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Scalar conservation and boundedness in simulations of compressible flow

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ABSTRACT

With the proper combination of high-order, low-dissipation numerical methods, physics-based subgrid-scale models, and boundary conditions it is becoming possible to simulate many combustion flows at relevant conditions. However, non-premixed flows are a particular challenge because the thickness of the fuel/oxidizer interface scales inversely with Reynolds number. Sharp interfaces can also be present in the initial or boundary conditions. When higher-order numerical methods are used, there are often aphysical undershoots and overshoots in the scalar variables (e.g. passive scalars, species mass fractions or progress variable). These numerical issues are especially prominent when low-dissipation methods are used, since sharp jumps in flow variables are not always coincident with regions of strong variation in the scalar fields: consequently, special detection mechanisms and dissipative fluxes are needed. Most numerical methods diffuse the interface, resulting in artificial mixing and spurious reactions. In this paper, we propose a numerical method that mitigates this issue. We present methods for passive and active scalars, and demonstrate their effectiveness with several examples.

1. Motivation

Accurate computations of scalar fields in high Reynolds number compressible flows pose several numerical challenges. Thin interfaces must be resolved without excessive numerical diffusion: this requires the use of relatively high-order, low dissipation schemes that promise to resolve these high wavenumber features. In addition, it is often crucial that the physical bounds on the scalar values set by the initial and boundary values of the simulation are not violated. For instance, we would like to ensure that the mass fractions of chemical species are individually in the range $[0, 1]$ and to sum to unity; naively correcting deviations from this can result in a scheme that does not conserve mass. The use of spatially high-order methods in reacting flow calculations often results in local undershoots and overshoots in the species mass fractions, causing aphysical results. This results in mass fraction or other scalar non-conservation, and for reacting cases, these errors can cause temperatures to exceed the adiabatic flame temperature. In other cases, we would like to ensure that scalar concentrations are everywhere strictly in some range of prescribed values. This includes passive scalar fields, mass fractions of chemical species and transported turbulence quantities, among many other examples.

While the use of high-order, low-dissipation schemes for the computation of compressible flow is now fairly commonplace, the issue of ensuring scalar boundedness has received less attention, and is the focus of this paper. Consider the usual

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inviscid conservation equations for mass, momentum, and energy along with the equation for the evolution of a scalar in compressible flow

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = 0 \tag{1}$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} \tag{2}$$

$$\frac{\partial E}{\partial t} + \frac{\partial (E+p) u_j}{\partial x_j} = 0 \tag{3}$$

$$\frac{\partial \rho \phi}{\partial t} + \frac{\partial \rho \phi u_j}{\partial x_j} = 0, \tag{4}$$

where the total energy, $E = p/(\gamma - 1) + \rho(u^2 + v^2 + w^2)/2$, the pressure is defined by $p = \rho RT$ and $\gamma = C_p/C_v$ is the ratio of specific heats of the gas. Combining equations (1) and (4), it is easy to show that

$$\frac{\partial \phi}{\partial t} + u_j \frac{\partial \phi}{\partial x_j} = 0,$$

implying that for the inviscid equations, in the absence of source terms, ϕ is a purely convected quantity which should be bounded by initial and boundary values. We would like to ensure that the numerical method for solving equations (1)–(4) respects this in a discrete sense.

Note that preserving the positivity of density and pressure (or internal energy) while solving the above equations is a related numerical issue that has been the subject of several discussions in the literature. Given initial conditions with positive density and pressure, a positivity preserving scheme will produce solutions which also have positive density and pressure: these schemes usually have an additional CFL constraint that guarantees this property. Of course, this CFL restriction should not be excessive for the methods to be useful. Perthame [1] constructed positivity preserving Boltzmann type schemes for the Euler equations. Perthame and Shu [2], in a pioneering paper demonstrated that higher-order positive schemes in space and time could be built from one-dimensional, first-order building blocks and specially constructed high-order reconstructions. In a similar vein, Linde and Roe [3] showed that, given a first order one-dimensional positive scheme, one can construct a second order, multidimensional MUSCL type scheme that is also positive: notably, the analysis uses a generic finite-volume formulation that should work for unstructured meshes as well. The notion of positivity preservation has played an important role in the construction of several popular approximate Riemann solvers as well: we mention, in particular, its influence on the HLLE [4] and AUSM [5] schemes.

In a series of recent papers, Zhang and Shu [6–8], building on the idea in Perthame and Shu [2], and incorporating the idea of a 'linear-scaling limiter' from Liu and Osher [9], developed genuinely high-order finite volume and discontinuous Galerkin schemes that satisfy the strict maximum principle for scalar conservation laws and the positivity principle for the Euler equations, when certain CFL conditions are satisfied. Hu, Adams and Shu [10] later constructed a positive flux-limiter scheme for the Euler equations which also produces positive solutions, under a slightly less restrictive CFL condition.

Note that artificial viscosity methods based on the paper by von Neumann and Richtmyer [11] form the basis for a distinct and increasingly popular set of numerical schemes that can be used to address some of these issues. We refer the reader to section 3.3 in the review paper by Pirozzoli [12] for background and relevant references. In the context of the issues discussed in this paper, we mention the work of Cook and Cabot [13] who use a sensitive detector formed using high order derivatives to create a low dissipation artificial viscosity method. Fiorina and Lele [14] and Cook [15] extended the method to multi-species calculations by augmenting the physical diffusivity coefficients with artificial ones. We note that the artificial diffusion term for species diffusivity in Cook's [15] formulation is sensitized to global mass fraction bounds via the use of Heaviside functions (equation 18 in [15]).

Let us assume that we have a finite volume code that satisfactorily solves the mass, momentum and energy equations. The method may or may not be strictly positivity preserving for the density and pressure (the code should stop with an error message of some sort if the density or pressure assume negative values). The fluxes in the method should satisfy the entropy condition in order to prevent physically ambiguous solutions. For time accurate, unsteady simulations, the dissipation terms in the fluxes may be damped by a shock-detecting switch to localize the numerical diffusion. Given this common framework, we would like to add additional transport equations describing, for example, passive scalars, multiple chemical species (perhaps in lieu of the total mass conservation equation), or advected variables that feed into a turbulence model. The key question we examine in this paper relates to achieving bounded (maximum-principle satisfying) schemes that also have low levels of dissipation for these fields.

It should be noted that, for compressible flow as well as flows with strong density variation, numerical methods that aim to preserve the maximum principle for fields determined by (4) should take into account (1) (the variation of the density field) as well: these equations are strongly coupled and the discretization should respect this.