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Efficient partially implicit integration method for stiff chemistry in high-fidelity simulations of turbulent reacting flows[1] HAO WU, MATTHIAS IHME, Stanford University — High-fidelity turbulent reactive flow simulations are typically associated with small time step sizes ($h \leq 10^{-8}$ sec) due to the CFL condition imposed by the fine gird. Although the step size is not sufficiently small to allow fully explicit time integration in the presence of stiff chemistry, it makes the use of classical implicit multi-step ODE solvers (e.g. VODE) an inefficient approach in combustion simulations due to the reduced number of internal iterations and excessive implicitness. In this study, an improved 4th-order Rosenbrock-Krylov (ROK4L) scheme is developed for the system of chemical reactions. This class of schemes replaces the Jacobian matrix by its low-rank Krylov approximation, thus introducing partial implicitness. The scheme is improved in both accuracy and efficiency by fulfilling additional order conditions and reducing the number of function evaluations. The ROK4L scheme is demonstrated to possess superior efficiency in comparison to CVODE due to the minimal degree of implicitness for small time-step sizes and the avoidance of other overhead associated with the start-up process of multi-step methods.

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