

An Adaptive Finite Element Method for Combustion Problems^{1 2}

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Abstract: We develop an adaptive finite element algorithm for reactive flow simulations. The underlying equations are the Navier-Stokes equations for low-Mach-number flows and an additional system of convection-diffusion-reaction equations for the chemical species. Especially in combustion problems the reaction terms are very stiff and nonlinear. This set of equations represents a complicated system of PDEs which is solved usually on parallel computers due to the high numerical cost of memory and computing time. Adaptive methods lead to an important reduction of the computational cost for this type of equations if a good error estimator is available.

Our adaptive process is based on an *a posteriori* error estimate. We use duality arguments in order to control the error in functionals of the solution like, e.g., line-averaged radical concentrations in a stationary flame front. By solving a linearized dual problem, we determine weights multiplying the local residuals in the error estimate. This provides information about the global error propagation, which is used in a criterion for local mesh adaptation.

1 Introduction

The Navier-Stokes equations including Arrhenius-type chemical production terms for the simulation of reactive flow problems lead to an extremely complex nonlinear system of PDEs. The use of adaptive meshes for this kind of problems is crucial in reducing the numerical cost. The adaptive process should not only be efficient, but also reliable in order to allow for quantitative error control. Especially for comparisons between numerical and experimental results (e.g., laser measurements in flames) error control for relevant quantities is desirable. In this note, we show how the general approach of Becker and Rannacher [BR96] of error control for finite element schemes can be applied to stationary combustion problems.

The underlying equations describe the conservation of mass, momentum, energy and species mass fractions. We use the equations in the primitive variables, p for pressure, u for the velocity, T the temperature and w_i the species mass fractions,

$$\begin{aligned}\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) &= 0, \\ \rho \frac{\partial u}{\partial t} + (\rho u \cdot \nabla) u + \nabla \cdot \tau + \nabla p &= \rho \cdot f_e,\end{aligned}$$

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$$\begin{aligned}
\rho \frac{\partial T}{\partial t} + \rho u \cdot \nabla T - \frac{1}{c_p} \nabla \cdot (\lambda \nabla T) &= \frac{1}{c_p} f_T(T, w), \\
\rho \frac{\partial w_i}{\partial t} + \rho u \cdot \nabla w_i + \nabla \cdot j_i &= f_i(T, w), \quad i = 1, \dots, N_s, \\
p &= \rho R T,
\end{aligned} \tag{1}$$

involving several well-known physical coefficients. Due to the exponential dependence on temperature (Arrhenius law) and polynomial dependence on w , the source terms $f_i(T, w)$ are highly nonlinear. In general, these zero-order terms lead to a coupling between all chemical species mass fractions. For accurate modeling of the underlying chemical processes, a large number of chemical species is necessary, (e.g., $N_s \sim 30 - 40$ for a methane flame). This leads to very high numerical cost. The use of adaptive meshes is particularly important for capturing thin reaction zones.

Our application is directed to low-Mach-number flow. This implies that the flow is hydrodynamically incompressible while strong heat release leads to thermodynamical changes. We apply the approximation for low-Mach-number combustion [Maj84], splitting the total pressure $p(x, t)$ in two parts, the thermodynamic part $P_{th}(t)$, which is uniform in space, and the hydrodynamic part $p_{hyd}(x, t)$, which is several magnitudes smaller than P_{th} and is neglected in the equation of state (1). This approximation implies that acoustic waves are eliminated.

2 Finite Element Discretization

Our discretization is based on conforming finite elements on quadrilateral meshes $\mathcal{T} = \{K\}$. The trial space consists of continuous and piecewise bilinear functions (Q_1 -elements) for all variables. It is well known that the original Galerkin formulation is not stable for the Stokes system, because the Babuska-Brezzi condition is not fulfilled [GR86]. We stabilize the formulation by introducing additional least-square terms in the equation for the pressure [HFB86]. For convection dominated flow, we use streamline diffusion for velocity, temperature and all chemical species, see [TV96, FF92, Bec95] for more details.

Let $U = (p, u, T)$ denote the discrete solution in the finite element space V_h . We neglect here the chemical species w , since the corresponding equations are similar to the equation for the temperature. The discrete equations for the low-Mach-number model in the stationary case read

$$a_h(U; \varphi) := a(U; \varphi) + s_h(U; \varphi) = F_h(\varphi) \quad \forall \varphi = (q, v, r) \in V_h,$$

where a denotes the original semi-linear form

$$\begin{aligned}
a(U; \varphi) &= (\nabla \cdot u, q) - (T^{-1} u \cdot \nabla T, q) + (\rho u \cdot \nabla u, v) + (\mu \nabla u, \nabla v) \\
&\quad - (p, \nabla \cdot v) + (\rho c_p u \cdot \nabla T, r) + (\lambda \nabla T, \nabla r) - (f_T(T), r),
\end{aligned}$$

and s_h the stabilization terms

$$\begin{aligned} s_h(U; \varphi) &:= \sum_{K \in \mathcal{T}} \delta_K \cdot (\rho u \cdot \nabla u - \nabla \cdot (\mu \nabla u) + \nabla p, \nabla q + \rho u \cdot \nabla v)_K \\ &+ \sum_{K \in \mathcal{T}} \gamma_K \cdot (\rho c_p u \cdot \nabla T - \nabla \cdot (\lambda \nabla T) - f_T(T), \rho u \cdot \nabla r)_K. \end{aligned}$$

The parameters δ_K and γ_K are chosen according to the mesh size h_K and the balance between convection and diffusion on each cell K . The functional F_h includes the stabilization terms due to consistency and is, therefore, mesh dependent, too. The mesh handling in our adaptive process is done by the finite element library DEAL [BKS].

3 Solver

The discretized equations are solved by a Quasi-Newton method. The resulting linear equations are solved by restarted GMRES iterations with multi-grid preconditioning (V-cycle). The smoothing operator consists of a block-ILU decomposition in streamline direction. The blocks are adjusted to the underlying equations. For combustion problems, the coupling between several chemical species is based mainly on the zero-order source terms. Coupling between distinct species on different mesh points is neglected in the blocks. This leads to a substantial reduction of memory requirement and CPU time for problems with detailed chemistry and many species. For more details see [Bra98].

4 Adaptivity

The error indicators used in reactive flow computations are usually based on estimation of the local interpolation error. For scalar equations, such an error indicator η_{ind} has the following form

$$\eta_{ind} = C \sum_{K \in \mathcal{T}} h_K^4 \cdot |D_h^2 u_h(x_K)|,$$

where $D_h^2 u_h(x_K)$ is a suitable difference quotient in order to approximate the second derivatives. For vector equations, $U = \{U^i\}$, the corresponding indicator reads

$$\eta_{ind} = C \sum_{K \in \mathcal{T}} \sum_{i=1}^m \omega_i h_K^4 |D_h^2 U_h^i(x_K)|,$$

where ω_i are unknown weights. The appropriate choice of these weights is usually based on mere heuristic arguments. It is clear that such an indicator can detect the position of a front and will, therefore, lead to a refinement in reaction zones. The obvious disadvantage is the absence about global error

propagation. Furthermore, a quantitative error control is not possible with this kind of error indicator.

The *a posteriori* error estimates coming from the literature are usually not appropriate for reactive flow problems, because they are mostly based on the energy norm for elliptic problems. For this kind of computations, it is also quite natural that certain local error quantities rather than a global error norm are to be controlled.

We now present our approach of error control for a functional J of the solution. The functional can represent, e.g., the maximal temperature, point values of temperature or a species mass fraction or a line average over certain components of the system. The stopping criterion for the adaptive iteration is

$$|J(U) - J(U_h)| < TOL,$$

for a given tolerance TOL . We assume J to be linear, although the approach can be extended to nonlinear functionals, see [BR96].

The Galerkin orthogonality for the semi-linear form a_h with Frechét derivative a'_h reads

$$0 = a_h(U, \phi) - a_h(U_h, \phi) = \underbrace{\int_0^1 a'_h(U_h + te; e, \phi) dt}_{=: L(U, U_h; e, \phi)} \quad \forall \phi \in V_h, \quad (2)$$

where $e = U - U_h$ is the error. In the error estimation, we utilize the following dual problem

$$Z \in V : \quad L(U, U_h; \phi, Z) = J(\phi) \quad \forall \phi \in V.$$

Assuming the existence of a corresponding dual solution Z and taking $\phi = e$, we obtain an exact error representation. Further, using the Galerkin orthogonality (2) of the dual solution results in

$$J(e) = L(U, U_h; e, Z - i_h Z),$$

where $i_h Z$ is an arbitrary approximation of Z in V_h . This error identity is converted into an *a posteriori* error estimate of the form

$$|J(e)| \leq \sum_K \omega_K \rho_K,$$

where the element-wise residuals ρ_K and weights ω_K are defined by

$$\begin{aligned} \rho_K &:= \|\rho u \cdot \nabla u + \nabla \cdot \tau + \nabla p\|_K + \text{“jump-terms”} + \dots \\ \omega_K &:= \max\{h_K^{-1} \|Z - i_h Z\|_K, h^{-1/2} \|Z - i_h Z\|_{\partial K}\} \leq C_I h_K \|D^2 Z\|_K. \end{aligned}$$

The evaluation of the weights ω_K requires approximation, because the dual problem is posed on the continuous level and its coefficients depend on the

unknown solution U . We propose to use a numerical approximation of the form

$$\omega_K \simeq C_I h_K \|D_h^2 Z_h\|_K, \quad (3)$$

where Z_h is the solution of the perturbed discrete dual problem

$$Z_h \in V_h : \quad L(U_h, U_h; \phi, Z_h) = a'_h(U_h; \phi, Z_h) = J(\phi) \quad \forall \phi \in V_h.$$

For simplicity, this linear problem is solved on the same mesh on which the primal solution U_h has been obtained. The corresponding computational cost is equivalent to just one additional Newton step of the primal problem. This process leads to an alternating solution of primal and dual problem on a sequence of successively improved meshes and is called weighted-residual error estimate. For more details see [Bra98].

5 Refinement Strategies

We present two different strategies for mesh adaptation. Both are based on error estimators of the form

$$\eta = \sum_{K \in \mathcal{T}} \eta_K,$$

with local error indicators η_K . In the first strategy (so-called *numerous clausus*), in each refinement cycle the elements are ordered according to the size of the η_K . The refinement is performed for that fraction of elements which make up a considerable part of the estimated value η . The second strategy (so-called *mesh optimization*) takes additionally advantage of the special structure of our error estimator,

$$|J(e)| \sim \eta = \sum_{K \in \mathcal{T}} \omega_K \rho_K.$$

In this process, we consider the optimization problems

(a) *Minimize the number of cells N under the condition $\eta \leq TOL$, or*

(b) *Minimize η under the condition $N \leq N_{max}$*

for a given tolerance TOL or a maximal number of nodes N_{max} . We suppose that the number of elements and the estimator can be expressed by

$$\eta = \int_{\Omega} w \cdot h^{\alpha} dx \quad \text{and} \quad N = \int_{\Omega} h^{-d} dx,$$

where $\Omega \subset \mathbb{R}^d$ is the computational domain. The solution of the constrained optimization problem (a) is given by

$$\lambda = TOL^{1/\alpha} \cdot \left[\int_{\Omega} w^{d/(\alpha+d)} \right]^{-1/\alpha} \quad \text{and} \quad h = \lambda \cdot w^{-1/(\alpha+d)}.$$

For the optimization problem (b) the solution can be obtained in a similar way. In both cases, the ‘‘optimal’’ h_K^* for each K can now be explicitly determined. Because the weight function w is *a priori* unknown, it has to be approximated using the current solution U_h . This results in a feed-back process for the iterative generation of optimal mesh-size distributions.

6 Numerical Results

6.1 Flame-Sheet Model

As an application, we treat a simple flame-sheet model of an axi-symmetric methane diffusion flame [Smo91], see Figure 1. This model is chosen in order to compare our adaptive process with more classical strategies [Geh95]. The underlying equations consist of the equations for p , u and one flame-sheet variable S . The temperature and the species are explicitly determined by S . The simulation is performed in cylindrical coordinates.

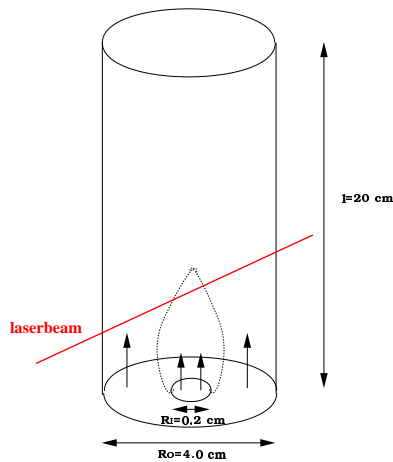


Figure 1: Model of a Bunsen burner

We consider two different functionals of the solution. In the first example, we control the mean value of the velocity u along the line Γ , which corresponds to the path of a laser beam. In the second example, we focus on the variable S , which describes the progress of the reaction :

$$J_1(e) = \int_{\Gamma} u(x) dx - \int_{\Gamma} u_h(x) dx \quad , \quad J_2(e) = \int_{\Gamma} S(x) dx - \int_{\Gamma} S_h(x) dx .$$

Figures 2 and 3 show the behavior of the true error and the corresponding estimator and demonstrate the efficiency and reliability of our approach. The reference solution is generated by a computation on an adaptively refined mesh with more than 85.000 nodes and 14 refinement levels.

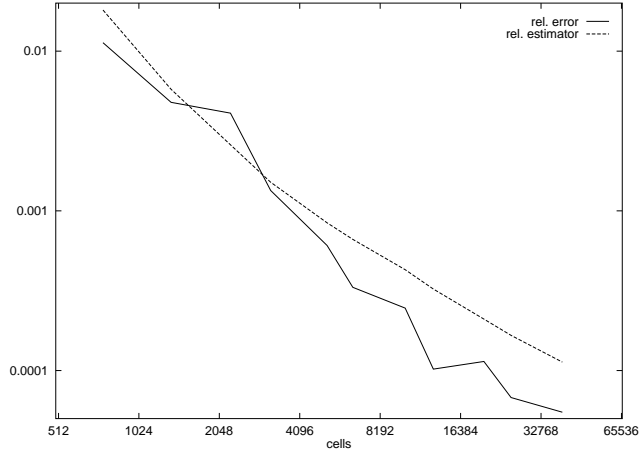


Figure 2: Efficiency of the weighted-residual error estimator for $J_1(e)$

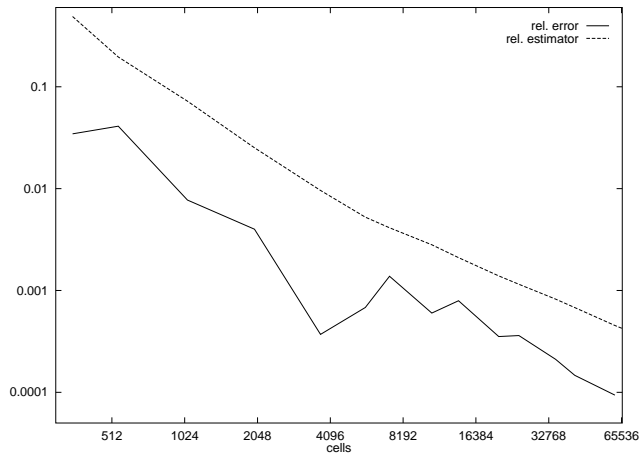


Figure 3: Efficiency of the weighted-residual error estimator for $J_2(e)$

For the estimation of $J_1(e)$, the error is underestimated on coarse grids. This can be explained by the nonlinear behavior of the underlying equation, which requires an approximation of the dual problem. On finer grids, the estimated and the true error are nearly proportional. The proportionality factor can be brought closer to 1 by calibrating the interpolation constant C_I in (3).

Turning to the efficiency of the new approach in generating economical meshes, we compare three different refinement strategies: (1) uniform refinement of tensor grids, (2) adaptive refinement based on a curvature criterion, and (3) adaptive refinement based on the weighted-residual error estimator. In the last one, we use the *mesh-optimization strategy* described above, while for the error indicator based on the second derivatives of u and S we

choose the *numerus-clausus strategy*, since the *mesh-optimization strategy* is not applicable.

For the calculation on the globally refined mesh, we start from an anisotropic mesh, taking into account the singularities of the solution. In this case, the calculations show that the error changes its sign and does not decrease monotonically when mesh refinement is taking place. This is due to the non-linearity, and indicates the difficulty in using extrapolation arguments for error prediction.

In Figure 4, we compare the relation between resulting error and the number of cells for the three refinement strategies considered. To achieve an error of 0.1%, the new approach needs only 25% of the cells of the classical error indicator and less than 10% of the number of cells required by global mesh refinement.

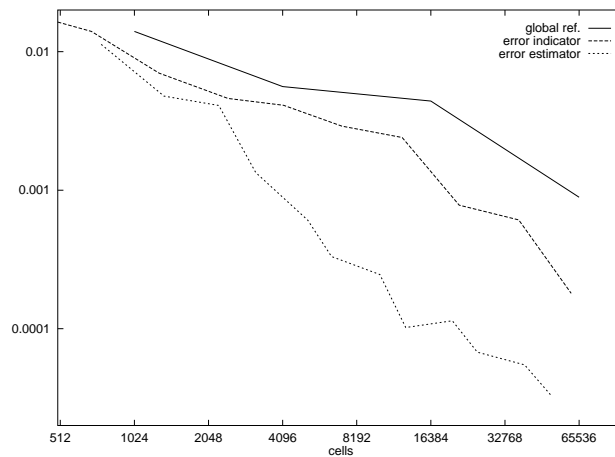


Figure 4: Comparison of the relative errors e_{rel} for control of $J_1(e)$

In Figure 5, we show the CPU times elapsed for the control of $J_1(e)$. The new approach shows a better performance, even though we need additional time for solving the dual problem. However, because the dual problem is linear, it consumes only approximately 10-15% of the CPU time of the whole calculation. In total, we save approximately 50% of the computing time for tolerances less than 0.1%. Furthermore, we have a quantitative error estimate. Finally, we show in Figure 6.1 three locally refined grids obtained by the new approach. On the grid with 25312 cells, we clearly see the effect of the local nature of the error functional considered, i.e., the strong refinement near the horizontal line Γ . [Bra98].

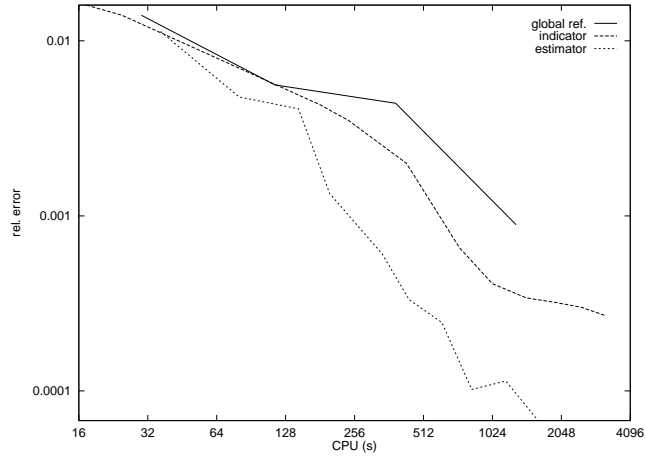
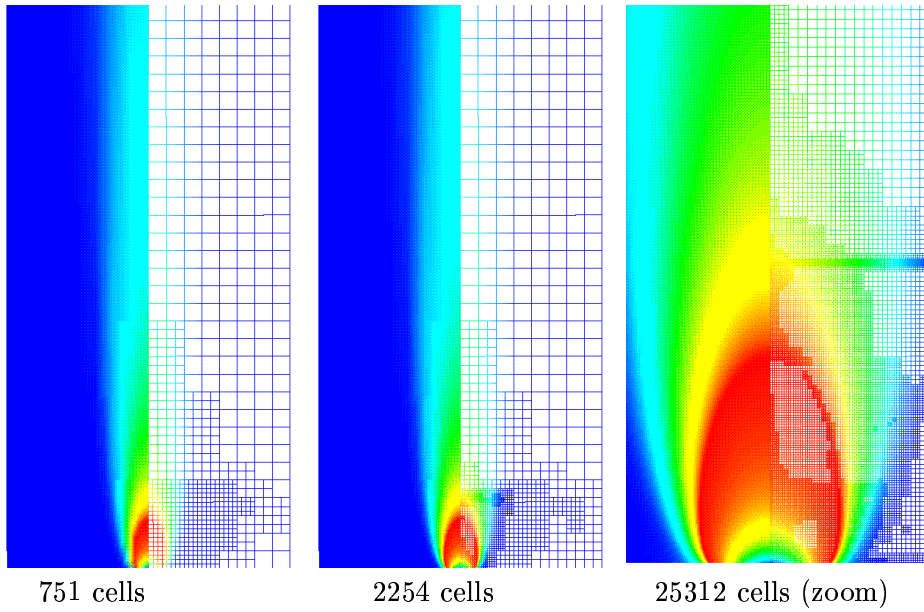
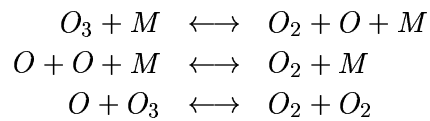


Figure 5: Comparison of CPU times



6.2 Detailed Chemistry

We present numerical results for a combustion model describing an ozone decomposition flame with three species: ozone O_3 , oxygen molecules O_2 and oxygen atoms O . The underlying reaction mechanism consists of six (three bidirectional) elementary reactions [War78]:



Here, M denotes an arbitrary third body, i.e., one of the three considered species. The formation of the stable O_2 molecules leads to the main part of heat release. Transport coefficients for viscosity, thermal conductivity and diffusion are evaluated using the kinetic models with coefficients based on the data bases of the Sandia National Laboratories [KRM87]. The geometry consists of two flat plates with an inflow of a cold mixture of ozone and oxygen molecules ($w_{O_3} = 0.2$, $w_{O_2} = 0.8$, $T = 298 K$).

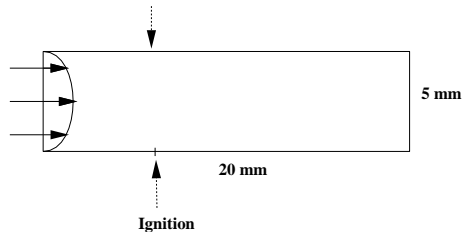


Figure 6: Geometry for the ozone decomposition

The flame is ignited by the hot walls. The hottest point of the wall is indicated by the arrows in Figure 6. The quantity we wish to control is the average value of w_{O_3} , because this is a good quantity in order to capture the correct position of the flame front. The underlying error functional is

$$J(u) = \int_{\Omega} w_{O_3} dx .$$

The calculation uses quasi-time stepping, until a stationary solution is reached. We cannot expect to get quantitative error control *during* the time stepping, because our error estimate is based on a stationary solution. However, we obtain an error estimate for the limiting steady-state on the basis of the local error indicators η_K derived from the estimator η .

In order to validate the quantitative error control for stationary solutions, in this example, we compute the stationary solution in each adaptation step. For this solution, we compare the true error with the bound obtained by the estimator η . The comparison of our approach with more classical approaches in terms of computation time is questionable, because it depends crucially on the parameters in the algorithm. Numerical tests indicate that the performance (error related to CPU time) mainly depends on the strategy of nesting the time-step iteration and the adaptive iteration.

Because the value $J(u)$ cannot be obtained analytically, we compute it numerically on a extremely refined mesh with 43800 nodes and 10 levels of refinement.

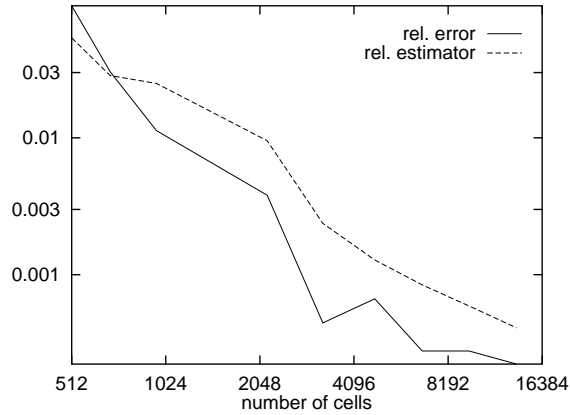


Figure 7: Relative error and estimator as a function of the number of cells

In Figure 7, we present the obtained values for the error e_{rel} and the estimator η_{rel} . In this example with detailed chemistry, we additionally get a reliable and efficient error estimate. For very coarse grids, the error is underestimated. This can be expected, because the nonlinear operator is not well represented on coarse grids. Due to the change of the sign of the error, the absolute value of $e = u - u_h$ oscillates. This leads to an overestimation of the error by η (e.g., for 3257 cells). However, the asymptotic behavior of e is very well predicted by η , because the two quantities are nearly proportional to each other.

Figure 8 shows the obtained temperature profile. We automatically get a strong refinement in the reaction zone. However, the grid is also moderately refined upstream of the reaction front. In Figure 9 we show several grids obtained by the adaptive process and the corresponding mass fraction of oxygen atoms (O).

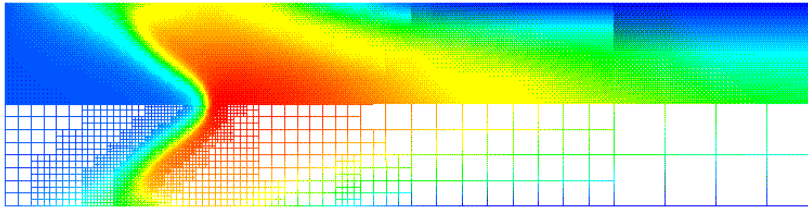


Figure 8: Temperature profile

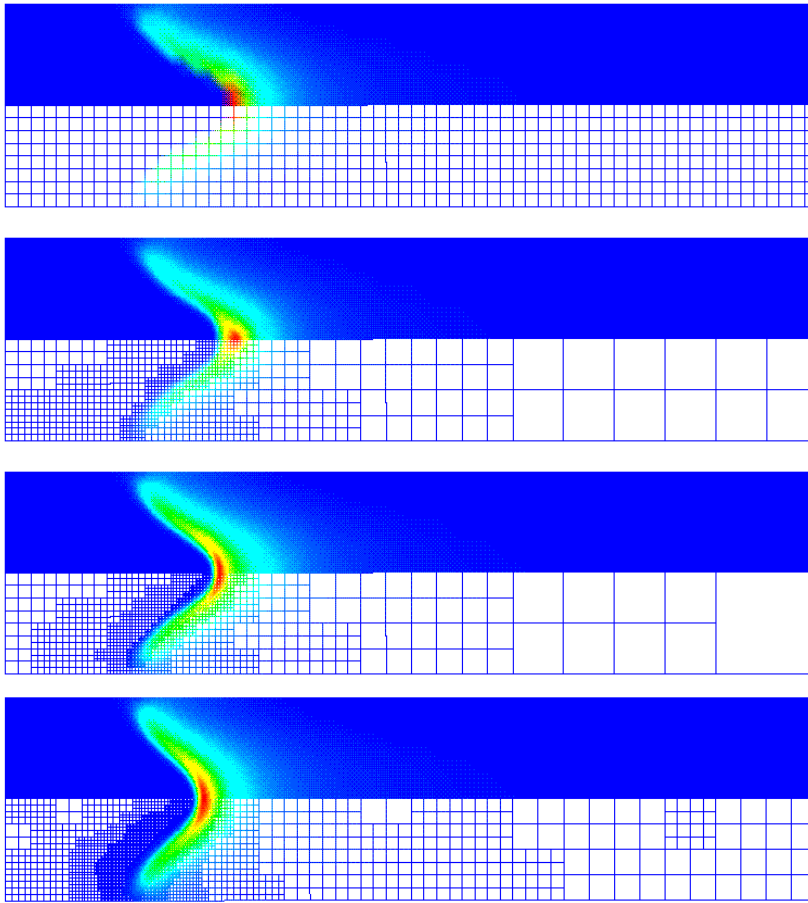


Figure 9: *O*-atoms on 512, 1004, 2288 and 8018 cells

References

- [BBR97a] M. Braack, R. Becker, and R. Rannacher. *Adaptive Finite Elements for Reactive Flows*. In *Enumath, Second European Conference on Numerical Mathematics and Advanced Applications*. Enumath, 1997.
- [BBR97b] M. Braack, R. Becker, and R. Rannacher. *An adaptive finite element method for combustion problems*. In *Third Summer Conference, Numerical Modelling in Continuum Mechanics*. Charles University, Prague, 1997.
- [Bec95] R. Becker. *An Adaptive Finite Element Method for the Incompressible Navier-Stokes Equation on Time-dependent Domains*. Dissertation, Heidelberg University, 1995.
- [BKS] R. Becker, G. Kanschat, and F.-T. Suttmeier. *DEAL Home Page*. IWR, Universität Heidelberg, <http://gaia.iwr.uni-heidelberg.de/DEAL/>.
- [BR96] R. Becker and R. Rannacher. *A feed-back approach to error control in finite element methods: Basic analysis and examples*. East-West J. Numer. Math., 4(4):237–264, 1996.
- [Bra98] M. Braack. *An Adaptive Finite Element Method for Reactive Flow Problems*. Dissertation, Heidelberg University, 1998.
- [FF92] L.P. Franca and S.L. Frey. *Stabilized finite element methods: II. The incompressible Navier-Stokes equations*. Comp. Meth. Appl. Mech. Eng., 99:209–233, 1992.
- [Geh95] E. Gehrke. *Parallele Methoden zur numerischen Simulation reaktiver Strömungen am Beispiel laminarer Diffusionsflammen*. Dissertation, Heidelberg University, 1995.
- [GR86] V. Girault and P.-A. Raviart. *Finite Elements for Navier Stokes Equations*. Springer-Verlag, Berlin, 1986.
- [HFB86] T. J. R. Hughes, L. P. Franca, and M. Balestra. *A new finite element formulation for computational fluid dynamics: V. Circumvent the Babuska-Brezzi condition: A stable Petrov-Galerkin formulation for the Stokes problem accommodating equal order interpolation*. Comp. Meth. Appl. Mech. Eng., 59:89–99, 1986.
- [KRM87] R.J. Kee, F.M. Rupley, and J.A. Miller. *The Chemkin thermodynamic data base*. Sandia Report, SAND87-8215.UC4, 1987.
- [Maj84] A. Majda. *Compressible Fluid Flow and Systems of Conservation Laws in Several Space Variables*. Springer-Verlag, New York, 1984.
- [Smo91] M. D. Smooke. *Numerical Modeling of Laminar Diffusion Flames*. Progress in Astronautics and Aeronautics, Vol. 135, 1991.
- [TV96] L. Tobiska and R. Verfürth. *Analysis of a streamline diffusion finite element method for the Stokes and Navier-Stokes equations*. SIAM J. Numer. Anal., 33(1):107–127, 1996.
- [War78] J. Warnatz. *Calculation of the structure of laminar flat flames I: Flame velocity of freely propagating ozone decomposition flames*. Ber. Bunsengesellschaft. Phys. Chem., 82:193–200, 1978.