

Adaptive time-space algorithms for the simulation of multi-scale reaction waves

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Numerical simulations of multi-scale phenomena are commonly used for modeling purposes in many applications such as combustion, chemical vapor deposition, or air pollution modeling. In general, all these models raise several difficulties created by the high number of unknowns, the wide range of temporal scales due to large and detailed chemical kinetic mechanisms, as well as steep spatial gradients associated with very localized fronts of high chemical activity. Furthermore, a natural stumbling block to perform 3D simulations with all scales resolution is either the unreasonably small time step due to stability requirements or the unreasonable memory requirements for implicit methods. In this work, we introduce a new resolution strategy for multi-scale reaction waves based mainly on time operator splitting and space adaptive multiresolution, in the context of very localized and stiff reaction fronts. It considers high order time integration methods for reaction, diffusion and convection problems, in order to build a time operator splitting scheme that exploits efficiently the special features of each problem [1, 2, 3]. Based on recent theoretical studies of numerical analysis, such a strategy leads to a splitting time step which is not restricted neither by fast scales in the source term nor by restrictive stability limits of diffusive or convective steps, but only by the physics of the phenomenon. Moreover, this splitting time step is dynamically adapted taking into account a posteriori error estimates, carefully computed by a second embedded and economic splitting method [4]. The main goal is then to perform computationally very efficient as well as accurate in time and space simulations of the complete dynamics of multi-scale phenomena under study, considering large simulation domains with conventional computing resources and splitting time steps purely dictated by the physics of the phenomenon and not by any stability constraints associated with mesh size or source time scales.

Références

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