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Efficient numerical simulation of three-dimensional Bethe-Zel'dovich-Thompson fluid flows

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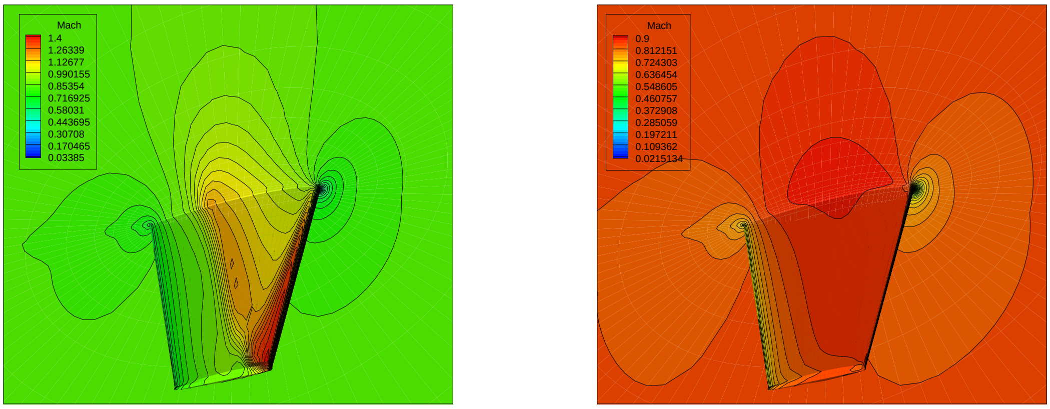
ABSTRACT

Dense gases are defined as single-phase vapors of molecularly complex fluids close to saturation conditions, with properties significantly deviating from the ideal gas law. At these conditions, real gas effects play a crucial role in the gasdynamic behavior of the fluid. The study of the complicated dynamics of compressible flows of dense gases is strongly motivated, among other reasons, by their potential technological advantages as working fluids in energy-conversion cycles. Specific interest has been developed in a particular class of dense gases, known as the Bethe-Zel'dovich-Thompson fluids, which exhibit nonclassical gasdynamic behaviors in a range of thermodynamic conditions above the liquid/vapor coexistence curve, such that the Fundamental Derivative of Gasdynamics $\Gamma = 1 + \frac{\rho}{a}\left(\frac{\partial a}{\partial \rho}\right)_s$, with ρ the fluid density, a the sound speed, and s the entropy, becomes negative. At these conditions, the well-known compression shocks of the perfect gas theory violate the entropy inequality, over a certain range of temperatures and pressures in the vapor phase, and are therefore inadmissible. BZT properties are theoretically predicted in fluids possessing large heat capacities and formed by complex, heavy molecules, such as some commercially available heat transfer fluids. The non-classical phenomena typical of BZT fluids have several practical outcomes: prominent among them is an active research effort to reduce losses caused by wave drag and shock/boundary layer interactions in turbomachines and nozzles, with particular application to Organic Rankine Cycles (ORCs). The present paper contributes to this effort through the development of an efficient numerical solver for studying BZT fluid flows in general geometries.
Previous works by the first two authors have been devoted to the development of an inviscid structured grid finite-volume solver (SGS) based on a Jameson type numerical scheme extended to third-order accuracy, coupled with a four-stage Runge-Kutta time-integration and including local time stepping, implicit residual smoothing and multigrid to efficiently drive the solution to the steady state [1] [2]. The use of a scalar dissipation term simplifies the scheme implementation with the complex equations of state (such as Martin Hou's) retained to describe the dense gas behaviour. Recently, a 2D inviscid unstructured grid solver (UGS) for dense gas flows has been developed [3] using the HLL scheme, extended to second-order with a MUSCL-type linear

reconstruction process where the gradient estimates required at each cell center are obtained through a least-square technique. The HLL scheme has been retained because of its accuracy properties and easy extension to complex equations of state. Fast convergence to steady state is provided by a matrix-free implicit stage allowing the use of large CFL numbers and solved by an inexpensive point-relaxation technique. The numerical flux through the boundary edges is computed using an inflow / outflow characteristic-based condition to define the ghost-cell states at the far-field boundary and a mirror boundary condition to define the ghost-cell states at the wall. The comparisons between SGS and UGS performed in [3] have provided a convincing cross-validation of the available dense gas flow solvers for 2D configurations.

The present contribution is focused on the development of an efficient 3D extension of the existing UGS for dense gas flows described using Martin-Hou's equation of state. This 3D version will include a quadratic least-square-based reconstruction ensuring 3rd-order accuracy on general grids and low-Mach preconditioning to speed up convergence in low-speed regions; it will be applied to the computation of inviscid BZT flows over an ONERA M6 wing for a variety of operating conditions associated with more or less pronounced dense gas effects. The results will be analyzed both from the viewpoint of physical accuracy and numerical efficiency since 3D shape optimization implying numerous direct simulations is targeted next. A grid convergence study will be performed and the computed flow patterns will be compared with those previously obtained using SGS in [4].



(a) Perfect gas: $M_{max} = 1.37$, $C_L = 0.329$.

(b) Dense gas: $M_{max} = 0.9$, $C_L = 0.301$

Figure 1: Inviscid flow at $M_\infty = 0.84$ and $\alpha = 3.06°$ over the ONERA M6 wing. Mach number contours computed using the 2nd-order HLL scheme on a coarse grid made of 48×10^3 hexahedral elements. (a) Perfect gas flow displaying a typical λ-shock structure. (b) Dense gas (fluorocarbon PP10) flow at operating conditions (far-field over critical values): $p_\infty/p_c = 1$, $\rho_\infty/\rho_c = 0.752$ ($\Gamma_\infty = 0.416$).

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