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Exact Jacobians for implicit Navier–Stokes simulations of equilibrium real gas flows

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ABSTRACT

This paper documents the extension of several widespread flux schemes, used in finite-volume Navier–Stokes solvers, for the simulation of flows whose fluid properties must be estimated with complex thermophysical models. Exact Jacobian matrices for the convective fluxes are derived with no assumption on the fluid equations of state model for Liou's AUSM$^+$, Toro et al.'s HLLC, and Kurganov and Tadmor's central scheme. The Jacobians of the diffusive fluxes are expressed using the formulation proposed by Pulliam and Steger, resulting in additional terms due to the viscosity and thermal conductivity variations. An efficient look-up table approach is thoroughly studied and proposed as an alternative to the direct solution of the equation of state model for the fluid thermophysical property evaluation. The newly introduced schemes are validated and tested in terms of accuracy and convergence rate on a series of one- and two-dimensional test cases. The results indicate that the Jacobian must be based on the same flux formulation as the one used on the right-hand side of the implicit equation to achieve numerically converged solutions.

1. Introduction

Nowadays, computational fluid dynamics (CFD) is a widely used tool for the analysis and design of many engineering applications, as well as for the study of the physics of complex flows. Most of the numerical techniques applicable to compressible flows developed throughout the years have been derived under the assumption that the fluid complies with the ideal gas model. However, several assumptions (e.g., constant specific heats, ideal gas law) do not hold if a fluid state is close to its vapor–liquid critical point or at high temperatures and low pressures. There is a wide variety of flows for which real gas effects are predominant and must be considered, some of them being hypersonic flows, reacting flows, and supercritical flows. It is therefore of paramount importance to include a complex thermophysical description of the fluid when such numerical simulations are to be performed.

The topic of adapting standard numerical techniques to be applicable for real gas flows using the finite volume Godunov method [1] has been proposed in the 1980s by several authors. Colella and Glaz [2] were among the first to study the numerical solution of the Riemann problem of gasdynamics for a real fluid. Further contributions are the pioneering work of Glaister [3–6], Montagné and co-workers [7,8], and Gallouët and co-workers [9,10]. They extended Roe's approximate Riemann solver [11], and some variants of the original scheme, with a complex equations of state. A generalization of the

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Roe linearization for high temperature reacting flows was introduced by Mottura et al. [12]. Other splitting schemes such as Steger–Warming's [13], van Leer's [14], Osher's [15], and Liou's AUSM$^+$ [16] were considered by Liou et al. [17], Suresh and Liou [18], and Edwards and co-workers [19,20]. Central difference schemes were studied by Saurel et al. [21] and later by Merkle et al. [22]. Recently, the increasing interest in transcritical fluids as the working medium for energy conversion applications (e.g., organic Rankine cycle and supercritical CO_2 Brayton cycle turbines) drove the scientific community to further develop numerical schemes for the simulation of complex three-dimensional flows of real gases, see for example Colonna and co-workers [23–25], Cinnella and co-workers [26–28], Boncinelli et al. [29], and Cirri et al. [30].

The aim of this paper is to provide a complete methodology for incorporating complex thermophysical models in several well established inviscid and viscous flux schemes for the Navier–Stokes equations. The inviscid flux schemes considered are the AUSM$^+$ scheme introduced by Liou [16], the HLLC scheme of Toro et al. [31], and the central scheme of Kurganov and Tadmor (KT) [32]. No assumption on the equation of state model is assumed. The description of the Roe solver is included for the purpose of comparison and its implementation is taken from Colonna and Rebay [23]. The diffusive fluxes and their implicit formulations are discretized following Pulliam and Steger [33]. Additional terms in the Jacobian caused by temperature-dependent viscosity and thermal conductivity are highlighted and discussed. Furthermore, a look-up table (LUT) interpolation is proposed and comprehensively evaluated. A detailed assessment of the LUT accuracy, consistency, and computational efficiency with respect to direct solution of the equation of state model is given to provide a solid basis for its use.

The focus of the numerical experiments presented is on the dense gas region, therefore high temperature phenomena such as dissociation are excluded from the analysis. Furthermore, only single phase flows are considered in the numerical modeling. However, the methods proposed in this work can be applied to model two-phase vapor–liquid flows when the assumption of the homogeneous mixture can be made, see for example Refs. [34,35].

The paper is structured as follows. Section 2 describes the analysis of the LUT interpolation method and the evaluation of its performance compared to the direct calculation of fluid properties using EoS models. The formulation of the convective and diffusive numerical fluxes and the expression of the Jacobians for both is provided in Sections 3 and 4. A series of one- and two-dimensional test cases is presented in Section 5 and convergence histories are also reported. Finally, conclusions are drawn in Section 6. The appendices give the generic expressions of the pressure derivatives needed for the fluxes and the Jacobians (Appendix A), and the strategy adopted to obtain the exact solution of the Riemann problem of gasdynamics for a real gas (Appendix B).

2. Look-up tables for fluid property evaluations

The main limitation of CFD simulations for the analysis of fluids governed by complex thermodynamics is the computational effort required for their thermophysical property evaluation. This issue can be the bottle-neck of the use of real gas flow simulations within the framework of uncertainty quantification or numerical optimization. If real gas equations of state models are adopted, various levels of approximation are possible, whereby high accuracy implies large computational cost. In order to reduce the latter an approximate property evaluation must be considered instead of a direct solution of the equation of state. A LUT interpolation provides the best features in terms of efficiency, simplicity, and flexibility. A grid is generated over a range for two independent thermodynamic variables (e.g., temperature and density), and all the thermophysical properties of interest are stored in its nodes. The table can be accessed specifying any pair of properties, and the cell identification can be easily done with standard search algorithms. If the tabulated region encompasses the vapor–liquid equilibrium (VLE) region, we split the grid into two sub-grids, one for the single phase and one for the VLE region. This is done because of the discontinuity across the saturation lines of thermophysical properties such as pressure derivatives and the speed of sound. The accuracy, consistency, and computational cost of table interpolation are analyzed in the following sections.

2.1. Accuracy

The comparison of the results of three table interpolation schemes is described hereafter, namely the bilinear, the 3rd order Lagrange polynomial, and the least-squares gradient interpolation schemes. The accuracy of the property interpolation is assessed in the supercritical region of carbon dioxide CO_2 (similar results can be obtained with different fluids), where several thermophysical properties show a nonlinear behavior, e.g. density, specific heats, thermal conductivity, and viscosity. Interpolated values for 40,000 random input states are compared with the values obtained from the solution of the thermodynamic model, namely the multiparameter EoS for technical applications of Span and Wagner type [36–38]. The thermodynamic model is expressed in terms of the reduced Helmholtz free energy as a function of the reduced density and of the inverse of the reduced temperature. The model parameters (12 in total) are optimized fitting a large set of high accuracy experimental data. The average relative interpolation error is shown in Fig. 1 as a function of the number of discretization nodes for the single edge of the table. The convergence rate for the three schemes is not affected by the different choice of input variables. As expected, the polynomial interpolation shows the best accuracy and convergence. Similar results and trends are obtained if values calculated in other thermodynamic regions are compared. It is worth mentioning that a limited number of discretization nodes (around 100 for each dimension in the presented case) leads to a level of accuracy acceptable for many practical applications.