheme (because the numerical solutions are point values): third-order accurate for linear equations and second-order accurate for nonlinear equations [16, 17]. Note that this should not be considered as a failure of the scheme design because it is just a simplified version of the original finite-difference scheme of Van Leer [16] without flux reconstruction and it is deliberately designed this way in this work for developing practical and efficient schemes with low dispersion and dissipation. As we will show later, the scheme can achieve higher than third-order accuracy (for linear equations) with these explicit gradients replaced by higher-order implicit gradient formulas. In effect, the resulting schemes are high-order conservative finite-difference schemes approximating the flux divergence in a conservative manner by a flux difference, rather than the finite-volume scheme approximating the integral form of the governing equations. Therefore, the quadratic reconstruction scheme does not limit the order of accuracy of the resulting scheme: it is used as a stepping stone towards a higher-order difference approximation. High-order explicit gradient formulas may be employed instead of implicit gradient methods, but such will significantly extend the residual stencil and require complicated algorithms near boundaries. Implicit gradients do not involve such complications near boundaries, and also have been found to generate schemes much lower dispersion and dissipation that high-order explicit gradients.

3.1.4. High-order implicit gradients: Novel IG4 and IG6 schemes

To construct fourth-order conservative upwind finite-difference schemes, we consider implicit gradients, where the derivatives, $Q'$ and $Q''$, in Equation (10) are computed by using high-order implicit gradient methods (compact finite difference schemes) proposed in Ref. [6] and therefore the reconstruction procedure is named as implicit gradient (IG) approach. In our case, we employ compact schemes of Lele [6] and are listed in [6]. In this work, we considered difference schemes for the first derivatives with $\alpha$ in Equation (13) contains the spatial derivatives $Q'_j$ while the right hand side contains the function values $\hat{Q}$ at the cell center $x_j$, respectively. Compact finite difference schemes of different orders of accuracy are derived by matching the Taylor series coefficients with different constraints on the parameters $\alpha$, $\beta$, $a$, $b$ and $c$ and are listed in [6]. In this work, we considered difference schemes for the first derivatives with the following parameters,

$$\beta = 0, \quad a_1 = \frac{2}{3}(\alpha + 2), \quad b_1 = \frac{1}{3}(4\alpha - 1), \quad c = 0,$$

$$\beta = -\frac{1 + 3\alpha}{12}, \quad a = \frac{2}{9}(8 - 3\alpha), \quad b = \frac{1}{18}(-17 + 57\alpha), \quad c = 0.$$  

By substituting $\alpha = \frac{2}{11}$ in Equation (14a) we obtain the optimised fourth-order compact derivative (see Fig. 2 in Ref. [6]) and is denoted by CD4. For $\alpha = \frac{1}{4}$ in Equation (14b), we obtain the sixth-order compact derivative and is denoted by CD6, and can be written as:

$$\frac{5}{14}Q'_{j-1} + \frac{5}{14}Q'_j + \frac{5}{14}Q'_{j+1} = \frac{b_1}{4\Delta x} \left( \hat{Q}_{j+2} - \hat{Q}_{j-2} \right) + \frac{a_1}{2\Delta x} \left( \hat{Q}_{j+1} - \hat{Q}_{j-1} \right),$$
$$\frac{1}{3}Q'_{j-1} + \frac{1}{3}Q'_j + \frac{1}{3}Q'_{j+1} = \frac{b_1}{36\Delta x} \left( \hat{Q}_{j+2} - \hat{Q}_{j-2} \right) + \frac{7}{9\Delta x} \left( \hat{Q}_{j+1} - \hat{Q}_{j-1} \right).$$
where \( j = 1, 2, 3, \ldots, N - 1 \). Unlike the second-order central differences given by the Equations (11), which depend only on values at \( j - 1, j \), and \( j + 1 \), compact finite differences depend on all the nodal values of the domain and therefore mimic the global dependence of the spectral methods. This global dependence results in a tridiagonal system of equations that the Thomas algorithm can easily invert. Near the boundary cells, lower-order one-sided difference formulas are used to approximate derivatives \( Q_0 \) and \( Q_N \). The following third-order formulas are considered for both the CD4 and CD6 schemes in the present work.

\[
Q_0' + 2Q_0'' = \frac{1}{\Delta x} (-\frac{5}{2}Q_0 + 2Q_1 + \frac{1}{2}Q_2),
\]
\[
Q_N' + 2Q_{N-1}'' = \frac{1}{\Delta x} (\frac{5}{2}Q_N + 2Q_{N-1} + \frac{1}{2}Q_{N-2}),
\]
\[
Q_{j+1/2}^r = \frac{1}{2}Q_{j+1/2}^l + \frac{5}{6}Q_{j+1} - \frac{5}{6}Q_j + \frac{1}{6}Q_{j-1/2},
\]
\[
Q_{j-1/2}^r = \frac{1}{2}Q_{j-1/2}^l + \frac{5}{6}Q_j - \frac{5}{6}Q_{j-1} + \frac{1}{6}Q_{j-1/2},
\]

3.1.5. Accuracy and properties of IG4, and IG6

The schemes with high-order gradients are both fourth-order accurate for linear equations despite the use of the quadratic reconstruction formula \([9]\) and the sixth-order method \([15b]\) for derivatives. Generally, schemes based on the quadratic reconstruction are third-order accurate at best. However, the use of high-order gradients makes it possible to go beyond third-order accuracy. To prove this, we apply the schemes to a linear convection equation \( \dot{Q} + F_x = 0 \) with \( F = Q \).

\[
\frac{dQ_j}{dt} = -\frac{1}{\Delta x} [F_{j+1/2} - F_{j-1/2}],
\]
where
\[ F_{j+1/2} = \frac{1}{2} \left[ F(Q_{j+1/2}^R) + F(Q_{j+1/2}^L) \right] - \frac{1}{2} (Q_{j+1/2}^R - Q_{j+1/2}^L) = Q_{j+1/2}^L, \]  \hspace{1cm} (22)
and perform a Fourier analysis, which is especially useful for analyzing schemes with implicit gradients. Consider a Fourier mode: \( \hat{Q}_\beta = \hat{Q}_0 \exp(i\beta x/\Delta x) \), where \( \hat{Q}_0 \) is the amplitude, \( \beta \) is the frequency, \( \Delta x \) is the mesh spacing of a uniform grid, and \( i = \sqrt{-1} \). Substituting it into the semi-discrete form \((21)\), we find
\[
\frac{d\hat{Q}_0}{dt} = F_{\text{exact}} \hat{Q}_0, \tag{23}
\]
where \( F_{\text{exact}} \) denotes the exact convection operator:
\[
F_{\text{exact}} = -\frac{i\beta}{\Delta x}. \tag{24}\]
This is the operator approximated by numerical schemes. Below, we derive the corresponding operators for the explicit and implicit gradients schemes, and measure the error by the leading deviation from the exact operator in the expansion for smooth components. The Fourier analysis is also useful for analyzing the dispersion and dissipative properties, which we will discuss subsequently.

Explicit gradients: Baseline scheme:

First, we consider the explicit scheme with Equation \((12)\). Substituting the Fourier mode into the residual computed with the explicit gradients, we obtain
\[
\frac{d\hat{Q}_0}{dt} = F_{\text{EG}} \hat{Q}_0, \tag{25}
\]
where
\[
F_{\text{EG}} = \left( \cos \beta - 1 \right)^2 + \frac{\sin \beta(\cos \beta - 4)}{3} i. \tag{26}\]
Expanding it for a small \( \beta \approx O(\Delta x) \), we obtain
\[
F_{\text{EG}} = -\frac{\beta}{\Delta x} \left[ i + \frac{\beta}{12} + \frac{\beta^4}{30} i - \frac{\beta^5}{72} + \frac{\beta^6}{252} i + \cdots \right], \tag{27}
\]
which shows, compared with the exact operator \((24)\), that the leading error is third-order as expected: \( O(\beta^3) = O(\Delta x^3) \). The third-order error appears in the real part, which indicates the error is dissipative. The leading dispersive error is fourth-order. As we will show next, implicit gradients lead to a negative leading real part (stable) and have significantly better dispersion and dissipation properties.

Implicit gradients: IG4 and IG6:

For the IG4 and IG6 schemes, we first derive the gradient and the second derivative. Consider a Fourier mode for the gradient: \( Q_{\beta x} = G_0 \exp(i\beta x/\Delta x) \), where \( G_0 \) is the amplitude, and substitute it into CD4 \((15a)\) to get
\[
\frac{5}{7} \cos \beta G_0 + G_0 = \sin \beta \cos \beta + 11 \sin \beta \frac{\Delta x}{7} Q_0 i, \tag{28}\]
which can be solved for \( G_0 \):
\[
G_0 = \frac{\sin \beta \cos \beta + 11}{\Delta x(5 \cos \beta + 7)i} Q_0. \tag{29}\]
Similarly, for the second derivative, substituting \( Q_{\beta xx} = H_0 \exp(i\beta x/\Delta x) \), where \( H_0 \) is the amplitude, and substituting it into the CD4 \((18a)\), solving it for \( H_0 \), and substituting Equation \((29)\), we obtain
\[
H_0 = -\frac{(\sin \beta \cos \beta + 11)^2}{\Delta x^2(5 \cos \beta + 7)^2} Q_0. \tag{30}\]
Finally, substituting the Fourier modes, \( Q_\beta, Q_\beta x, \) and \( Q_\beta xx \), into the IG4 scheme and eliminating \( G_0 \) and \( H_0 \) by the above equations, we obtain
\[
F_{\text{IG4}} = \left( \cos \beta - 1 \right)^2 (\cos^3 \beta - 7 \cos^2 \beta + 11 \cos \beta - 5) \frac{12(5 \cos \beta + 7)^2}{12(5 \cos \beta + 7)^2} - \sin \beta(\cos^4 \beta - 8 \cos^3 \beta + 78 \cos^2 \beta + 728 \cos \beta + 929) i, \tag{31}\]
which is expanded as
\[ F^{IG4} = -\frac{\beta}{\Delta x} \left[ i + \frac{\beta^4}{720} i + \frac{\beta^6}{12096} i + \frac{\beta^7}{6912} + \cdots \right]. \] (32)

Clearly, it shows that it is fourth-order accurate with a leading fourth-order dispersive error and a sixth-order dissipative error. Note that there are no third- and fifth-order dissipative errors, i.e., no real part of \( O(\beta^3) \) and \( O(\beta^5) \), in contrast to the result for the explicit scheme (27). It indicates that the use of implicit gradients effectively removed the third- and fifth-order dissipative errors and produced a significantly low-dissipation scheme.

Similarly, for the IG6 scheme, we first derive the amplitudes of the Fourier modes for the gradient and the second derivative by substituting the Fourier modes and solving the resulting equations for \( G_0 \) and \( H_0 \). The results are
\[ G_0 = \frac{\sin \beta (\cos \beta + 14)}{3 \Delta x (2 \cos \beta + 3)} Q_0, \] (33)
and
\[ H_0 = -\frac{\sin^2 \beta (\cos \beta + 14)^2}{9 \Delta x^2 (2 \cos \beta + 3)^2} Q_0. \] (34)

Then, substituting the Fourier modes, \( Q^\beta \), \( Q_x^\beta \), and \( Q_{xx}^\beta \), into the IG6 scheme and eliminating \( G_0 \) and \( H_0 \) by the above equations, we obtain
\[ F^{IG6} = \frac{(\cos \beta - 1)^2 (\cos^3 \beta - 7 \cos^2 \beta + 26 \cos \beta - 20)}{108 (2 \cos \beta + 3)^2} - \frac{\sin \beta (\cos^4 \beta - 8 \cos^3 \beta + 105 \cos^2 \beta + 1070 \cos \beta + 1532)}{108 (2 \cos \beta + 37)^2} i, \] (35)
which is expanded as
\[ F^{IG6} = -\frac{\beta}{\Delta x} \left[ i + \frac{\beta^4}{720} i + \frac{\beta^5}{1440} - \frac{\beta^6}{5040} i + \frac{17 \beta^7}{86400} + \cdots \right]. \] (36)

Therefore, the IG6 scheme is also fourth-order accurate with the leading fourth-order dispersive error. Note that there is a fifth-order dissipative error, which does not exist in IG4. Therefore, IG4 is expected to be less diffusive than IG6. Again, we emphasize that the order of accuracy of the scheme with implicit gradients is not necessarily determined by either the order of the reconstruction polynomial or the order of accuracy of the gradient algorithms. As we have just shown, the order of accuracy of the implicit-gradient-based schemes are not intuitive and needs to be analyzed correctly to reveal their accuracy and properties.

Before we discuss the dispersion and dissipation properties, we present, for comparison, the Fourier analysis for the C5 scheme based on the implicit solution reconstruction (20a). We begin by substituting \( Q_\beta = Q_0 \exp(i\beta/\Delta x) \) for the cell-center solution and \( Q_{x\beta} = Q_0 \exp(i(\beta(x/\Delta x - 1/2))) \) for the face value. Solving the result for the amplitude \( Q_0 \), we obtain
\[ Q_0 = \frac{\cos(\beta/2) \left\{ 4 \cos^4(\beta/2) + 50 \cos^2(\beta/2) + 21 \right\} - 4i \sin(\beta/2)}{12 \cos^4(\beta/2) + 12 \cos^2(\beta/2) + 1} Q_0. \] (37)

Then, we substitute \( Q_\beta = Q_0 \exp(i\beta/\Delta x) \) for the cell-center solution and \( Q_{x\beta} = Q_0 \exp(i(\beta(x/\Delta x - 1/2))) \) with \( Q_0 \) given by the above equation for the face value into the semi-discrete equation (21), we obtain
\[ F^{C5} = -\frac{8 \sin^6(\beta/2) - i \sin \beta \left\{ 4 \cos^4(\beta/2) + 50 \cos^2(\beta/2) + 21 \right\}}{36 \left\{ \cos^4(\beta/2) + \cos^2(\beta/2) + 1/12 \right\}}. \] (38)

Expanding it, we find
\[ F^{C5} = -\frac{\beta}{\Delta x} \left[ i + \frac{\beta^5}{600} + \frac{\beta^6}{7000} i + \cdots \right], \] (39)
which shows that the C5 scheme is fifth-order accurate.

Dispersion and dissipation properties:

Fig. 2 shows the dispersion and dissipation properties of the IG4, IG6, MUSCL and C5 schemes, i.e., imaginary and real parts of Equations (31), (35), (26), and (38), respectively. Figure 2(a) shows that the dispersion property of the IG4 is better than IG6. The dispersion property of the IG4 scheme is very close to that of the C5 scheme. Also, as can be seen in Figure 2(b), the proposed schemes have superior dissipation in comparison with the C5 scheme. These properties are also confirmed later by the inviscid Taylor-Green simulations (Example 1.11 in numerical results). Comparison is also made with the MUSCL scheme, Equation (12) which uses explicit gradients. It can be seen that explicit gradients are much more dispersive and dissipative.
than the implicit gradients considered here.

Figure 2: Dispersion and Dissipation properties of the linear upwind schemes.

Note that the accuracy analysis is valid only for linear equations. For nonlinear equations, all the schemes are second-order accurate at best as long as the averaged flux is evaluated with reconstructed solutions: $|F(Q^L_{j+1/2}) + F(Q^R_{j+1/2})|/2$ [16, 17]. To preserve the high order of accuracy for nonlinear equations, the averaged flux needs to be evaluated by flux reconstruction $[F^L_{j+1/2} + F^R_{j+1/2}] / 2$, where $F^L_{j+1/2}$ and $F^R_{j+1/2}$ are computed by a direct flux reconstruction scheme, e.g., by applying the kappa scheme to the fluxes. See Ref. [18] for efficient flux reconstruction techniques based on solution derivatives (not using flux derivatives). Alternatively, one may reinterpret the numerical solution values as cell averages and apply a single-point high-order flux quadrature formula proposed in Refs. [27, 32], or a multiple-point flux quadrature formula with a dimension-by-dimension solution reconstruction [33]. However, it has been demonstrated that linearly high-order schemes can produce solutions with dramatically higher resolution than conventional second-order schemes for practical turbulent flows at a lower cost [10, 11, 12, 13]. The same has been demonstrated for flows with shock waves in Ref. [14]. The development of a genuinely high-order version of IG4 and the comparison with the linearly higher-order version proposed in this paper is left as future work.

3.2. Shock-capturing via BVD algorithm: IG4MP and IG6MP

The novel schemes, IG4 and IG6, derived in the earlier section, are linear in nature and therefore lead to oscillations for flows involving material interfaces and shocks. In this section, we describe the shock-capturing scheme using the BVD algorithm, previously presented in [9], extended to the IG schemes for both single and multi-component flows. By comparing two different polynomials, the BVD algorithm selects the reconstruction polynomial with minimum numerical dissipation by evaluating the Total Boundary Variation (TBV) given by the Equation (40) for each cell for each primitive variable:

$$TBV_j = |U^L_{j-\frac{1}{2}} - U^R_{j-\frac{1}{2}}| + |U^L_{j+\frac{1}{2}} - U^R_{j+\frac{1}{2}}|.$$  \hspace{1cm} (40)

For a given cell, the terms on the right-hand side of Equation (40) represent the amount of numerical dissipation introduced in the numerical flux in Equation (40). The BVD algorithm compares the TBVs of the concerned polynomials and selects the one that is least dissipative at an interface. In the smooth regions of the flow, the IG6 or IG4 linear schemes will be used, and in the presence of discontinuities, the BVD algorithm will turn to the MP5 scheme [34]. The combination of IG4 and MP5 is denoted as IG4MP and, the combination of IG6 and MP5 is denoted as IG6MP in this paper, respectively. Both schemes are denoted together as IGMP schemes.

Physically, the density and pressure should be positive, and failure to preserve these variables’ positivity may cause a blow-up of the numerical solutions. The reconstructed states, $L$ and $R$, obtained by IG4MP, IG6MP and even MP5 methods, may sometimes lead to unphysical values for density and pressure. In the present paper, we use the order reduction strategy of Titarev and Toro [33]. We note that in the test cases we have addressed, the IG4MP and IG6MP schemes failed in very few cells, even after using the BVD algorithm, and in relatively few time steps, this choice is justified. If the MP5 reconstruction also produced unphysical values in the worst-case scenario, the reconstructed states are reduced to first-order (FO) accurate reconstructions given by Equations (6). In the following, reconstruction procedure only in the $x$-direction is discussed. Due to the dimension-by-dimension approach, the other directions are handled the same way and the procedure is summarized below:
Step i. Evaluate the interface values by using the implicit gradient approach:

(a) Compute the first and second derivatives of the primitive variables by implicit gradient methods.
(b) Form the reconstructed states by substituting the derivatives in the Equation (19), either IG4 or IG6, for each primitive variable

\[
\begin{aligned}
U_{j+1/2}^{IG4} &= \hat{U}_j + \frac{1}{2}U_j' + \frac{1}{12}U_j'' \\
U_{j-1/2}^{IG4} &= \hat{U}_j - \frac{1}{2}U_j' + \frac{1}{12}U_j''
\end{aligned}
\]  

(41)

Step ii. Evaluate the interface values using MP5 scheme, necessary for the BVD algorithm. The steps involved are as presented in Appendix A.

Step iii. Calculate the TBV values for each cell \( I_j \) by using the implicit gradient reconstruction for IG4,

\[
TBV_{j}^{IG4} = |U_{j-\frac{1}{2}}^{L,IG4} - U_{j-\frac{1}{2}}^{R,IG4}| + |U_{j+\frac{1}{2}}^{L,IG4} - U_{j+\frac{1}{2}}^{R,IG4}|
\]  

for IG6,

\[
TBV_{j}^{IG6} = |U_{j-\frac{1}{2}}^{L,IG6} - U_{j-\frac{1}{2}}^{R,IG6}| + |U_{j+\frac{1}{2}}^{L,IG6} - U_{j+\frac{1}{2}}^{R,IG6}|
\]  

and MP5 scheme:

\[
TBV_{j}^{MP5} = |U_{j-\frac{1}{2}}^{L,MP5} - U_{j-\frac{1}{2}}^{R,MP5}| + |U_{j+\frac{1}{2}}^{L,MP5} - U_{j+\frac{1}{2}}^{R,MP5}|
\]  

Step iv. Modify all the interface values at \( j - \frac{1}{2}, j - \frac{1}{2}, j + \frac{1}{2} \) and \( j + \frac{3}{2} \), both \( L \) and \( R \) according to the following algorithm, for each primitive variable, to obtain non-oscillatory results. For the IG4MP scheme we have

\[
\begin{aligned}
U_{j-\frac{1}{2}}^{IG4} &= U_{j+\frac{1}{2}}^{MP5} \\
U_{j+\frac{1}{2}}^{IG4} &= U_{j+\frac{3}{2}}^{MP5}
\end{aligned}
\]  

if \( TBV_{j}^{MP5} < TBV_{j}^{IG4} \)

(45)

and for the IG6MP scheme we obtain,

\[
\begin{aligned}
U_{j-\frac{1}{2}}^{IG6} &= U_{j+\frac{1}{2}}^{MP5} \\
U_{j+\frac{1}{2}}^{IG6} &= U_{j+\frac{3}{2}}^{MP5}
\end{aligned}
\]  

if \( TBV_{j}^{MP5} < TBV_{j}^{IG6} \)

(46)

where \( K = L \) or \( R \).

Step v. For each reconstructed state, \( K \), we check the following conditions for positivity of pressure and density

\[
\rho^K \leq 0 \quad \text{or} \quad p^K \leq 0.
\]  

(47)

If conditions given by Equations (47) are not satisfied we decrease the order of reconstruction and the procedure is as follows,

\[
U^K = \begin{cases} 
U^K_{\text{IG4MP or IG6MP}}, \\
U^K_{\text{MP5}}, \\
\text{default}
\end{cases}
\]  

(48)

\[
\begin{aligned}
&\text{if } U^K_{\text{IG4MP or IG6MP}} \text{ fails,} \\
&\text{if } U^K_{\text{MP5}} \text{ fails,}
\end{aligned}
\]

where, \( U^K_{\text{FO}} \) is the first order approximation computed using Equation (8).

Step vi. Evaluate the conservative variables, \( Q_{j+\frac{1}{2}}^L, Q_{j+\frac{1}{2}}^R \), from the primitive variables, \( (U_{j+\frac{1}{2}}^L, U_{j+\frac{1}{2}}^R) \) obtained from the above procedure, and compute the interface flux \( \mathbf{F}_{\text{Riemann}}^{j+\frac{1}{2}} \).
Remark 3.3. The choice of MP5 scheme as a candidate polynomial for shock-capturing has been arrived at by testing several different combinations of linear and nonlinear schemes. It is also possible to use a third-order reconstruction with the minmod limiter and THINC, and readers are referred to Appendix A and B of Ref. [9]. The BVD algorithm used here is similar to the one used in Ref. [9] where the combination of the C5 and MP5 schemes for parameter α is shown in Table I which is also based on the previous analysis from Ref. [9]. In this paper, we compare the developed IGMP schemes with the HCOUS5 scheme presented in Ref. [9], which combines C5 and MP5 schemes using the BVD algorithm. Time integration is performed with a CFL = 0.2 for all the test cases.

3.3. Riemann solver

Riemann solvers approximate the convective flux after the obtaining reconstructed states at the interface as explained in the earlier section. This section illustrates how the HLLC Riemann solver [22, 23] approximates convective fluxes. For simplicity, only the HLLC approximations for both single and multicomponent flows in the x-direction are illustrated in this section. The HLLC flux in x-direction is given by:

\[
\vec{F}_{xK} = \vec{F}_K + S_K (\vec{Q}_{\ast K} - \vec{Q}_K),
\]

where \( L \) and \( R \) are the left and right states respectively. With \( K = L \) or \( R \), the star state quantities are defined as:

\[
\vec{Q}_{\ast K} = \left( \frac{S_K - u_K}{S_K - S_*} \right) \begin{bmatrix} ρ_K \\ ρ_K S_* \\ ρ_K v_K \\ ρ_K w_K \\ E_k + (S_* - u_K) \left( \frac{ρ_K S_*}{S_K - S_*} + \frac{ρ_K}{ρ_K - ρ} \right) \end{bmatrix}.
\]

In the above expressions, the waves speeds \( S_L \) and \( S_R \) can be obtained as suggested by Einfeldt [23], \( S_L = \min(u_L - cL, \bar{u} - \bar{c}) \) and \( S_R = \max(u_R + cR, \bar{u} + \bar{c}) \), where \( \bar{u} \) and \( \bar{c} \) are the Roe averages from the left and right states. Batten et al. [22] provided a closed form expression for \( S_* \) which is as follows:

\[
S_* = \frac{p_R - p_L + ρ_L u_n L (S_L - u_{nL}) - ρ_R u_n R (S_R - u_{nR})}{ρ_L (S_L - u_{nL}) - ρ_R (S_R - u_{nR})}.
\]

3.4. Temporal integration

Finally, the semi-discrete approximation of the Euler equations is temporally integrated. The conserved variables are integrated in time using the following third-order TVD Runge-Kutta scheme [35]:

\[
\begin{align*}
\hat{\vec{Q}}^{(1)} &= \vec{Q}^n + \Delta t \text{Res} (\hat{\vec{Q}}^n), \\
\hat{\vec{Q}}^{(2)} &= \frac{3}{4} \vec{Q}^n + \frac{1}{4} \hat{\vec{Q}}^{(1)} + \frac{1}{4} \Delta t \text{Res} (\hat{\vec{Q}}^{(1)}), \\
\hat{\vec{Q}}^{n+1} &= \frac{1}{3} \vec{Q}^n + \frac{2}{3} \hat{\vec{Q}}^{(2)} + \frac{2}{3} \Delta t \text{Res} (\hat{\vec{Q}}^{(2)}),
\end{align*}
\]

where \( \vec{Q} \) and \( \text{Res} \) denote global vectors of the numerical solutions and residuals. The \((j,i,k)\) component of \( \text{Res} \) is given by the right-hand side of Equation [4]. The superscripts \( n \) and \( n+1 \) denote the current and the subsequent time-steps, and superscripts \((1)\) \(- (2)\) correspond to intermediate steps, respectively. The time step \( \Delta t \) is taken as:

\[
\Delta t = \text{CFL} \times \left( \min_{\text{cells}} \left( \frac{Δx}{|u + c|}, \frac{Δy}{|v + c|} \right) \right),
\]

where \( c \) is the speed of sound and given by \( c = \sqrt{γ p/ρ} \). The value of \( α \) in Equation [20] puts a restriction on the CFL (Courant-Friedrichs-Lewy) number such that \( \text{CFL} \leq 1/(1+α) \) (see Suresh and Hyunh [34] for further details). The values considered various schemes for parameter \( α \) is shown in Table I which is also based on the previous analysis from Ref. [9]. In this paper, we compare the developed IGMP schemes with the HCOUS5 scheme presented in Ref. [9], which combines C5 and MP5 schemes using the BVD algorithm. Time integration is performed with a CFL = 0.2 for all the test cases.
### 4. Results

#### 4.1. Order of accuracy

**Example 4.1. Accuracy of the proposed schemes**

First of all, we present the order of accuracy (OOA) of the new schemes by convecting the initial profile given by equation (55) in the domain \( x, y \in [-1, 1] \). The solution is obtained at time \( t = 2 \), and the time-step is varied as a function of the grid size as \( \Delta t = \text{CFL} \Delta x^2 \).

\[
(\rho, u, v, p) = (1 + 0.5 \sin(x + y), \ 1.0, \ 1.0) \tag{55}
\]

This exact solution effectively linearizes the Euler equations \([16, 17]\) and therefore we expect fourth-order accuracy for the new schemes, which are linearly fourth-order accurate as proved. The OOA’s are presented in Table 2 indicates that the new schemes are fourth-order accurate in space.

| \( N \) | HOCUS5 OOA | IG6MP OOA | IG4MP OOA |
|---|---|---|---|
| 10^2 | 3.14E-04 | - | - |
| 20^2 | 1.79E-05 | 4.14 | 4.59E-05 | 3.71 |
| 40^2 | 6.78E-07 | 4.72 | 2.54E-06 | 4.18 |
| 80^2 | 2.30E-08 | 4.88 | 1.77E-07 | 3.84 |

We have the following observations regarding order of accuracy:

- The order accuracy of the IG schemes is consistent with the mathematical proof provided in section \([3.1.4]\). Therefore it is possible to obtain fourth-order accuracy with the kappa scheme given by the Equation (9).

- \( L_2 \) norm errors given in Table 2 also indicates that the absolute error of the IGMP schemes is higher than the fifth-order HOCUS5 scheme. However, as it will be shown in the following examples, the IGMP schemes will give better resolution than the HOCUS5 scheme. Hu et al. \([35]\) optimized the linear schemes for favourable spectral properties satisfying the dispersion-dissipation relation but such optimization lead to order degeneration. Even though the proposed schemes are only fourth-order accurate, they have superior dispersion and dissipation properties, evident from all the earlier test cases.

Next, we consider the nonlinear test case proposed by Yee et al.\([37]\), where an isentropic vortex is convected in an inviscid free stream. The computations are carried out on a computational domain of \([0, 10] \times [0, 10]\) with periodic boundary conditions on all sides where the final time is \( t=10 \). An isentropic vortex is added to the mean flow, and the initial flow field is as follows:

\[
\rho = \left[ 1 - \frac{(\gamma-1)\beta^2}{\gamma\pi} e^{(1-r^2)} \right]^{\frac{1}{\gamma-1}}, \quad r^2 = \bar{x}^2 + \bar{y}^2,
\]

\[
(u, v) = (1, 1) + \frac{\beta}{\pi} e^{\frac{1}{2}(1-r^2)} (-\bar{y}, \bar{x}), \quad \bar{x} = x - x_{vc}, \quad \bar{y} = y - y_{vc},
\]

\[
p = \rho^\gamma,
\]

where \((x_{vc}, y_{vc}) = (5,5)\) are the coordinates of the center of the initial vortex and \( \beta = 5 \). Note that this problem can still be linearized if the parameter \( \beta \) is small, and the choice \( \beta = 5 \) is made to avoid it. See Ref.\([16, 17]\) for details. Results are summarized in Table 3. We can observe clearly from Table 3 that the proposed schemes are only second-order accurate as expected.

| \( N \) | HOCUS5 OOA | IG6MP OOA | IG4MP OOA |
|---|---|---|---|
| 25^2 | 3.03E-03 | - | - |
| 50^2 | 6.48E-04 | 2.22 | 6.34E-04 | 2.26 |
| 100^2 | 1.64E-04 | 1.99 | 1.64E-04 | 2.00 |
| 200^2 | 4.10E-05 | 2.00 | 4.10E-05 | 2.00 |

Zhang et al. demonstrated in Ref.\([14]\) that the finite-volume WENO method with mid-point rule is only second-order accurate for nonlinear systems, and Gaussian integral rule is necessary for high-order accuracy.
However, they also noted that the resolution characteristics are often comparable for flows involving discontinuities despite the difference in the order of accuracy. In the present paper, we are also interested in flows involving discontinuities. Also, such linearly high-order schemes have been demonstrated to serve as very low-dissipation schemes for practical turbulent-flow simulations \cite{10, 11, 12, 13}. As mentioned earlier, the developed schemes can be easily made to preserve high-order accuracy for nonlinear problems by applying economical high-order flux reconstruction techniques \cite{13}. In the following sections, we will demonstrate that the developed schemes do indeed serve as very low-dissipation/dispersion schemes for strongly nonlinear problems with shock waves.

4.2. One-dimensional Euler equations

In this subsection, we consider the test cases for the one-dimensional Euler equations.

Example 4.2. Shock tube problems

The two shock-tube problems proposed by Sod \cite{38} and Lax \cite{39}, are solved by the proposed schemes, IG6MP and IG4MP. The solutions are obtained by setting the specific heat ratio to be $\gamma = 1.4$, and are compared with that of results from exact Riemann solver \cite{40}. The initial conditions for the Sod test case and the Lax problem are given by the following initial conditions (57), and (58), respectively.

\[
(\rho, u, p) = \begin{cases} (0.125, 0, 0.1), & 0 < x < 0.5, \\ (1, 0, 1), & 0.5 \leq x < 1, \end{cases} \quad (57)
\]

\[
(\rho, u, p) = \begin{cases} (0.445, 0.698, 3.528), & 0 < x < 0.5, \\ (0.5, 0, 0.571), & 0.5 \leq x < 1. \end{cases} \quad (58)
\]

First, the Sod test case is used to assess the shock-capturing ability of the scheme. The initial condition is evolved for time $t = 0.2$, and the solution is shown for 200 cells. Fig. 3 shows the density and velocity profiles for both the proposed schemes, and the HOCUS5 scheme. The solutions by all the schemes are in good agreement with the exact solution in addition to the absence of overshoots in regions of discontinuities.

![Figure 3: Numerical solution for Sod problem in Example 4.2 for $N = 200$ points, where dashed line: reference solution; green stars: IG6MP; blue squares: IG4MP; red circles: HOCUS5.](image)

Second, we used 200 cells for the Lax problem, and the solution is obtained at time $t = 0.14$. Fig. 4 presents the density and velocity of the new schemes and the HOCUS5 scheme. The IG4MP scheme resolves well the features of the flow while avoiding oscillations.
Figure 4: Numerical solution for Lax problem in Example 4.2 for $N = 200$ cells, where dashed line: reference solution; green stars: IG6MP; blue squares: IG4MP; red circles: HOCUS5.

Example 4.3. Shu-Osher problem

Third, we consider the Shu-Osher problem [41], which is a one-dimensional idealization of shock-turbulence interaction, that simulates the interaction of a right moving shock wave for a given Mach number ($M = 3$) superimposed with a perturbed density field. The initial condition for this problem are

$$(\rho, u, p) = \begin{cases} 
(3.857143, 2.629369, 10.3333), & -5 < x < -4, \\
(1 + 0.2\sin(5x), 0, 1), & -4 \leq x < 5.
\end{cases} \quad (59)$$

The solution is obtained for a time $t = 1.8$ for two different grids of 150 and 300 cells. The reference solution is obtained using the WENOZ scheme [42] on a fine grid of 1600 cells. The solution for density profile is shown in Fig. 5. It is observed that both IGMP schemes perform well in capturing the post-shock oscillations in density. Notably, both the proposed schemes capture the peaks and troughs of the density very well and better than the HOCUS5 scheme.
**Example 4.4.** *Blast wave problem*

In this one-dimensional test case, we consider the blast wave problem by [43]. This problem simulates the interaction of two blast waves with reflective boundaries on both ends of the domain. The initial condition is given by equation (60). The simulation is performed for a time of $t = 0.038$, on a grid size of 800 cells. The exact solution is obtained by the WENOZ scheme on a fine grid of 1600 points. From Fig. 6, it can be observed that both the schemes perform well compared to the HOCUS5 solution, particularly in capturing the peak density profile.

$$\begin{align*}
(\rho, u, p) &= \begin{cases}
(1.0, 0.0, 1000) & 0.0 < x < 0.1, \\
(1.0, 0.0, 0.01) & 0.1 < x < 0.9, \\
(1.0, 0.0, 100) & 0.9 < x < 1.0.
\end{cases}
\end{align*}$$

(60)
Example 4.5. *Titarev-Toro problem*

The last one-dimensional test case we consider is the shock-entropy wave problem of Titarev-Toro [33]. In this test, a high-frequency sinusoidal wave interacts with a shock wave. The test case reflects the ability of the scheme to capture the extremely high-frequency waves. The initial conditions are given by equation (61) on a domain of $[-5,5]$,

$$(\rho, u, p) = \begin{cases} (1.515695, 0.523326, 1.805), & x < -4.5, \\ (1 + 0.1 \sin(20\pi x), 0, 1), & x \geq -4.5. \end{cases} \quad (61)$$

We used 1000 cells to simulate the problem for time $t = 5$, and compared with the reference solution obtained from a WENOZ simulation on a fine grid size of 3000 cells. The results obtained presented in Fig. 7 indicate that both the schemes can accurately capture the high-frequency wave. Specifically, we observe that the IGMP schemes capture the linear region significantly better than the HOCUS5 scheme.

4.3. *Multi-dimensional test cases for Euler equations*

In this section, we present the numerical results of the proposed method for multi-dimensional test cases.
Example 4.6. 2D shock-entropy wave test

In this test case we consider the two-dimensional shock-entropy wave interaction problem proposed in [44]. The initial conditions for the test case are as follows,

\[
\begin{align*}
(\rho, u, v, p) = & \begin{cases} 
(3.857143, 2.629369, 0, 10.3333), & x \leq -4, \\
(1 + 0.2 \sin(10x \cos \theta + 10y \sin \theta), 0, 0, 1), & \text{otherwise},
\end{cases}
\end{align*}
\]

with \( \theta = \pi/6 \) over a domain of \([-5, 5] \times [-1, 1]\). The initial sine waves make an angle of \( \theta \) radians with the \( x \) axis. Initial conditions are modified as in [45] with a higher frequency for the initial sine waves compared to that of [44] to show the benefits of the proposed method. Mesh size of \( 400 \times 80 \) is chosen and the flow is developed for time \( t = 1.8 \). The reference solution is computed on a fine mesh of \( 1600 \times 320 \) by using the WENOZ scheme. Density contour plots shown in Fig. 8 indicate that the proposed schemes significantly improve the resolution of the flow structures. The local density profile along \( y = 0 \) is presented in Fig. 8(d). The results demonstrate that IG6MP and IG4MP retain the desirable shock-capturing features in the MP5 scheme while capturing the high-frequency region better than the HOCUS5 scheme.

Example 4.7. Riemann Problem

In this test case we consider the Riemann problem of [46] described as configuration 3. The initial conditions of the problem are given by equation (63) with constant states of the primitive variables along the lines \( x = 0.8 \), and \( y = 0.8 \) in the domain \( x, y \in [0, 1] \). This produces four shocks at the interfaces of the four quadrants. Also, the small-scale complex structures generated along the slip-lines due to the Kevin-Helmholtz instabilities serve to assess the numerical dissipation of the scheme. Non-reflective boundary conditions are employed on all four boundaries. The test case is run for a time \( t = 0.8 \) on a grid of size \( 400 \times 400 \).

\[
\begin{align*}
(\rho, u, v, p) = & \begin{cases} 
(1.5, 0, 0, 1.5), & \text{if } x > 0.8, \ y > 0.8, \\
(33/62, 4/\sqrt{11}, 0, 0.3), & \text{if } x \leq 0.8, \ y > 0.8, \\
(77/558, 4/\sqrt{11}, 4/\sqrt{11}, 9/310), & \text{if } x \leq 0.8, \ y \leq 0.8, \\
(33/62, 0, 4/\sqrt{11}, 0.3), & \text{if } x > 0.8, \ y \leq 0.8.
\end{cases}
\end{align*}
\]
The results are presented for the IG6MP and the IG4MP schemes, and the density contours are presented in Fig. 9. The proposed schemes resolve better rollup behaviour along the slip lines compared to the HOCUS5 scheme. This richness of the fine structures indicate low numerical dissipation features for both the proposed schemes. Specifically, the guitar-like shape of the jet is well captured.

![Density Contours](image)

**Figure 9:** Density contours of the Riemann problem in Example 4.7 for different schemes on a grid size of 400 × 400.

**Example 4.8. Rayleigh-Taylor instability**

Rayleigh-Taylor instability occurs at the interface between fluids with different densities when acceleration is directed from the heavy fluid to the light one. In this test case, two initial gas layers with different densities are subjected to unit magnitude’s gravity, where the resulting acceleration is directed towards the lighter fluid. A small disturbance of the contact line triggers the instability. This problem has been extensively studied using high order shock-capturing schemes in the literature, see, e.g. [47], with the following initial conditions,

\[
(\rho, u, v, p) = \begin{cases} 
(2.0, 0, -0.025 \sqrt{\frac{5\rho}{4\pi}} \cos(8\pi x), 2y + 1.00), & 0 \leq y < 0.5, \\
(1.0, 0, -0.025 \sqrt{\frac{5\rho}{4\pi}} \cos(8\pi x), 1y + 3/2), & 0.5 \leq y \leq 1.0,
\end{cases}
\]

over the computational domain [0, 1/4] × [0, 1]. Reflective boundary conditions are imposed on the right and left boundaries via ghost cells. The flow conditions are set to \(\rho = 1\), \(p = 2.5\), and \(u = v = 0\) on top boundary.
and $\rho = 2$, $p = 1.0$, and $u = v = 0$ on bottom boundary with the specific heat ratio, $\gamma$, of 5/3. The source term $S = (0, 0, \rho, \rho v)$ is added to the Euler equations. We performed simulations on a uniform mesh of resolution $120 \times 480$ and the computations are conducted until $t = 1.95$.

![Density contours](image)

Fig. 10 shows the density distribution of the Rayleigh-Taylor instability problem. We can observe that the implicit gradient schemes produced more small vortices in the shear layer, indicating that they have better resolution to capture small scale features of the flow.

**Example 4.9. Kelvin Helmholtz instability**

The Kelvin-Helmholtz (KH) instability occurs where there is a velocity difference across the interface between two fluids, and it plays an important role in the evolution of the mixing layer and the transition to turbulence. Consider the following initial conditions over a periodic domain of $[0, 1] \times [0, 1]$,

\[
\begin{align*}
p &= 2.5, \\
\rho(x,y) &= \begin{cases} 
2, & \text{if } 0.25 < y \leq 0.75, \\
1, & \text{else,}
\end{cases} \\
u(x,y) &= \begin{cases} 
0.5, & \text{if } 0.25 < y \leq 0.75, \\
-0.5, & \text{else.}
\end{cases} \\
v(x,y) &= 0.1 \sin(4\pi x) \left\{ \exp \left[ -\frac{(y-0.75)^2}{2\sigma^2} \right] + \exp \left[ -\frac{(y-0.25)^2}{2\sigma^2} \right] \right\}, \text{ where } \sigma = 0.05/\sqrt{2}. \tag{65}
\end{align*}
\]

The computational domain is discretized with 512 cells in each direction, and the final time is taken to be $t = 0.8$. The numerical solutions are computed using the IGMP schemes are depicted in Fig. 19. We can observe that the IGMP schemes capture complex structures and small-scale vortices.
Figure 11: Numerical results of Kelvin-Helmholtz instability test case, Example 4.9, by different schemes on a grid size of 512 × 512.

**Example 4.10. Double Mach reflection**

Next, we consider the double-Mach reflection problem proposed by [43], and is typically used to test resolution capability of numerical schemes. In this test case, an unsteady planar shock-wave of Mach 10 impinges on an inclined surface of 30 degrees to the horizontal axis. This inclined surface is simplified by tilting the shock-wave to avoid modelling the oblique no-slip physical wall boundary. The near-wall jet structure and the vortex structures appearing from the contact discontinuity that emerges from the triple-point indicate the proposed scheme’s numerical dissipation. Post-shock flow conditions are set at the left boundary, and zero gradient conditions are applied at the right boundary. At the bottom boundary, reflecting boundary conditions are applied at the upper at $y = 1$ and is time-dependent. The computational domain is taken as $x \in [0, 3], y \in [0, 1]$ and the simulation is performed for time $t = 0.2$ on a grid of $768 \times 256$ cells.

\[
(\rho, u, v, p) = \begin{cases} 
(8, 8.25 \cos 30^\circ, -8.25 \sin 30^\circ, 116.5), & x < 1/6 + \frac{y}{\tan 60^\circ}, \\
(1.4, 0, 0, 1), & x > 1/6 + \frac{y}{\tan 60^\circ}.
\end{cases}
\]  

(66)

Observations made from Figs. 12 and 13 indicate that the IG4MP and the IG6MP schemes have better resolution of the KH instabilities than the HOCUS5 scheme. Notably the resolution of the shear layers along the slip lines and the near-wall jet region are well resolved. It can be noted that the current IG4MP scheme is
slightly better in resolving the shear layer along the slip line than the IG6MP scheme.

Figure 12: Density contours in the blown-up region around the Mach stem for Example 4.10 on a grid size of 768 × 256.
Example 4.11. Inviscid Taylor-Green Vortex

Next, we consider the three-dimensional inviscid Taylor-Green vortex problem, with initial conditions given by equation (67) and are applied to the domain of size \( x, y, z \in [0, 2\pi) \). Periodic boundary conditions are applied for all boundaries. The ratio of the specific heats of the gas is taken as \( \gamma = 5/3 \). The simulations are performed for a time \( t = 10 \) on a grid size of \( 64 \times 64 \times 64 \).

\[
\begin{pmatrix}
\rho \\
u \\
v \\
w \\
p
\end{pmatrix} = \begin{pmatrix}
1 \\
\sin x \cos y \cos z \\
\cos x \sin y \cos z \\
0 \\
100 + \frac{(\cos (2x)+2)(\cos (2x)+\cos (2y))}{16}
\end{pmatrix}.
\tag{67}
\]

This flow problem is essentially incompressible as the mean pressure is chosen to be very large. The Taylor-Green vortex is the simplest problem for analyzing the nonlinear transfer of kinetic energy among the different scales of the flow. It contains several physical processes that are key to understanding turbulence. The vortices in the initial flow stretch and produce smaller-scale features with time. This problem can be used as a test to examine the scale-separation ability of different schemes to under-resolved flow. We compare the ability of different schemes to preserve kinetic energy and also the growth of enstrophy in time, i.e., the sum of vorticity of all the vortex structures, indicating the schemes ability to preserve as many structures as possible. The enstrophy can be described as the integral of the square of the vorticity that can be computed as the integral of the magnitude of vorticity, \( \Omega \), over the whole domain.
\[
\text{Enstrophy} = \sum_{\text{cells}} \|\vec{\omega}\| \quad (68)
\]

Fig. 14: Normalised kinetic energy and enstrophy for different schemes presented in Example 4.11 on grid size of 64\(^3\). Solid line with circles: exact solution; solid blue line: IG4; solid green line: IG6; solid cyan line: C5; dashed blue line: IG4MP; dashed green line: IG6MP; dashed red line: MP5-6E; dashed black line: MP5-4T; dashed cyan line: HOCUS5.

5. Conclusions

In this paper, linearly high-order implicit gradient schemes have been developed based on a quadratic solution reconstruction combined with implicitly computed solution derivatives. Although the developed schemes are fourth-order accurate only for linear equations and the formal order of accuracy reduces to second-order for
nonlinear equations, they still act as very low-dissipation/dispersion schemes and are capable of producing highly-resolved solutions even for problems with shock waves. Important contributions and observations of the paper are summarized as follows

1. We proposed a novel approach of computing the cell interface values for cell-centered conservative framework where the gradients of reconstruction polynomials are computed by compact finite differences. The resulting upwind schemes have superior dissipation and dispersion than the compact reconstruction approach.
2. We have shown that fourth-order accuracy can be achieved with a quadratic solution reconstruction if the derivatives are computed implicitly.
3. We demonstrated that linearly high-order schemes can still serve as very low-dissipation/dispersion schemes for highly nonlinear problems with discontinuous solutions.
4. Problem independent shock-capturing technique via the BVD algorithm gave superior results for several benchmark test cases involving shocks and small scale features.
5. Results obtained by IG4MP are superior to IG6MP scheme, even though they they share the same stencil, due its superior dispersion and dissipation properties.

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Appendix

A. Fifth-order monotonicity-preserving scheme

In this Appendix the procedure for fifth-order monotonicity-preserving scheme of [34] is documented. For brevity, we only explain the procedure for the left interface values, $U_{j+1/2}^{L,MP}$, since the right interface values, $U_{j+1/2}^{R,MP}$, can be obtained via symmetry. The steps involved are as follows.

$$U_{j+1/2}^{L,MP} = \begin{cases} U_{j+1/2}^{\text{Linear}} & \text{if } (U_{j+1/2}^{\text{Linear}} - \hat{U}_j) (U_{j+1/2}^{\text{Linear}} - U_{j+1/2}^{MP}) \leq 10^{-20}, \\ U_{j+1/2}^{\text{Nonlinear}} & \text{otherwise}, \end{cases}$$

(69)

where

$$U_{j+1/2}^{\text{Linear}} = \frac{1}{60} (2\hat{U}_{j+2} - 13\hat{U}_{j+1} + 47\hat{U}_j + 27\hat{U}_{j+1} - 3\hat{U}_{j+2}),$$

$$U_{j+1/2}^{\text{Nonlinear}} = U_{j+1/2}^{\text{Linear}} + \min\text{mod} \left( \min_{j+1/2} (U_{j+1/2}^{\text{Linear}}) - U_{j+1/2}^{\text{Linear}}, \max_{j+1/2} (U_{j+1/2}^{\text{Linear}}) - U_{j+1/2}^{\text{Linear}} \right),$$

$$U_{j+1/2}^{MP} = U_j + \min\text{mod} \left( \hat{U}_{j+1} - \hat{U}_j, \alpha \left( \hat{U}_j - \hat{U}_{j-1} \right) \right),$$

$$U_{j+1/2}^{\text{min}} = \max \left[ \min \left( \hat{U}_j, \hat{U}_{j+1} \right), \min \left( \hat{U}_j, U_{j+1/2}^{UL}, U_{j+1/2}^{LC} \right) \right],$$

$$U_{j+1/2}^{\text{max}} = \min \left[ \max \left( \hat{U}_j, \hat{U}_{j+1} \right), \max \left( \hat{U}_j, U_{j+1/2}^{UL}, U_{j+1/2}^{LC} \right) \right],$$

$$U_{j+1/2}^{MD} = \frac{1}{2} \left( \hat{U}_j + \hat{U}_{j+1} \right) - \frac{1}{2} d_{j+1/2}^{MD},$$

$$U_{j+1/2}^{UL} = \hat{U}_j + 4 \left( \hat{U}_j - \hat{U}_{j-1} \right),$$

$$U_{j+1/2}^{LC} = \frac{1}{2} \left( 3\hat{U}_j - \hat{U}_{j-1} \right) + \frac{4}{3} d_{j-1/2}^{MD},$$

$$d_{j+1/2}^{MD} = \min\text{mod} (4d_j - d_{j+1}, 4d_{j+1} - d, d_j, d_{j+1}),$$

$$d_j = \hat{U}_{j-1} - 2\hat{U}_j + \hat{U}_{j+1},$$

where

$$\min\text{mod}(a, b) = \frac{1}{2} (\text{sign}(a) + \text{sign}(b)) \min(|a|, |b|),$$

(71)

Similar to the Ref. [9] the above mentioned MP5 reconstruction involves the transforming of primitive variables into characteristic variables and readers are referred to section 2.3 in [9].

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