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Higher order implicit time-stepping for low-Mach number reactive flow simulations

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Low-Mach number reactive flow computations with detailed chemistry are numerically challenging. Explicit time integration schemes are often preferred in this context due to their simplicity. These methods severely limit the time-step sizes due to numerical stability constraints, the stiffness of source terms, and the mesh resolution required to capture steep spatial gradients in the reactive zones. With finite-rate chemistry, species transport typically dominates the overall cost due to strong disparities in characteristic timescales, with advection being much slower than diffusion and reaction. Implicit time integration schemes can offer a promising alternative, allowing for larger time-step sizes in the absence of stability constraints. In a previous study conducted within a finite-volume code [1], we evaluated implicit time integration schemes for scalar advection-diffusion-reaction problems and showed that accurate results can be achieved at a lower cost with an appropriate choice of numerical schemes [2,3].
This work explores and evaluates multiple strategies to develop a cost-effective framework for the accurate simulation of low-Mach number reactive flows with an implicit time integration. An implicit time advancement method for multi-species transport using a multicomponent diffusion model [4] is proposed. Picard iterations are used to solve the resulting non-linear coupled equations and ensure discrete mass conservation. To further improve efficiency, operator splitting techniques can be employed to decouple stiff reaction terms from grid-coupled advection and diffusion operators. Source terms are integrated in each control volume based on the local thermochemical state assuming a constant pressure and mass reactor and using stiff ODE integrator packages such as VODE [5]. The performance of various implicit time-stepping approaches is assessed on freely propagating one-dimensional laminar flames. As part of this assessment, it is observed that splitting errors can quickly overshadow discretization errors.

References

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