Explicit discontinuous spectral element method with entropy generation based artificial viscosity for shocked viscous flows

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Abstract

A spatio-temporal adaptive artificial viscosity (AV) based shock-capturing scheme is proposed for the solution of both inviscid and viscous compressible flows using a high-order parallel Discontinuous Spectral Element Method (DSEM). The artificial viscosity and artificial thermal conduction coefficients are proportional to the viscous and thermal entropy generating terms, respectively, in the viscous entropy conservation law. The magnitude of AV is limited based on the explicit stable CFL criterion, so that the stable artificial viscous time step size is greater than the convective stable time step size. To further ensure the stability of this explicit approach, an adaptive variable order exponential filter is applied, if necessary, in elements where the AV has been limited. In viscous flow computations a modified Jameson's sensor (Ducros *et al.*, JCP **152** (2)) limits the AV to small values in viscous shear regions, so as to maintain a high-order resolution in smooth regions and an essentially non-oscillatory behavior near sharp gradients/shocks regions. We have performed a systematic and extensive validation of the algorithm with one-dimensional problems (inviscid moving shock and viscous shock-structure interaction), two-dimensional problems (inviscid steady and unsteady shocked flows and viscous shock-boundary layer interaction), and a three-dimensional supersonic turbulent flow over a ramped cavity. These examples demonstrate that the explicit DSEM scheme with adaptive artificial

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viscosity terms is stable, accurate and efficient.

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1 The development of accurate and efficient algorithms for the simulation
2 of high-speed flows in complex geometry has challenged the scientific com-
3 munity for several decades. While much progress has been made, the efficient
4 and accurate Direct Numerical Simulation (DNS) and Large Eddy Simulation
5 (LES) of dynamic environments that include viscous phenomena, turbulence,
6 shocks and their nonlinear interactions in a complex geometry continues to
7 present major challenges. In general, the community agrees, as the first step,
8 that high-order/resolution numerical schemes are necessary to resolve and
9 understand small scale flow phenomena and its interaction with shocks with
10 limited computational resources.

11 Many high-order/resolution shock-capturing nonlinear schemes have been
12 designed for application on structured meshes with simple geometry. Most
13 noticeably, one of such nonlinear methods is the high-order Weighted Es-
14 sentially Non-oscillatory (WENO) scheme [1, 2] that combines an essen-
15 tially non-oscillatory shock capturing ability with high resolution of small
16 scales. For complex geometry, WENO can be applied in combination with
17 the immersed boundary method [3, 4] and adaptive mesh refinement [5,
18 6] or through a multi-block mapping approach [7]. For the simulation of
19 multi-dimensional compressible turbulent flows in complex geometry, how-
20 ever, WENO schemes for unstructured mesh (for example [8–11]) are still
21 at their infancy. Moreover, WENO is overly dissipative and computationally
22 inefficient for turbulent flow computation [12–14]. Hybrid numerical schemes
23 that hybridize the nonlinear WENO scheme with low dissipative and more
24 efficient linear (for example, finite difference, spectral, Fourier continuation
25 and compact) schemes [2, 15–17] have been developed in recent years, but
26 are yet to be extended to applications with complex geometry.

27 The literature of high-order shock-capturing methods for unstructured
28 meshes is much less extensive than that of structured mesh. High-order dis-
29 continuous Galerkin (DG) or more general Discontinuous Spectral Element
30 Method (DSEM) represent a class of an unstructured mesh method that has
31 received much attention in terms of shock-capturing recently. DSEM com-
32 bines the advantages of low dispersion and dissipation, boundary fitting for
33 complex geometry and an h/p adaptive mesh approach for high-resolution

of small-scale structures. DSEM is cost effective as compared to high-order WENO schemes (see [18] for a brief overview).

In order to suppress Gibb's oscillations near shocks with higher-order basis functions that DSEM relies on, slope limiters are often employed. The bulk of literature reports on the development and augmentation of explicit Runge Kutta Discontinuous Galerkin (RKDG) methods with min-mod slope limiters introduced by Cockburn [19, 20]. The concept of slope limiting is enhanced in [21] by applying a discontinuity detector based on a posteriori error estimates of the solution jump over neighbouring element interfaces [22, 23]. Works presented in [24–26] report on the usage of both shock detector and slope limiters on unstructured meshes. A dynamic p -adaptive gradient based limiting is discussed in [27–29] for unstructured mesh. A positivity-preserving limiter is used in [30] to enforce the minimum entropy principle. Positivity preserving limiting is also proposed in conjunction with 2D mixed element unstructured meshes in [31, 32]. In general, limiters are less robust as compared to WENO reconstruction in their control of spurious oscillations in flows with strong shocks. As mentioned in [33], RKDG type implementation experiences difficulty in reducing the residual in steady-state problems. RKDG method combined with WENO limiters are producing promising results [34–40]. However, the performance of these schemes in 3D complex shock-turbulence interactions in complex geometry is yet to be established. The design and application of multi-dimensional limiters for broader application is still an open issue.

A cost-effective alternative to limiting is the artificial viscosity (AV) approach (see [41–44]) where artificial higher, even-order differential terms are added to the equations to dissipate the high frequency waves or smoothen the small scale structures. The major consequence of such approach is that the stable time step required by an explicit time stepping scheme (for example, Runge-Kutta scheme) must be additionally restricted by artificial viscous terms. For shocked flows, the artificial coefficients could become quite large and the resulting time step must be becoming very small just for maintaining the numerical stability.

In the context of DSEM and DG, a number of AV approaches have been developed. A summary of them is presented in Table 1. In the first part of the table, references are listed that have focused on DG and scaled the artificial viscosity in a number of ways based on additional PDE and ODE solutions. The second half of the table lists the contributions pertaining to the entropy viscosity approach. In [45, 46] the concept of an AV scaled

with the entropy residual (entropy viscosity) was introduced for Continuous/Discontinuous Galerkin method suitable for structured or unstructured mesh. The applicability of the AV in collocation type DSEM methods can be found in [47, 48]. Implementation and validation of DSEM has generally been restricted to inviscid flows in two-dimensions. The viscous three-dimensional flow interaction with shocks has not been addressed (as can be deduced from Table 1), which is the main focus of this study.

We develop and assess a high-order parallel DSEM algorithm using an adaptive artificial viscosity approach (DSEM-AV) that captures shocks and provides high-order resolution for both two- and three-dimensional viscous compressible turbulent flows in complex geometries. We propose an estimation of AV scaled with the non-negative entropy generation term in the viscous entropy equation (as opposed to the inviscid entropy residual [45]). The artificial viscosity and thermal conductivity coefficients are designed to be proportional to the entropy generation by viscous and thermal dissipation. To detect high gradients and shocks in each element, a modified Jameson’s (Ducros) shock sensor [61] is employed and the AV coefficients are limited to reduce artificial dissipation in viscous shear regions in order to capture small scale structures such as Kelvin-Helmoltz instability. To remove the severe viscous time step restriction related to a large AV when using an explicit Runge-Kutta scheme, the magnitude of AV is limited to ensure that the stable CFL and viscous time step conditions are of the same order regardless of the AV. To enhance the stability of the numerical scheme in elements containing a strong shock, a spatial-adaptive variable order exponential filter is also used. We have performed a systematic and extensive validation of the DSEM-AV with one-dimensional problems (inviscid moving shock, and viscous shock-structure interaction), two-dimensional problems (inviscid steady and unsteady shocked flows, and viscous shock-boundary layer interaction), and a three-dimensional supersonic turbulent flow over a ramped cavity. These examples demonstrate that the explicit DSEM-AV with adaptive artificial viscosity terms is stable, accurate and efficient.

The paper is organized as follows. After a brief description of the governing equations and 3D DSEM formulation in Sec. 1, the details of the new proposition of artificial viscosity and spectral filter are addressed in Section 2. A wide range of one- and two-dimensional problems is presented as validation to establish the applicability of the formulation, and the results of the three-dimensional supersonic ramped cavity are presented in Sec. 3. Conclusions are given in Sec. 4.

Reference	Method/Specification	Cases
2002, Vegt & Ven [49]	DG + AV (pressure jump/residual based) + AMR	2D inviscid
2006, Hartman [50]	DG + FE residual based AV + AMR	2D inviscid/NS
2006, Persson & Peraire [51]	DG + piecewise AV + smoothness indicator	2D inviscid
2007, Touil <i>et al.</i> [52]	DSEM + spectral level set (Godunov element)	1D inviscid
2010, Barter & Darmofal [33]	DG + PDE model of AV	1D/2D inviscid
2011, Bassi <i>et al.</i> [53]	DG + pressure gradient based AV	2D NS (transonic)
2011, Klöckner <i>et al.</i> [54]	DG + piecewise AV (like in [51])	2D NS
2011, Atkins <i>et al.</i> [55]	DG + ODE of AV (modified form of [33])	1D/2D inviscid
2013, Nazarov <i>et al.</i> [56]	FE + Residual based AV	2D inviscid/3D implicit LES
2013, Yücel <i>et al.</i> [57]	DG + piecewise (like in [51])	2D reaction-diffusion
2013, Reisner <i>et al.</i> [58]	C-method + parabolic regularization (PDE)	1D inviscid
2011, Guermond <i>et al.</i> [45]	FE/DG/Fourier + Entropy viscosity	1D/2D inviscid
2013, Zingan <i>et al.</i> [46]	DG + Entropy viscosity	1D/2D inviscid
2013, Delchini <i>et al.</i> [59]	FE + Entropy viscosity	1D inviscid
2014, Berry <i>et al.</i> [60]	Entropy viscosity	1D single/two phase flow
2014, Abbassi <i>et al.</i> [48]	DSEM + modified Entropy viscosity	1D/2D inviscid

Table 1: A short review of existing literature of artificial viscosity in conjunction with high-order methods. NS: Navier-Stokes, AMR: Adaptive mesh refinement, PDE: Partial differential equation, ODE: Ordinary differential equation

110 1. Numerical method

111 In this section, a brief description is given of the governing equations and
 112 a flavor of the DSEM that uses a staggered, Chebyshev collocation method to
 113 approximate the compressible Navier-Stokes equations. The DSEM method
 114 has been extensively discussed and used for the solution of *smooth* flows [62–
 115 66]. We shall present several numerical techniques used in extending the
 116 DSEM to *non-smooth* flows that contain both small scale smooth structures
 117 and large scale high gradients/shocks. A spatial-temporal adaptive artificial
 118 dissipation is devised by means of a combination of artificial viscosity
 119 and thermal conductivity coefficients scaled with viscous entropy generation
 120 terms. We will also discuss the limiting of the artificial dissipation in such
 121 a way that the stable time step for an *explicit* Runge-Kutta time stepping
 122 scheme can be maintained. An adaptive method that adjusts the dissipation
 123 through a shock sensor and a variable order exponential filter is presented
 124 that enhances accuracy and stability of the nonlinear PDEs.

125 1.1. Governing equations

126 The non-dimensional governing Navier-Stokes conservation laws for a
 127 compressible fluid are given by

$$\frac{\partial \mathbf{Q}}{\partial t} + \nabla \cdot \mathcal{F}^a(\mathbf{Q}) - \frac{1}{Re_f} \nabla \cdot \mathcal{F}^v(\mathbf{Q}) = 0, \quad (1)$$

and

$$\mathbf{Q} = \begin{pmatrix} \rho \\ \rho \mathbf{u} \\ \rho E \end{pmatrix}, \quad \mathcal{F}^a(\mathbf{Q}) = \begin{pmatrix} \rho \mathbf{u} \\ \rho \mathbf{u} \mathbf{u} + p \bar{\delta} \\ (\rho E + P \bar{\delta}) \mathbf{u} \end{pmatrix}, \quad \mathcal{F}^v(\mathbf{Q}) = \begin{pmatrix} 0 \\ \bar{\tau} \\ \bar{\tau} \mathbf{u} + \frac{\kappa}{(\gamma-1)M_f^2 Pr_f} \nabla T \end{pmatrix},$$

128 where $\mathbf{Q}$ is the conservative variable, $\mathcal{F}^a$ and $\mathcal{F}^v$ are the inviscid and viscous
 129 fluxes, respectively, ρ is the density, $\mathbf{u}$ is the velocity vector, and E is the
 130 total internal energy. P and T are the static pressure and temperature,
 131 respectively. γ is the ratio of specific heats. δ is the Kronecker delta tensor.
 132 M_f, Re_f and Pr_f are the reference Mach number, Reynolds number, and
 133 Prandtl number, respectively, and κ is the thermal conductivity. The viscous
 134 shear stress tensor is given by,

$$\bar{\tau} = 2\mu \bar{\mathcal{S}} + \left(-\frac{2}{3}\mu\right) (\nabla \cdot \mathbf{u}) \bar{\delta}, \quad (2)$$

135 where $\bar{S} = \frac{1}{2} (\nabla \mathbf{u} + (\nabla \mathbf{u})^\mathbb{T})$ is the symmetric part of the velocity gradient
 136 tensor and the superscript $\mathbb{T}$ identifies a transpose. μ is the non-dimensional
 137 viscosity which is taken unity throughout. The ideal gas equation of state,
 138 $p = \rho T / (\gamma M_f^2)$, closes the equations. In this study, we take $\gamma=1.4$, $M_f = 1$
 139 and $Pr_f = 0.72$ for all cases reported here.

140 1.2. Three-dimensional DSEM: staggered formulation

141 In the nodal collocation formulation of the DSEM, the approximation
 142 begins with the subdivision of the physical domain into K hexahedral phys-
 143 ical elements, $\Omega_k, k = 1, \dots, K$). Each physical element is then mapped
 144 by an iso-parametric transformation (a linear blending formula) to a unit
 145 cubic computational element in the computational domain. Hence, in each
 146 computational element, Eqn. (1) becomes,

$$\frac{\partial \tilde{\mathbf{Q}}}{\partial t} + \tilde{\nabla} \cdot \tilde{\mathcal{F}} = 0, \quad (3)$$

147 where $\tilde{\mathbf{Q}} = |\bar{J}| \mathbf{Q}$, $\tilde{\nabla} \cdot \tilde{\mathcal{F}} = \frac{\partial \tilde{\mathbf{f}}}{\partial \xi} + \frac{\partial \tilde{\mathbf{g}}}{\partial \eta} + \frac{\partial \tilde{\mathbf{h}}}{\partial \zeta}$ and

$$(\tilde{\mathbf{f}}, \tilde{\mathbf{g}}, \tilde{\mathbf{h}})^\mathbb{T} = |\bar{J}|^{-1} (\mathbf{f}^a - \frac{1}{Re_f} \mathbf{f}^v, \mathbf{g}^a - \frac{1}{Re_f} \mathbf{g}^v, \mathbf{h}^a - \frac{1}{Re_f} \mathbf{h}^v)^\mathbb{T}, \quad (4)$$

148 with $|\bar{J}| = x_\xi(y_\eta z_\zeta - y_\zeta z_\eta) - x_\eta(y_\xi z_\zeta - y_\zeta z_\xi) + x_\zeta(y_\xi z_\eta - y_\eta z_\xi)$ being the
 149 determinant of the Jacobian matrix of the domain transformation.

150 In the staggered grid, spectral formulation, the solution $\tilde{\mathbf{Q}}$ is collocated
 151 at the Chebyshev-Gauss quadrature points while the fluxes are collocated
 152 at the Chebyshev-Lobatto quadrature points. In one dimensional domain
 153 $0 \leq \xi \leq 1$, the Gauss (g) points $\xi_{i+1/2}$ and the Lobatto (l) points ξ_i of the
 154 $N - 1$ and N degree Chebyshev polynomial, respectively, are defined by,

$$\xi_{i+1/2} = \frac{1}{2} \left[1 - \cos \left(\frac{i + \frac{1}{2}}{N + 1} \right) \pi \right] \quad i = 0, 1, \dots, N - 1. \quad (5)$$

$$\xi_i = \frac{1}{2} \left[1 - \cos \left(\frac{i\pi}{N} \right) \right] \quad i = 0, 1, \dots, N. \quad (6)$$

155 In three dimensions, the Gauss points, denoted by the superscript ggg , is
 156 determined by the tensor product of the three one-dimensional Cartesian
 157 grids (see Fig. 1). Assuming an equal number of collocation points in each

Figure 1: Gauss and Lobatto points in a mapped reference domain for a P2 element. Symbols, filled circle: *ggg*, open square: *lgg*, open circle: *glg*, open triangle *ggl*.

158 direction, the solution values $\tilde{\mathbf{Q}}$ collocated on the *ggg* point can be expressed
 159 as

$$\tilde{\mathbf{Q}}(\xi, \eta, \zeta) = \sum_{i=0}^{N-1} \sum_{j=0}^{N-1} \sum_{k=0}^{N-1} \tilde{\mathbf{Q}}_{i+1/2, j+1/2, k+1/2}^{ggg} h_{i+1/2}(\xi) h_{j+1/2}(\eta) h_{k+1/2}(\zeta), \quad (7)$$

160 where $h_{p+1/2}(\xi)$ is the Lagrange interpolation polynomial of degree at most
 161 $N - 1$ defined on the Gauss (*g*) points $\xi_{m+1/2}$, $m = 0, \dots, N - 1$,

$$h_{p+1/2}(\xi) = \prod_{m=0, m \neq p}^{N-1} \frac{\xi - \xi_{m+1/2}}{\xi_{p+1/2} - \xi_{m+1/2}}, \quad p = 0, \dots, N - 1. \quad (8)$$

162 Similarly, the fluxes are collocated on the Lobatto (*l*) points but evaluated at
 163 the Gauss (*g*) points. For example, the ξ -direction flux, $\tilde{\mathbf{f}}$ is approximated on
 164 the Lobatto-Gauss-Gauss grid (*lgg*). The η -direction flux $\tilde{\mathbf{g}}$ and ζ -direction $\tilde{\mathbf{h}}$
 165 are collocated on Gauss-Lobatto-Gauss (*glg*) grid and Gauss-Gauss-Lobatto
 166 (*ggl*) grid, respectively. Once the fluxes are all computed at the respective
 167 Lobatto points and then interpolated at the *ggg* points, a classical fourth-
 168 order explicit Runge-Kutta time stepping scheme is applied to march the
 169 resulting ODE in time with a stable CFL condition (see below).

170 At the heart of the DSEM algorithm, there are two main operations that
 171 interpolate and differentiate a function and transfer the information from one
 172 set of quadrature points to the others. These are

- 173 1. Interpolate a function $\mathbf{F}$ from the Gauss (g) points to Lobatto (l) points
 174 using the interpolating polynomial of Eqn. (8) as

$$\begin{aligned}
 \mathbf{F}^{lgg}(\xi_i, \eta_{j+1/2}, \zeta_{k+1/2}) &= \sum_{p=0}^{N-1} \mathbf{F}_{p+1/2, j+1/2, k+1/2}^{ggg} h_{p+1/2}(\xi_i), \\
 \mathbf{F}^{glg}(\xi_{i+1/2}, \eta_j, \zeta_{k+1/2}) &= \sum_{p=0}^{N-1} \mathbf{F}_{i+1/2, p+1/2, k+1/2}^{ggg} h_{p+1/2}(\eta_j), \\
 \mathbf{F}^{ggl}(\xi_{i+1/2}, \eta_{j+1/2}, \zeta_k) &= \sum_{p=0}^{N-1} \mathbf{F}_{i+1/2, j+1/2, p+1/2}^{ggg} h_{p+1/2}(\zeta_k).
 \end{aligned} \tag{9}$$

- 175 2. Differentiate a function $\mathbf{F}$ on Gauss (g) points based on the Lobatto
 176 (l) points given in Eqn. (9), namely,

$$\begin{aligned}
 \partial_\xi \mathbf{F}^{ggg}(\xi_{i+1/2}, \eta_{j+1/2}, \zeta_{k+1/2}) &= \sum_{p=0}^N \mathbf{F}_{p, j+1/2, k+1/2}^{lgg} \partial_\xi q_p(\xi_{i+1/2}), \\
 \partial_\eta \mathbf{F}^{ggg}(\xi_{i+1/2}, \eta_{j+1/2}, \zeta_{k+1/2}) &= \sum_{p=0}^N \mathbf{F}_{i+1/2, p, k+1/2}^{glg} \partial_\eta q_p(\eta_{j+1/2}), \\
 \partial_\zeta \mathbf{F}^{ggg}(\xi_{i+1/2}, \eta_{j+1/2}, \zeta_{k+1/2}) &= \sum_{p=0}^N \mathbf{F}_{i+1/2, j+1/2, p}^{ggl} \partial_\zeta q_p(\zeta_{k+1/2}),
 \end{aligned} \tag{10}$$

177 where $q_p(\xi)$ is the Lagrange interpolation polynomial of degree at most
 178 N defined on the Lobatto (l) points along the ξ direction.

179 The DSEM algorithm is then summarized as follows:

- 180 1. On the Gauss (g) points,
- 181 • Interpolate $\mathbf{Q}$ from the Gauss (g) points to Lobatto (l) points
 182 using Eqn. (9).
- 183 2. On the Lobatto (l) points,
- 184 • Determine the advective fluxes $\mathbf{f}^a$, $\mathbf{g}^a$ and $\mathbf{h}^a$ using their respective
 185 $\mathbf{Q}$ obtained in Step 1.
 - 186 • Use a Roe approximate Riemann solver to compute the flux using
 187 the two solutions, $\mathbf{Q}$, from the neighboring elements.

- 188 • Apply desired boundary condition for boundary adjacent elements
- 189 • Compute the derivatives of $\mathbf{Q}$, $\mathbf{Q}'$, on Gauss (g) points using Eqn.
- 190 (10) and then interpolate them back onto the Lobatto (l) points
- 191 using Eqn. (9).
- 192 – Determine the viscous flux according to Eqn. (1.1). To con-
- 193 struct a continuous approximation, the average of the viscous
- 194 fluxes are used on either side of the interface as the interface
- 195 value.
- 196 – Apply Neumann boundary condition for boundary adjacent
- 197 elements.
- 198 • Determine the mapped fluxes $\tilde{\mathbf{f}}$, $\tilde{\mathbf{g}}$ and $\tilde{\mathbf{h}}$ using the metric terms
- 199 of Eqn. (4).
- 200 • Compute spatial derivatives of fluxes at ggg using Eqn. (10).
- 201 3. On the Gauss (g) points,
- 202 • Apply a fourth-order low-storage Runge-Kutta time stepping scheme
- 203 to update $\mathbf{Q}$ to the next Runge-Kutta stage.
- 204 4. Repeat from process above or terminate based on a given termination
- 205 criteria.

206 2. Artificial viscosity

207 Given a hyperbolic conservation law, the general idea of an artificial vis-
 208 cosity method is to add a high even-order dissipation term (with an appro-
 209 priate sign) to stabilize the numerical scheme in regions where the solution
 210 gradients are high relative to the grid spacing, i.e. shock regions. The arti-
 211 ficial viscosity must be positive to ensure a dissipative behavior. In a well-
 212 posed scheme, the artificial viscosity should vanish for mesh size $\Delta h \rightarrow 0$ or
 213 in regions where the gradient is small relative to the grid spacing. To satisfy
 214 these conditions, Guermond et al. [45] scaled the artificial viscosity with the
 215 entropy pair inequality or entropy residual, ($R(D_h) = |D_h|$). The entropy
 216 residual is theoretically (not necessarily numerically) always greater equal to
 217 zero and it tends to zero in regions where the solution is smooth. For the
 218 Euler equations or an inviscid ideal gas flow, the entropy is a function of the
 219 thermodynamic state variables and satisfies the inequality of the second law

220 of thermodynamics. $D_h = \frac{\partial \rho s}{\partial t} + \nabla \cdot \rho s \mathbf{u} \geq 0$, where s is the entropy. Irre-
 221 versible phenomena such as shock-waves lead to entropy production, while in
 222 smooth, inviscid and isentropic flows, the entropy residual is zero. The resid-
 223 ual, hence, is an excellent candidate for scaling of the artificial viscosity. In
 224 [45] the so-called entropy viscosity was used in conjunction with continuous
 225 Galerkin method. It was extended for discontinuous Galerkin method [46]
 226 and later also exploited for Euler equations and the staggered-grid DSEM
 227 [48].

228 In viscous flow environments or Navier-Stokes simulations, the governing
 229 equations are not hyperbolic, but have a mixed hyperbolic-parabolic charac-
 230 ter. A physical viscous dissipation changes the characteristics of equations
 231 and physics. Notably, entropy is generated in areas where viscous stresses
 232 are significant such as near walls typically or in general shear regions. In
 233 these areas the flow can be smooth, but the entropy residual defined for the
 234 inviscid Euler equations is positive because of viscous entropy generation
 235 contributions. With the “inviscid” entropy viscosity definition, the solution
 236 is hence excessively dissipated. This is not desirable in turbulence simula-
 237 tions or simulation where subtle mixing of small scales is of importance. In
 238 viscous flows, the entropy behavior and its scaling with artificial viscosity,
 239 hence, requires a revisit.

240 To start, in viscous compressible flow, the entropy does not satisfy an
 241 inequality, but the entropy conservation equation [67]. **The non-dimen-**
 242 **sional form of this transport equation is derived in Appendix A and is given**
 243 **as**

$$\begin{aligned} \frac{\partial \rho s}{\partial t} + \nabla \cdot \rho s \mathbf{u} - \frac{1}{Pr_f Re_f (\gamma - 1) M_f^2} \nabla \cdot \left(\frac{\kappa}{T} \nabla T \right) \\ - \frac{1}{Re_f} \left(\frac{\Phi}{T} \right) - \frac{1}{Re_f Pr_f (\gamma - 1) M_f^2} \left(\frac{\Gamma}{T} \right) = 0. \end{aligned} \quad (11)$$

244 with

$$\Phi = 2(\bar{\bar{S}} - \frac{1}{3}\bar{\bar{\delta}}\bar{\bar{S}})(\bar{\bar{S}} - \frac{1}{3}\bar{\bar{\delta}}\bar{\bar{S}}), \quad (12)$$

$$\Gamma = \frac{\kappa}{T} \nabla T \cdot \nabla T. \quad (13)$$

245 This equation suggests the use of Eqn. (12) as a residual for viscous flow
 246 [68] instead of the inviscid entropy residual. However, Eqn. (12) is not an

inequality constraint, but a conservation law. In addition to the inviscid terms, the viscous entropy conservation equation contains an additional diffusion transport (second term) and the entropy generation term arising from viscous and thermal dissipations (third term). Combined with the inviscid convective term the second term represents the divergence of an entropy flux vector q_i/T [67]) while the third term measures the irreversibility associated with shock waves and dissipative phenomena. The entropy generation term is $\frac{\Phi + \Gamma}{T} \geq 0$ and in accordance with the second law of thermodynamics known as *Clausius-Duhem's inequality*. With this the entropy inequality $\frac{\partial \rho s}{\partial t} + \nabla \cdot \left(\rho s \mathbf{u} - \frac{\kappa}{T} \nabla T \right) \geq 0$ follows. Within the continuum assumption, hence, it makes sense to scale the artificial viscosity with the entropy generation terms, which is what we propose and validate in this investigation.

We scale the momentum and thermal conductivity separately with the viscous and conductive entropy generating terms Φ and Γ (non-dimensional), respectively, which are both non-negative. The separate scaling is intuitive physically. It improves resolution of physical phenomena where one form of entropy generation is more prominent than the other. Moreover it provides flexibility to change the influence of momentum and energy dissipation if needed. In test below, for example, we find that a lower thermal conductivity in areas of contact discontinuities yields a sharper capturing of such discontinuities.

Normalizing with the modulus of the entropy norm [45], the non-dimensional artificial viscosity (AV) coefficients are given by

$$\hat{\mu}_h = C_\mu \frac{\rho(\Delta h)^2}{\|\rho s - \bar{\rho s}\|_\infty} \left[\frac{\Phi}{T} \right], \quad (14)$$

$$\hat{\kappa}_h = C_\kappa \frac{\rho(\Delta h)^2}{\|\rho s - \bar{\rho s}\|_\infty} \left[\frac{1}{Pr_f(\gamma - 1)M_f^2} \frac{\Gamma}{T} \right], \quad (15)$$

where C_μ and C_κ are model parameters, and Δh is the mesh size. $\bar{\rho s}$ is the spatial average of ρs given by,

$$\rho s = \frac{\rho}{\gamma(\gamma - 1)M_f^2} \ln \left(\frac{p}{\rho^\gamma} \right).$$

Following [45], $\|\rho s - \bar{\rho s}\|_\infty$ is the globally (to the computational domain) computed supremum based on the global average entropy.

275 With this definition, two primary properties of the artificial viscosity
 276 are satisfied: Firstly, since the entropy generation term is always positive
 277 (theoretically and numerically), the artificial dissipation is positive. Secondly,
 278 μ_h and κ_h scale with the grid spacing and vanish with $\Delta h \rightarrow 0$. With this
 279 formulation, the artificial viscous and thermal dissipations can be added to
 280 the existing viscous flux in the NS equations simply as follows

$$\frac{1}{Re_f} \left(\begin{array}{c} 0 \\ \frac{\partial}{\partial x} \left[\frac{4}{3} (\hat{\mu}_h Re_f + \mu) \frac{\partial u}{\partial x} \right] \\ \frac{\partial}{\partial x} \left[\frac{4}{3} u (\hat{\mu}_h Re_f + \mu) \frac{\partial u}{\partial x} \right] + \frac{\partial}{\partial x} \left[\frac{(\hat{\kappa}_h Re_f + \kappa)}{(\gamma - 1) M_f^2 Pr_f} \frac{\partial T}{\partial x} \right] \end{array} \right), \quad (16)$$

281 in the x -direction, for example.

282 2.1. Limiting entropy generation in viscous zones

283 In viscous regions of the flow, such as boundary layers and free shear
 284 flows, the entropy generation by viscous and thermal dissipations can be
 285 considerable. The artificial viscosity that is scaled with this generation can
 286 thus also be large and potentially lead to an overly dissipated solution in those
 287 regions. To reduce the artificial dissipation in viscous regions, we employ a
 288 modified Jameson's shock sensor [61, 69] (referred here as Ducros sensor)

$$\theta = \frac{(\nabla \cdot \mathbf{u})^2}{(\nabla \cdot \mathbf{u})^2 + (\nabla \times \mathbf{u})^2 + \epsilon}, \quad (17)$$

289 to identify regions with high dilatation, that is, regions with shock waves.
 290 The sensor θ is within the interval $[0, 1]$, and $\epsilon = 10^{-12}$ is a small number to
 291 avoid division by zero. The value of θ is close to unity near shocks and is
 292 small for rotation or shear dominated regions. We modify the AV coefficients
 293 with the Ducros sensor as follows

$$\begin{aligned} \mu_h &= \hat{\mu}_h \theta \mathcal{H}(-\nabla \cdot \mathbf{u}), \\ \kappa_h &= \hat{\kappa}_h \theta, \end{aligned} \quad (18)$$

294 where $\mathcal{H}$ is the Heaviside function, in order to reduce the contribution of
 295 artificial dissipation in rotation dominated regions. The negative dilatation
 296 switch essentially removes the contribution of the coefficients in the expan-
 297 sion regions and contact discontinuities, where the divergence of the flow may

298 be significantly negative and the related increase in AV can have an impact
 299 on the solution. Expansions regions, however, are always smooth and non-
 300 entropy changing (expansion shocks do not exist in the physical world) and
 301 hence a contribution from AV is not desired. The Heaviside function $\mathcal{H}(\ast)$
 302 ensures that the AV is small in isentropic expansion fans and contact dis-
 303 continuities. In Sec. 3 below, the effectiveness of the switch is demonstrated
 304 with several benchmark problems.

305 2.2. Explicit time stepping and limiting AV

306 For explicit time stepping schemes, the viscous terms yield a restriction
 307 on the stable time step,

$$\Delta t_{vis} = \text{CFL}_{vis} \frac{(\Delta h)^2}{\nu_{eff}} Re_f, \quad (19)$$

308 where $\nu_{eff} = (\mu_h Re_f + \mu)/\rho$. This might result in an excessive small time
 309 step if the artificial dissipation is large. To alleviate the time step restriction,
 310 a computationally expensive implicit time stepping scheme in combination
 311 with small grid spacing is often employed when AV methods are used.

312 Instead, we limit the AV coefficients so that the inviscid time step

$$\Delta t_{inv} = \text{CFL}_{inv} \Delta h / (|\mathbf{u}| + \sqrt{T}), \quad (20)$$

313 is smaller (more restrictive) than the viscous time step. With $\nu_{eff} = \mu_h Re_f / \rho$
 314 and $\Delta t_{vis} \geq \Delta t_{inv}$, it follows that

$$\mu_{h,max} = C_m \rho \Delta h (|\mathbf{u}| + \sqrt{T}), \quad (21)$$

315 where $C_m \propto \text{CFL}_{vis} / \text{CFL}_{inv}$ represents one more model parameter for the
 316 upper bound of μ_h . Similarly, κ_h is bounded by the $\mu_{h,max}$.

317 In this work, we shall define and denote the model constants as $\mathbf{C}_{AV} =$
 318 (C_μ, C_κ, C_m) , and the artificial viscosity μ_h and thermal conductivity κ_h co-
 319 efficients as AV coefficients collectively. For brevity, we refer to the com-
 320 bination of the Ducros sensor with switch, simply just as modified Ducros
 321 sensor.

322 2.3. Adaptive localized spectral filtering

323 With the artificial viscosity limited by the convective time step, insuffi-
 324 cient dissipation may be available to eliminate high frequency errors from

the solution near strong shocks and to prevent instability. The stability of the scheme can be enhanced by applying an adaptive low pass filter to the conservative variables, that is localized around shocks. A low pass filter is an effective technique to remove the high frequency components from the solution in order to stabilize the scheme without affecting the spectral accuracy of the low frequency components of the solution and time step size.

Following Vandeven [70], we define a $\phi > 1$ order filter function $\sigma(k/N)$ as a $C^\infty[-1, 1]$ function satisfying

$$\begin{aligned} \sigma(0) &= 1, & \sigma(\pm 1) &= 0, \\ \sigma^{(j)}(0) &= 0, & \sigma^{(j)}(\pm 1) &= 0, \quad j \leq \phi, \end{aligned} \quad (22)$$

where $\sigma^{(j)}$ denotes the j -th derivative of σ .

The popular ϕ order Exponential filter is

$$\sigma\left(\frac{k}{N}\right) = \begin{cases} \exp\left(-\alpha\left(\frac{k-N_c}{N-N_c}\right)^\phi\right), & N_c < |k| \leq N, \\ 1 & , \quad |k| \leq N_c, \end{cases} \quad (23)$$

where $\alpha = -\ln \varepsilon$ with ε the machine zero, $0 \leq N_c < N$ the cutoff wave number (typically, $N_c = 0$) and $\phi > 1$ the order of the filter. Even though the exponential filter does not strictly adhere to the definition of the filter given above, it does behave asymptotically like one. For the ease of presentation, we discuss the results for the Fourier collocation method, since nothing essential is added in the Chebyshev cases.

Given the Fourier approximation

$$f_N(x) = \sum_{k=-N}^N a_k e^{i\pi k x},$$

we construct the following *filtered* sum by modifying the Fourier coefficients a_k by the filter $\sigma(k/N)$, that is,

$$f_N^\sigma(x) = \sum_{k=-N}^N \sigma\left(\frac{k}{N}\right) a_k e^{i\pi k x}. \quad (24)$$

The smoothing operation can be cast as a matrix-vector multiplication, where the filtering matrix $\mathbf{S}$ is created by substituting the definition of the coefficient

Figure 2: Transfer function of the ϕ -order exponential filter.

346 a_k into (24) and rearranging the order of the summation, that is

$$f_N^\sigma(x_k) = \sum_{j=0}^{2N-1} S_{kj} f_j, \quad (25)$$

347 where S_{kj} are the entries of the filtering matrix $\mathbf{S}$, or in the matrix form

$$\vec{f}_N^\sigma = \mathbf{S} \vec{f}_N. \quad (26)$$

348 An interesting fact about the exponential filter σ is that its order can be
 349 changed by adjusting the parameter ϕ . One does not have to provide a dif-
 350 ferent filtering function to obtain a filter of different order. In Fig. 2, the
 351 exponential filter with several orders ϕ in the wavenumber space are shown.
 352 By adapting the exponential filter strength in element with oscillatory solu-
 353 tions stability of the scheme can be improved without unnecessary smoothing
 354 in in shock-free smooth elements. We have designed a spatially adaptive lo-
 355 calized variable-order filtering technique, which adjusts the filter order ϕ as a
 356 function of entropy viscosity μ_h . If μ_h is limited by the time step restriction,
 357 then a higher filter strength (low order) is employed to reduce oscillations
 358 in the solutions. Otherwise, a very mild filter with high order is used to
 359 maintain the spectral accuracy of the solution.

360 2.4. Remarks

361 We offer the following remarks and observations on the numerical tech-
 362 niques used in the DSEM-AV for inviscid and viscous shocked flow.

- 363 • The proposed AV coefficients are cost effective as they can be directly
364 calculated on *ggg*, *lgg*, *glg* or *ggl* nodes as needed and used to included
365 in the viscous fluxes.
- 366 • Δh is the local minimum mesh size within an element.
- 367 • The μ_h and κ_h on *lgg*, *glg* or *ggl* points are needed for flux computation.
- 368 • In the present methodology no smoothing operation is necessary needed
369 to apply on μ_h or κ_h .
- 370 • Eqn. (16) reduces to the inviscid Euler formulation by setting transport
371 properties $\mu = \kappa = 0$.
- 372 • The inverse of the non-zero μ_h is a measure of effective local artificial
373 Reynolds number that is required to regularize a shock, effectively
374 creating a viscous shock, where physical viscosity accounts for the ir-
375 reversible entropy generation. In the numerical experiments below, we
376 conduct detailed test of the formulation versus an analytical viscous
377 shock solution.
- 378 • The AV model constants, $\mathbf{C}_{AV}$ should to be tuned for optimal stabi-
379 lization of a given problem. A systematic assessment of the model
380 parameters is presented in Sec. 3.
- 381 • h/p -adaptivity can potentially be implemented based on the magnitude
382 AV coefficients dictated by the entropy dissipation terms irrespective
383 of smooth/non-smooth zones additional to the shock stabilisation.

384 3. Results and discussion

385 In the following sub-sections, we validate the proposed artificial viscosity
386 approach, switch and adaptive spectral filter. We split the assessment of
387 the scheme into an inviscid and viscous flow discussion with one- and two-
388 dimensional benchmark problems. A three dimensional supersonic flow over
389 ramped cavity geometry is presented to illustrate the performance of the
390 viscous flow for a three-dimensional, large-scale, viscous, turbulent fluid flow
391 with shocks. A stable CFL=0.9 is taken unless stated otherwise.

3.1. Numerical experiments with inviscid flow

3.1.1. One-dimensional moving shock

We test the effect of model constants $\mathbf{C}_{AV}$ on shock capturing in a simple 1D moving shock benchmark. 500 P₃ elements are used with the following initial condition

$$(\rho, u, P) = \begin{cases} (1.4, 0, 1), & -0.5 \leq x < 0, \\ (2.36, 0.57, 2.12), & 0 < x \leq 0.5. \end{cases}$$

We vary $C_\mu = C_\kappa$ while keeping $C_m = 1$. The pressure P , and the AV coefficients μ_h and κ_h are shown in Fig. 3 at $t = 0.2$ when the shock is located at $x_s = 0.28$ according to inviscid exact solution (black dashed curve). Values of $C_\mu \approx O(1)$ and $C_m \approx O(1)$ are sufficient to stabilize the moving shock with only minor oscillations around the shock location (tested for polynomial order up to P₆ but omitted here). For large C_μ , μ_h is limited by its upper bound according to Eqn. (21). The blue curves (square symbols) identify the maximum allowable dissipation while keeping the explicit stable time step restriction. For $C_\mu = 1$, the maximum of $\mu_h \approx 9.82 \times 10^{-4}$, which implies an equivalent artificial local Reynolds numbers $Re_l \gtrsim 1018$ in the shock region. The general trends in the thermal conductivity coefficient κ_h are similar to those in μ_h but with a smaller magnitude.

Figure 3: 1D moving shock with variation of C_μ and C_κ (a) pressure P , (b) μ_h , (c) κ_h .

3.1.2. One-dimensional Sod problem

To demonstrate the performance of artificial dissipation with and without the modified Ducros switch in the presence of shocks, contact discontinuities

and expansion waves, we solve the one-dimensional Sod problem using 50 P_3 elements with initial condition

$$(\rho, u, P) = \begin{cases} (0.125, 0, 0.1), & -0.5 \leq x < 0, \\ (1, 0.75, 1), & 0 < x \leq 0.5 \end{cases}$$

407 We take $\mathbf{C}_{AV} = (1, 1, 1)$. Figure 4 shows the effect of the modified Ducros
 408 switch on the density and the AV coefficients. With the modified Ducros
 409 switch the prediction of the expansion fan is closer to the exact density so-
 410 lution as compared to the expansion fan predicted without the switch. The
 411 switch $\mathcal{H}(-\nabla \cdot \mathbf{u})$ in Eqn. (18) eliminates the contribution of μ_h in the ex-
 412 pansion region, which leads to the improved resolution. The resolution of the
 413 contact discontinuity region is in large determined by the entropy generation
 414 by the thermal dissipation term. Reducing the artificial thermal conductiv-
 415 ity coefficient κ_h around the contact discontinuity by lowering C_κ yields a
 416 sharper contact discontinuity (Fig. 5). It is clear that the independent mod-
 417 ification of μ_h and κ_h provides a flexible control that benefit the resolution
 418 of different physical behaviors, including shocks, contact discontinuities and
 419 expansion waves.

Figure 4: (Left) Density and (Right) AV coefficients of the one-dimensional Sod problem with 50 P_3 elements and $\mathbf{C}_{AV} = (1, 1, 1)$.

420 3.1.3. One-dimensional Mach 3 shock interaction with density wave

The performance of the AV formulation is further examined by considering the classical Mach 3 shock-density wave interacting with sinusoidal waves

Figure 5: (Left) Density and (Right) AV coefficients of the one-dimensional Sod problem with 50 P_3 elements and $\mathbf{C}_{AV} = (1, C_\kappa, 1)$.

in the density field [71],

$$(\rho, u, P) = \begin{cases} \left(\frac{27}{7}, \frac{4\sqrt{35}}{9}, \frac{31}{3} \right), & 0 \leq x < 1, \\ \left(1 + 0.2 \sin(5x), 0, 1 \right), & 1 \leq x \leq 10, \end{cases}$$

421 This simplified model mimics the interaction of a shock wave with turbulence.

422 Fig. 6 shows the density and the AV coefficients of the shock-density
 423 wave interaction with 200 P_3 elements, $\mathbf{C}_{AV} = (1, 0.5, 1)$ at time $t = 1.8$.
 424 The DSEM scheme captures the shocklets and resolves high frequency waves
 behind the main shock and compares well with the reference solution.

Figure 6: The density and AV coefficients of the shock-density wave interaction with 200 P_3 elements and $\mathbf{C}_{AV} = (1, 0.5, 1)$.

3.1.4. Mach 3 flow over a forward facing step

To validate the applicability of the DSEM-AV algorithm on a higher dimensional shocked problem, we simulate the two-dimensional Mach 3 flow over a forward facing step [72]. For details on the setup we refer to extensive descriptions in literature. We use 25,200 P_3 elements (each of size 0.01) and a CFL=0.75 with $\mathbf{C}_{AV} = (1.0, 0.5, 0.5)$. For time $t \leq 0.1$, we use a special treatment of the singular point at the expansion corner (which is common practice [72]); we use an eighth order exponential filter in each element and ($\phi = 4$) is used wherever μ_h reaches its local upper bound. Afterwards, the filter order is relaxed to $\phi = 64$ everywhere expect for a few elements in the corner region where we take $\phi = 4$ regardless of the size of μ_h . This initial spatial-adaptive filtering prevents instability stemming from the strong reflected bow shock from the corner of the step. Since this reflection is an artificial (unphysical) initialization artifact, the strong adaptive filter is required and justified only initially. At a later time the strong filter is only required around the equally artificial singular corner.

Figure 7: Mach 3 flow over a forward facing step : density field at time $t = 0.5, 1, 2, 3$ with the Ducros switch.

With the modified Ducros switch activated, the temporal evolution of the density field is shown in Fig. 7. The primary flow structures including the shock reflections, expansions are well captured, and perhaps most importantly, the Mach stem are visible in the same locations as reported in literature. As shown in Fig. 8, the AV coefficients trace the bow shock struc-

447 ture and its reflection from the top wall. In the step corner region μ_h and κ_h
 448 have nominal contributions required for stabilization, but the contributions
 449 are local and do not affect the global flow characteristics. The stability of
 450 the slip line that emanates from the Mach stem is generally known to be a
 451 good measure of the high resolution capability of a numerical scheme. If the
 452 dissipation over this slip line is small, then a Kelvin-Helmholtz instability
 453 appear. The slip line is stable for an overly dissipative scheme. With the
 454 modified Ducros switch deactivated, the slip line is stable because of the en-
 455 tropy generation by shear stresses in the slip line and the associated large,
 456 dissipative artificial viscosity. With the modified Ducros switch activated,
 457 the artificial dissipation in the shear regions reduces dramatically (see nu-
 458 merical schlieren in Fig. 9). As the result, the shear layer is resolved with
 459 the low dissipative and high resolution DSEM scheme and is unstable as is
 460 expected for a high-resolution scheme.

Figure 8: Mach 3 flow over a forward facing step : artificial viscosity μ_h and thermal conductivity κ_h coefficients with and without the modified Ducros switch.

461 3.2. Numerical Experiments with Viscous Flow

462 3.2.1. 1D Viscous shock-structure

463 When regularizing an *inviscid* shock wave with an artificial viscosity ap-
 464 proach, the shock dissipation that physically occurs on the scale of the molec-
 465 ular mean free path, is artificially smeared over a finite width on the order
 466 of the resolution of the continuum equations. Exactly like a real physical
 467 viscous shock, the shock jumps in the far-field correspond to the inviscid

Figure 9: Mach 3 flow over a forward facing step : comparison of numerical Schlieren of the temperature field with and without the modified Ducros switch.

Figure 10: Structure of 1D stationary shock with p-refinement, (a) pressure profiles, dotted line indicates inviscid jump and dashed black line is 1D NS exact solution, (b) μ_h and κ_h .

Rankine-Hugoniot relations, while the size of the dissipation zone widens with increasing dissipation or viscosity. To understand the relation between the physical dissipation and the artificial dissipation, we compare a regularized inviscid standing shock with an exact Navier-Stokes solution for the one-dimensional viscous shock problem ([73]). We initialize the computational domain $x \in [-0.1, 0.1]$ with the exact Navier-Stokes shock structure solution for an upstream Mach 2 flow and $Re_f = 1000$ using 100 P_n elements and a constant $\mathbf{C}_{AV} = (1, 1, 1)$. We converge the Euler solution to the steady-state solution, and then compare it to the Navier-Stokes solution.

The inviscid regularized shock matches best with the Navier-Stokes shock structure for P_4 elements (see Fig. 10a). With increasing resolution, i.e. a higher P_n , the shock is captured more sharply. That is, the shock thickness decreases with increasing order of the polynomial approximation for a given shock jump. With greater p -refinement the solution converges to the inviscid solution. The maximum of μ_h decreases from P_3 to P_6 elements (for P_3 : $\mu_h \approx 1.8 \times 10^{-3}$, P_4 : $\mu_h \approx 1.2 \times 10^{-3}$, and P_6 : $\mu_h \approx 6.4 \times 10^{-4}$), while the shock thickness increases. κ_h behaves similar to μ_h . The P_3 solution is smooth, whereas the P_4 and P_6 solution show minor oscillations.

The effective local Reynolds numbers for P_4 is approximately $Re_l = 1000$, also corresponding the viscous Navier-Stokes shock solution. This effective Reynolds number is similar to the one reported above in the moving shock discussion. The Reynolds number of 1000 hence appears general. This in turn hints towards a general relation between the regularization, the viscous shock and the constants $\mathbf{C}_{AV} = (1, 1, 1)$. We aim to explore this in future work.

3.2.2. 2D Blasius laminar boundary layer

To test the artificial viscosity reducing effect of the modified Ducros switch in a viscous, compressible flow regions, we consider a boundary layer flow over a flat plate under zero pressure gradient with an adiabatic wall boundary condition [74] which has an exact analytical solution. We simulate a Mach 2 flow at a Reynolds number of $Re_f = 2000$. The computational domain size is $[0, 4] \times [0, 1]$, which is initialized with the analytical compressible Blasius boundary layer profiles, with 100×20 P_3 elements. Stretched elements near the solid boundary are generated according to $y = L_y f(\eta, \beta)$, where L_y is the computational domain length in the wall normal direction, and the stretching

503 function is given by

$$f(\eta, \beta) = \frac{(\beta + 1) - (\beta - 1)\omega^{1-\eta}}{1 + \omega^{1-\eta}}, \quad \omega = \frac{(\beta + 1)}{(\beta - 1)}, \quad (27)$$

504 where $0 \leq \eta \leq 1$ and $\beta = 1.05$. In this case, $\mathbf{C}_{AV} = (1, 1, 0.15)$ and the final
505 time is $t = 72$.

506 The solution ρ, u, T and AV coefficients (μ_h, κ_h) profiles at the mid-section
507 of the domain are shown in Fig. 11. The viscous stresses inside the boundary
508 layer generate entropy which yields an increased artificial viscosity, μ_h , and
509 thermal conductivity, κ_h according to Eqns.(14) and (15), respectively. The
510 artificial viscosities are comparable in magnitude to the physical viscosity at
511 $\approx 5 \times 10^{-4}$ and can clearly not be ignored. With AV, the velocity u and
512 temperature T in the boundary layers are diffused more as compared to the
513 analytical solution. The velocity and thermal boundary layers have an in-
514 creased boundary layer thickness as compared to the analytical one. Because
515 of the increased displacement, the outer flow experiences changes by blockage
516 and boundary condition effects, resulting in a density ρ increase. The modi-
517 fied Ducros switch is close to zero inside the boundary layer where rotation
518 dominates dilatation. With activated modified Ducros switch, the artificial
519 dissipation inside the boundary layer is thus very small as compared to the
520 physical viscosity, and the analytical profiles of the viscous Navier-Stokes
521 equation are retrieved. Hence, the modified Ducros switch is an important
522 component in the overall DESM-AV algorithm for viscous flows.

523 3.2.3. 2D Shock-wave boundary layer interaction

To rigorously test the DSEM-AV scheme for the interaction between
shocks and viscous shear flows, we consider a benchmark problem of a shock
and a reflected shock interaction with a boundary layer in a shock tube [75–
77]:

$$(\rho, u, v, P) = \begin{cases} (120, 0, 0, \rho/\gamma), & 0 \leq x < 0.5, 0 \leq y \leq 0.5 \\ (1.2, 0, 0, \rho/\gamma), & 0.5 < x \leq 1, 0 \leq y \leq 0.5 \end{cases}$$

524 500×70 P₃ elements are used with stretching parameter $\beta = 1.05$ (Eqn. 27)
525 in wall normal direction. The top boundary is set to symmetric condition
526 while no-slip adiabatic wall boundary conditions are imposed on the remain-
527 ing boundaries. The Reynolds number is taken $Re_f = 1000$, with the AV
528 coefficients $\mathbf{C}_{AV} = (1, 0.1, 0.5)$ and the CFL=0.75. An adaptive spectral filter

Figure 11: Two-dimensional Blasius laminar boundary layer : ρ, u, T and AV coefficients (μ_h, κ_h) profiles at the mid-section of the domain.

Figure 12: Temporal evolution of the density field of the two-dimensional shock-boundary layer interaction for $Re_f = 1000$ with the modified Ducros switch. At $t = 0.4$, numerical Schlieren together with ϕ -order spectral filter is shown. Red patches are regions with $\phi = 16$ and $\phi = 64$ elsewhere.

is necessary with order $\phi = 16$ near the regions where $\max(\mu_h, \kappa_h)$ attains its local upper bound and $\phi = 64$ otherwise.

The accelerated flow behind the right moving normal shock leads to the formation of a boundary layer (see Fig. 12). At time $t = 0.4$, after reaching the downstream end of the shock tube, the normal shock reflects back and starts interacting with the boundary layer of the bottom wall. This yields a complex shockwave boundary interaction and associated λ shock, shocklets and vortices at the later time. The reflected shock is strong, which leads to the activation of the stronger adaptive filter, but only in within the immediate vicinity of the shock (Fig. 12a).

A comparison of the numerical Schlieren, and μ_h in Fig. 13 illustrates the effect of the modified Ducros switch on the viscous solution. Without the switch the initial boundary layer is thicker (not shown here, but also observed in the laminar boundary layer case above), which affects the shock-boundary layer interaction. With the switch activated the structures are richer and instabilities appear in the slip lines that are not present when the artificial viscosity stabilizes the flow in case of deactivated modified Ducros switch. When the switch is on, the vortices and associated μ_h are different in the vortex dominated boundary layer. Detailed shock-shock, shock-vortex and shock-boundary layer interactions are captured and the predicted structure of the foot of the lambda shock, triple point, coiled slip streams with activated modified Ducros switch and are well in accordance with the results in literature [75, 76].

3.3. Three dimensional supersonic turbulent flow with a ramped cavity

To demonstrate the applicability of the present methodology in a three-dimensional environment, we simulate the supersonic turbulent flow over a ramped cavity. The geometry of the cavity (see Fig. 14) is taken similar to that presented in [78]. The span-wise dimension and inflow boundary layer thickness are taken same as the step height (unity) of the cavity. The Reynolds number of the incoming flow is based on this reference length-scale. We use the compressible flat plate Mach 2 flow DNS database of [79] for $Re_f = 5000$ to initialize the mean three dimensional flow-field and the turbulent fluctuations are reconstructed with second-order statistics according to the stochastic model reported in [80]. The static temperature and pressure are set similar to that reported in [78]. Simulations are carried out with 613,800 P_3 elements, having 15 elements in span-wise direction. The AV model constants are $\mathbf{C}_{AV} = (0.1, 1, 0.15)$ together with the exponential filter

Figure 13: Numerical Schlieren and the artificial viscosity μ_h of the shock-boundary layer interaction at time $t=1$ without and with the modified Ducros switch.

Figure 14: Computational domain for three dimensional cavity configuration.

Figure 15: (Left) Instantaneous three-dimensional turbulent flow structures (iso-surface of Q flooded with streamwise velocity and pressure at different planes) at $t = 18t_{ft}$. (Right) Artificial viscosity μ_h .

order $\phi=32$. To resolve the near wall characteristics of the three-dimensional turbulent supersonic flow, elements are stretched in wall normal (y -axis) direction so that the first Gauss point satisfies $y^+ \approx 1$ for this case. The number of Gauss points within the boundary layer thickness (δ_{BL}) is about 40, and the number of Gauss points within 10% of δ_{BL} is 4.

Fig. 15 shows the general flow features at 18 flow-through times (t_{ft}). The positive iso-surfaces of the Q-criterion Q , defined by,

$$Q = (\Omega_{ij}\Omega_{ij} - \Xi_{ij}\Xi_{ij})/2, \quad (28)$$

where $\Omega_{ij} = (u_{ij} - u_{ji})/2$ and $\Xi_{ij} = (u_{ij} + u_{ji})/2$, highlight rotation dominated vortex structures in the flow-field. In this figure, the pressure contours visualize the unsteady oblique shock boundary layer interaction. The downstream stretched and elongated hairpin vortices (large scale structures of the turbulence) are well captured by the present simulation. The incoming three-dimensional turbulent boundary layer evolves as a growing shear layer in the cavity section and impinges with the trailing edge of the cavity, producing an oblique shock wave. The oscillation of the oblique shock wave is closely coupled with the vortex shedding of the shear layer. The distribution of μ_h (see Fig. 15) highlight the major shock structures and the controlled artificial dissipation obtained inside the boundary layer. The downstream dissipation appears relatively larger in shock interacted compression regions of the downstream boundary layer. The magnitude of κ_h is similar but with a lower value than that of μ_h (not shown).

587 4. Conclusions

588 An explicit, shock-capturing, high-order, three-dimensional parallel DSEM-
 589 AV flow solver is developed for the simulation of viscous, turbulent flows
 590 with shocks in complex geometry. The shock-capturing framework depends
 591 on four critical components that include (i) a new artificial viscosity (AV)
 592 method that scales the AV with the non-negative entropy generation terms of
 593 the viscous entropy transport equation, (ii) a limiting operation using a mod-
 594 ified Ducros switch to reduce AV in viscous, shear dominated flow regions,
 595 (iii) an AV limiter to ensure that the explicit stable time step restricted by
 596 the convective CFL number is obeyed, and (iv) an adaptive localized variable
 597 order exponential filter that enhances the stability of the numerical scheme
 598 in regions with strong shocks.

599 The DSEM-AV scheme is systematically tested for inviscid and viscous
 600 flow benchmarks in one- and two-dimensions. A three-dimensional super-
 601 sonic flow over a ramped cavity illustrates the performance of the scheme
 602 for a geometric complex domain and for the complex interaction of shocks
 603 turbulence and viscous shear regions.

604 The AV coefficients require some tuning to obtain the optimal results,
 605 but generally, we find that the AV model constants C_μ related to μ_h can be
 606 taken as unity and C_κ related to κ_h to be between 0.1 and 1, which affects
 607 the capturing of shear dominated flows and contact discontinuities. The AV
 608 model constant C_m related to the explicitly time step limiting of AV ranges
 609 from 0.15 and 1. The usage of variable order exponential filter enhances the
 610 stability of the DSEM-AV for problems with strong shocks and singularities.

611 We find that the activation of the modified Ducros sensor significantly
 612 reduces the AV in shear regions and expansion fans. With the reduced AV,
 613 the DSEM scheme captures shear instabilities with higher resolution and fine
 614 scale structures that are otherwise dissipated.

615 We show that for a flow with a Reynolds number of 1000, a physical
 616 Navier-Stokes viscous shock matches well with an essentially non-oscillatory
 617 regularized shock with AV. The inverse of the AV, $1/\mu_h$, which represents an
 618 effective artificial Reynolds, is shown to be close to 1000 also. This finding
 619 hints that there is relation between the level of dissipation required, and
 620 hence the model constants, an essentially non-oscillatory shock capturing.
 621 and/or the general identification of trouble cells. We aim to explore this in
 622 future work.

623 The present AV proposition is not limited to DSEM and is expected to

624 easily extend to other high-order compressible explicit solvers to deal with
625 complex compressible flows involving shocks and turbulence. Detailed study
626 and analysis will be conducted in future with three-dimensional shock tur-
627 bulence interactions. We will also explore the application of the DSEM-AV
628 based scheme to high speed turbulent flows with chemical reaction.

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639 Reference

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Appendix A. Non-dimensionalization of the entropy transport equation

The transport equation of specific entropy s^* in dimensional form and index notation [67] is given by

$$\frac{\partial \rho s^*}{\partial t^*} + \frac{\partial \rho^* s^* u_j^*}{\partial x_j^*} - \frac{\partial}{\partial x_j^*} \left(\frac{\kappa^*}{T^*} \frac{\partial T^*}{\partial x_j^*} \right) - \frac{\Phi^* + \Gamma^*}{T^*} = 0, \quad (\text{A.1})$$

893 where,

$$\begin{aligned}\Phi^* &= \tau_{ij}^* \frac{\partial u_i^*}{\partial x_j^*} = 2\mu^* S_{ij}^* S_{ij}^* - \frac{2}{3}\mu^* S_{kk}^* S_{ii}^* + \mu_b^* S_{kk}^* S_{ii}^*, \\ \Gamma^* &= \frac{\kappa^*}{T^*} \frac{\partial T^*}{\partial x_j^*} \frac{\partial T^*}{\partial x_j^*},\end{aligned}\tag{A.2}$$

$$S_{ij}^* = \frac{1}{2}(u_{ij}^* + u_{ji}^*).\tag{A.3}$$

894 For $\mu_b = 0$, Φ^* becomes

$$\Phi^* = 2\mu^*(S_{ij}^* - \frac{1}{3}\delta_{ij}S_{kk}^*)(S_{ij}^* - \frac{1}{3}\delta_{ij}S_{kk}^*).\tag{A.4}$$

895 Following the non-dimensionalization of the Navier-Stokes in Eqns. 1, we
896 have

$$c_f = \sqrt{\gamma R T_f},\tag{A.5}$$

$$M_f = u_f/c_f = 1,\tag{A.6}$$

$$Re_f = \frac{L_f u_f \rho_f}{\mu_f},\tag{A.7}$$

$$Pr_f = \frac{\mu_f C_p}{\kappa_f},\tag{A.8}$$

$$s_f = u_f^2/T_f,\tag{A.9}$$

$$\frac{u_f^2}{C_p T_f} = M_f^2(\gamma - 1).\tag{A.10}$$

897 Now for any property ψ^* , the non-dimensional ψ is given by $\psi^* = \psi\psi_f$, where
898 ψ_f is the reference property. The terms in Eqn. A.1 therefore are expressed

899 as,

$$\begin{aligned}
\frac{\partial \rho s^*}{\partial t^*} &= \left(\frac{\rho_f s_f}{t_f} \right) \frac{\partial \rho s}{\partial t} \\
&= \left(\frac{\rho_f s_f u_f}{L_f} \right) \frac{\partial \rho s}{\partial t} \\
\frac{\partial \rho^* s^* u_j^*}{\partial x_j^*} &= \left(\frac{\rho_f s_f u_f}{L_f} \right) \frac{\partial \rho s u_j}{\partial x_j} \\
\frac{\partial}{\partial x_j^*} \left(\frac{\kappa^*}{T^*} \frac{\partial T^*}{\partial x_j^*} \right) &= \left(\frac{\rho_f s_f u_f}{L_f} \right) \left(\frac{1}{Re_f Pr_f (\gamma - 1) M_f^2} \right) \frac{\partial}{\partial x_j} \left(\frac{\kappa}{T} \frac{\partial T}{\partial x_j} \right) \\
\frac{\Phi^*}{T^*} &= \left(\frac{\rho_f s_f u_f}{L_f} \right) \frac{1}{Re_f} \frac{\Phi}{T} \\
\frac{\Gamma^*}{T^*} &= \left(\frac{\rho_f s_f u_f}{L_f} \right) \left(\frac{1}{Re_f Pr_f (\gamma - 1) M_f^2} \right) \frac{\Gamma}{T}
\end{aligned}$$

900 The non-dimensional form in index notation then follows as

$$\begin{aligned}
\frac{\partial \rho s}{\partial t} + \frac{\partial \rho s u_j}{\partial x_j} - \frac{1}{Pr_f Re_f (\gamma - 1) M_f^2} \frac{\partial}{\partial x_j} \left(\frac{\kappa}{T} \frac{\partial T}{\partial x_j} \right) \\
- \frac{1}{Re_f} \left(\frac{\Phi}{T} \right) - \frac{1}{Re_f Pr_f (\gamma - 1) M_f^2} \left(\frac{\Gamma}{T} \right) = 0,
\end{aligned} \tag{A.11}$$

901 which becomes Eqn. 11 in vector form.