A Modular Two Scale Capturing/Tracking Scheme for Turbulent Premixed Flames

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1 Introduction

Turbulent premixed combustion remains a challenging topic due the interaction of many different time and length scales. All these length scales are often not representable on a discrete numerical grid. Therefore, the reactive Navier Stokes equations are filtered, dividing the solutions into resolved (macroscopic) parts and unresolved (microscopic) parts, where the latter need closure. In this paper we focus on two key points of the multiple scale problem, namely (i) the consistent coupling of large and small scale state and (ii) the subtile interaction of numerics and the model for the unresolved scales. In the next section we present a strategy that couples the reactive macro and micro physics in an adaptive way. In section three we propose a turbulent subgrid closure, that seems to be less sensitive to the numerical scheme and the discrete grid than standard applied models. The reason for this is the explicit closure dependency from the large scale information instead of the small scale solution, which is influenced by numerics. In section four an examplary result ist shown.

2 The Modular Flame Tracking Concept

The deflagration capturing/tracking hybrid scheme of *Smiljanovski et al.* [6] allows a robust representation of turbulent high speed combustion. A deflagration is considered as a reactive discontinuity, which is embedded in a compressible surrounding flow. The flame surface is represented as the level set of a dynamically evolving scalar function. Flame flow coupling is realized by explicitly invoking Rankine-Hugoniot type jump conditions at the front. While the original scheme uses the standard Rankine-Hugoniot conditions and an explicit burning rate law expressing the net unburnt gas mass consumption as a function of the unburnt gas conditions, *Schmidt* and *Klein* [4] extend the idea to propagating flame structures which are attached in normal direction to the large scale front. The modular algorithmic structure allows the incorporation of a variety of internal flame structure descriptions. This ultimately enables one to capture turbulent combustion processes within any of the regimes in the Borghi diagram. In this paper we want to extend the modular idea to an "adaptivity in complexity".

Not only in the level set concept, the turbulent burning velocity, s_t, is a key parameter that summarizes the net effects of unresolved turbulence chemistry interactions. In principle, there are two different

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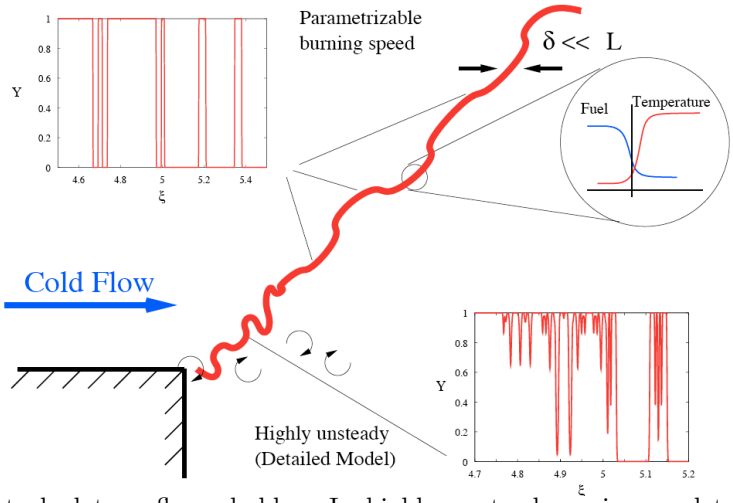

Figure 1: Flame attached to a flame holder: In highly unsteady regions a detailed flame structure computation, yielding the turbulent burning speed, is performed (lower right structure computed with LEM); if a parallel running parameterization yields comparable results, we switch off the costly online computation (upper left calculation, performed with LEM, switches to parameterization from eq. (1))

ways to get it, (i) by supplying a burning rate law that parameterizes s_t by resolved motions, or (ii) a lower order online calculation of the chemistry turbulence interaction in the turbulent flame brush. What is used during a calculation should in principle be the best possible compromise between numerical cheapness and physical sounding. The hierarchy of model complexity we use starts with a parameterization of s_t using the idea of [1]. Next level of complexity is GLEM [3] with prescribed laminar burning speed, going up till a LEM or ODT [2] simulation using a reduced tabulation technique [5]. This is a sample choice that might be exchanged in a modular fashion. The hierarchy can be interpreted as several levels of complexity, that are coupled to the overall capturing/tracking scheme in an adaptive fashion. The final goal is an algorithm that in the initial stages of a computation locally runs all the different modules. When a lower order module yields comparable results (to a defined error margin), one switches off the more expensive ones. In the end, only in flow regions where the turbulence/chemistry interaction appears to be not describable with a relatively simple parameterizations, the more expensive superparameterizations yield s_t and additional quantities. Depending on the setup the unexpensive parameterization is used in the major part of the grid. The used parameterized for s_t, that has originally been derived for the flame surface density concept, reads

$$\hat{s_t} = s_l^0 \left(1 + \min\left[\frac{\Delta}{\delta_l^0}, \Gamma \frac{u'_\Delta}{s_l^0}\right]\right)^\beta . \tag{1}$$

Laminar flame thickness δ_l^0 and laminar flame speed s_l^0 are calculated a priori for a given premixed system. The velocity fluctuation u'_Δ at the filter scale Δ is locally given by the scaling function described in the next section. Expression for the parameter β and the more complex function Γ are taken from [1]. A sketch of the adaptive idea is given in Figure 1.

3 The Two Scale Model

Filter Scale: The present developments are based on the reactive Euler equations in conservation form. Here the following notation is used: ρ is the density, $\boldsymbol{v}$ the flow velocity, p the pressure, Q the specific heat release, E the sum of internal and kinetic energy and γ the isentropic coefficient. To make

a difference between integral and filter scale terms, we mark the latter by a hat and the first by an over-bar. With these conventions the governing equations read

$$\begin{aligned}
\frac{\partial}{\partial t}\hat{\rho} + \nabla\cdot(\hat{\rho}\hat{\boldsymbol{v}}) &= 0 \\
\frac{\partial}{\partial t}(\hat{\rho}\hat{\boldsymbol{v}}) + \nabla\cdot(\hat{\rho}\hat{\boldsymbol{v}}\circ\hat{\boldsymbol{v}} + \mathbf{I}\hat{p}) &= f(\hat{\rho},\hat{\boldsymbol{v}},\hat{\nu_t}) \\
\frac{\partial}{\partial t}(\hat{\rho}\hat{E}) + \nabla\cdot\left([\hat{\rho}\hat{E}+\hat{p}]\hat{\boldsymbol{v}}\right) &= f(\hat{\rho},\hat{\boldsymbol{v}},\hat{E},\hat{p},\hat{\nu_t})
\end{aligned} \tag{2}$$

with the equation of State

$$\hat{\rho}\hat{E} = \frac{\hat{p}}{\gamma-1} + \frac{1}{2}\hat{\rho}\hat{\boldsymbol{v}}\cdot\hat{\boldsymbol{v}} + \hat{\rho}\sum_{i=1}^{N_{spec}} Q_i\hat{Y}_i. \tag{3}$$

The terms on the rhs, written in compact form as $f(\cdot)$, are source terms due to closure of chemistry and turbulence. The turbulent kinematic viscosity $\hat{\nu_t}$ stands symbolically for a gradient diffusion type closure. Balance laws for the species mass fractions Y_i are added in a standard way.

The flame surface on the filter level is calculated as the level set $G = 0$ of a scalar function, $G(\vec{x},t)$.

$$\hat{G}_t + (\hat{\boldsymbol{v}} + \hat{s}_t\hat{\boldsymbol{n}})\cdot\nabla G = 0. \tag{4}$$

Flame-flow coupling is achieved analogously to ideas of *Smiljanovski et al.* [6] and *Schmidt and Klein* [4].

Integral Scale: The unresolved terms of equation system (2), which is solved on a filter scale Δ, still need closure. Therefore, we modify a former two scale ansatz proposed by *Willems* and *Peters* [7]. They propose a closure that is motivated by Kolmogorov's theory of turbulence. We follow their way, but propose a formulation that removes some inconsistencies of the original formulation, while having the side benefit of being in principle independent of the numerical scheme. The key issue is to solve an additional model for the integral length and time scales, yielding the same solution when the grid is refined below the integral scale of turbulence. In the present development we chose for simplicity a standard $k-\epsilon$-model for the integral scale l_t

$$\begin{aligned}
\frac{\partial}{\partial t}(\overline{\rho}\overline{k}) + \nabla\cdot\left(\overline{\rho}\overline{k}\overline{\boldsymbol{v}}\right) &= f(\overline{\rho},\overline{\boldsymbol{v}},\overline{\nu_t}) \\
\frac{\partial}{\partial t}(\overline{\rho\epsilon}) + \nabla\cdot(\overline{\rho\epsilon}\overline{\boldsymbol{v}}) &= f(\overline{\rho},\overline{\nu_t}).
\end{aligned} \tag{5}$$

Here, k is the turbulent kinetic energy and ϵ is its dissipation. Since integral scales frequently are non isotropic, a more physical model would be of anisotropic nature. Extending the algorithm in such a way is work in progress. Since equations (5) are not grid dependent they are solved on the filter level. This increases the costs of the algorithm, but makes it much more easy to handle.

Two Scale Coupling: Thinking of the Kolmogorov picture of cascading energy from integral scales down to small scales, we close the unresolved motion (kin. viscosity $\hat{\nu_t}$) by a scaling function $f(\Delta,l_t)$

$$\hat{\nu_t} = c_\nu\frac{\overline{k}^2}{\overline{\epsilon}}\cdot(1-f(\Delta,l_t))^2 \quad \text{with } f(\Delta,l_t) = \begin{cases} 1-(\frac{\Delta}{l_t})^{2/3} & \text{for } \frac{\Delta}{l_t}\le 1 \\ 0 \text{ for } \frac{\Delta}{l_t} > 1 \end{cases}$$

relating turbulent viscosities $\hat{\nu_t}$ to the integral scales [7]. Although the equation system for the filter scale is in closed form, there are no relations for the integral density and velocity fields, $\overline{\rho}$ and $\overline{\boldsymbol{v}}$. We get $\overline{\phi}\in[\overline{\rho},\overline{\boldsymbol{v}}]$, e.g. by instantaneous diffusion of the filtered $\hat{\rho}$ and $\hat{\boldsymbol{v}}$ field to the l_t scale via integration of $\frac{\partial}{\partial t^*}\hat{\phi} = \frac{\overline{k}-\hat{k}}{\overline{\epsilon}}\nabla\cdot\left(\overline{\nu_t}\nabla\hat{\phi}\right)$ over the pseudo time interval $[0 < \underbrace{\frac{t}{(\tau-\tau_\Delta)}}_{t^*} < 1]$. Other methods to couple the two scales are under investigation.

To summarize, the advantage of our idea compared to standard subgrid closure models are, (i) the computation of equations for integral scale turbulence quantities, that yield the same solution for different (smaller and smaller) grid sizes, and (ii) the closure terms on the filter scale depend of the converging large scale model and *not* of fine scale solutions, which are directly influenced by numerics!

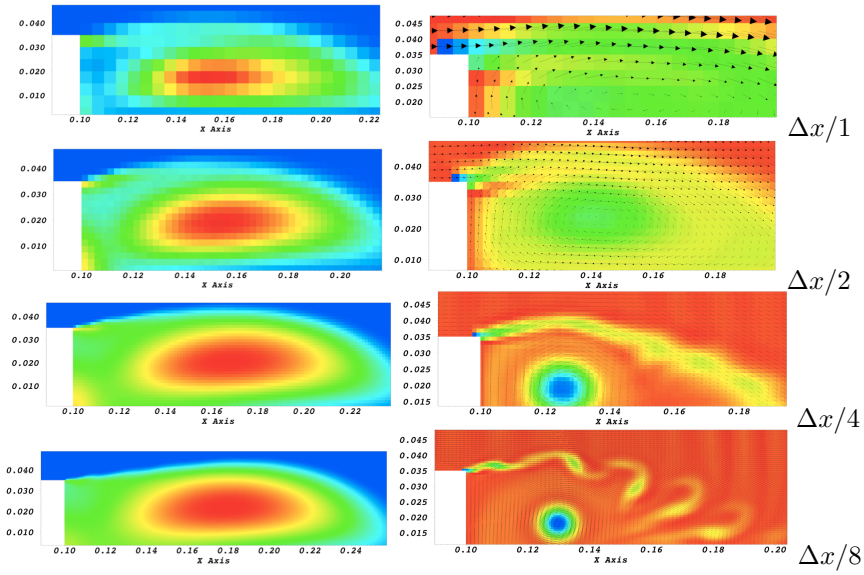

Figure 2: Unsteady flow over a backward facing step: plots of the integral length scale (left) and the vorticity on the filter scale (right) for different filter sizes $\Delta x/n$ at a fixed time level, where Δx is the grid size of the coarsest grid. Grid is refined by a factor of two from top to bottom

4 Results

First we want to illustrate the underlying concept of the two scale model. Therefore we calculate a flow over a step, that could also be seen as a characteristic burner outlet configuration. In Figure 2 results for the integral length and the vorticity on the filter scale are plotted for sucessivly refined grids at a fixed time. It becomes obvious that, as hoped, the solution on the integral scale converges. A scaling function relates the grid converged integral solution to the filter scale closure, thus the chosen numerical discretization does not directly influence the closure. Numerics only influence the lhs of (2), making it possible to distinguish between modelling and numerical error. Several examples for reactive cases of flame holder and swirl stabilized flames, as well as for the adaptivity concept are presented in the talk.

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