CAPTURING SHOCKS AND TURBULENCE SPECTRA IN
COMPRESSIBLE FLOWS. PART 2: A NEW HYBRID
PPM/WENO METHOD.

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Abstract. In the Part 1 of the present paper [12] the performance of several
different low and high-order finite-volume methods were assessed by inves-
tigating how well they can capture the turbulent spectra of a compressible
flow where small smooth turbulent structures interact with shocks and dis-
continuities. The comparisons showed that a second-order Godunov method
with PPM interpolation provides results virtually the same as a fourth-order
WENO scheme but at a significant lower cost. However, it is shown that the
PPM method fails to provide an accurate representation in the high-frequency
range of the spectra. In the present paper we show that this specific issue
comes from the slope-limiting procedure and a novel hybrid PPM/WENO
method is developed, which has the ability to capture the turbulent spectra
with the accuracy of a formally high-order method, but at the cost of the
second-order Godunov method. Overall, it is shown that virtually the same
physical solution can be obtained much faster by refining a simulation with the
second-order method and carefully chosen numerical procedures, rather than
running a coarse high-order simulation.

1. Introduction

Many compressible flows of interest are turbulent. The objective of the present
study is to explore the utility of higher-order discretization approaches for the sim-
ulation of such flows. The asymptotic rate of convergence of the numerical error
of higher-order methods for simplified problems with smooth solutions is well doc-
umented in the literature. As the resolution increases, higher-order methods will
eventually provide more accurate solutions than lower-order methods. However in
most Computational Fluid Dynamics (CFD) applications, particularly those involv-
ing turbulent flow, the solution is well-resolved well before reaching the asymptotic
regime of the numerical method (see discussion in [1]). This issue is exacerbated
for compressible flow. The solution can include shock waves that require a diffusive
treatment to prevent the appearance of spurious nonphysical oscillations in the so-
lution, reducing the order of accuracy of the numerical method employed. Thus,
this means that the minimum resolution required to capture the physics of such
flow accurately cannot be assumed a priori.

More critically, it is emphasized that the performance of a numerical method
should not be defined only by the order of the convergence of the error for smooth

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solutions. A better measure for the actual accuracy is the ability of the numerical method to adequately resolve both the inertial range and the dissipation range of the turbulent energy spectrum. In order to assess the potential computational advantage of using a higher-order method for turbulent flows to obtain a desired accuracy, simulations of the decay of homogeneous isotropic turbulence are performed with different finite-volume schemes and on different mesh resolutions.

The purpose of the Part 1 of the present paper [12] was to study the actual performance of several different low and high-order finite-volume methods by investigating how well they can capture the turbulent spectra of a compressible flow where small smooth turbulent structures interact with shocks and discontinuities. Comparisons revealed that a second-order Godunov method with PPM interpolation provides essentially the same results as a fourth-order WENO scheme but a significant lower cost. In the conclusion of Part 1 of the present paper [12], it is emphasized that virtually the same physical solution can be obtained much faster by refining a simulation with the second-order method, rather than running a coarse high-order simulation. However, the results show that the refinement of the mesh presents some limit when using the second-order Godunov procedure with PPM interpolation. Indeed, it is found that when the mesh is fine enough, a non-physical pile-up of energy appears in the high-frequency range of the turbulent spectra. After an intensive trial and error process, it has been found that the limiting procedures employed by the PPM to ensure monotonicity are responsible to this pile-up of energy in the high-frequency range of the spectra.

The present Part 2 of the paper proposes to replace the interpolation and limiting procedures in the PPM algorithm by a WENO interpolation. The WENO interpolation is formally fifth-order and has been proven to be robust for capturing discontinuities, preventing the algorithm from relying on many numerical parameters. The original PPM method as well as the new hybrid PPM/WENO method proposed here are implemented in the PeleC code developed in the Center for Computational Sciences and Engineering (CCSE) group[1] at Lawrence Berkeley National Laboratory, USA. The PeleC code is a second-order Adaptive Mesh Refinement (AMR) finite-volume solver for reacting and non-reacting fluid simulations with complex geometry and multi-phase support. The simulations performed in the present paper only use of fraction of the capability of the software, namely the Godunov-based integration procedure on a single level mesh grid.

Note also that comparisons are also made with the RNS code [3], which employs a fourth-order finite-volume WENO strategy. The codes are implemented in the AMReX framework[2] it facilitates the development of a generic post-processing chain as well as the assessment of computing costs via embedded profiling functionality. Note that while the AMReX library is developed for AMR applications, only single level mesh grids are considered in the present paper.

The remainder of the present paper is organized as follows. In section 2 the set of equations solved by the code are presented, while in section 3 the PPM algorithm as it is implemented in the PeleC code is presented, followed by the description of the new hybrid PPM/WENO procedure. In the results section 4 the new hybrid PPM/WENO strategy is confronted to the original PPM method with slope-limiting, as well as to the fourth-order finite-volume WENO method. It
is found that the novel hybrid PPM/WENO method has the ability to capture the turbulent spectra with the accuracy of a high-order method, but at the cost of a second-order Godunov method.

2. Governing equations

As explained in the companion paper, the PeleC software employed in the present study was initially devoted to the simulation of combustion problems. However, as only non-reacting problems with no specific mixture composition are investigated in the present study, the set of multicomponent reacting Navier-Stokes equations are significantly simplified and are given by

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) &= 0, \\
\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) + \nabla p &= \nabla \cdot \mathbf{\tau}, \\
\frac{\partial \rho E}{\partial t} + \nabla \cdot [(\rho E + p) \mathbf{u}] &= \nabla \cdot (\lambda \nabla T) + \nabla \cdot (\mathbf{\tau} \cdot \mathbf{u}),
\end{align*}
\]

where $\rho$ is the density, $\mathbf{u}$ is the velocity, $p$ is the pressure, $E = e + \mathbf{u} \cdot \mathbf{u}/2$ is the total energy, $T$ is the temperature and $\lambda$ is the thermal conductivity. The viscous stress tensor is given by

\[
\mathbf{\tau} = \eta (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) + (\zeta - \frac{2}{3} \eta) (\nabla \cdot \mathbf{u}) \mathbf{I},
\]

where $\eta$ and $\zeta$ are the shear and bulk viscosities.

The system is closed by an equation of state (EOS) that specifies $p$ as a function of $\rho$ and $T$. An ideal gas mixture for the EOS is assumed:

\[
p = \rho T \mathfrak{R},
\]

where $\mathfrak{R}$ is the gas constant. Here we set $C_p$ and $C_v$ the heat capacity at constant pressure and volume, respectively, to follow an ideal gas law proportional to the ratio of the specific heats $\gamma$ so that equation (5) is equivalent to the following relation:

\[
e = p / (\gamma - 1) \rho
\]

where $e$ is the specific internal energy and $\gamma$ is set to $\gamma = 1.4$.

Note that for the ease of simplicity, the system presented at equations (1) to (3) is recast in the form of

\[
\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \mathbf{F} = \mathbf{S},
\]

where $\mathbf{U}$ is the vector of conservative variables, while $\mathbf{F}$ represents the convective flux vector and $\mathbf{S}$ the diffusive terms, respectively.

3. Numerical methods

The solution is advanced from time $n$ to time $n + 1$ with the following second-order Godunov method:

\[
\begin{align*}
\mathbf{U}^+ &= \mathbf{U}^n - \Delta t \nabla \cdot \mathbf{F}^{n+1/2} + \Delta t \mathbf{S}^n, \\
\mathbf{U}^{n+1} &= \mathbf{U}^+ + \frac{1}{2} \Delta t (\mathbf{S}^* - \mathbf{S}^n),
\end{align*}
\]
where $\Delta t = t^{n+1} - t^n$ is the time step. The second step at equation (9) is a correction of the solution to ensure second-order accuracy by effectively time-centering the diffusion source terms. The conserved state vector $U$ is stored at cell centers and the flux vectors are computed on cell edges.

The convective flux vector $F$ that appears in equation (8) is constructed from time-centered edge states computed with a conservative, shock-capturing, unsplit Godunov method, which makes use of the Piecewise Parabolic Method (PPM) [7], characteristic tracing and full corner coupling [2, 11]. As the present paper proposes a modification of the PPM method, for ease of exposition the whole algorithm will be detailed in 1D for the Euler equations. It is emphasized that the algorithm can be extended to multi-dimensional problems and multi-component flows. Moreover, since the publication of the original paper [7] presenting the PPM method, several modifications have been proposed in the literature (see [11, 6, 5]). Consequently, the algorithm implemented in the code PeleC incorporates some of the variants, but it is emphasized that these changes only slightly differ from the original PPM method. Many variants have been tested through this study, and while not reported in the present paper, none change fundamentally the results.

### 3.1. System of primitive variables.

The conservative equation (7) is rewritten in terms of primitive variables, such that:

\[
\frac{\partial Q}{\partial t} + A \frac{\partial Q}{\partial x} = S_Q.
\]

Here $Q$ is the primitive state vector, $A = \partial F/\partial Q$ and $S_Q$ are the viscous source terms reformulated in terms of the primitive variables.

In one dimension, this comes:

\[
\begin{pmatrix}
\rho \\
u \\
p \\
p e
\end{pmatrix}_t + \begin{pmatrix}
u & \rho & 0 & 0 \\
0 & u & \frac{1}{\rho} & 0 \\
0 & 0 & \rho e^2 & u \\
0 & \rho e + p & 0 & u
\end{pmatrix} \begin{pmatrix}
\rho \\
u \\
p \\
p e
\end{pmatrix}_x = S_Q
\]

Note that here, the system of primitive variables has been extended to include an additional equation for the internal energy, denoted $e$. This avoids several calls to the equation of state, especially in the Riemann solver step.

The eigenvalues of the matrix $A_x$ are given by:

\[
\Lambda (A_x) = \{u - c, u, u, u + c\}.
\]

The right column eigenvectors are:

\[
r_x = \begin{pmatrix}
1 & 1 & 0 & 1 \\
-\frac{c}{\rho} & 0 & 0 & \frac{c}{\rho} \\
0 & 0 & \rho e^2 & 0 \\
h & 0 & 1 & h
\end{pmatrix}.
\]

The left row eigenvectors, normalized so that $1_x \cdot r_x = I$ are:

\[
1_x = \begin{pmatrix}
0 & -\frac{c}{2e} & \frac{c}{2e} & 0 \\
1 & 0 & -\frac{1}{h} & 0 \\
0 & 0 & \rho e^2 & 0 \\
0 & \frac{c}{2e} & -\frac{c}{2e} & 0
\end{pmatrix}.
\]
Note that here, \( c \) and \( h \) are the sound speed and the enthalpy, respectively.

3.2. Edge state prediction. As discussed at the beginning of section 3, the fluxes are reconstructed from time-centered edge state values. Thus, the primitive variables are first interpolated in space with the PPM method, then a characteristic tracing operation is performed to extrapolate in time their values at \( n + 1/2 \).

3.2.1. Interpolation and slope limiting. Basically the goal of the algorithm is to compute a left and a right state of the primitive variables at each edge in order to provide inputs for the Riemann problem to solve.

First, the average cross-cell difference is computed for each primitive variable with a quadratic interpolation as follows:

\[
\delta q_i = \frac{1}{2} (q_{i+1} - q_{i-1}) .
\]

In order to enforce monotonicity, \( \delta q_i \) is limited with the van Leer method:

\[
\delta q_i^* = \min (|\delta q_i|, 2|q_{i+1} - q_i|, 2|q_i - q_{i-1}|) \sgn(\delta q_i) ,
\]

and the interpolation of the primitive values to the cell face \( q_{i+\frac{1}{2}} \) is estimated with:

\[
q_{i+\frac{1}{2}} = q_i + \frac{1}{2} (q_{i+1} - q_i) - \frac{1}{6} (\delta q_{i+1}^* - \delta q_i^*) .
\]

In order to enforce that \( q_{i+\frac{1}{2}} \) lies between the adjacent cell averages, the following constraint is imposed:

\[
\min (q_i, q_{i+1}) \leq q_{i+\frac{1}{2}} \leq \max (q_i, q_{i+1}) .
\]

The next step is to set the values of \( q_{R,i-\frac{1}{2}} \) and \( q_{L,i+\frac{1}{2}} \), which are the right and left state at the edges bounding a computational cell. Here, a quartic limiter is employed in order to enforce that the interpolated parabolic profile is monotone. The procedure proposed by [11] is adopted, which slightly differs from the original one proposed in [7]. In [11], this specific procedure is followed by the imposition of another limiter based on a flattening parameter to prevent artificial extrema in the reconstructed values. In the present paper, the order of imposition of the different limiting procedures is reversed.

First, the edge state values are defined as:

\[
q_{L,i+\frac{1}{2}} = q_{i+\frac{1}{2}} ,
\]

\[
q_{R,i-\frac{1}{2}} = q_{i-\frac{1}{2}} ,
\]

Then the flattening limiter is imposed as follows:

\[
q_{L,i+\frac{1}{2}} \leftarrow \chi_i q_{L,i+\frac{1}{2}} + (1 + \chi_i) q_i ,
\]

\[
q_{R,i-\frac{1}{2}} \leftarrow \chi_i q_{R,i-\frac{1}{2}} + (1 + \chi_i) q_i ,
\]

where \( \chi_i \) is a flattening coefficient computed from the local pressure, and its evaluation is presented in appendix A.

Finally, the monotonization is performed with the following procedure:

\[
q_{L,i+\frac{1}{2}} = q_{R,i-\frac{1}{2}} = q_i \quad \text{if} \quad \left( q_{L,i+\frac{1}{2}} - q_i \right) \left( q_i - q_{R,i-\frac{1}{2}} \right) > 0 ,
\]

\[
q_{L,i+\frac{1}{2}} = 3q_i - 2q_{R,i-\frac{1}{2}} \quad \text{if} \quad |q_{L,i+\frac{1}{2}} - q_i| \geq 2|q_{R,i-\frac{1}{2}} - q_i| ,
\]

\[
q_{R,i-\frac{1}{2}} = 3q_i - 2q_{L,i+\frac{1}{2}} \quad \text{if} \quad |q_{R,i-\frac{1}{2}} - q_i| \geq 2|q_{L,i+\frac{1}{2}} - q_i| .
\]
3.2.2. Piecewise Parabolic Reconstruction. Once the limited values \( q_{R,i-\frac{1}{2}} \) and \( q_{L,i+\frac{1}{2}} \) are known, the limited piecewise parabolic reconstruction in each cell is done by computing the average value swept out by parabola profile across a face, assuming that it moves at the speed of a characteristic wave \( \lambda_k \). The average is defined by the following integrals:

\[
I^{(k)}_+ (q_i) = \frac{1}{\sigma_k \Delta x} \int_{(i+1/2)\Delta x}^{(i+1/2)\Delta x + \sigma_k \Delta x} q_i^\sigma (x) \, dx,
\]

\[
I^{(k)}_- (q_i) = \frac{1}{\sigma_k \Delta x} \int_{(i-1/2)\Delta x}^{(i-1/2)\Delta x - \sigma_k \Delta x} q_i^\sigma (x) \, dx,
\]

with \( \sigma_k = |\lambda_k| \Delta t / \Delta x \), where \( \lambda_k = \{ u - c, u, u + c \} \), while \( \Delta t \) and \( \Delta x \) are the discretization step in time and space, respectively, with the assumption that \( \Delta x \) is constant in the computational domain.

The parabolic profile is defined by

\[
q_i^\sigma (x) = q_{R,i-\frac{1}{2}} + \xi (x) \left[ q_{L,i+\frac{1}{2}} - q_{R,i-\frac{1}{2}} + q_{i,6} (1 - \xi (x)) \right]
\]

with

\[
q_{i,6} = 6q_i - 3 \left( q_{R,i-\frac{1}{2}} + q_{L,i+\frac{1}{2}} \right),
\]

and

\[
\xi (x) = \frac{x - x_{i-\frac{1}{2}}}{\Delta x}, \quad x_{i-\frac{1}{2}} \leq x \leq x_{i+\frac{1}{2}}.
\]

Substituting equation (29) in equations (26) and (27) leads to the following explicit formulations:

\[
I^{(k)}_+ (q_i) = q_{L,i+\frac{1}{2}} - \frac{\sigma_k}{2} \left[ q_{L,i+\frac{1}{2}} - q_{L,i+\frac{1}{2}} - \left( 1 - \frac{2}{3} \sigma_k \right) q_{i,6} \right],
\]

\[
I^{(k)}_- (q_i) = q_{R,i-\frac{1}{2}} + \frac{\sigma_k}{2} \left[ q_{L,i+\frac{1}{2}} - q_{L,i+\frac{1}{2}} + \left( 1 - \frac{2}{3} \sigma_k \right) q_{i,6} \right].
\]

3.2.3. Characteristic tracing and flux reconstruction. The next step is to extrapolate in time the integrals \( I^{(k)}_{\pm} \) to get the left and right edge states at time \( n + 1/2 \). This procedure is complex, especially in multi-dimensions where transverse terms are taken into account; the complete detailed procedure can be found in [11]. In 1D, the left and right edge states are computed as follows:

\[
q_{L,i+\frac{1}{2}}^{n+\frac{1}{2}} = I^{(k=u+c)}_+ - \sum_{k: \lambda_k > 0} \beta_k l_k \cdot \left[ I^{(k=u+c)}_+ - I^{(k)}_+ \right] f_k + \frac{\Delta t}{2} S^n_i,
\]

\[
q_{R,i-\frac{1}{2}}^{n+\frac{1}{2}} = I^{(k=u-c)}_- - \sum_{k: \lambda_k < 0} \beta_k l_k \cdot \left[ I^{(k=u-c)}_- - I^{(k)}_- \right] f_k + \frac{\Delta t}{2} S^n_i.
\]

where

\[
\beta_k = \begin{cases} \frac{1}{2}, & \text{if } \lambda_k = 0, \\ 1, & \text{otherwise,} \end{cases}
\]
and $l_k$ and $r_k$ are the left row and right column of the matrices defined at equations (13) and (14) for each eigenvalue $k$. Note that here, $S^n_i$ represents any source terms at time $n$ to include in the characteristic tracing operation.

Finally, the time-centered fluxes are computed using an approximate Riemann problem solver. Here the HLLC algorithm [15] is employed. At the end of this procedure the primitive variables are centered in time at $n + 1/2$, and in space at the edges of a cell. This is the so-called Godunov state and the convective fluxes can be computed to advance equation (8).

3.3. The hybrid PPM/WENO method. As shown in the Part 1 [12], the PPM method presented above gives good results for a small computational time compared to a costly fourth-order finite-volume WENO strategy. However, for fine meshes, the PPM method exhibits a significant pile-up of energy in the high-frequency range of the spectra, which is undesirable and limits mesh refinement. During the study of turbulent spectra in [12], it has been found that the pile-up of energy at the high-frequencies was sensitive to the slope-limiting procedure presented at section 3.2.1. As many variants can be found in the literature, an attempt to tweak this procedure was tried, for example by playing with the numerical parameters (see appendix A) or by removing the slope limiting operation completely. Also, the procedure given in [6] was tested. For all cases, the results were very similar and the impact on the pile-up of energy was modest and not satisfying.

After an intensive trial and error process, it became apparent that the interpolation and slope-limiting procedure described in section 3.2.1 was not robust, leading to poor results in the high-frequency range. Here we consider replacing this whole procedure by a WENO interpolation.

The WENO strategy [10] as well as several popular variants [9, 4, 13] have been presented and tested in [12]. As the WENO-Z [4] appears to be the most robust and gives satisfying results for a small computational cost compared to other WENO methods, only the WENO-Z method will be presented and tested below.

Basically, for a given cell $i$, the general principle of a WENO method is to provide a shock-capturing, high-order approximation of the variable $q$ interpolated on the left and the right side of a face, denoted $q_{i+1/2}^L$ and $q_{i+1/2}^R$. In the remainder of this section, the procedures to evaluate $q_{i+1/2}^L$ are provided, but a simple mirror-symmetric change on the procedure will provide $q_{i-1/2}^R$.

A fifth-order polynomial approximation of $q_{i+1/2}^L$ is constructed through a convex combination of the values $q_{i+1/2}^k$ interpolated with a third degree polynomial on a three point stencil $k$, such that:

\[(37) \quad q_{i+1/2}^L = \sum_{k=0}^{2} \omega_k q_{i+1/2}^k.\]

Here, $\omega_k$ are non-linear weights balancing the contribution of each stencil, and are defined as

\[(38) \quad \omega_k = \frac{\alpha_k}{\sum_{l=0}^{2} \alpha_l}, \quad \alpha_k = d_k \left(1 + \frac{\tau_5}{\beta_k + \epsilon}\right)^p,\]

where

\[(39) \quad \tau_5 = |\beta_0 - \beta_2|.\]
Here $d_k$ are the so-called optimal weights because they reconstruct the fifth-order upstream central scheme for the 5-point stencil, $\beta_k$ are the smoothness indicators, $\alpha_k$ are refereed as the unnormalized weights and $\epsilon$ is a parameter set to avoid a division by zero. The parameter $p$ controls the adaption rate. According to [3], a large value of $p$ leads to unnecessarily dissipation in the smooth regions of the flow. In the present study, and in order to be consistent with the study presented in Part 1 [12], the parameter is set to $p = 1$ for all the test cases. Moreover, as suggested by [3], $\epsilon$ is set to $\epsilon = 10^{-40}$.

The smoothness indicators $\beta_k$ are given by:

\begin{align}
\beta_0 &= \frac{13}{12} (q_{i-2} - 2q_{i-1} + q_i)^2 + \frac{1}{4} (q_{i-2} - 4q_{i-1} + 3q_i)^2, \\
\beta_1 &= \frac{13}{12} (q_{i-1} - 2q_i + q_{i+1})^2 + \frac{1}{4} (q_{i-1} - q_{i+1})^2, \\
\beta_2 &= \frac{13}{12} (q_i - 2q_{i+1} + q_{i+2})^2 + \frac{1}{4} (3q_i - 4q_{i+1} + q_{i+2})^2.
\end{align}

The optimal weights are:

\begin{align}
d_0 &= \frac{1}{10}, \quad d_1 = \frac{6}{10}, \quad d_2 = \frac{3}{10},
\end{align}

and $q_{i+\frac{1}{2}}$ is given by:

\begin{align}
q_{i+\frac{1}{2}} &= \frac{1}{6} \omega_0 (2q_{i-2} - 7q_{i-1} + 11q_i) \\
&\quad + \frac{1}{6} \omega_1 (-q_{i-1} + 5q_i + 2q_{i+1}) + \frac{1}{6} \omega_2 (2q_i + 5q_{i+1} - q_{i+2}).
\end{align}

Once $q_{i+\frac{1}{2}}$ and $q_{i-\frac{1}{2}}$ are evaluated through the WENO-Z procedure, the PPM algorithm continues exactly the same as in section 3.2.2. In other words, the purpose of the hybrid PPM/WENO method is only to replace the procedure in section 3.2.1. One should note that the WENO-Z method is employed here for its performance, but it is emphasized that any other WENO reconstruction methods can be employed. For the ease of exposition, the hybrid method will be called PPM/WENO in the remainder of the paper, but one has to keep in mind that the WENO-Z method has been used for the reconstruction at faces.

4. Results

In the following section, the hybrid PPM/WENO method is tested and compared to the original PPM method with slope limiting described in section 3.2.1 as well as the fourth-order finite-volume WENO method [14] implemented in the RNS code and discussed in the companion paper [12]. We recall here that both PPM methods are implemented in the PeleC code that uses a general second-order Godunov procedure (see section 3). Moreover, as discussed above in section 3.3, only the WENO-Z variant is tested in the present paper. The test cases consist on the Shu-Osher test case and the decay of compressible homogeneous isotropic turbulence. These test cases are described in the Part 1 of the present paper [12] and for conciseness will not be reiterated here. Note that in Part 1, the convection of a smooth 2D vortex is investigated to highlight the asymptotic rate of convergence of the numerical methods. Because for this specific test case the hybrid PPM/WENO method proposed in this paper presents virtually the same behavior as the original
PPM method, for conciseness the results are not reported here. Note also that PeleC is part of the Pele Suite of codes, which are publicly available and may be freely downloaded[3] and that all the test cases presented in the Part 1 and Part 2 of the paper are available from the PeleC distribution.

4.1. Strong shock test case: Shu-Osher. The purpose of the Shu-Osher test case is to simulate the one-dimensional propagation of a normal shock wave interacting with a fluctuating entropy wave, generating a flow field containing both small scale structures as well as discontinuities. Similarly to the simulations in the Part 1 of the paper, the solution is advanced in time to \( t = 1.8 \), and for all numerical methods investigated, the mesh is progressively refined from \( N_x = 256 \) to \( N_x = 2048 \). The convergence is measured using the \( L^1 \)-norm of the difference of the density between the final computed solution and a reference solution defined to be the solution computed with the second-order Godunov method with PPM interpolation and slope limiting, and with a very fine mesh \( N_x = 32768 \). In all simulations the CFL number is set to 0.5.

The density field at \( t = 1.8 \) computed with \( N_x = 256, 512, 1024 \) and 2048 is shown in figures 1 to 4 respectively. In these figures, the blue square, red circle and purple cross represents the fourth-order finite-volume WENO method with the WENO-Z variant, the original PPM method with slope limiting and the hybrid PPM/WENO method developed in the present paper, respectively (see legend in figure 1b). Note also that the panels (a) and (b) in figure 1, figure 2 and figure 3 present the full domain and a zoom in the domain, respectively, while figure 4 is only a zoom in the domain.

For a coarse mesh \((N_x = 256)\), a close look at figure 1b reveals that the fourth-order finite-volume WENO method is able to capture the correct phase of the waves, despite a damping of the amplitude. The second-order Godunov method with the original PPM interpolation and the slope limiting procedure does not accurately capture the correct profile of density. However, the hybrid PPM/WENO method presents a profile very similar to the one captured by the fourth-order finite-volume method. It turns out that changing the slope-limiting procedure in the PPM method to the WENO interpolation makes the second-order Godunov method recover the correct profile of density. This can be explained by the fact that the shock is better resolved by the WENO interpolation and that the slope limiting procedure introduces spurious wiggles in the density waves.

As seen in figure 2b, a mesh refinement by a factor 2 makes all the method accurately capture the phase of the density waves. However the original PPM method with slope-limiting (red circle symbols) shows a damping of the amplitude, while the hybrid PPM/WENO method solution correctly captures both the phase and the amplitude, and is very close to the solution computed with the fourth-order finite-volume WENO method.

As the mesh is further refined, all the methods tend to collapse to the same solution. However, as can be seen in figure 3 for a fine mesh \((N_x = 2048)\), the fourth-order finite-volume WENO method shows a slight damping of the amplitude of the density wave, whereas the second-order Godunov method with PPM interpolation and slope-limiting exhibits some smooth high-frequency oscillations. The best solution is the one computed with the second-order Godunov method and

[3] https://amrex-combustion.github.io/
the hybrid PPM/WENO method. The shape and amplitude of the density are closer to the reference solution.

The convergence rate is evaluated by computing the $L^1$-norm of the error on the density profile. The error $\epsilon_\rho$ is reported in figure 5 and the convergence rate computed with a curve fitting method is reported in table 1. Similarly to the study performed in the Part 1 of the present paper [12], all numerical methods collapse to less than first-order accuracy because of the presence of the discontinuity.

Overall, the present study suggests that reaching a correct approximation of a flow solution can be achieved by a second-order Godunov method and replacing the slope-limiting procedure by a WENO interpolation. In the following section, a more realistic three-dimensional compressible turbulent flow is simulated to investigate the capabilities of the hybrid PPM/WENO method to accurately capture turbulent spectra when both shocks and small structures interact in the same domain.

![Figure 1. Shu-Osher test case: profile of density for $N_x = 256$.](image)

The circle, square and cross symbols represent the PPM with slope limiting, 4th-order WENO-Z and the hybrid PPM/WENO methods, respectively.

### Table 1. Shu-Osher test case: convergence rate of the $L^1$-norm of the error on the density.

| Method                  | $O(\epsilon_\rho)$ |
|-------------------------|---------------------|
| PPM with slope-limiting | 0.92                |
| 4th-order WENO-Z        | 0.89                |
| Hybrid PPM/WENO         | 0.96                |

#### 4.2. Three-dimensional isotropic compressible turbulence decay.

The present test case consists on the simulation of the decay of a compressible isotropic turbulent field with the presence of eddy shocklets. Recall that Part 1 [12] of the paper is devoted to the comparison between a second-order Godunov method with PPM interpolation and slope-limiting procedure, and with the finite-volume WENO method (see [14]) with different WENO variants. Results presented in Part 1 show that all the methods give very similar results in terms of capturing the turbulent
Figure 2. Shu-Osher test case: profile of density for $N_x = 512$. The circle, square and cross symbols represent the PPM with slope limiting, 4th-order WENO-Z and the hybrid PPM/WENO methods, respectively.

Figure 3. Shu-Osher test case: profile of density for $N_x = 1024$. The circle, square and cross symbols represent the PPM with slope limiting, 4th-order WENO-Z and the hybrid PPM/WENO methods, respectively.

spectra. For the temporal evolution of physical quantities, some differences exist when the mesh is very coarse, but all the results collapse quickly to the same solution as the mesh is refined. Because the second-order Godunov method is far less costly than the fourth-order finite-volume WENO method, it is advocated in the conclusion of the companion paper [12] that an accurate solution can be obtained faster by using the second-order Godunov method with PPM interpolation together with a finer mesh resolution, and that the use of a high-order finite-volume method is questionable due to the high computational cost for little improvement to the solution. However, it is also pointed out that the major drawback of the second-order PPM method is the poor representation in the high-frequency range of the spectra when the mesh is fine enough to resolve very small scale structures of
Figure 4. Shu-Osher test case: profile of density for $N_x = 2048$. The circle, square and cross symbols represent the PPM with slope limiting, 4th-order WENO-Z and the hybrid PPM/WENO methods, respectively.

Figure 5. Shu-Osher test case: $L^1$-norm of the error on the density.
the turbulence. As explained in section 3.3, it has been found that the issue with the original PPM method is the slope-limiting procedure, and we propose in the present paper to replace it by a WENO interpolation.

Recall that the numerical set-up is exactly the same as in the Part 1 of the present paper. Figures 6a to 6d present the temporal evolution of the kinetic energy, the enstrophy, the variance of temperature and the dilatation from \( t = 0 \) to \( t/\tau = 4 \). Figures 7a to 7d present the spectra taken at \( t/\tau = 4 \) for the kinetic energy, the vorticity, the dilatation and the density. In these figures, the circle, cross and square symbols represent the second-order Godunov with PPM interpolation and slope-limiting, the second-order Godunov method with the hybrid PPM/WENO procedure, and the fourth-order finite-volume WENO strategy, respectively. The red, blue, purple and orange colors represent simulations performed with \( N_x = 64 \), \( N_x = 128 \), \( N_x = 256 \) and \( N_x = 512 \), respectively. It is emphasized that these figures contain a significant number of curves. For clarity, a zoom on the high-end of the spectra is shown in figures 8 to 11 for each mesh resolution.

From the temporal evolution of physical quantities presented in figure 6, it is clear that the second-order Godunov method, with either the PPM interpolation method with slope limiting or the hybrid PPM/WENO method, gives virtually the same results, with the exception of the very coarse mesh where some slight differences exist. In any case, for the same mesh resolution, the fourth-order finite-volume WENO method provides a better solution.

However, the analysis of the spectra does not show the same trend. The spectra presented in figures 5 to 11 for each mesh resolution show that the second-order Godunov method with the hybrid PPM/WENO reconstruction method is able to reproduce virtually the same spectra as the fourth-order finite-volume WENO method. As already presented in the Part 1 of the present paper, the second-order Godunov method with the original PPM method and slope-limiting exhibits a significant pile-up of energy in the high-frequency range. Replacing the slope-limiting procedure by the WENO reconstruction method recovers a monotone spectra close to the reference solution.

As explained in the Part 1 of this paper, the present HIT test case is interesting because it features both shock waves and smooth turbulence structures. As demonstrated in the previous sections and in the Part 1, while the numerical methods follow their theoretical order of convergence when the solution is smooth, they all collapse to first-order in the presence of a discontinuity. In the context of the HIT present simulations, the overall rate of convergence is estimated by computing the \( L^1 \)-norm of the error on the \( x \)-velocity profile. The error \( \epsilon_u \) is reported in figure 12 and the convergence rate computed with a best-fitting curve method is reported in table 2. Overall, all methods exhibit second-order accuracy.

Table 3 presents the average of the computational time for the evaluation of the routines involved in the computation of the hyperbolic convection term, divided by the number of calls during the whole simulation. This nondimensionalization is adopted here because the second-order Godunov procedure requires only one evaluation of the convection term, whereas the finite-volume WENO method is implemented with a Runge-Kutta time integration procedure that requires many calls by time iteration. Also, the simulations are performed with the same mesh resolution of \( N_x = 256 \) and with the same parallelization over 512 MPI process. It turns out that the fourth-order finite-volume WENO method is about 200 times
more computationally expensive than the second-order Godunov method. For the Godunov method, the new hybrid PPM/WENO method proposed in the present paper has roughly the same computational cost as the original PPM method with slope-limiting.

From the results presented in this section, it becomes apparent that an accurate representation of a compressible turbulent flow can be achieved faster with a second-order accurate Godunov method, together with the new hybrid PPM/WENO strategy for the reconstruction of physical values at faces that can achieve the same spectra resolution as a more complex and costly high-order method. In this test case, it appears that the use of a fourth-order finite-volume WENO method is unnecessary in practice.

Figure 6. Time series of selected physical quantities for simulations performed with Godunov/PPM and WENO schemes with different mesh resolution. The circle, square and cross symbols represent the Godunov/PPM, 4-order WENO-Z and the hybrid PPM/WENO methods, respectively. The red, blue, purple and orange colors represent simulations performed with $N_x = 64$, $N_x = 128$, $N_x = 256$ and $N_x = 512$, respectively.
Figure 7. Spectra of selected physical quantities for simulations performed with Godunov+PPM and WENO schemes with different mesh resolution. The circle, square and cross symbols represent the Godunov/PPM, 4–order WENO-Z and the hybrid PPM/WENO methods, respectively. The red, blue, purple and orange colors represent simulations performed with \( N_x = 64 \), \( N_x = 128 \), \( N_x = 256 \) and \( N_x = 512 \), respectively.

Table 2. HIT convergence rate

| Method                    | \( O(\epsilon_p) \) |
|---------------------------|-----------------------|
| PPM with slope-limiting   | 2.15                  |
| 4th-order WENO-Z          | 2.22                  |
| Hybrid PPM/WENO           | 2.08                  |

Table 3. HIT convergence rate

| Method                    | Nondimensional CPU time [s] |
|---------------------------|-------------------------------|
| PPM with slope-limiting   | \( 5.06 \times 10^{-3} \)    |
| 4th-order WENO-Z          | \( 1.1149 \)                |
| Hybrid PPM/WENO           | \( 5.03 \times 10^{-3} \)    |
5. Conclusions

The present Part 2 of the paper describes a novel hybrid PPM/WENO method that has been developed in the context of a second-order Godunov integration procedure. Similarly to the Part 1 of the present paper [12], a careful analysis is performed to assess the performance of the method and comparisons are made to the original PPM method as well as the fourth-order finite-volume WENO method. Results show that the hybrid PPM/WENO method has the ability to capture the turbulent spectra with the accuracy of a formally high-order method, but at the cost of the second-order Godunov method. Overall, it is shown that virtually the same physical solution can be obtained much faster by refining a simulation with the second-order method and carefully chosen numerical procedures, rather than running a coarse high-order simulation.

Appendix A. Slope-flattening procedure

In section 3.2.1 a flattening limiter is imposed at equations (21) and (22) through a flattening coefficient $\chi_i$. The coefficient $\chi_i \in [0, 1]$, where $\chi_i = 1$ indicates that no additional limiting takes place, whereas $\chi_i = 0$ means that the Godunov method is dropped to first-order accuracy. The computation of $\chi_i$ is performed as follows:
(A) Kinetic Energy

(B) Vorticity

(C) Dilatation

(D) Density

Figure 9. Zoom of figure 7 for results computed with mesh $N_x = 128^3$.

(1) First, a dimensionless measure of the shock resolution is computed with

$$\varsigma_i = \frac{p_{i+1} - p_{i-1}}{\max(p_{\text{small}}, |p_{i+2} - p_{i-2}|)}$$

where $p$ is the pressure and $p_{\text{small}}$ is a very small value to avoid a division by zero.

(2) Then the parameter $\tilde{\chi}_i$ is defined as

$$\tilde{\chi}_i = \min\{1, \max[0, a (\varsigma_i - b)]\}$$

where $a = 10$ and $b = 0.75$ are parameters set by the user. In order to confine $\tilde{\chi}_i$ in the range $[0, 1]$, $\tilde{\chi}_i = 0$ if either $u_{i+1} - u_{i-1} < 0$ or

$$\frac{p_{i+1} - p_{i-1}}{\min(p_{i+1}, p_{i-1})} \leq c$$

with $c$ a parameter set by the user, which take the value of $c = 1/3$ here.

(3) Finally $\chi_i$ is computed as follows:

$$\chi_i = \begin{cases} 1 - \max(\tilde{\chi}_i, \tilde{\chi}_{i-1}), & \text{if } p_{i+1} - p_{i-1} > 0, \\ 1 - \max(\tilde{\chi}_i, \tilde{\chi}_{i+1}), & \text{otherwise.} \end{cases}$$
Figure 10. Zoom of figure 7 for results computed with mesh \( N_x = 256^3 \).

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REFERENCES

1. A. Almgren, A. Aspden, J. Bell, and M. Minion, On the Use of Higher-Order Projection Methods for Incompressible Turbulent Flow, SIAM J. Sci. Comput. 35 (2013), no. 1, B25–B42.
2. A. S. Almgren, V. E. Beckner, J. B. Bell, M. S. Day, L. H. Howell, C. C. Joggerst, M. J. Lijewski, A. Nonaka, M. Singer, and M. Zingale, CASTRO: A New Compressible Astrophysical Solver. I. Hydrodynamics and Self-gravity, Astrophys. J. 715 (2010), no. 2, 1221.
Figure 11. Zoom of figure 7 for results computed with mesh $N_x = 512^3$.

Figure 12. HIT convergence study.
3. Ghulam M. Arshed and Klaus A. Hoffmann, *Minimizing errors from linear and nonlinear weights of WENO scheme for broadband applications with shock waves*, J. Comput. Phys. **246** (2013), 58–77.

4. Rafael Borges, Monique Carmona, Bruno Costa, and Wai Sun Don, *An improved weighted essentially non-oscillatory scheme for hyperbolic conservation laws*, J. Comput. Phys. **227** (2008), no. 6, 3191–3211.

5. P. Colella, M.R. Dorr, J.A.F. Hittinger, and D.F. Martin, *High-order, finite-volume methods in mapped coordinates*, J. Comput. Phys. **230** (2011), no. 8, 2952–2976.

6. Phillip Colella and Michael D. Sekora, *A limiter for PPM that preserves accuracy at smooth extrema*, J. Comput. Phys. **227** (2008), no. 15, 7069–7076.

7. Phillip Colella and Paul R Woodward, *The Piecewise Parabolic Method (PPM) for gasdynamical simulations*, J. Comput. Phys. **54** (1984), no. 1, 174–201.

8. Matthew Emmett, Emmanuel Motheau, Weiqun Zhang, Michael Minion, and John B. Bell, *A fourth-order adaptive mesh refinement algorithm for the multicomponent, reacting compressible Navier–Stokes equations*, Combust. Theory and Modelling **0** (2019), no. 0, 1–34.

9. Andrew K. Henrick, Tariq D. Aslam, and Joseph M. Powers, *Mapped weighted essentially non-oscillatory schemes: Achieving optimal order near critical points*, J. Comput. Phys. **207** (2005), no. 2, 542–567.

10. Guang-Shan Jiang and Chi-Wang Shu, *Efficient Implementation of Weighted ENO Schemes*, J. Comput. Phys. **126** (1996), no. 1, 202–228.

11. G.H. Miller and P. Colella, *A Conservative Three-Dimensional Eulerian Method for Coupled Solid–Fluid Shock Capturing*, J. Comput. Phys. **183** (2002), no. 1, 26–82.

12. Emmanuel Motheau and John Wakefield, *Capturing shocks and turbulence spectra in compressible flows. Part 1: Comparison of low and high-order finite-volume methods*, (Submitted for publication).

13. Zhen-Sheng Sun, Yu-Xin Ren, Cédric Larricq, Shi-ying Zhang, and Yue-cheng Yang, *A class of finite difference schemes with low dispersion and controllable dissipation for DNS of compressible turbulence*, J. Comput. Phys. **230** (2011), no. 12, 4616–4635.

14. V.A. Titarev and E.F. Toro, *Finite-volume WENO schemes for three-dimensional conservation laws*, J. Comput. Phys. **201** (2004), no. 1, 238–260.

15. E. F. Toro, M. Spruce, and W. Speares, *Restoration of the contact surface in the HLL-Riemann solver*, Shock Waves **4** (1994), no. 1, 25–34.

16. Bram van Leer, *Towards the ultimate conservative difference scheme. V. A second-order sequel to Godunov’s method*, J. Comput. Phys. **32** (1979), no. 1, 101–136.