HYBRID COMPACT-WENO FINITE DIFFERENCE SCHEME WITH CONJUGATE FOURIER SHOCK DETECTION ALGORITHM FOR HYPERBOLIC CONSERVATION LAWS

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Abstract. For discontinuous solutions of hyperbolic conservation laws, a Hybrid scheme, based on the high order nonlinear characteristic-wise weighted essentially non-oscillatory conservative finite difference (WENO) scheme and the high resolution spectral-like linear compact finite difference (Compact) scheme, is developed for capturing shock and strong gradients accurately and resolving smooth scale structures efficiently. The key issue in any hybrid scheme is the design of an accurate, robust, and efficient high order shock detection algorithm that is capable of determining the smoothness of the solution at any given grid point. The conjugate Fourier partial sum and its derivative are investigated for its applicability as a shock detector due to its unique property, namely, the conjugate Fourier partial sum converges to the location and strength of an isolated jump. For a non-periodic problem, the data is first evenly extended before the derivative of the conjugate Fourier partial sum and its mean are computed. The mean allows one to partition the domain into subdomains containing strong gradients or smooth solutions. The locations of shocks are then accurately identified and flagged for special treatment using the WENO scheme. The matrix-matrix multiply (MXM), Even-Odd decomposition (EOD) and Cosine/Sine fast transform (CFT) algorithms of the conjugate Fourier (cF) analysis are derived, and their advantages and disadvantages in their implementations, usage and technical issues are discussed in detail. The conjugate Fourier shock detector and its iterative version for detecting jumps of large difference in scales are presented. The Hybrid-cF scheme is applied to 1D shock-density wave interaction problem, 2D Riemann IVP problems, and 2D Mach 10 double Mach reflection problems. The preliminary results are in good agreement with those obtained in the literature. They demonstrate the spatial and temporal adaptivity of the Hybrid-cF scheme for problems containing strong shocks, multiple developing shocklets, and high frequency waves. A speedup of the CPU times with factor up to 2-3 is obtained showing the potential efficiency of the Hybrid-cF scheme over the pure WENO-Z scheme.

Key words. Conjugate Fourier, WENO, Compact, Hybrid, Hyperbolic, Shock detection, Riemann

AMS subject classifications. 65P30, 77Axx

1. Introduction. The nonlinear system of hyperbolic conservation laws (PDE) can be written compactly as

\[
\frac{\partial Q}{\partial t} + \nabla \cdot F(Q) = 0,
\]

where \(Q\) and \(F(Q)\) are the conservative variables and flux respectively, together with appropriate initial conditions and boundary conditions in a Cartesian domain. It is well-known that the solution of (1.1) can develop finite time singularities, such as shocks, contact waves and rarefaction waves, at some later time even if the solution is a smooth function initially. The solution of such nonlinear system could also create

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both fine complex smooth and large strong gradient flow structures dynamically in space and time.

Characteristic-wise Weighted Essentially Non-Oscillatory conservative finite difference (WENO) nonlinear schemes on an equidistant stencil, as a class of high order/high resolution nonlinear scheme for solutions of hyperbolic conservation laws in the presence of shocks and small scale structures, was initially developed by [19] (for details and history of WENO scheme, see [2, 3, 33] and references therein). However, there are certain disadvantages of using WENO schemes for some classes of hyperbolic conservation laws. The WENO scheme is fairly complex to implement and computationally expensive. In order to guarantee essentially non-oscillatory capturing of shocks and resolving high gradient structures, the scheme requires the setup of the Roe-averaged eigensystem, the positive and negative splitting of the fluxes, the forward and backward projections of split fluxes between the characteristic and physical spaces, the computation of the smoothness indicators and nonlinear weights for each projected flux. (Parallel implementation of the WENO scheme will certainly help in reducing the overall CPU time.) These steps make the WENO scheme at least four to five times more expensive than other nonlinear shock capturing schemes (for example, TVD, PPM). In addition, the WENO scheme is, in general, too dissipative for certain classes of problems (for example, compressible turbulence) [18, 20] and has limited its wider adoption in its pure form.

A natural remedy to alleviate some of these difficulties is to use a linear scheme in place of the nonlinear WENO scheme in smooth regions of the solution wherever possible. Some often used linear schemes are the central scheme (CFD) [5, 11] that has a strong dispersive error, the bandwidth optimized central scheme (BFD) that increases the resolution at a cost of a reduced order of accuracy, and the compact scheme (Compact) that requires solving a system of banded matrix equations [1, 31]. Therefore, a spatial and temporal switching between a WENO scheme for non-smooth stencils and a linear scheme for smooth stencils (hybridization) must be designed by employing a measure of smoothness of the solution at each grid point and time. In the last two decades, many shock detection methods have been developed. Li et al. [26, 27] showed the comparison among several different low order smoothness indicators used in a hybrid upwind-WENO scheme for solving hyperbolic conservation laws and shallow water equations. Costa et al. [5, 6] described the arbitrary order multi-resolution (MR) analysis by Harten [17] for identifying the non-smooth and smooth stencils. In general, high order MR analysis is preferable to a low order shock detector in the high order hybrid scheme for its efficiency (with its \(O(N)\) floating point operations count) and much improved resolving power in differentiating high frequency waves and discontinuities.

By treating a discontinuity as an edge of an object in an image, tools for edge detection in image processing can be directly applied as well. In [12] and their later works, Gelb et al. described the theoretical justification and an algorithm, based on the conjugate Fourier partial sum with concentration factors, for edge detection of a piecewise smooth function given its Fourier coefficients.

In a limit, the conjugate Fourier partial sum converges to the associated jump function\(^1\) at a rate of \(O(1/\log N)\), where \(N\) is the number of Fourier modes. A few numerical techniques, such as modifying the concentration factor and nonlinear enhancement procedures, were developed to accelerate the convergence rate, to re-

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\(^1\)The jump function (defined formally in Lemma 2.1) is identically zero everywhere, except at discontinuity locations, where it is equal to the jump height.
move oscillations, and to recover edges in a piecewise smooth function [12, 14]. The method has also been applied to solving 1D Euler equations using a Legendre collocation method with (adaptive) spectral vanishing viscosity [13, 36]. Jung et al. [21] deployed an iterative algorithm based on the modification of the scaling coefficient $\epsilon$ in the multiquadric radial basis functions to approximate a piecewise discontinuous function, thus avoiding the Gibbs phenomenon. To our knowledge, the methods described above are mainly used in the detection of edges and none other than the high order MR algorithm has been applied in solving hyperbolic conservation laws with hybrid schemes. In this study, we will investigate the applicability of the conjugate Fourier (cF) method as the shock detector in the high order hybrid Compact-WENO scheme for solving hyperbolic PDEs and discuss its accuracy, efficiency and other implementation issues. The algorithmic implementation of the conjugate Fourier method (matrix-multiply algorithm (MXM), Even-odd decomposition algorithm (EOD) and Cosine/Sine fast transform algorithm (CFT)) and an effective strategy that works in partitioning the domain and detecting edges are given in detail. Numerical examples of one-dimensional extended shock-density wave interaction problem, two-dimensional Riemann initial value problems and Mach 10 double Mach reflection problems are presented. This study shows the potential of the cF method and can spur further development of these techniques in the hybrid scheme for high speed shocked flows.

This paper is organized as follows. In Section 2, we briefly review the conjugate Fourier method and describe the conjugate Fourier edge detection algorithm in detail. Examples are given for edge detection of the Shepp-Logan phantom image and the efficiency of various conjugate Fourier algorithms are presented. In Section 3, the one-dimensional and two-dimensional shocked problems are simulated to investigate the performance (accuracy and speed) of the Hybrid-cF schemes. Concluding remarks are given in Section 4.

2. Hybrid Scheme. In this study, an improved fifth order characteristic-wise weighted essentially non-oscillatory conservative finite difference nonlinear scheme (WENO-Z) and a high order spectral like compact linear scheme (Compact) are employed for solutions of multi-dimensional system of hyperbolic conservation laws in the Cartesian domain discretized with an uniformly spaced grid.

For the fifth order WENO-Z5 finite difference nonlinear scheme used here, we take the sensitivity parameter $\epsilon = \Delta x^4$ with power parameter $p = 2$ [7]. For the sixth order compact finite difference linear scheme, see [25] for details. We should noted that the derivative of fluxes at the boundary for the boundary closure of the Compact scheme is computed via the WENO-Z5 scheme. The temporal scheme is the third order TVD Runge-Kutta scheme [33]. Readers are referred to [2, 3, 25, 33] and references therein for further details regarding their algorithmic implementations.

The key issue in any spatially adaptive scheme is how to quantify the smoothness of a numerical solution at each uniformly spaced grid point $x_i$. Since both the Compact scheme and the WENO scheme are high order/resolution schemes, the measure of the smoothness of the solution must also be of high order in order to differentiate a high frequency wave from a high gradient/shock. The high order information obtained allows one to apply an appropriate numerical spatial scheme (such as the Compact scheme for high-frequency waves and the WENO scheme for shocks) adaptively at a given spatial location $x$ and dynamically at a given time $t$.

Two high order shock detection algorithms on a uniform grid are considered, namely,

- the Lagrangian polynomial based multi-resolution (MR) analysis; and
the trigonometric polynomial based conjugate Fourier (cF) analysis.

The Lagrangian polynomial based multi-resolution (MR) analysis [17] has been extensively studied and successfully applied to the Hybrid schemes [5, 6]. The high order trigonometric polynomial based conjugate Fourier (cF) analysis together with a high order concentration factor has been used for detection of discontinuities in functions and edges in images [12, 14, 15, 35] but seldom used in the context of numerical PDE. In [15], theoretical development of the shock detection using continuous and discrete conjugate Fourier series was reviewed in detail. Below, we will briefly introduce the idea of conjugate Fourier analysis and then develop a shock detector to identify shocks and discontinuities in the solution of hyperbolic PDE. Readers are referred to [9, 10, 29] for the detailed theory of the conjugate Fourier series.

2.1. Conjugate Fourier (cF) Analysis. A truncated Fourier series expansion of a \(2\pi\)-periodic function \(f(x) \in L^2[0, 2\pi]\) with \(2N + 1\) terms is

\[
f_N(x) = \frac{1}{2} a_0 + \sum_{k=1}^{N} (a_k \cos kx + b_k \sin kx),
\]

where the Fourier coefficients \(a_k\) and \(b_k\) are defined as

\[
a_k = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \cos kx \, dx, \quad b_k = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \sin kx \, dx,
\]

respectively, and its corresponding conjugate Fourier series is

\[
\tilde{f}_N(x) = \sum_{k=1}^{N} (a_k \sin kx - b_k \cos kx).
\]

They are the Fourier partial sum and conjugate Fourier partial sum, or simply Fourier and conjugate Fourier, respectively, for short when their meanings are clear in the context of the statement.

It is well-known that the finite sum of the Fourier series in the Fourier expansion of a piecewise smooth function generates \(O(1)\) numerical oscillations in the neighborhood of a discontinuity (Gibbs phenomenon). The \(\approx 8.9\%\) overshoot and undershoot of the jump do not decay even as the number of Fourier modes \(N\) increases. The numerical oscillations often destabilize numerical schemes for solving a time-dependent hyperbolic PDE and reduce the high order scheme to first order at most. There were many past studies in post-processing the oscillatory data to recover spectral accuracy of the solution when solved with spectral methods (see [16, 24] and website\(^2\) for research that has been done in the past decades.) with some degree of success. For the Hybrid scheme we are developing, our goal is to treat the discontinuities as edges and to design a simple yet effective procedure to detect and to identify discontinuities, including discontinuities in its first derivative, using the conjugate Fourier and/or its derivative.

The key aspect of the procedure lies in the relationship between the conjugate Fourier and the location and jump of a discontinuity. We recall the support of the conjugate Fourier \(\tilde{f}_N(x)\) (2.3) approaches the singular support of a piecewise smooth function \(f(x)\) as \(N \to \infty\) as shown in the following lemma [12].

\(^2\)http://www.cscamm.umd.edu/people/faculty/tadmor/Gibbs\_phenomenon/
**Lemma 2.1.** Let $f(x)$ be a $2\pi$-periodic piecewise smooth function, except at a single jump discontinuity at $x = \xi$ with an associated jump

$$[f](\xi) := f(\xi^+) - f(\xi^-).$$  \hfill (2.4)

Then

$$-\pi \log N \tilde{f}_N(x) \to [f](x)\delta_\xi(x) = \begin{cases} [f](\xi), & x = \xi, \\ 0, & \text{otherwise}, \end{cases}$$  \hfill (2.5)

where $\delta_\xi$ is the Dirac distribution located at $\xi$.

This is known as the concentration property of $\tilde{f}_N(x)$. Readers are referred to [12] for details of the proof. It can be seen in Lemma 2.1 that the convergence rate is only $O(1/\log N)$. The convergence rate can be increased to $O(\log N/\log N)$ [12] and faster in smooth regions away from discontinuities using a high order admissible concentration factor. A low pass filter and a minmod algorithm can be added to the conjugate Fourier together with a concentration factor to suppress oscillations near a jump and away in smooth regions, and that significantly reduces the chance of false identification of a discontinuity near a jump at an expense of enlarging the support around it.

In this work, we employ the hybrid finite difference scheme in solving the hyperbolic conservation laws on a uniformly spaced grid. The continuous Fourier coefficients will be approximated by the discrete Fourier coefficients with the data being sampled on a uniformly spaced grid domain with grid spacing $\Delta x$ using $N + 1$ grid points (see below). For simplicity, we shall use the same notations $a_k$ and $b_k$ as the discrete Fourier coefficients in the following discussion.

For problems containing high frequency waves and shocks, a high-pass filter will be employed to maintain the effectiveness of the conjugate Fourier shock detection algorithm (see below). The variable-order high-pass Exponential filter

$$\sigma_k = \begin{cases} 1 - \exp \left(-\alpha \frac{k - k_0}{N - k_0} \right), & |k| > k_0, \\ 0, & |k| \leq k_0, \end{cases}$$  \hfill (2.6)

where $k_0 = 0$ is the cutoff wave number, $\alpha = -\ln \varepsilon$ such that $\sigma_N = 1 - \varepsilon$ (typically, $\varepsilon = 10^{-16}$ is the machine zero), and $\gamma = 16$ is the order of the filter. Note that, if no high-pass filter is used, $\sigma_k = 1$. A high-pass filter removes waves with low- and mid-frequency from the data while keeping all the high frequency waves mostly intact. With a carefully chosen filter order $\gamma$, the filter will reduce the shock strength slightly, but it will not affect the location of the shocks. In practice, we find that it is more convenient and effective in detecting a location of a jump discontinuity of a function and its first and higher derivatives by using the derivative of the conjugate Fourier,

$$\hat{f}_N(x) = (\tilde{f}_N)'(x) = \sum_{k=1}^{N} k(a_k \cos kx + b_k \sin kx).$$  \hfill (2.7)

Together with a high-pass filter, one has the final form

$$\tilde{f}_N(x) = \sum_{k=1}^{N} \tilde{\tau}_k(a_k \sin kx - b_k \cos kx), \quad \tilde{\tau}_k = \sigma_k S_k,$$  \hfill (2.8)

$$\hat{f}_N(x) = \sum_{k=1}^{N} \hat{\tau}_k(a_k \cos kx + b_k \sin kx), \quad \hat{\tau}_k = k\sigma_k S_k,$$  \hfill (2.9)
where $S_k = \sin \left( \frac{k \Delta x}{2} \right) / \left( \frac{k \Delta x}{2} \right)$, and $\tilde{\tau}_k$ and $\hat{\tau}_k$ are the concentration factors using the notation of Gelb and Tadmor [12]. An example of the conjugate Fourier $\tilde{f}_N(x)$ and its derivative $\hat{f}_N(x)$ of a square function $f(x)$ with increasing resolution $N = 20, 40, 80$ is shown in Fig. 2.1. The locations and jumps of the discontinuities of the square function are well captured and estimated with high accuracy. In this work,

**Fig. 2.1.** (Left) The square function $f(x_i)$, (Middle) its conjugate Fourier $\tilde{f}_N(x_i)$ and (Right) its derivative of conjugate Fourier $\hat{f}_N(x_i)$ with $N = 20, 40, 80$.

we are concerned mainly about obtaining an accurate location of high gradients and discontinuities so that the WENO reconstruction procedure can capture shocks in an essentially non-oscillatory manner. Unless noted otherwise, we will only employ the high-pass filter $\sigma_k$ when it is absolutely needed.

When solving PDE, the solutions are often non-periodic in space. In order to apply the conjugate Fourier shock detection algorithm as described below to such data, we first perform an even extension of the solution. In this case, the odd discrete Fourier coefficients are identically equal to zero, that is, $b_k = 0$, due to the even symmetric property of the extended solution in an evenly extended domain. As a result, we will only need the even discrete Fourier coefficients $a_k$ in computing the discrete conjugate Fourier and/or its derivative, which can be computed using either the Matrix-Matrix Multiply (MXM), Even-Odd Decomposition (EOD) or Cosine/Sine Fast Transform (CFT) algorithms, as described below.

**2.1.1. Matrix-Matrix Multiply (MXM) Algorithm.** The discrete Fourier coefficient $a_k$, with the data $f_i = f(x_i)$ sampled at the Fourier Gauss-Lobatto collocation points $x_i = \pi i/N$, $i = 0, \ldots, N$, becomes,

$$a_k = \frac{2}{N c_k} \sum_{j=0}^{N} \frac{1}{c_j} f_j \cos k x_j, \quad \text{(2.10)}$$

where $c_j = 1, j = 1, \ldots, N - 1$ and $c_0 = c_N = 2$. By substituting (2.10) into (2.3) and (2.9), one has

$$\tilde{f}_N = S \vec{f}, \quad \hat{f}_N = D \vec{f}, \quad \text{(2.11)}$$

where $\vec{f}$ is a vector of length $N + 1$ with elements $f_i$, and the elements of the $(N + 1) \times (N + 1)$ matrices $S$ and $D$ are, respectively,

$$S_{i,j} = \frac{2}{N c_j} \sum_{k=1}^{N} \frac{\tilde{\tau}_k}{c_k} \cos(k x_j) \sin(k x_i), \quad D_{i,j} = \frac{2}{N c_j} \sum_{k=1}^{N} \frac{\hat{\tau}_k}{c_k} \cos(k x_j) \cos(k x_i). \quad \text{(2.12)}$$
This approach, with $O(N^2)$ floating point operations, is called the Matrix-Multiply algorithm (MXM) and can be represented graphically as

$$
\vec{f} \rightarrow \vec{S} \rightarrow \vec{f}_N, \quad \vec{f} \rightarrow \vec{D} \rightarrow \vec{f}_N. \quad (2.13)
$$

### 2.1.2. Even-Odd Decomposition (EOD) Algorithm

It is easy to see that $\mathbf{S}$ (or $\mathbf{D}$) is a centro-anti-symmetric (centro-symmetric) matrix with $S_{i,j} = -S_{N-i,N-j}$ ($D_{i,j} = D_{N-i,N-j}$). By exploiting the centro-anti-symmetric properties of $\mathbf{S}$, we can devise an efficient algorithm known as the Even-Odd Decomposition (EOD) algorithm [8, 34] to reduce the floating point operations count by nearly half, thus speeding up the CPU computation time by up to 35% when compared with the MXM algorithm.

Assuming that $N$ is even, for $i, j = 0, \ldots, N/2$, one has

$$
\hat{f}_N(x_i) = \sum_{j=0}^{N/2-1} (D_{i,j} + D_{i,N-j}) e_j + \sum_{j=0}^{N/2-1} (D_{i,j} - D_{i,N-j}) o_j + D_{i,N/2} e_{N/2}, \quad (2.14)
$$

where the even $e_j$ and odd $o_j$ functions are defined as

$$
e_j = \frac{f_j + f_{N-j}}{2}, \quad o_j = \frac{f_j - f_{N-j}}{2}, \quad j = 0, \ldots, N/2, \quad (2.15)
$$

respectively. By defining two smaller even $\mathbf{E}$ and odd $\mathbf{O}$ matrices of size $(N/2 + 1) \times (N/2 + 1)$, with elements,

$$
E_{i,j} = \begin{cases} 
D_{i,j} + D_{i,N-j}, & \text{if } j = 0, \ldots, N/2 - 1, \\
D_{i,N/2}, & \text{if } j = N/2,
\end{cases}
\quad O_{i,j} = \begin{cases} 
D_{i,j} - D_{i,N-j}, & \text{if } j = 0, \ldots, N/2 - 1, \\
0, & \text{if } j = N/2.
\end{cases} \quad (2.16)
$$

(2.14) can be written compactly as

$$
\hat{f}_N(x_i) = \mathbf{E} \vec{e} + \mathbf{O} \vec{o}, \quad i = 0, \ldots, N/2, \quad (2.17)
$$

$$
\hat{f}_N(x_i) = \mathbf{E} \vec{e} - \mathbf{O} \vec{o}, \quad i = N/2, \ldots, N. \quad (2.18)
$$

A similar procedure can be devised for odd $N$ (see [4]) and for computing the conjugate Fourier of a function.

This approach, with $O(N + N^2/2)$ floating point operations, is called Even-Odd Decomposition (EOD) algorithm and can be represented graphically as

$$
\vec{f} \rightarrow \left\{ \begin{array}{c}
\vec{e} \rightarrow \mathbf{E} \vec{e} \\
\vec{o} \rightarrow \mathbf{O} \vec{o}
\end{array} \right\} \rightarrow \hat{f}_N, \quad \vec{f} \rightarrow \left\{ \begin{array}{c}
\vec{e} \rightarrow \mathbf{E} \vec{e} \\
\vec{o} \rightarrow \mathbf{O} \vec{o}
\end{array} \right\} \rightarrow \hat{f}_N. \quad (2.19)
$$

### 2.1.3. Cosine/Sine Fast Transform (CFT) Algorithm

For a large number of grid points $N$ as often needed in numerical PDE, both the MXM and EOD algorithms are not only computationally expensive in setting up the matrices and require a large amount of memory for storing the large matrices but also slow in computing the conjugate Fourier and/or its derivative. A more efficient algorithm can be developed by recognizing that both conjugate Fourier $\hat{f}_N$ and its derivative $\hat{f}_N$ can be computed via cosine (sine) Fast Transform algorithm (CFT) [8], which would result in a substantial saving in CPU time for sufficiently large $N$. Recalling that, given a data vector $\vec{f}$ with length $N + 1$, the discrete even Fourier coefficients

$$
a_k = \frac{2}{N c_k} \sum_{j=0}^{N} e_j f_j \cos k x_j, \quad (2.20)
$$
with \( c_j = 1, j = 1, \ldots, N - 1 \) and \( c_0 = c_N = 2 \), can be computed efficiently by the cosine fast transform algorithm, provided that the transform length \( N \) consists of a product of small prime numbers raised to some powers (for example, \( N = 2^{k_1}3^{k_2}5^{k_3}7^{k_4} \cdots \)), and is most efficient if \( N = 2^{k_1} \). Next, the Fourier coefficients \( a_k \) are modified by \( \tilde{\tau}_k \) (\( \hat{\tau}_k \)) to obtain the modified Fourier coefficients, for example, \( \tilde{a}_k = \tilde{\tau}_k a_k \) (\( \hat{a}_k = \hat{\tau}_k a_k \)). Finally, \( \tilde{f}_N \) (\( \hat{f}_N \)) can be found by the inverse sine (cosine) fast transforms SFT (CFT) with coefficients \( \tilde{a}_k \) (\( \hat{a}_k \)).

This approach, with \( O(5N \log N) \) floating point operations, is called Cosine/Sine fast transform (CFT) algorithm and can be represented graphically as

\[
\begin{align*}
\tilde{f} & \xrightarrow{\text{CFT}} a_k \times \tilde{\tau}_k \xrightarrow{\text{Inverse SFT}} \tilde{f}_N, \\
\hat{f} & \xrightarrow{\text{CFT}} a_k \times \hat{\tau}_k \xrightarrow{\text{Inverse CFT}} \hat{f}_N.
\end{align*}
\]  

(2.21)  

(2.22)

**Fig. 2.2.** The CPU timings (in seconds) of the conjugate Fourier analysis with the MXM, EOD and CFT algorithms as a function of number of grid points \( N \).

The CPU timings (in seconds) of the conjugate Fourier analysis with the MXM, EOD and CFT algorithms as a function of grid points (resolution) \( N \) are shown in Fig. 2.2. For small \( N < 256 \), all three algorithms spend almost the same amount of CPU time with the CFT algorithm being the fastest among them. For large \( N > 256 \), the CPU times consumed by the MXM and EOD algorithms grow like \( O(N^2) \) with the EOD algorithm being the faster between them. The CPU timing of the CFT algorithm, on the other hand, grows like \( O(N \log N) \) and is substantially smaller than the CPU timing of both the MXM and EOD algorithms. Hence, the CFT algorithm, though complex in its implementation, is most efficient and recommended for large scale computing.

**2.1.4. Remarks, Comments And Cautions.** Before we proceed to describe the conjugate Fourier shock detection algorithm, we offer the following remarks regarding the algorithms and their applicability.

**Remark 2.2.** The MXM algorithm is most straightforward to implement, while the EOD algorithm is only slightly more complicated. The CFT algorithm, requires the most programming effort and the use of an optimized fast Fourier transform (FFT) library. For a casual user of the conjugate Fourier analysis and/or a small problem size \( N \), the MXM algorithm is probably the best choice for the ease of programming and prototyping. Otherwise, the CFT algorithm probably is preferred if efficiency and
speed of computing are an issue.

Remark 2.3. The MXM and EOD algorithms have flexibility that allows one to compute the conjugate Fourier or its derivative at any given grid point, while the CFT algorithm requires one to compute the conjugate Fourier and/or its derivative at all \( N + 1 \) grid points all at once.

Remark 2.4. Both MXM and EOD algorithms employ the BLAS 3 level subroutine \texttt{DGEMM} to perform the matrix-matrix multiply operation, while the CFT algorithm uses the vectorized version of the fast Fourier transform package \texttt{VFFTPack} written by P. N. Swarztrauber of NCAR. These subroutines as well as the compact scheme, the WENO scheme, the conjugate Fourier analysis, and the multi-resolution analysis are all included in the high performance software library HOPEpack developed by W. S. Don and his collaborators.

Furthermore, all the computations presented in this study are performed on a desktop computer with 8 cores i7-2600 processor and 8 GB memory running under the redhat Linux operating system.

Remark 2.5. As a programming note, unless \( N \) or high-pass filter changes, the matrices \( S \) and \( D \) of the MXM algorithm (\( E \) and \( O \) of the EOD algorithm) can be computed once and stored for later use. Otherwise, these matrices must be recomputed before their use.

Remark 2.6. A major caveat of an even extension of an arbitrary non-periodic function, for example, a linear function, is that the first or higher derivatives of the function at the boundary might not be continuous in an evenly extended domain. The derivative of the conjugate Fourier at the boundary, though small, will not be zero, even if the function is smooth. This might cause the conjugate Fourier shock detection algorithm to mis-classify the boundary point as a non-smooth stencil (depending on some user defined parameters). To remedy this scenario, for example, in a domain \([x_{00}, x_{01}] \times [y_{00}, y_{01}]\), one can first pre-process the data by subtracting a bilinear interpolation polynomial,

\[
s = \frac{(x - x_{00})}{(x_{01} - x_{00})}, \quad t = \frac{(y - y_{00})}{(y_{01} - y_{00})},
\]

\[
g(x, y) = (1 - t)(1 - s)f_{00} + (1 - t)sf_{01} + t(1 - s)f_{10} + stf_{11},
\]

where \( x_{ij}, y_{ij} \) and \( f_{ij} \) are the four corner coordinates of the original domain and their function values, before activating the conjugate Fourier shock detection algorithm. The regularity of the boundary can be further increased by using interpolation polynomial with higher degree of smoothness, for example, a bicubic-spline.

In the Hybrid Compact-WENO scheme, the derivative of the fluxes at boundary points are computed by the WENO scheme regardless of the smoothness of the boundary points. So an even extension of the solution does not pose a challenge for the problems we have tested. In a more general case, one can always require the numerical flux at the boundary points of the domain be computed by the WENO scheme regardless of its smoothness to avoid this issue at the expense of a slightly increased computational time.

Remark 2.7. Since we are mostly interested in solving large scale time dependent hyperbolic PDE which calls for the conjugate Fourier edge detection algorithm at every time step, it is preferable to employ the most efficient CFT algorithm to compute the conjugate Fourier and/or its derivative in order to keep the computational overhead as small as possible.

Remark 2.8. For a periodic problem, similar to a non-periodic problem, one could easily devise the MXM, EOD and FFT algorithms for computing the conjugate
Fourier and/or its derivative and the remarks discussed above are also generally valid.

2.2. Conjugate Fourier Shock Detection Algorithm. We shall define a key parameter $F_{\text{mean}}$ and a definition that plays a major role in our conjugate Fourier shock detection algorithm.

- Knowing the derivative of the conjugate Fourier, we define its mean as
  \[
  F_{\text{mean}} = \frac{1}{N+1} \sum_{j=0}^{N} |\hat{f}_N(x_j)|. \tag{2.23}
  \]
  This is a critical quantity that will be used in partitioning the domain into subdomains containing one or more discontinuities which will be subjected to further detailed analysis.

- We shall define a set of consecutive grid points in a non-overlapping subdomain
  \[
  \Omega_n = \{x_i \mid |\hat{f}_N(x_i)| > F_{\text{mean}}, \, i = i_n, i_n + 1, ..., i_n + s, s > 1\}, \tag{2.24}
  \]
  where $n = 1, 2, \ldots$ is an integer index of the subdomain.

To develop an effective and robust shock detection algorithm, we assume that discontinuities are singular rare events (finite number of them) with a measure zero and compactly supported and the function is otherwise sufficiently smooth. As a discontinuity forms, increasing more energy is being accumulated in the high frequency range in order to maintain a steady steep slope at the jump locations where the characteristic curves are converging. The mean value $F_{\text{mean}}$ gives a measure of the average energy of the function being examined, in which the energy contributed by the discontinuities are being amortized over the whole domain. This separation of scales allows the algorithm to identify the number of discontinuities as well as the location and strength of large jumps in the function with reasonably good accuracy and efficiency, as demonstrated in the examples shown.

We will first describe a general conjugate Fourier shock detection algorithm that works well for most problems containing discontinuities with jumps of similar order of strengths. In situations where there is a large difference in the jump strength between small and large discontinuities, an iterative version of the shock detection algorithm is given and an example using the Shepp-Logan phantom image is used to demonstrate its robustness.

**Algorithm 1 (Conjugate Fourier Shock Detection Algorithm)**

1. Compute the derivative of conjugate Fourier $\hat{f}_N(x_j)$ and its mean value $F_{\text{mean}}$.
   Use either the MXM, EOD or CFT algorithms to compute $\hat{f}_N$ with either no filtering ($\sigma_k = 1$) or, if needed, the high-pass Exponential filter (2.6) to reduce the influence of the low frequency modes.

2. Normalize $\hat{f}_N(x_j)$ with its maximum absolute value $\max_l(\hat{f}_N(x_l))$.

3. Modify the subdomains $\Omega_n$ into subdomains $\Omega_{n}^{\text{mod}}$.
   By comparing $\hat{f}_N(x_j)$ with its mean value $F_{\text{mean}}$:
   \[
   I_j^* = \begin{cases} 
   1, & |\hat{f}_N(x_j)| > F_{\text{mean}} \text{ (Jump subdomain),} \\
   0, & \text{otherwise (Smooth subdomain).} \end{cases} \tag{2.25}
   \]
   In the application, a buffer zone of width $2r$ centered at each $j^*$ is created and set them all to 1. The subdomains corresponding to the index belong to $I_j^*$ form $\Omega_{n}^{\text{mod}}$. (In this study, we take $r = 3$ as $2r - 1$ is the order of the WENO scheme.)
4. Generate the WENO Flag at each grid point in the Jump subdomain. Within each \( \Omega_{n}^{\text{mod}} \), we mark the locations of the minimum and maximum values of \( \hat{f}_{N} \) as \( i_{\text{min}} \) and \( i_{\text{max}} \) respectively. By defining \( i_{0} = \min(i_{\text{min}}, i_{\text{max}}) \) and \( i_{1} = \max(i_{\text{min}}, i_{\text{max}}) \), the WENO Flag at each grid point will then be decided accordingly as

\[
\text{Flag}_{i} = \begin{cases} 
1, & i \in [i_{0}, i_{1}] \quad \text{Non-smooth WENO stencils}, \\
0, & \text{otherwise} \quad \text{Smooth Compact stencils}. 
\end{cases}
\]  

(2.26)

For brevity, the conjugate Fourier shock detection algorithm and multi-resolution shock detection algorithm will be referred as cF shock detector and MR shock detector, respectively, in the following discussions.

**Remark 2.9.** Optionally, a check for constant will be performed by examining the absolute difference between the minimum and maximum values of the whole data vector, \( \Delta f_{\text{max}} = |\max_{i} |f_{i}| - \min_{i} |f_{i}| |. If \( \Delta f_{\text{max}} < \epsilon_{0} \) (typically, machine zero \( \epsilon \)), we shall assumed that no discontinuity exists and the cF shock detector will not be operated on this data vector.

To demonstrate the performance of cF shock detector for finding discontinuities in a piecewise smooth function and its derivative, we consider the following test function

\[
f(x) = \begin{cases} 
\frac{1}{6}[G(x, \beta, z - \delta) + 4G(x, \beta, z) + G(x, \beta, z + \delta)], & x \in [-0.8, -0.6], \\
1, & x \in [-0.4, -0.2], \\
1 - [10(x - 0.1)], & x \in [0, 0.2], \\
\frac{1}{6}[F(x, \alpha, a - \delta) + 4F(x, \alpha, a) + F(x, \alpha, a + \delta)], & x \in [0.4, 0.6], \\
0, & \text{else},
\end{cases}
\]  

(2.27)

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

where \( z = 0.7, \delta = 0.005, \beta = \frac{\log 2}{36\delta^2}, a = 0.5 \) and \( \alpha = 10 \). This function consists of a smooth Gaussian, a discontinuous Heaviside function, a piecewise linear triangle function and a smooth elliptic function. In Fig. 2.3, we show both the derivative of

**Fig. 2.3.** (Left) The derivative of conjugate Fourier \( \hat{f}_{N}(x_{i}) \) and (Right) the multi-resolution coefficients \( d_{i} \) for the test function Eq. (2.27) with \( N = 256 \).
\( N = 256 \). Notice that the strength of the jump of the \( \text{Heaviside} \) function is well predicted by the conjugate Fourier \( \hat{f}_n \) using the cf shock detector but not by the MR shock detector. From the figure, we can see that, comparing with the MR analysis, conjugate Fourier analysis gives a very large value at the discontinuities of the \( \text{Heaviside} \) function, the corners of the piecewise linear triangle function and the smooth elliptic function, along with some oscillations in the neighborhoods of these shapes. Using the mean \( F_{\text{mean}} \), the cf shock detector partitions the domain into several subdomains containing jumps of the function and its derivatives accurately, which will be further analyzed to pinpoint their estimated jump locations.

2.3. Iterative Conjugate Fourier Shock Detection Algorithm. In the example above, we presented the performance of the cf shock detector for a function with different forms of shapes. We note that the jumps of different shapes are of similar order in size and support. Often, the solution, for example, in a high speed compressible turbulence flow, contains not only both fine smooth structures and discontinuities, but also disparate scales. In this situation, the mean \( F_{\text{mean}} \) will still be too large for the shock detection algorithm to identify the relatively small jump discontinuities. The Algorithm 1 described above will fail to detect those small jumps. Thus, an iterative algorithm is developed to improve the shock detection capability of Algorithm 1 by subtracting large jumps incrementally from the solution until all relevant jumps have been identified. The iterative algorithm described below is very accurate in identifying most if not all relevant jump discontinuities subject to certain limitations, however, it is computationally expensive. Thus, the iterative algorithm should only be used sparingly and when necessary.

Algorithm 2 (Iterative Conjugate Fourier Shock Detection Algorithm)

1. Compute the conjugate Fourier \( A_i = \hat{f}_n(x_i) \) and its derivative \( B_i = \tilde{f}_n(x_i) \) of the function \( f(x) \).
2. Search for an index \( i^* \) such that \( A^* = |A_i| \) is the maximum.
3. If \( A^* > \epsilon_{cF} \), then
   - Set the WENO Flag using the cf shock detector with \( B_i \).
   - Determine the index \( j^* = i^* - 1 \) or \( j^* = i^* + 1 \) such that \( |A_{j^*}| \) is the next maximum.
   - Set the height of the jump to be \( H^* = \frac{1}{2}\left( [f](x_{i^*}) + [f](x_{j^*}) \right) / (1 + \epsilon_{\text{Gibbs}}) \).
   - Subtract a \( \text{Heaviside} \) function \( H(x, x_{i^*}, H^*) \) with jump \( H^* \) at \( x_{i^*} \) from \( f(x) \).
   - Repeat the procedure from Step 1 until the maximum number of iterations \( CF_{\text{max}} \) has reached.

We take the parameters \( \epsilon_{cF} = O(\Delta x) \), \( \epsilon_{\text{Gibbs}} = 0.09 \), and \( CF_{\text{max}} = 100 \).

To illustrate the performance of the iterative cf shock detector, we find the WENO Flag in the x- and y-directions of the Shepp-Logan phantom image, which is used as a benchmark two-dimensional piecewise smooth data set that models a MRI image of a human brain. It is very challenging for a shock detection algorithm to detect the small structures enclosed inside the head-bone as the heights of the head-bone range between 1 and 2 while the heights of the small scale soft tissues range between 1.01 and 1.02. The ratio of the jumps from large to small structures is of order of hundreds. We applied the iterative cf shock detector on the modified Shepp-Logan phantom image (with a bilinear function added) with resolutions \( N = 128 \) and \( N = 256 \), and the results are shown in Fig. 2.4. The small scale structures cannot be detected even at a relatively high resolution \( N = 256 \) using the cf shock detector. However, they are well identified by the iterative cf shock detector even at a
lower resolution $N = 128$. Good results had also been obtained by a similar iterative algorithm based on the radial basis function (RBF) method [21, 22, 23].

Fig. 2.4. The discontinuities $\text{Flag}_y$ as detected by (Left) the cF shock detector with $N = 256$; (Middle) Iterative cF shock detector with $N = 256$; and (Right) $N = 128$.

Remark 2.10. In all the examples as well as those not shown in the numerical results section below, only the cF shock detector is employed.

2.4. The Hybrid Compact-WENO Finite Difference Scheme. Now, together with all the numerical algorithms (Compact scheme, WENO scheme, and shock detectors), we have all the tools to build the hybrid Compact-WENO finite difference scheme. For the details of the hybrid scheme, see [5, 28, 30] and references therein.

Algorithm 3 (Hybrid Compact-WENO scheme)
1. Perform the conjugate Fourier or multi-resolution analysis on one or more suitable variable(s) (Typically, density $\rho$) once at the beginning of a time stepping scheme.
2. Set a WENO Flag using the shock detection algorithm.
3. Create a buffer zone around each grid point $x_i$ such that all the grid points inside the buffer zone are flagged as non-smooth stencils.
   This condition prevents the computation of the derivative of the fluxes by the Compact scheme using a non-smooth functional values. If, for example, a grid point $x_i$ is flagged as a non-smooth stencil, then its neighboring grid points $\{x_{i-m}, \ldots, x_i, \ldots, x_{i+m}\}$ will also be designated as non-smooth stencils that is, $\{\text{Flag}_j = 1, j = i - m, \ldots, i, \ldots, i + m\}$. (Typically, $m = r$.)
4. Compute the derivative of the fluxes at each cell center by
   • (Non-smooth WENO subdomain): the WENO scheme.
   • (Smooth Compact subdomain): the Compact scheme.

In other words, the computational domain is subdivided into non-smooth WENO subdomains and smooth Compact subdomains based on the shock detection algorithm in which the WENO-Z scheme and the Compact scheme will be applied respectively.

In the following discussion, we shall denote the Hybrid scheme using the cF shock detector as the Hybrid-cF scheme and the MR shock detector as the Hybrid-MR scheme, and collectively refer to both schemes as the Hybrid scheme. We shall also denote $N_{\text{flag}}$ ($N_{\text{cf}}$ and $N_{\text{mr}}$) as the number of stencils including those within the buffer zone that are flagged as non-smooth WENO stencils by a shock detector.

3. Numerical Experiments. We consider the two-dimensional Euler equations for gas dynamics in strong conservation form:

$$Q_t + F_x + G_y = 0,$$  \hspace{1cm} (3.1)
where the conservative variables $\mathbf{Q} = (\rho, \rho u, \rho v, E)^T$, the fluxes $\mathbf{F} = (\rho u, \rho u^2 + P, \rho uv, (E + P)u)^T$ and $\mathbf{G} = (\rho v, \rho uv, \rho v^2 + P, (E + P)v)^T$ in the $x$ and $y$ directions, respectively, and the equation of state (EOS) is $P = (\gamma - 1) \left( E - \frac{1}{2} \rho (u^2 + v^2) \right)$, $\gamma = 1.4$. The $\rho, u, v, P,$ and $E$ are the density, velocity in $x$- and $y$-direction, pressure and total energy respectively. Readers are referred to [3, 28, 30] and references contained therein for details of the spatial schemes and the third order TVD Runge-Kutta time stepping scheme used in the Hybrid scheme. The CFL condition for stability is $CFL = 0.45$.

In the following numerical experiments, we present a few preliminary results obtained by the Hybrid-cF scheme in solving a system of hyperbolic conservation laws. The density and pressure, along with the Flag showing the stencils using the WENO scheme for computing the fluxes in both directions, of a few classical one- and two-dimensional shocked problems are shown. The CPU timing (in seconds) and the speedup factor of the Hybrid-cF scheme using the MXM, EOD and CFT algorithms and the Hybrid-MR scheme over the pure WENO scheme are given showing the efficacy of the Hybrid scheme. The one-dimensional extended shock-density wave interaction problem is simulated with the Hybrid-cF scheme showing the effective spatiotemporal adaptivity of the scheme. The two-dimensional classical Riemann initial value problems and the Mach 10 double Mach reflection (DMR) problem are shown to demonstrate that the performance of the Hybrid scheme can be extended to a higher dimensional problem. With the exception of the one-dimensional extended shock-density wave interaction, where the $\gamma = 16$ order high pass Exponential filter is employed for the cF shock detector, no filter (that is, $\sigma_k = 1$) is needed in obtaining the results shown. Other standard test cases have been conducted with similar performances metrics. Hence, their results are not shown.

### 3.1. One-Dimensional Extended Shock-Density Wave Interaction Problem

To demonstrate the spatial and temporal adaptivity of the Hybrid-cF scheme, we simulated the one-dimensional Euler equations in an extended domain for a longer time with an initial condition

$$(\rho, u, P) = \begin{cases} (\frac{27}{4}, \frac{4\sqrt{3}}{9}, \frac{31}{5}) , & -5 \leq x < -4, \\ (1 + \varepsilon \sin(kx), 0, 1) , & -4 \leq x \leq 15, \end{cases}$$

where $x \in [-5, 15]$, $\varepsilon = 0.2$ and $k = 5$.

The non-linearity of the Euler equations generates both large fine scale structures and localized shocklets. The high frequency waves behind the main shock are smooth functions but often mis-identified as a strong gradient by a lower order shock detection algorithm when the solution is slightly under-resolved. In Fig. 3.1, the density $\rho$ and WENO Flag (red squares and line) as computed by the Hybrid-cF scheme with $N = 800$ at times $t = 2.5$ and $t = 5$ respectively, are shown. The absolute values of derivative of the conjugate Fourier partial sum and its mean $F_{\text{mean}}$ of the density as computed by the Hybrid-cF scheme are also presented at the corresponding times. The results show that the cF shock detector coupled with its $F_{\text{mean}}$ have accurately identified the locations of the main shock and the temporally evolving shocklets, and correctly classified the high frequency wave as smooth fine scale structures behind the main shock. The Hybrid-cF scheme deploys the WENO-Z5 scheme to compute the flux gradient in an essentially non-oscillatory manner while the high resolution Compact scheme is used for resolving the high frequency waves efficiently. In order to reduce the influence from the large fine scale structures behind the shock on the cF shock detector, the $\gamma = 16$ order high-pass Exponential filter is employed in this example. The WENO flag counts are $N_{\text{flag}}^{cF}(t = 2.5) = 54$ (6%) and $N_{\text{flag}}^{cF}(t = 5) = 110$.
The temporal evolution of the mean is also given in Fig. 3.1 to show the adaptivity of the cF shock detector in response to the formation of shocklets and high gradients, and the general trend in the solution in time.

3.2. Two-Dimensional Riemann Initial Value Problem. To examine the performance of the Hybrid scheme for higher dimensional problems, we solve the classical Riemann initial value problem with initial data in the form

\[ Q = (P, \rho, u, v) = \begin{cases} 
Q_1 = (P_1, \rho_1, u_1, v_1), & \text{if } x > x_0 \text{ and } y \geq y_0, \\
Q_2 = (P_2, \rho_2, u_2, v_2), & \text{if } x \leq x_0 \text{ and } y \geq y_0, \\
Q_3 = (P_3, \rho_3, u_3, v_3), & \text{if } x \leq x_0 \text{ and } y \leq y_0, \\
Q_4 = (P_4, \rho_4, u_4, v_4), & \text{if } x > x_0 \text{ and } y < y_0.
\end{cases} \]

According to [32], there are 19 genuinely different admissible configurations for polytropic gas, separated by the three types of one-dimensional centered waves, namely, rarefaction-\((\overrightarrow{R})\), shock-\((\overleftarrow{S})\), and contact-wave \((J^\pm)\). The arrows \((\overrightarrow{\cdot})\) and \((\overleftarrow{\cdot})\) indicate forward and backward waves, and the superscript \(J^+\) and \(J^-\) refer to negative and positive contacts respectively. We refer readers to [32] for details. We have performed calculations on all 19 configurations with the same resolution of 400 \times 400 as used in [32]. Here, we will only show the three representative results of configurations \((3, 5, 12)\) as computed by the Hybrid-cF scheme. The performance of the Hybrid-cF scheme with other configurations are similar and their results are omitted here.

The density with flooded contours and lines of these three configurations are shown in Fig. 3.2–3.4 respectively. The large scale structures of the flow agree well with those in the literature. We remark that the WENO Flag in \(x\)- and \(y\)-directions are very sharp with only a few grid points contained in each segment showing the
accuracy of the cF shock detector. Table I presents the CPU timings along with the speedup factor in the simulation of two-dimensional Riemann initial value problem with configuration 3 computed by the pure WENO-Z5, Hybrid-cF (including MXM, EOD and CFT algorithms), and Hybrid-MR schemes. From the results, we can see that the Hybrid schemes are substantially faster than the pure WENO-Z5 scheme with speedup factor increased from 1.5 to 3.0 as the resolution increased. The cF shock detector with the CFT algorithm has a slight speed advantage over the EOD algorithm at high resolutions and is a definite win over the MXM algorithm. The Hybrid-MR scheme is always slightly faster than the Hybrid-cF scheme as the amount of work required for detecting discontinuities is $O(N)$ and $O(N \log N)$, respectively. Methods to further reduce the CPU time required for the cF shock detector, such as restricting the shock detection algorithm to be activated only around potential discontinuities, is under study and will be reported in the future.

<table>
<thead>
<tr>
<th>$N \times M$</th>
<th>WENO-Z5</th>
<th>Hybrid</th>
<th>Hybrid-MR</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>MXM $r$</td>
<td>Hybrid-cF $r$</td>
<td>Hybrid-MR $r$</td>
</tr>
<tr>
<td>128 x 128</td>
<td>57</td>
<td>41</td>
<td>1.4</td>
</tr>
<tr>
<td>256 x 256</td>
<td>489</td>
<td>262</td>
<td>1.9</td>
</tr>
<tr>
<td>512 x 512</td>
<td>4426</td>
<td>2065</td>
<td>2.1</td>
</tr>
</tbody>
</table>

*Table I* The CPU timings (in seconds) and speedup factors $r$ of two-dimensional Riemann initial value problem with configuration 3 computed by the pure WENO-Z5, Hybrid-cF and Hybrid-MR schemes with $\epsilon_{MR} = 5 \times 10^{-3}$.

3.3. Two-Dimensional Mach 10 Double Mach Reflection Problem. To illustrate the efficiency of the Hybrid scheme in a more practical problem, we applied both Hybrid schemes to solve the two-dimensional Mach 10 double Mach reflection (DMR) problem. The problem and its numerical results are well documented in the literature [37].

We run both the Hybrid-cF and Hybrid-MR schemes with resolution 800 x 200 uniform cells to a final time $t_f = 0.2$. The density flooded contours and lines are shown in Fig. 3.5. The large scale structures (for example, the triple point, the incident shock, the reflected shock, a Mach stem and a slip plane) of the flow agree very well with each other and with those in the literature. In Fig. 3.6, the small scale structures (for example, the small vortical rollups along the slip line and the large mushroom shaped vortical rollup at the tip of the jet) around the region $x \in [2.15, 2.9]$ behind the incident shock are shown. Besides some expected minor discrepancies in the small scale vortical rollups along the slip line and the jet at high resolution, the fine scale structures agree very well with each other between the Hybrid schemes at the given resolution. The WENO Flag in $x$- and $y$-directions of the Hybrid schemes are shown in Fig. 3.7. Generally speaking, the Hybrid-cF scheme captures the high gradients more accurately and sharply than the Hybrid-MR scheme.

4. Conclusion. We have developed the Hybrid Compact-WENO finite difference scheme with the conjugate Fourier shock detection algorithm (Hybrid-cF) for solving hyperbolic conservation laws with discontinuous solution in a non-periodic Cartesian domain. We utilize the derivative of the conjugate Fourier partial sum and its mean to partition the physical domain robustly into non-smooth and smooth sub-domains. The shock locations are then identified and flagged for special treatment
\textbf{Configuration 3} : \(( R_{21}, R_{32}, R_{34}, R_{41} ), ( x_0, y_0 ) = ( 0.8, 0.8 ), t_f = 0.8. \)

\[ Q = \begin{cases} 
( 1.5, 1.5, 0, 0 ) \\
( 0.3, 0.5323, 1.206, 0 ) \\
( 0.029, 0.138, 1.206, 1.206 ) \\
( 0.3, 0.5323, 0, 1.206 ) 
\end{cases} \]

\begin{tabular}{cc}
Density $\rho$ & Pressure $P$ \\
\hline
Flag$_x$ & Flag$_y$ \\
\end{tabular}

\textbf{Fig. 3.2}, Two dimensional Riemann initial value problem with configuration 3: Density $\rho$, Pressure $P$, Flag$_x$ and Flag$_y$ in $x$- and $y$-directions respectively.

using the WENO scheme. The matrix-matrix multiply (MXM), Even-Odd decomposition (EOD) and Cosine/Sine fast transform (CFT) algorithms for computing the discrete conjugate Fourier partial sum and its derivative are derived. We have addressed the respective advantages and disadvantages in their implementations, usages and speeds along with other technical issues. We then present the cF shock detector and its iterative version for problems with jumps of large difference in scales. The iterative cF shock detector is able to identify edges of the small scale structures in the Shepp-Logan phantom image clearly even at a lower resolution.

The Hybrid-cF scheme is then applied to one- and two-dimensional hyperbolic conservation laws. The simulation of the 1D extended shock-density wave interaction problem and 2D classical Riemann IVP problems demonstrate the spatial and temporal adaptivity of the Hybrid-cF scheme in solving a problem containing strong shock, multiple developing shocklets, and high frequency waves behind the strong shock.
Configuration 5: \((J_{21}, J_{32}, J_{34}, J_{41}), (x_0, y_0) = (0.5, 0.5), t_f = 0.23\).

\[
Q = \begin{cases} 
(1, 1, -0.75, -0.5) \\
(1, 2, -0.75, 0.5) \\
(1, 1, 0.75, 0.5) \\
(1, 3, 0.75, -0.5)
\end{cases}
\]

<table>
<thead>
<tr>
<th>Density (\rho)</th>
<th>Pressure (P)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flag(_x)</td>
<td>Flag(_y)</td>
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</table>

Fig. 3.3. Two dimensional Riemann initial value problem with configuration 5: Density \(\rho\), Pressure \(P\), Flag\(_x\) and Flag\(_y\) in \(x\)- and \(y\)-directions respectively.

The 2D Mach 10 double Mach reflection problem is also simulated to show that the Hybrid-cF scheme works as well as the Hybrid-MR scheme. These preliminary results are in good agreement with those obtained in the literature and can potentially be very useful for certain classes of shocked flows containing both discontinuities and small scale structures, such as high speed compressible turbulent flows. Furthermore, a speedup up to 2 or more in CPU timings is achieved with Hybrid-cF (CFT) scheme when compared with the pure WENO-Z5 scheme.

In our future work, we plan to use the high order shock detectors to classify discontinuities of different types, such as contact waves, shocks, rarefaction waves and material interfaces, and to apply appropriate numerical techniques to obtain the best possible solution. We are also planning to apply the Hybrid-cF scheme for simulating compressible turbulence and chemically reactive multi-components multi-phase flows, and to study the related theoretical and practical issues (non-uniform, finite volume or...
Configuration 12 : \((\vec{S}_{21}, J_{32}^+, J_{34}^+, \vec{S}_{41})\), \((x_0, y_0) = (0.5, 0.5)\), \(t_f = 0.25\).

\[
Q = \begin{cases} 
(0.4, 0.5313, 0, 0) \\
(1, 1, 0.7276, 0) \\
(1, 0.8, 0, 0) \\
(1, 1, 0, 0.7276)
\end{cases}
\]

<table>
<thead>
<tr>
<th>Density (\rho)</th>
<th>Pressure (P)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\text{Flag}_x)</td>
<td>(\text{Flag}_y)</td>
</tr>
</tbody>
</table>

Fig. 3.4. Two dimensional Riemann initial value problem with configuration 12: Density \(\rho\), Pressure \(P\), \(\text{Flag}_x\) and \(\text{Flag}_y\) in \(x\)- and \(y\)-directions respectively.

finite element grids, parallellization), and to explore alternative advanced techniques in identifying discontinuities.
Fig. 3.5. The density contour flood and lines of the Mach 10 double Mach shock reflection problem as computed by (Left) the Hybrid-cF scheme and (Right) the Hybrid-MR scheme at time \( t_f = 0.2 \).

Fig. 3.6. The zoom in of the density of the Mach 10 double Mach shock reflection problem as computed by (Left) the Hybrid-cF scheme and (Right) the Hybrid-MR scheme at time \( t_f = 0.2 \).

Acknowledgments. We appreciate the careful reading and valuable suggestions made to the contents of the manuscript by the reviewers and Dr. Oleg Schilling of Lawrence Livermore National Laboratory. The authors would also like to thank Qing Cheng of Xiamen University for the preliminary work done in the conjugate Fourier method during the summer workshop in Advanced Research in Applied Mathematics and Scientific Computing 2014 at the School of Mathematical Sciences of Ocean University of China.

References


Hybrid-cF  Hybrid-MR

WENO Flag in $x$

WENO Flag in $y$

**Fig. 3.7.** Distribution of the WENO flags $\text{Flag}_x$ and $\text{Flag}_y$ in $x$- and $y$-directions respectively, of the Hybrid-cF and Hybrid-MR schemes at time $t_f = 0.2$.  


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