# Simulation of combustion with detailed chemistry

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The mathematical model for reactive flows and detonations for an inviscid compressible fluid consists of the Euler equations of gas dynamics, additional equations for the transport of the species and source terms in the equation for the conservation of energy. The kinetics of the chemical reaction is modeled by the Arrhenius law. In this contribution we consider the hydrogen oxygen reaction in 2D. The model is based on 9 different species and 48 elementary reactions. The algorithm is a finite volume code on an unstructured grid in 2D. In order to get a sufficient resolution of the detonation front and the chemical reaction we have to do the calculation on a locally refined grid in the neighborhood of the detonation front. Since the front is moving the refined part of the mesh has to follow the front. The process of dynamical mesh refinement is based on grid indicators, which are designed similar to theoretical results for a posteriori error estimators, which we have obtained for weakly coupled systems of conservation laws. The discretization is based on an operator splitting for the PDEs for the flow and the ODEs for the reaction. In addition to the local, dynamical grid refinement in space we use a time step control for the ODE solver.

The code has been validated for special problems with known exact solutions and applied for different applications in 2D: detonations in tubes and detonations in tubes with obstacles. The detonation cells of the well-known Strehlow experiment and the transition from detonation to deflagration is shown.

This code will be parallelized under MPI and will be generalized to 3D. The general structure of the parallel code has been established already for an MHD code in 3D. In the lecture I will show a video of the results for an atmospheric flow on the sun. The reactive part is based on a joint paper with my former PhD student T. Gessner and the part, concerning the parallelization is due to C. Rohde and my PhD students A. Dedner and M. Wesenberg.

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