Preliminary Results: A GPU-Oriented NASA–Roe Flux Solver

Thermally Perfect Gas Dynamics in PeleC/AMReX

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Motivation

For compressible reacting-flow simulations at high temperature, the use of a calorically perfect-gas approximation inside the convective flux calculation may become inconsistent with the temperature-dependent thermodynamics used by the equation of state and chemistry. This inconsistency is potentially important in strong-shock problems, where a localized temperature error can strongly alter chemical induction times.

The present work explores a Roe-type approximate flux formulation (*NASA–Roe*) for thermally perfect gases represented by NASA polynomial thermodynamics. The objective is to retain much of the computational efficiency and GPU suitability of conventional linearized Riemann solvers while treating the temperature-dependent thermodynamics more consistently.

Solvers Compared

Four flux solvers are considered.

PeleC Riemann. "Riemann" denotes the default convective Riemann solver used in the present PeleC configuration. It is used here as the baseline and evaluates the flux through a linearized approximate treatment based on a calorically perfect (γ-law) gas model.

GodunovPG. GodunovPG is an exact thermally perfect-gas Riemann solver implemented following the framework of Xu, Yang, and Liu [1]. It evaluates the star state using the NASA-polynomial thermodynamics. The resulting nested ODE integrations and iterative star-state solution make it computationally expensive for routine CFD use.

Taylor_2_Fast. Taylor_2_Fast replaces the ODE integrations in GodunovPG by a second-order Taylor approximation, avoiding direct numerical integration. This substantially reduces the cost, but the algorithm still contains significant control-flow branching and requires iterative matching of u^* and p^*, which is unfavorable for massively parallel GPU execution.

NASA–Roe. NASA–Roe was developed from these observations as a low-branch, Roe-type approximate solver for NASA-polynomial thermodynamics. It removes the expensive ODE integrations and star-state iterations from the flux evaluation and is therefore designed to map efficiently to GPU execution.

Computational Cost

Representative end-to-end runtimes from the current benchmark suite were 3.64 s for PeleC Riemann, 4.32 s for NASA–Roe, 156.96 s for Taylor_2_Fast, and 2548.22 s for GodunovPG. Thus, NASA–Roe is only 18.7% slower than the baseline Riemann solver, while remaining approximately 36 times faster than Taylor_2_Fast and 590 times faster than GodunovPG. For simulations in which detailed chemical kinetics dominate the total computational cost, this level of convective-flux overhead is expected to have little effect on the overall wall-clock time.

Strong-Shock Collision Test

A symmetric one-dimensional collision of two pre-formed strong shocks is used as a controlled stress test. The two shocks have identical strength ($M_s = 5.4$) and propagate inward toward one another. The thermodynamic state and species composition are initialized from the equilibrium products behind a CJ detonation of a stoichiometric $2H_2 + O_2$ mixture, using the Li–Dryer mechanism without argon. The chemical composition is then frozen throughout this diagnostic calculation in order to isolate differences arising from the hydrodynamic and thermodynamic flux treatments. The calculation uses the Fuego/NASA equation of state and second-order PLM reconstruction.

This configuration is intended as a controlled one-dimensional representation of the severe thermodynamic and numerical conditions that can arise when a detonation-generated strong shock interacts with a reflecting wall in multidimensional reactive-flow simulations.

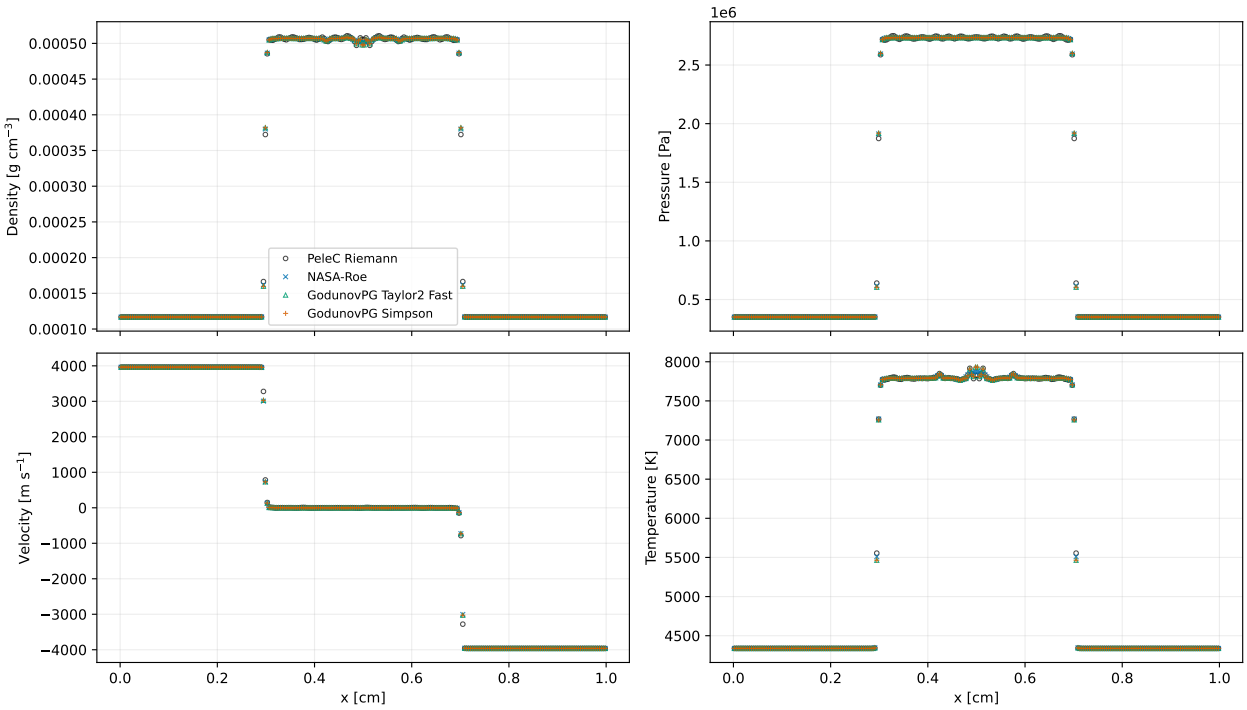

Figure 1: Symmetric collision of two pre-formed shocks at $M_s = 5.4$. The initial thermodynamic state and composition correspond to the equilibrium products behind a CJ detonation of stoichiometric $2H_2 + O_2$. Density, pressure, velocity, and temperature are compared for PeleC Riemann, NASA–Roe, Taylor_2_Fast, and GodunovPG. The species composition is frozen during this diagnostic test so that differences between the solutions originate from the hydrodynamic/thermodynamic flux treatment rather than chemical kinetics.

Preliminary Observation and Open Question

Following the shock collision, the baseline PeleC Riemann solution develops visible oscillations in the high-temperature region. The different thermally perfect-gas solvers also exhibit different post-collision temperature responses. In contrast, NASA–Roe produces a substantially smoother temperature distribution near the collision region. The different solvers tend to generate temperature perturbations of different signs near the point of collision, whereas the NASA–Roe formulation appears to balance these competing tendencies. Corresponding entropy diagnostics indicate a nearly uniform entropy distribution around the collision point for NASA–Roe.

This behavior is potentially important for multidimensional reactive-flow simulations. Numerical temperature overshoots generated when a strong shock or detonation wave interacts with a reflecting boundary can substantially shorten local chemical induction times and may therefore cause artificial early ignition or alter the predicted onset of DDT.

The present result, however, should not yet be interpreted as evidence that NASA–Roe is intrinsically more accurate. In particular, the suppression of the post-collision oscillations may partly result from additional numerical dissipation introduced by the approximate solver. An important subject of the ongoing investigation is therefore to determine whether the observed behavior originates primarily from a more consistent treatment of temperature-dependent thermodynamics, from increased numerical dissipation, or from a combination of the two. Nevertheless, the combination of strong-shock stability and low computational cost makes the formulation worth further investigation.

References

[1] L. Xu, W. Yang, and T. Liu, "An interface treatment for two-material multi-species flows involving thermally perfect gases with chemical reactions," *Journal of Computational Physics*, vol. 448, 110707, 2022. doi:10.1016/j.jcp.2021.110707.