Variable high-order overset grid methods for mixed steady and unsteady multiscale viscous hypersonic nonequilibrium flows

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1. Motivation and objectives
The simulation of multiscale turbulence with strong shocks and flows containing both steady and unsteady components requires mixing of numerical methods and switching on appropriate schemes in the appropriate subdomains of the flow fields. The development and validation of the time-accurate, unsteady, variable high-order solver ADPDIS3D for tackling this kind of flows on multiblock overlapping (overset) grids is supported by a grant from the Department of Energy (DOE) SciDAC program through the Science Application Partnership (SAP) initiative. A unique feature of the solver is its ability to perform Direct Numerical Simulation (DNS), resolving all scales of the flow fields, and Large Eddy Simulation (LES), modeling the small turbulent scales, in non-trivial geometries through the use of overset curvilinear grids. ADPDIS3D contains (1) a large number of high-order finite difference schemes and shock-capturing schemes that can be used to perform accurate unsteady computations for flow speeds ranging from nearly incompressible to hypersonics, (2) many innovative low dissipative algorithms that adaptively use numerical dissipation from shock-capturing schemes as postprocessing filters on non-dissipative high-order centered schemes (Sjögreen & Yee 2009b), (Yee et al. 2008), (Yee & Sjögreen 2009), (Yee et al. 2010). Those filter schemes were especially designed for improved accuracy over standard high-order shock-capturing schemes in resolving turbulence with strong shocks and density variations. For multi-dimensional curvilinear grids, the metrics are evaluated at the same high order as the spatial base scheme with high-order freestream preservation (Vinokur & Yee 2000). Recently, these filter schemes were proved to be well-balanced (Wang et al. 2010), i.e., they exactly preserve certain non-trivial steady-state solutions of the chemical nonequilibrium governing equations. With this added property the filter schemes can minimize spurious numerics in reacting flows containing both steady shocks and unsteady turbulence with shocklet components better than standard non-well-balanced shock-capturing schemes. While low dissipative sixth-or higher-order shock-capturing filter methods are appropriate for unsteady turbulence with shocklets, third-order or lower shock-capturing methods are more effective for strong (nearly) steady shocks in terms of convergence. In order to minimize the shortcomings of low order and high-order shock-capturing schemes for the subject flows, ADPDIS3D can utilize overset grids with different types of spatial schemes and orders of accuracy on different chosen grid blocks as an efficient method in combating the difficulty. The modular overset grid framework allows for an optimum synthesis of these new algorithms in such a way that the most appropriate spatial discretizations can be tailored for each particular region of the flow. In addition, ADPDIS3D provides operational interfaces for (1) the MUTATION library (version 1.3, Thierry Magin, private communication) for more accurate transport, chemical and thermodynamics properties for nonequilibrium
flows than standard table look up and mixture rules, and (2) the overset grid generator Ogen (Henshaw 1998) that is part of the Overture platform (Brown et al. 2010). Ogen can be used to generate overlapping grids for high-order accurate approximations that use wide stencils and require high-order accurate interpolation.

Important applications for the proposed solver include: (1) simulation of turbulent hypersonic flows around space vehicles, involving strong steady (or nearly steady) shocks with possible complex turbulence/shocklet interactions near the shoulder and/or in the wake region at different angles of attack; (2) study of the leading edge heat shield due to surface irregularities and/or isolated surface singularities such as very small openings; (3) numerical modeling of the heliosphere, space weather forecasts, supernova explosions and inertial confinement fusion.

The objective of the current paper † is a further validation of the overset grid capability for high-speed chemical nonequilibrium flows. The current investigation, which is a follow-up on previous work by (Sjögreen & Yee 2009b), (Lani et al. 2010a), (Wang et al. 2009), (Wang et al. 2010), (Lani et al. 2010b), extends the use of variable order methods for both inviscid and viscous chemical nonequilibrium flows with strong shocks on 2D and 3D multiblock overlapping grids. A 5-species and one-temperature air model in chemical nonequilibrium is considered in all cases. Second-order TVD, fifth- or higher-order WENO schemes are applied on and around the bow shock in combination with fourth-order or sixth-order filter schemes elsewhere (Yee et al. 2008). Unlike the standard pseudo time-marching to the steady state, in order to assess the capability of unsteady computations, the computations are time accurate even though the chosen test cases are laminar.

The paper is organized as follows: first, the governing equations and the numerical methodology are described; second, some numerical computations using variable order methods on inviscid and viscous test cases in conditions of chemical nonequilibrium are discussed. The latter also include a preliminary result of a mixed steady/unsteady nonequilibrium 3D computation with variable order numerical schemes on an Apollo-like Crew Exploration Vehicle (CEV). This is a work in progress of the first several stages of a multistage validation process for the nonequilibrium implementation.

2. Flow solver

2.1. Governing equations

The system of governing equations for a gas mixture in thermodynamic equilibrium and chemical nonequilibrium can be expressed in conservative form as:

$$\frac{\partial U}{\partial t} + \left( \frac{\partial F_k(U)}{\partial x_k} \right)_k + \left( \frac{\partial G_k(U)}{\partial x_k} \right)_k = S(U), \quad k = 1, \ldots, 3, \tag{2.1}$$

where $U = (\rho_s, \rho v, \rho E)^T$ are the conservative variables, and $\rho_s$ the partial densities with $s = 1, \ldots, N_s$ for a mixture of $N_s$ species. The convective and diffusive fluxes, $F_k$ and $G_k$ are

$$F_k = \begin{pmatrix} \rho s v_k \\ \rho v_k v_l + p \delta_{kl} \\ \rho v_k H \end{pmatrix}, \quad G_k = \begin{pmatrix} \rho s v_{sk} \\ -\tau_{kl}v_l + q_k + \sum_s \rho_s v_{sk} h_s \\ -\tau_{kl}v_l + q_k + \sum_s \rho_s v_{sk} h_s \end{pmatrix}, \quad l = 1, \ldots, 3. \tag{2.2}$$

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where \( h_s \) and \( H \) are the species and total enthalpy per unity mass, \( v \) are the velocity components and \( v_{sk} \) are the diffusion velocities. \( S(U) \) in Eq. 2.1 represents the mass production/destruction term. More details on the thermodynamic, transport and chemical properties, as provided by MUTATION 1.3, can be found in (Wang et al. 2009), (Lani et al. 2011), (Magin & Degrez 2004), (Park 1993).

2.2. Finite difference discretizations

In spite of the large number of low dissipative high-order schemes contained in AD-PDIS3D that have been extensively validated for a perfect gas and for several 1D and 2D nonequilibrium flow test cases (Sjögreen & Yee 2009b), (Yee et al. 2008), (Yee & Sjögreen 2009), (Yee et al. 2010), (Wang et al. 2010), the present study only considers Harten-Yee TVD (Yee 1989), fifth- and seventh-order well-balanced WENO-Lax Friedrichs (WENO5-LF, WENO7-LF) (Wang et al. 2009), (Wang et al. 2010), fourth-order or sixth-order filter central finite difference schemes (Yee et al. 2008) for the numerical experiments in this paper. In particular, WENO-LF schemes have been used in blocks enclosing the bow shock to discretize the convective fluxes, whereas the dissipative portion of WENO5 has been utilized elsewhere as a high-order nonlinear filter for sixth-order central base schemes (WENO5f). In viscous computations, a central discretization of the same order as the convection flux derivatives is used for the viscous flux derivatives. In all simulations a pointwise evaluation of the source term has been applied. The explicit second- or fourth-order Runge-Kutta method is used in a time-accurate mode for the time discretization. Due to the explicit time-accurate computation, a very large number of iterations should be expected to reach steady state. Since time accuracy is not a concern for the 2-D blunt body flow as it consists of a major bow shock and smooth flow on the remainder of the flow field, fourth-order (RK4) Runge-Kutta schemes have been employed for the test cases. With a sufficiently fine grid, unsteady features of the Apollo-like CEV flow field, if they exist, can be observed with this time-accurate approach.

2.2.1. Well-balanced high-order filter schemes for reacting flows

Part of the inaccuracy in Direct Numerical Simulations (DNS) and Large Eddy Simulations (LES) of turbulent flow using standard high-order shock-capturing schemes is due to the fact that this type of computation involves long time integrations. Standard stability and accuracy theories in numerical analysis are not applicable to long time wave propagations and/or long time integrations (Stuart & Humphries 1998). Modern shock-capturing schemes were originally developed for rapidly evolving unsteady shock interactions and short time integrations. Any numerical dissipation inherent in the scheme, even for high-resolution shock-capturing schemes that maintain their high-order accuracy in smooth regions [e.g., fifth- and seventh-order WENO schemes (WENO5 and WENO7)] (Jiang & Shu 1996), will be compounded over long time integration leading to smearing of turbulence fluctuations to unrecognizable forms. Current trends in the containment of numerical dissipation in DNS and LES of turbulence with shocks are summarized in (Yee & Sjögreen 2009), (Yee et al. 2008). Here, the performance of the high-order nonlinear filter schemes with preprocessing and postprocessing steps in conjunction with the use of a high-order non-dissipative spatial base scheme (Yee & Sjögreen 2009) is briefly summarized.

Preprocessing step. Before the application of a high-order non-dissipative spatial base scheme, the preprocessing step to improve stability splits inviscid flux derivatives of the governing equation(s) in the following three ways, depending on the flow type and the desire for rigorous mathematical analysis or physical argument.
• Entropy splitting of (Olsson & Oliger 1994) and (Yee et al. 2000), (Yee & Sjögreen 2002): The resulting form is non-conservative and the derivation is based on entropy norm stability with numerical boundary closure for the initial value boundary problem.
• The system form of the splitting by (Ducros et al. 2000): This is a conservative splitting and the derivation is based on physical arguments.
• Tadmor entropy conservation formulation for systems (Sjögreen & Yee 2009a): The derivation is based on mathematical analysis. It is a generalization of Tadmor’s entropy formulation to systems and has not been fully tested on complex flows.

Postprocessing step. After the application of a non-dissipative high-order spatial base scheme on the split form of the governing equations, in order to further improve nonlinear stability from the non-dissipative spatial base scheme, the postprocessing step of (Yee & Sjögreen 2007), (Yee & Sjögreen 2009), (Sjögreen & Yee 2000) is applied. The solution is non-linearly filtered by a dissipative portion of a high-order shock-capturing scheme with a local flow sensor. These flow sensors provide locations and amounts of built-in shock-capturing dissipation. To be more precise, the idea of these nonlinear filter schemes for turbulence with shocks is that, instead of relying solely on very high-order high-resolution shock-capturing methods for accuracy, the filter schemes (Yee et al. 1999), (Yee et al. 2000), (Sjögreen & Yee 2000), (Yee & Sjögreen 2007) take advantage of the effectiveness of the nonlinear dissipation contained in good shock-capturing schemes as stabilizing mechanisms at locations where needed. Such a filter method consists of two steps: a full-time step using a spatially high-order non-dissipative base scheme, followed by a postprocessing filter step. The postprocessing filter step consists of the products of wavelet-based flow sensors and nonlinear numerical dissipations. The flow sensor is used in an adaptive procedure to analyze the computed flow data and indicate the location and type of built-in numerical dissipation that can be eliminated or further reduced. The nonlinear dissipative portion of a high-resolution shock-capturing scheme can be any TVD, MUSCL, ENO, or WENO scheme. By design, the flow sensors, spatial base schemes and nonlinear dissipation models are stand alone modules. Therefore, a whole class of low dissipative high-order schemes can be derived with ease.

Properties of the method. Some attributes of the high-order filter approach are:
• Spatial Base Scheme: high-order and conservative (no flux limiter or Riemann solver is involved).
• Physical Viscosity: The contribution of physical viscosity, if it exists, is automatically taken into consideration by the base scheme in order to minimize the amount of numerical dissipation to be used by the filter step.
• Efficiency: The filter step requires one Riemann solve per dimension per time step, independent of time discretizations (less CPU time and fewer grid points than their standard shock-capturing scheme counterparts).
• Accuracy: Containment of shock-capturing numerical dissipation via a local wavelet flow sensor.
• Well-balanced scheme: These nonlinear filter schemes are well-balanced for certain chemical reacting flows (Wang et al. 2010).
• Parallel Algorithm: Suitable for most current supercomputer architectures.

2.2.2. Variable high-order multiblock overset grid methods
For over two decades, second- and third-order shock-capturing schemes employing time-marching to the steady state have enjoyed much success in simulating many transonic, supersonic and hypersonic steady aeronautical flows containing strong shocks. In the presence of mixed steady and unsteady multiscale viscous flows, low order (third-order
or lower) time-accurate methods are not effective in accurately simulating, e.g., unsteady turbulent fluctuations containing shocklets. At the same time, high-order schemes with good unsteady shock-capturing capability suffer from an inability to converge to the proper steady shocks effectively. Attempts to improve the convergence rate of high-order methods for strong steady shocks involve order reduction near steep gradient regions or added numerical dissipation of the scheme in the vicinity of the shocks, thus degrading the true order of the scheme in other parts of the flow. Although extreme grid refinement in conjunction with low order schemes can be used on the unsteady turbulence part of the flow field, increases in CPU time and instability and stiffness of the overall computations are inevitable. One method to effectively overcome these difficulties for mixed steady and unsteady viscous flows is a multiblock overset grid with a different order and different type of numerical scheme on different blocks.

Stable SBP (summation-by-parts) energy norm numerical boundary procedures (Olsson 1995) for high-order central spatial schemes are employed at physical boundaries. Second-, third- and fourth-order Lagrangian interpolations are options in the solver ADPDIS3D to be used for interpolating grid point values among the block overlapping regions (Chesshire & Henshaw 1990). For stability, in most of the computations, a second-order interpolation is preferred. In the presence of physical viscosity and curvilinear grids, matching high-order spatial scheme such as the inviscid terms for viscous flux derivatives and metric evaluations with freestream preservation are used (Vinokur & Yee 2000), respectively. The multiblock option can, e.g., easily accommodate low order shock-capturing schemes in regions of steady shocks and high-order schemes in regions containing unsteady turbulence and shocklets. See (Sjögren & Yee 2009b), (Sjögren et al. 2009) for details.

3. Overset grid numerical results for chemical nonequilibrium flows

Before embarking on multiscale problems containing mixed steady and unsteady shock/turbulence interactions, we first illustrate a few simple blunt body test cases to validate the high-order overlapping approach. The test cases were chosen to contain a strong bow shock without any mixed unsteady components in the flow. Furthermore, in order to validate the proposed variable high-order multiblock overlapping grid methods, only two different orders of schemes are used as an illustration.

3.1. A 2D chemical nonequilibrium flow past a cylinder

A 2D test case simulating high-speed air flow around a 1 m radius cylinder has been chosen for the inviscid and viscous numerical experiments. The free stream and wall conditions (for the viscous case) are given in Table 1. This test case was computed by Peter Gnoffo (private communication) and further studied by Xiaowen Wang from the UCLA SciDAC team. The physico-chemical model used in the present work does not consider thermal nonequilibrium as in Xiaowen Wang’s study, but uses more sophisticated and computationally expensive thermodynamic and transport properties (see Section II.A for details) as opposed to energy fitting polynomials and mixture rules. The chemical reaction rate coefficients for characterizing the neutral air mixture are taken from (Park 1993) by neglecting reactions involving ions and electrons. The performance of TVD, WENO5 and WENO7 on a single block and overset meshes for the inviscid case can be found in (Lani et al. 2011). Here, some results with mixed WENO5 and sixth-order filter central scheme on the overset mesh are presented for the inviscid case. Finally, a simulation of higher-order filter schemes for the viscous case is included. Since this
Table 1. Free stream and wall conditions for Gnoffo’s test case.

<table>
<thead>
<tr>
<th>$M_\infty$</th>
<th>$\rho_\infty$ (kg/m$^3$)</th>
<th>$U_\infty$ (m/s)</th>
<th>$T_\infty$ (K)</th>
<th>$T_w$ (K)</th>
<th>$Re_\infty$</th>
</tr>
</thead>
<tbody>
<tr>
<td>17.64</td>
<td>0.0001</td>
<td>5000</td>
<td>200</td>
<td>553.3</td>
<td>37634.8</td>
</tr>
</tbody>
</table>

is a time-accurate approach, the residual tracking has not been used as a convergence criterion. However, simulations are computed for long enough (typically up to 500,000 iterations and 1,000,000 iterations for inviscid and viscous cases respectively, using a CFL number up to 0.8, depending on the case) to allow the flow to be fully established.

3.1.1. Inviscid case: mixed WENO5 and 6$^{th}$-order central filter scheme (WENO5fi)

Results using variable high-order methods have been computed on two three-block overset meshes, one coarse and one twice as fine in all directions. WENO5-LF was used for the shock block, while a sixth-order central discretization with dissipative portion of the corresponding WENO scheme as a non-linear filter (WENO5fi) (Yee et al. 2008) was used on the body and background blocks. Figures 1 and 2 illustrate the temperature isolevels and stagnation line profiles for the two meshes. The shock and the overall flowfield are well captured even on the coarse overset mesh. A smooth transition between blocks has been achieved. Figures 3 and 4 show pressure and temperature fields, respectively, computed on the fine mesh by the variable high-order method for the three different cases WENO5-LF, WENO5-LF-WB and TVD schemes on the shock block. Although their pressure isolines are indistinguishable, some small differences can be identified in the temperature isolines between WENO schemes and TVD within the shock block. The difference increases while moving far from the stagnation region where the mesh is less aligned with the flow.

3.1.2. Viscous case: mixed TVD and 4$^{th}$-order central filter schemes

The interested reader is referred to (Lani et al. 2010b) for a preliminary validation of Gnoffo’s test case in viscous conditions on single and overset block grids with a TVD scheme. This subsection presents the same viscous test case on a three-block overset grid configuration with, in particular, $201 \times 120$ points in the shock block and $123 \times 240$ points in the boundary layer block. Figure 5 shows the grid. The grid used is far from being optimal. A stretched boundary grid with a better grid aspect ratio should be used. The grid spacing on the wall is 0.0008 (m). Figure 6 shows the temperature obtained with a mixed approach, where the second-order TVD scheme is used on the shock grid and the fourth-order centered approximation, filtered nonlinearly with the dissipative portion of the TVD scheme (D04+TVDfi) in conjunction with Ducros et al. splitting a preprocessing step discussed in Section I, is used on the boundary layer grid.

Figure 7 shows the close-up boundary-layer grid with high aspect ratio overlapping with the background grid. Figure 8 displays iso-density contours of the solution by the TVD scheme. Figures 9 and 10 show solutions obtained with different fourth-order schemes on the boundary layer grid, while keeping the TVD scheme on the other grids. Figure 9 shows the solution with the fourth-order spatial central scheme and sixth-order constant linear dissipation (D04+AD6) on the boundary grid. Figure 10 shows the result by the same fourth-order central spatial scheme on the boundary grid but with the nonlinear
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*Figure 1.* Temperature isolevels (in K) on the coarse (grey dashed isolines) and fine (black solid isolines) overset meshes: sixth-order central filtered (WENO5fi) is applied on body and background blocks, WENO5-LF on the shock block. Part of the background block has been left out.

*Figure 2.* Temperature stagnation line profiles on the coarse (dashed lines) and fine (solid lines) overset meshes: sixth-order central filtered (WENO5fi) is applied on body and background blocks, WENO5-LF on the shock block.

*Figure 3.* Pressure isolevels (in Pa) on the overset mesh: sixth-order central filtered (WENO5fi) is applied on body and background block, WENO5-LF (black solid isolines), WENO5-LF-WB (grey dashed isolines), TVD (black long dashed isolines) on the shock block.

*TVD filter as a postprocessing step (D04ss+TVDfi) instead of the sixth-order linear dissipation. D04ss+TVDfi also employs the Ducros et al. splitting as a preprocessing step as described previously in section I. The solution shown is converged, but it appears that the number of grid points was insufficient to obtain accuracy in the high-aspect ratio overlapping boundary grid region. It is expected that one or two levels of grid refinement.*
Figure 5. Upper half of the three-block overset mesh used for the mixed order viscous computation. Boundaries for shock and body blocks are highlighted in white.

Figure 6. Temperature contours and isolines with fourth-order central with TVD filter.

Figure 7. Boundary layer grid at one segment of the boundary.

Figure 8. Density isolines: second-order TVD scheme is used in the boundary layer block.

will overcome the inaccuracy problem. The grid refinement study will be included in a forthcoming paper.

3.2. 3D chemical nonequilibrium example: Apollo-like CEV computation

Improved CFD predictability of future CEV afterbody flowfields in various flight conditions are of great importance for future aerospace explorations. In light of the fact that future CEV has increased in size and weight, and consequently has higher Reynolds numbers over the previously considered configurations, the ability to better characterize the base heating and the role of transition and turbulence in future aerothermodynamic design (MacLean et al. 2009) remains a pacing item for aerothermodynamicists. Here, the preliminary investigation on a CEV-like geometry started in (Sjögreen & Yee 2009b) is continued but in conditions (see Table 2) taken from (Sinha et al. 2004), and corre-
Table 2. Free stream and wall conditions for the CEV simulation.

<table>
<thead>
<tr>
<th>( h ) (km)</th>
<th>( M_\infty )</th>
<th>( \rho_\infty ) (kg/m(^3))</th>
<th>( U_\infty ) (m/s)</th>
<th>( \alpha ) ((^\circ))</th>
<th>( T_\infty ) (K)</th>
<th>( T_w ) (K)</th>
<th>( Re ) (10(^6))</th>
</tr>
</thead>
<tbody>
<tr>
<td>35</td>
<td>16</td>
<td>0.0082</td>
<td>5000</td>
<td>0</td>
<td>237</td>
<td>553.3</td>
<td>1.76</td>
</tr>
</tbody>
</table>

The first step of the investigation consists of a time-accurate Navier-Stokes computation without any turbulence model but including chemical nonequilibrium effects. The same neutral five-species model used for the 2D case is utilized here, with reaction rate coefficients derived from (Park 1993). Thermodynamics and transport properties are described in (Lani et al. 2011). For a low enough Reynolds number and with a fine enough grid to resolve all scales, the simulation could be considered as a DNS computation.

3.2.1. Viscous flow: TVD scheme

A six-block 3D viscous overset mesh consisting of 26.5M nodes was used as a first step in the investigation. In order to keep the computational cost affordable, the size of the first cell on the wall has been set to 0.003 (m). A snapshot of the overset mesh, featuring all six blocks around and on the capsule, is depicted in Figure 11. To obtain a benchmark flow field, the TVD scheme was applied to four blocks and a first-order Roe scheme was applied on the two blocks containing the shock. The flow conditions for this test case are listed in Table 2.

Figure 12 shows that all the typical features of this kind of flow are well detected [see a perfect gas solution from (Sinha et al. 2004), (Yee et al. 2008) for a qualitative comparison]. After undergoing a severe compression through the bow shock, the flow heats up to about 6000 K in the stagnation region. The strong expansion around the aft
causes the temperature to drop considerably and the laminar boundary layer to separate at the beginning of the conical afterbody. A thick rake of shear layers forms, enclosing a large recirculation region which extends up to the neck region about one and a half capsule diameters further, where a weak recompression shock wave forces the flow to return parallel to the axis.

4. Conclusions

In the present paper, variable high-order methods have been applied to the simulation of hypersonic flows in chemical nonequilibrium on multiblock overlapping meshes. In order to validate the time-accurate nonequilibrium flow implementation, a time-accurate approach has been conducted on 2D and 3D inviscid and viscous chemical nonequilibrium laminar flows with strong shocks before embarking on multiscale problems containing both steady and unsteady shock/turbulence interactions. All the considered test cases are laminar flows with a strong steady bow shock.

A fourth-order or sixth-order central space discretization has been successfully combined with upwind TVD or WENO schemes for 2D inviscid and viscous cases, where the lower order has been confined only to the block including the bow shock. The variable high-order method has been further validated in the case of the high-speed flow over the 3D CEV space vehicle, under realistic flight conditions. The results of a preliminary viscous computation with TVD schemes have been shown and will be the basis for future analyses where high-order filter schemes are used away from the shock to better resolve critical flow features such as the laminar boundary layer up to the capsule shoulder, the flow separation on the conical afterbody, the shock/shear interaction occurring in the neck region and the overall wake dynamics.

Representative test cases with mixed steady and unsteady turbulence with strong shocks components that can benefit fully from the present high accuracy approach will be presented in forthcoming papers.
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