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EFFICIENCY AND ROBUSTNESS OF IMPLICIT MULTIGRID METHODS FOR TURBULENT COMBUSTION

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Even with recent advances in computing power availability, the computational costs of combustion simulations involving detailed chemical kinetics and turbulence modeling may prove infeasible as more elaborate models, including hundreds of chemical species, are developed. Therefore, convergence acceleration methods, such as multigrid, are highly sought in the context of reacting flows. However, finite-rate chemistry models currently pose a significant challenge for standard multigrid methods due to the strong non-linearity of chemical source terms and the stiffness of detailed chemical kinetics that normally cause divergence of multigrid schemes. To overcome these difficulties, extensive artificial stabilization is employed by the few researchers who applied multigrid in combustion simulations [1, 2]. While stabilization techniques increase the stability of multigrid simulations of combustion, they may also hinder convergence rates and lower robustness due to dependence on user-supplied parameters.

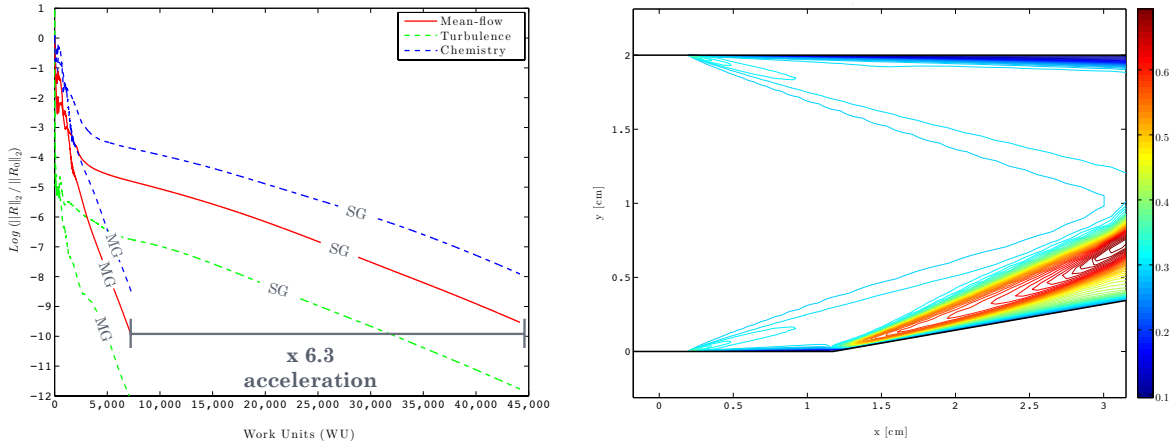
In this work, several key aspects affecting the efficiency and robustness of multigrid methods for combustion are discussed, and a new, robust multigrid method is proposed.

Since chemical reaction zones are usually very narrow, discretizations on the coarse grid levels of the multigrid hierarchy may not sufficiently resemble those obtained on the fine grid. As a result, the coarse-grid-correction is not guaranteed to drive toward a correct fine-grid solution. To tackle this issue, a modified defect correction procedure is devised, and successfully applied in this work for the first time in the context of reacting flows. The procedure is based on use of alternate, stable discretizations of convection and diffusion operators on coarse levels, while still retaining the accuracy of the fine-grid solution.

Furthermore, straightforward numerical treatment of turbulence and chemistry model

equations, disregarding the issue of positivity, may result in stall or divergence due to the appearance of non-physical values of turbulence quantities or species densities. Artificial limiting in which corrections that result in loss of positivity are neglected may deteriorate convergence rates. In this work, a novel prolongation operator is proposed to avoid loss of positivity due to coarse-grid corrections. Positivity of the solution on each level of the multigrid hierarchy is guaranteed by the unconditionally positive-convergent (UPC) time integration implicit scheme. Necessary extensions and improvements for use with chemical kinetics models are presented.

The advantages of a decoupled implicit method where the chemistry and turbulence model equations are solved separately from the Navier-Stokes equations, are examined with regards to the conventional, fully coupled method, which incurs heavy computational costs, especially if the modeled reaction mechanism is very large. To maximize the computational savings offered by a decoupled implicit method, simplifications to the large, highly populated analytic chemical kinetics source term Jacobian are sought. It is shown that a diagonal approximation of the full implicit operator significantly reduces the computational cost, without significantly affecting stability and convergence in steady-state combustion simulations. **The proposed multigrid method is robust thanks to being nearly free of stabilization techniques that are commonly used to avoid numerical difficulties, and efficient since it only scales linearly with the number of chemical species.**



(a) Multigrid (MG) vs. Single-grid (SG) Convergence

(b) Density Contours

Figure 1: Simulation of Mach 4 internal turbulent combustion of hydrogen-air in a 10°-ramped duct

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