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Entropy stable wall boundary conditions for the three-dimensional compressible Navier–Stokes equations

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ABSTRACT

Non-linear entropy stability and a summation-by-parts framework are used to derive entropy stable wall boundary conditions for the three-dimensional compressible Navier–Stokes equations. A semi-discrete entropy estimate for the entire domain is achieved when the new boundary conditions are coupled with an entropy stable discrete interior operator. The data at the boundary are weakly imposed using a penalty flux approach and a simultaneous-approximation-term penalty technique. Although discontinuous spectral collocation operators on unstructured grids are used herein for the purpose of demonstrating their robustness and efficacy, the new boundary conditions are compatible with any diagonal norm summation-by-parts spatial operator, including finite element, finite difference, finite volume, discontinuous Galerkin, and flux reconstruction/correction procedure via reconstruction schemes. The proposed boundary treatment is tested for three-dimensional subsonic and supersonic flows. The numerical computations corroborate the non-linear stability (entropy stability) and accuracy of the boundary conditions.

1. Introduction

During the last twenty years, scientific computation has become a broadly-used technology in all fields of science and engineering due to a million-fold increase in computational power and the development of advanced algorithms. However, the great frontier is in the challenge posed by high-fidelity simulations of real-world systems, that is, in truly transforming computational science into a fully predictive science. Much of scientific computation's potential remains unexploited—in areas such as engineering design, energy assurance, material science, Earth science, medicine, biology, security and fundamental science—because the scientific challenges are far too gigantic and complex for the current state-of-the-art computational resources [1].

In the near future, the transition from petascale to exascale systems will provide an unprecedented opportunity to attack these global challenges using modeling and simulation. However, exascale programming models will require a revolutionary approach, rather than the incremental approach of previous projects. Rapidly changing high performance computing (HPC) architectures, which often include multiple levels of parallelism through heterogeneous architectures, will require new paradigms to exploit their full potential. However, the complexity and diversity of issues in most of the science community are such that increases in computational power alone will not be enough to reach the required goals, and new

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algorithms, solvers and physical models with better mathematical and numerical properties must continue to be developed and integrated into new generation supercomputer systems.

In computational fluid dynamics (CFD), next generation numerical algorithms for use in large eddy simulations (LES) and hybrid Reynolds-averaged Navier–Stokes (RANS)–LES simulations will undoubtedly rely on efficient high-order accurate formulations (see, for instance, [2–21]). Although high order techniques are well suited for smooth solutions, numerical instabilities may occur if the flow contains discontinuities or under-resolved physical features. A variety of mathematical stabilization strategies are commonly used to cope with this problem (e.g., filtering [22], weighted essentially non-oscillatory (WENO) [23], artificial dissipation, over-integration, and limiters [2]), but their use for practical complex flow applications in realistic geometries is still problematic.

A very promising and mathematically rigorous alternative is to focus directly on discrete operators that are non-linearly stable (entropy stable) for the compressible Navier–Stokes equations. These operators simultaneously conserve mass, momentum, energy, and enforce a secondary entropy constraint. This strategy begins by identifying a non-linear neutrally stable flux for the Euler equations. An appropriate amount of dissipation can then be added to achieve the desired smoothness of the solution. Regardless of whether dissipation is added, enforcing a semi-discrete entropy constraint enhances the stability of the base operator.

The idea of enforcing entropy stability in numerical operators is quite old [24], and is commonly used for low-order operators [25,26]. An extension of these techniques to include high-order accurate operators recently appears in references [27–30] and provides a general procedure for developing entropy conservative and entropy stable, diagonal norm summation-by-parts (SBP) operators for the compressible Navier–Stokes equations. The strong conservation form representation allows them to be readily extended to capture shocks via a comparison approach [25,28]. The generalization to multi-domain operators follows immediately using simultaneous-approximation-term (SAT) penalty type interface conditions [31], whereas the extension to three-dimensional (3D) curvilinear coordinates is obtained by using an appropriate coordinate transformation which satisfies the discrete geometric conservation law [32]. See LeFloch and Rohde [33] for a more comprehensive discussion on high order schemes and entropy inequalities. Therein, the focus is on the approximation of under-compressive, regularization-sensitive, non-classical solutions of hyperbolic systems of conservation laws by high-order accurate, conservative, and semi-discrete finite difference methods.

Several major hurdles remain, however, on the path towards complete entropy stability of the compressible Navier–Stokes equations including shocks. A major obstacle is the need for solid wall viscous boundary conditions that preserve the entropy stability property of the interior operator. In fact, practical experience indicates that numerical instability frequently originates at solid walls, and the interaction of shocks with these physical boundaries is particularly challenging for high order formulations. An important step towards entropy stable boundary conditions appears in the work of Svärd and Özcan [34]. Therein, entropy stable boundary conditions for the compressible Euler equations are reported for the far-field and for the Euler no-penetration wall conditions, in the context of finite difference approximations.

The focus herein is on building non-linearly stable wall boundary conditions for the compressible Navier–Stokes equations; primarily a task of developing stable wall boundary conditions for the viscous terms. At the semi-discrete level, the proposed boundary treatment mimics exactly the boundary contribution obtained by applying the entropy stability analysis to the continuous, compressible Navier–Stokes equations. Furthermore, the new technique enforces the Euler no-penetration wall condition as well as the remaining no-slip and thermal wall conditions in a weak sense (using the SAT approach). The thermal boundary condition is imposed by prescribing the heat entropy flow (or heat entropy transfer), which is the primary means for exchanging entropy between two thermodynamic systems connected by a solid viscous wall. Note that the entropy flow at a wall is a quantity that in some experiments is directly or indirectly available (e.g., through measurements of the wall heat flux and temperature in some supersonic or hypersonic wind tunnel experiments), or can be estimated from geometrical parameters and fluid flow conditions for the problem at hand. For fluid–structure interaction simulations, (e.g., supersonic and hypersonic flow past aerospace vehicles, heat-exchangers), the entropy flow can be numerically computed at no additional cost while numerically solving the coupled systems of partial differential equations of the continuum mechanics and fluid dynamics.

Historically, most boundary condition analysis for the compressible Navier–Stokes equations is performed at the linear level by linearizing about a known state; a rich collection of literature is available [35–38]. The non-linear wall boundary conditions developed herein are fundamentally different from those derived using linear analysis and cannot rely on a complete mathematical theory. In fact, a fundamental shortcoming that limits further development of any entropy stable boundary conditions is the incomplete development of the analysis at the continuous level for proving well-posedness of the compressible Navier–Stokes equations. Nevertheless, the boundary conditions proposed herein is extremely powerful because they provide a mechanism for ensuring the non-linear stability in the L^2 norm of the semi-discretized compressible Navier–Stokes equations. In fact, they allow for a priori bounds on the entropy function at the continuous and semi-discrete level when imposing "solid viscous wall" boundary conditions. The new boundary conditions are easy to implement and compatible with any diagonal norm SBP spatial operator, including finite element (FE), finite volume (FV), finite difference (FD) schemes and the more recent class of high-order accurate methods which include the large family of discontinuous Galerkin (DG) discretizations [39] and flux reconstruction (FR) schemes [40].

The robustness and accuracy of the complete semi-discrete operator (i.e., the entropy stable interior operator coupled with the new boundary conditions) is demonstrated by computing subsonic and supersonic flows past a 3D square cylinder without any stabilization technique (e.g., artificial dissipation, filtering, limiters, over-integration, de-aliasing, etc.), a feat