A POSTERIORI METHODS WITH AUTOMATIC DISSIPATION ADJUSTMENT FOR THE SIMULATION OF COMPRESSIBLE FLOWS

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ABSTRACT

In this work, a generalized framework for the numerical computations of the compressible Euler and Navier–Stokes equations is presented in order to increase the accuracy of any numerical scheme that uses a numerical flux that can be rewritten as a central term plus some dissipation term. The key idea is to regulate the numerical dissipation introduced by the scheme in real-time according to some estimate of the high-frequency content in the flow. This technique is called adaptive dissipation, and has been applied successfully to the calculation of incompressible turbulent flows. In the present case, and due to the compressibility effects, the methodology may present some stability problems, in order to remedy this behavior, we couple the adaptive dissipation methodology with an *a posteriori* procedure that guarantees that the solution remains physical at all times. We validate the proposed methodology with a finite volume and a finite difference scheme, with some one- and three-dimensional test cases, obtaining solutions that are physical and in really good agreement with the ones that can be found in the literature.

Keywords: high-order methods, compressible flows, implicit large eddy simulation, computational fluid dynamics, a posteriori*, shock capturing, turbulent flows.*

1 INTRODUCTION

Understanding compressible turbulence is paramount not only from a purely scientific standpoint, but also from an engineering and practical point of view. In turbulent flows of interest in engineering processes such as supersonic aircraft design, high-temperature reactive flows, or inertial confinement fusion; it is not computationally possible nowadays to simulate the entire range of scales that are present in the flow, since this number scales grows faster than $O(\mathrm{Re}^{11/4})$, being Re the Reynolds number [1]. Given this severe computational limitation, large eddy simulation (LES) is the most practical approach in order to simulate these flows. Since LES simulations do not solve the complete range of scales of the flow, the effect of the unresolved scales should be adequately modeled in order to get the most accurate solution on a given grid. This is a very challenging task, due to the complexity of the involved physical processes. To this end, subgrid scale (SGS) models where proposed and are still today a very active area for research. However, the vast majority of the SGS models where developed for incompressible flows, and using them in a compressible context not only does not account for the intermodal energy transfer which takes place in compressible turbulence, but also the physical mechanism driving this transfer is completely neglected. Another issue that arises is related to compressibility, the possible presence of shocks that makes the use of numerical stabilization mandatory, which may lead to unwanted extra dissipation (see [2]–[4]).

The main issue is how to introduce the right amount of numerical dissipation that stabilizes the simulation while not interfering with vorticial dynamics. The accuracy in LES computations depends on several factors that are intertwined, namely: temporal and spatial

WIT Transactions on Engineering Sciences, Vol 128, © 2020 WIT Press
www.witpress.com, ISSN 1743-3533 (on-line)
doi:10.2495/AFM200011

discretization scheme, resolution and quality of the grid and the accuracy of the SGS model (if used). Moreover, the numerical dissipation of a particular scheme is a key to determine whether it is suitable for LES simulations. In this context, Implicit LES (ILES) proposes the use of the truncation error of the discretization schemes for modeling the effect of SGS on the resolved scales. In general, only high-order schemes that are specifically tailored for turbulent calculations can be applied successfully to ILES [5].

The most used methods for simulation of compressible flows are based in the use of Riemann solvers [6]. One of these is the approximate Riemann solver of Roe [7], which can be extended to the computation of low-Mach flows after some corrections to the original method [8]. Self-adaptive upwind methods are proposed in order to reduce as much as possible the dissipation introduced by the Roe scheme [9]. In [10], an Automatic Dissipation Adjustment (ADA) method for low Mach computations using the low-Mach Roe scheme was presented, and in [11] this methodology was extended to compressible transonic and supersonic flows. In this method, the energy ratio (ER) criterion from [12] is used to automatically adjust the amount of viscosity introduced by the numerical flux.

In this work, we aim show how to extend the ADA method for the computation of compressible flows with shock waves, regardless of the type of numerical scheme. In order to address the problem of stabilization due to shocks we propose to use the *a posteriori* paradigm (see [13], [14]). The ER criterion adjusts the dissipation in the smooth zones of the flow, while the *a posteriori* framework preserves the stability by increasing the dissipation if the simulation fails or oscillations are produced. Thus, we determine numerically and in runtime if the scheme should introduce more dissipation or not, avoiding the use of specific shock sensors that predict the shock position in the next iteration. The only requirement in order to apply the proposed methodology is that the numerical flux has to be expressed as the sum of a central plus a dissipative part. We will show that the proposed methodology can greatly increase the accuracy of the original numerical methods. To do that, in this work we focus on a third-order finite volume and the WENO5 finite difference schemes.

The paper is structured as follows. In Section 2 the governing equations are presented. In Section 3 the formulation of the proposed methodology is exposed, and in Section 4 some numerical tests are presented to show the accuracy of the proposed methodology. Finally, the conclusions are drawn.

2 GOVERNING EQUATIONS

In this work, we solve the three-dimensional Euler equations with the compressibility hypothesis. Although, without loss of generality, the same procedure can be applied to the Navier–Stokes equations, since the methodology explained here only affects the inviscid part of the equations. Using vector notation, the Euler system can be expressed as

$$\frac{\partial \mathbf{U}}{\partial \tau} + \frac{\partial \mathbf{F}}{\partial x} + \frac{\partial \mathbf{G}}{\partial y} + \frac{\partial \mathbf{H}}{\partial z} = 0. \tag{1}$$

The vector quantities involved are related to the physical properties of the fluid, and they are computed as

$$\mathbf{U} = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ \rho E \end{pmatrix}, \mathbf{F} = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ \rho uw \\ u(\rho E + p) \end{pmatrix}, \mathbf{G} = \begin{pmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ \rho vw \\ v(\rho E + p) \end{pmatrix}, \mathbf{H} = \begin{pmatrix} \rho w \\ \rho uw \\ \rho vw \\ \rho w^2 + p \\ w(\rho E + p) \end{pmatrix}. \tag{2}$$

In eqn (2), **U** is the conserved variables vector, and **F**, **G** and **H** are the inviscid fluxes. The physical properties of the fluid are denoted as ρ, the density; p, the pressure; $\mathbf{V} = (u, v, w)$ the cartesian velocity vector, and $\rho E = \frac{p}{\gamma - 1} + \frac{1}{2}\rho(\mathbf{V} \cdot \mathbf{V})$, the total energy. Since we are working with ideal gases, we take the non-dimensional coefficient to be $\gamma = 1.4$. Please note that no explicit SGS model is employed in this work.

3 NUMERICAL METHOD

We present a novel methodology of application to the numerical computation of turbulent flows. It is based on the ADA model that regulates the amount of dissipation of the flow according to some measurement based on the energy ratio (ER). In order to guarantee that the scheme is robust and avoids oscillations that may cause the simulation to fail, we use the *a posteriori* paradigm. The ADA method acts as an implicit SGS model, whereas the *a posteriori* approach ensures the stability.

3.1 Automatic dissipation adjustment (ADA) method

The ADA method was first developed and applied to the computation of low Mach flows [10]. It is based on the local ER introduced in the context of the Truncated Navier–Stokes procedure [12]. In this work we extend the application of this methodology to the complete extent of Mach numbers flows. The method is implemented in the form of a multiplicative coefficient $\epsilon \in [0,1]$ that solely affects the dissipative part of the convective numerical flux. Thus, the reconstructed flux can be written as

$$f^{Rec} = \text{central} + \epsilon \cdot \text{dissipation}. \tag{3}$$

The only requirement, as previously stated, in order to apply the proposed methodology is that the numerical flux has to be expressed as the sum of a central plus a dissipative part. This methodology is very general and is not limited to a single family of schemes. In fact, this can be extended to any of the usual discretization techniques such as discontinuous galerkin, finite volume or finite difference formulations. Examples of the latter two, can be seen in [15] where the finite difference WENO5 is expressed in the form of eqn (9), and in [11] or [12] where the same is achieved with finite volume methods.

The key idea of the ADA method is to link the reduction of the dissipation part with the ER, which gives some insight of the well-resolved-ness of the fluid. For the case of compressible flow, the ER is defined to include the effect of compressibility as

$$\text{ER} = \frac{\sum_{i=1}^{3}(\rho u_i - \overline{\rho u}_i)^2}{\sum_{i=1}^{3}(\rho u_i - \widehat{\rho u}_i)^2}. \tag{4}$$

The variables ρu_i stand for each component of the momentum field. The variables with the overbar $\overline{(\cdot)}$ and hat $\widehat{(\cdot)}$ represent filtered fields obtained by using two different low-pass filter widths. In this work instead of using top-hat filters as in [16], we use moving least squares (MLS) based filters. An MLS approximation of a variable can be seen as a low-pass filtering of such variable. These filters can be consulted in [11], and we use a shape parameter κ equal to 4 and 3 respectively for the overbar and hat variables. Other kinds of filtering schemes could be also applied.

As previously stated, the ER can be seen as a ratio of the spatial high-frequency components of the momentum field for two different filters. In this work, we consider that when ER<0.5, the introduced numerical dissipation is excessive, so ϵ must be reduced.

Conversely, if ER > 0.55, it is considered that there is excessive energy at small scales of the flow, and it should be dissipated by increasing the value of ϵ. In order to adjust the parameter ϵ, we follow the rule proposed in [10], and we have calibrated the model using the Taylor–Green vortex test case. In general, we can write it as

$$\begin{cases} \mathrm{ER} < \mathrm{ER}_{\mathrm{inf}} & \epsilon \leftarrow \max\{(\epsilon - \phi), 0\} \\ \mathrm{ER}_{\mathrm{inf}} \leq \mathrm{ER} \leq \mathrm{ER}_{\mathrm{sup}} & \epsilon \text{ does not change} \\ \mathrm{ER} > \mathrm{ER}_{\mathrm{sup}} & \epsilon \leftarrow \min\{(\epsilon + \phi), 1\}. \end{cases} \tag{5}$$

The values of $\mathrm{ER}_{\mathrm{inf}}$ and $\mathrm{ER}_{\mathrm{sup}}$ in eqn (5) are scheme-dependent and must be calibrated beforehand. A small constant value of $\phi = 0.01$ is used to adjust the value of ϵ in a continuous and gradual manner. To ensure a single value of ϵ across the interface of cells i and j, we define $\epsilon_{ij} = \max\{\epsilon_i, \epsilon_j\}$ in order to ensure the robustness of the numerical scheme. Please note that everything explained so far is only valid for smooth flows, and there is no guarantee whatsoever that the scheme is robust enough, so in order to extend this methodology to compressible turbulent flows, we propose to combine the ADA methodology with the *a posteriori* paradigm [13], [14].

3.2 *A posteriori* paradigm

The use of the ADA method in the compressible flow framework is problematic since the algorithm of eqn (5) may not be fast enough to introduce dissipation in the presence of a shockwave. There may appear cases where even a value of $\epsilon = 1$ may not be enough to stabilize the solution, since schemes of higher order than 1 are not monotonic. Thus, it is required a method for stabilizing the computations with the minimum interference with the ADA methodology.

The key idea is to find, for each time step, the most accurate scheme available that is also robust enough. To this end, a *candidate solution* is formed with the highest-order scheme. Afterwards, the candidate solution is run through a series of detectors that check whether this solution is admissible or not according to certain criteria, which are described in the following. If any of the detectors flag the solution as invalid, it is recomputed using a lower-order scheme or different values of ϵ. This process can be as sophisticated as needed, generating a cascade of different schemes and combinations of ϵ values.

3.2.1 Employed detectors

Once a candidate solution is computed, it is run by the following chain of detectors:

- Physical admissibility detector (PAD): It checks that both the density and pressure of the solution at every cell is positive. In practice it also detects the NaN values. If a cell has a negative value of pressure or density, it is flagged and recomputed using a stable scheme, for instance a first-order finite volume or a fifth order finite difference WENO scheme. It is recommended to set $\epsilon = 1$, although other possibilities are presented in [11].
- Numerical admissibility detector (NAD) [17]: It is a relaxed version of the Discrete Maximum Principle (DMP). It checks whether the solution is monotonic and no new local extrema are created. If the double inequality

$$\min_{\boldsymbol{y} \in \mathcal{V}_i} \left(\mathbf{U}^{\mathrm{RK}}(\boldsymbol{y})\right) - \delta \leq \mathbf{U}^*(\boldsymbol{x}) \leq \max_{\boldsymbol{y} \in \mathcal{V}_i} \left(\mathbf{U}^{\mathrm{RK}}(\boldsymbol{y})\right) + \delta, \tag{6}$$

holds true, the solution is considered admissible. The δ parameter defined as

$$\delta = \max\left\{10^{-4}, 10^{-3} \cdot \left(\max_{\boldsymbol{y}\in\mathcal{V}_i}\left(\mathrm{U}^n(\boldsymbol{y})\right) - \min_{\boldsymbol{y}\in\mathcal{V}_i}\left(\mathrm{U}^n(\boldsymbol{y})\right)\right)\right\}, \tag{7}$$

allows a certain level of oscillations. This is allowed in order to keep a high accuracy when dealing with smooth extrema. $\mathcal{V}_i$ represents all the neighboring cells that are present in the MLS stencil.

- This chain of detectors can be extended in order to check any other desirable property.

The fulfilment of the NAD condition implies that the candidate solution value remains between the local minimum and the local maximum of that of the previous time step. In all the examples of this work, the NAD is checked only in one variable (density or energy), but it could be applied to the full vector of conservative variables as suggested by [14]. If a cell does not verify the NAD criterion, the cell is recomputed. There are several strategies on how to recompute this cell depending on the type of numerical scheme. One possible strategy is to find the new value of ϵ that takes into account the compressibility of the problem with a hyperbolic tangent limiter as in [11]. A more simplistic strategy is to recompute the cell exactly in the same way as if there was a PAD violation, that is, using the same scheme with $\epsilon = 1$.

4 NUMERICAL TEST CASES

In this section we test the proposed methodology against several common benchmark test cases in order to study if the proposed approach is stable. In this section we test the proposed approach for the resolution of under resolved turbulent flows in an Implicit LES approach. First, we address two 1D problems in order to show that the modification of the dissipation does not introduce dispersion errors. In all of the numerical examples presented here we have used a third-order TVD Runge–Kutta scheme [18] for time integration.

4.1 One-dimensional double shock test case

The objective of this test case is to show that the proposed scheme is as robust as the original scheme. In this test case, a left-going and a right-going shock collide, and the solution consists of a left-going shock that travels very slowly to the right, a contact discontinuity which travels to the right and a right traveling shock wave. The domain is set in [0,1], being $x = 0.5$ the separation between the initial left and right states, given as

$$(\rho, u, p) = \begin{cases} (6, 20, 450) \text{ if } x \leq 0.5 \\ (6, -6, 45) \text{ if } x > 0.5. \end{cases} \tag{8}$$

This test case is solved using a third-order finite volume solver with Roe flux, using the methodology explained in [11]. This scheme is labelled as FV-MLS-ADA. The results using the aforementioned scheme are compared with the original scheme with no ADA, labeled just as FV-MLS. We use 100 control volumes and run the simulation until $t = 0.02$. The exact solutions were computed using the NUMERICA software [19]. The results can be seen in Fig. 1.

We observe that the use of adaptive dissipation does not vary the results. This is the expected behavior for this test case, since in the zone of the shock we recover the original scheme, whereas in the rest of the domain, the dissipation introduced by the original scheme is low.

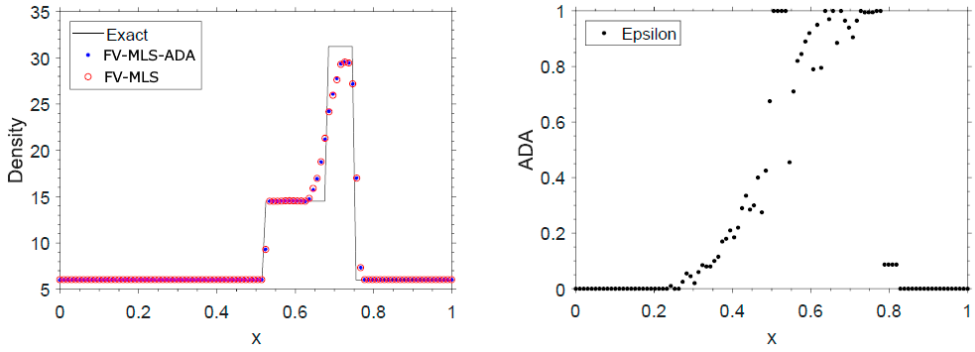

Figure 1: One-dimensional double shock test case results at $t = 0.02$. Comparison of the results using the adaptive dissipation and the numerical flux of Roe.

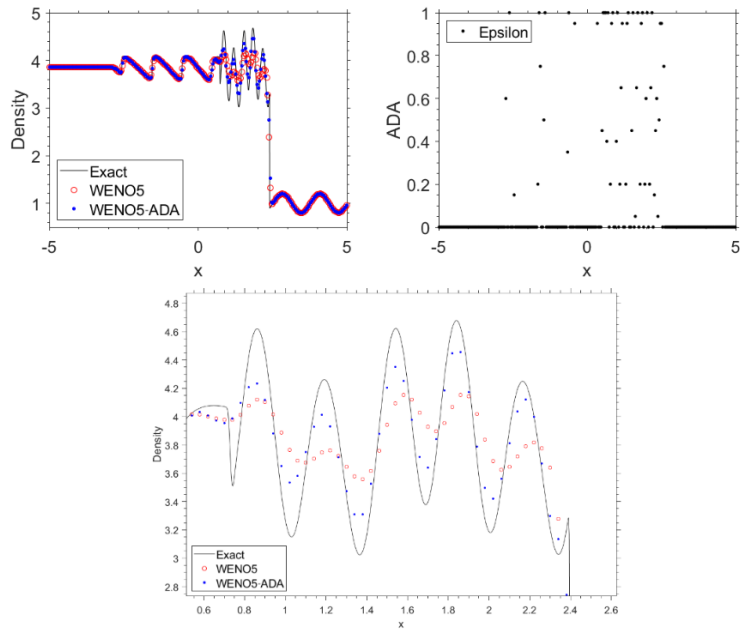

Figure 2: Shock/density oscillation interaction test case. Obtained results for a 250-point grid at $t = 1.8$ using a WENO5 finite difference scheme. The WENO5 ADA version obtains a sharper resolution than the original counterpart. Below, a zoomed plot of the density is seen.

4.2 Shock/density oscillation interaction test case

This is a classical benchmark proposed in [20]. It is Mach 3 shock wave interactive with upstream sinusoidal density waves. The domain is set in [–5, 5]. The solution is computed using a finite difference WENO 5 with the ADA and MOOD methodology explained in this work. This is possible because, as explained before, the WENO 5 can be put into a central

plus dissipation flux [15]. The solution is computed with a CFL number equal to 0.5 and the final time of the simulation is $t = 1.8$. We use a grid with 250 points, which is a coarse grid for this test case. The initial condition is given by

$$(\rho, u, p) = \begin{cases} (3.857143, 2.629369, 10.33333) & \text{if } x < -4 \\ (1 + 0.2\sin(5x), 0, 1) & \text{if } x \geq -4. \end{cases} \tag{9}$$

This test measures the ability of the schemes for capturing both small-scale smooth flow and shocks. It is a common benchmark in the context of turbulence solvers. The overall performance of the WENO5 ADA scheme can be seen in the upper part of Fig. 2 and with more detail for the density in the bottom part of Fig. 2. Since this test case is designed to be a turbulence benchmark, an important improvement can be observed in the oscillatory region, where the WENO5 ADA scheme performs better than its original counterpart. As seen in the presented one-dimensional test cases, the ADA mechanism delivers a really similar solution to that of the WENO5 scheme, achieving a sharper resolution around contact discontinuities and shocks. There are no phase or dissipation errors in the solutions obtained with the WENO5 ADA method.

4.3 Inviscid incompressible isotropic Taylor–Green vortex

This test case is the simplest model for the analysis of the nonlinear transfer of kinetic energy among the different scales of the flow. Despite its simplicity, it contains several key physical processes of turbulence. We solve the inviscid version of this test case in order to analyze the behavior under an infinite Reynolds number, until $t = 10$. This is intended to show the behavior of the proposed method for under-resolved simulations, and to examine its capabilities to reproduce the transition to turbulence.

The initial setup for this three-dimensional case is

$$\begin{aligned} \rho &= 1 \\ u &= \sin(x)\cos(y)\cos(z) \\ v &= -\cos(x)\sin(y)\cos(z) \\ w &= 0 \\ p &= 100 + \frac{(\cos(2x)+\cos(2y))(2+\cos(2z))-2}{16}. \end{aligned} \tag{10}$$

For very large Reynolds numbers, it is known that statistically isotropic turbulence develops following the Kolmogorov's law, $(-5/3)$ decay, of the kinetic-energy spectra within the inertial subrange around $t = 9$. A physically-consistent numerical method developed for implicit LES should recover this behavior. Since the density the density must remain constant in this case due to the incompressibility hypothesis, we use the kinetic energy as the variable to check for oscillations in the *a posteriori* framework.

Figs 3 and 4 present the results obtained by the proposed approach and the baseline schemes, using the third order FV-MLS scheme and the WENO 5 scheme. The results obtained by the proposed approach, are in excellent agreement with the reference solution. Both in terms of enstrophy and kinetic energy. The use of the ADA method allows to obtain comparable or better results than those obtained with higher-order schemes and closely reproduces the semi-analytical results of [21]. The spectrum obtained by the proposed methodology is in very good agreement with the expected theoretical Kolmogorov's law.

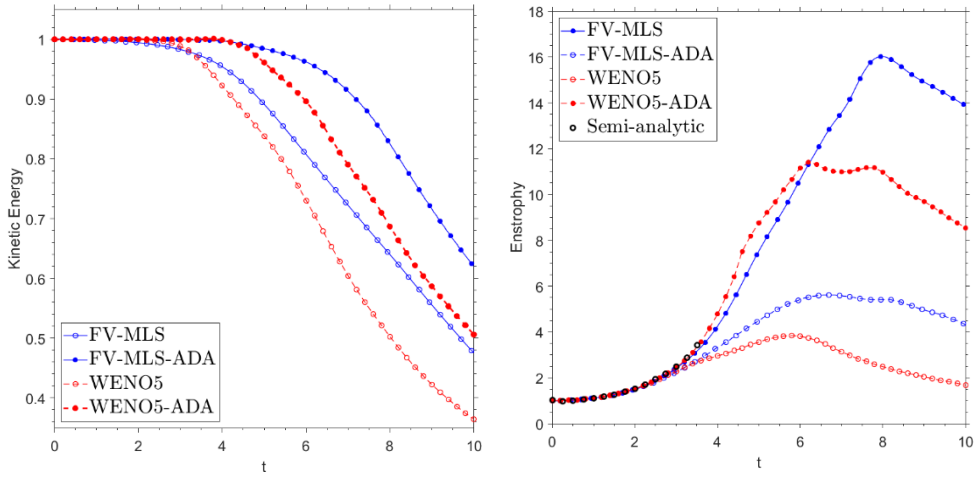

Figure 3: Incompressible isotropic Taylor–Green vortex. Evolution of the normalized total kinetic energy (left) and enstrophy (right). Results obtained for a 64^3 periodical grid for the WENO5 and FV-MLS schemes, with and without the ADA framework. Results from other schemes have been taken from [11].

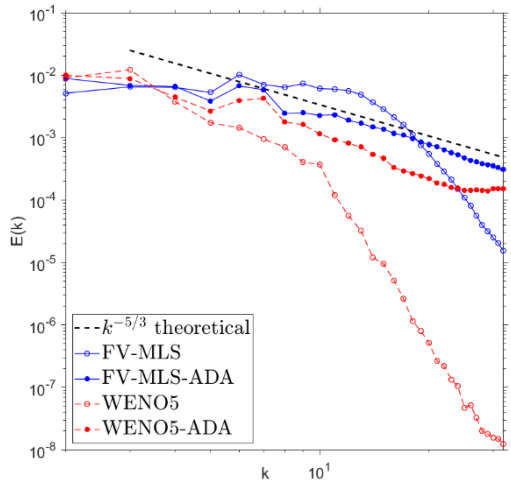

Figure 4: Incompressible isotropic Taylor–Green vortex. The 3D energy spectrum at the final time $t = 10$ compared with the Kolmogorov scaling of (–5/3).

5 CONCLUSIONS

In this work, we have presented a general framework of using an Adaptive Dissipation Algorithm (ADA) in combination with the *a posteriori* methodology to obtain improved accuracy for any numerical scheme whose numerical flux can be rewritten as a central plus a dissipative part. This is the cases of many finite volume and finite difference schemes, which are the ones tested here, but this framework can be extended to discontinuous galerkin

or any other numerical discretization that follows the aforementioned rule. We have tested some one-dimensional test cases where the ADA variants are at least as good as their original counterparts. In the case of the three-dimensional case, a notable increase of accuracy of the method is observed.

ACKNOWLEDGEMENTS

This work has been partially supported by FEDER funds of the European Union, Grant #RTI2018-093366-B-I00 of the Ministerio de Ciencia, Innovación y Universidades of the Spanish Government and by the Consellería de Educación e Ordenación Universitaria of the Xunta de Galicia (grants #GRC2014/039 and #ED431C 2018/41).

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