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Adaptive Time–Space Discretization for Combustion Problems

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ABSTRACT

We present a self-adaptive finite element method to solve combustion problems in 1D, 2D, and 3D. An implicit time integrator of Rosenbrock type is coupled with a multilevel approach in space. A posteriori error estimates are obtained by constructing locally higher order solutions involving all variables of the problem. Adaptive strategies such as step size control, spatial refinement and coarsening allow us to get economically an accurate solution. Various examples are presented to demonstrate practical applications of the proposed method.

INTRODUCTION

In the numerical simulation of combustion problems much attention has to be paid to different time scales forced by ignition or propagation processes, and to an efficient spatial resolution of steep solutions often arising when thin flame fronts propagate through the computational domain. In this situation, adaptive methods, such as step size control, spatial refinement and coarsening, or moving meshes are attractive to get an accurate solution economically [14, 4, 12, 10, 15]. One of the main questions in the area of adaptive algorithms is how to determine where small time steps and spatial refinement are necessary, and where large time steps and coarse meshes are sufficient. In addressing this issue, two approaches are mostly applied. The first is to use special engineering knowledge about physical and chemical properties of the model equations. Unfortunately, those criteria often request a tuning process for each new application.

The second approach is to use a posteriori estimates. Here the goal is to capture local discretization errors involving all variables of the model equations. Higher order solutions are constructed both in time and space [1, 7, 13], which can be utilized to adjust the time step and the local spatial resolution in order to keep the numerical error below a prescribed tolerance. This methodology is quite general, it can be applied to a large class of combustion problems governed by the same model.

Guided by this mathematical approach, we present an adaptive finite element method coupled with an implicit time integrator of Rosenbrock type. The algorithm has demonstrated its reliability for a variety of practical relevant unsteady problems. Selected examples including 1D, 2D, and 3D problems will be presented to illustrate practical applications of our mesh quality control techniques.

The implementation of adaptive finite element codes employing multilevel techniques require modern software design and programming languages. Dynamic tree structures are used to manage grid enhancement and robust coarsening as well. Our code KARDOS is based on the programming environment KASKADE [6] which is available at <ftp://ftp.zib.de/pub/kaskade>.

ADAPTIVE TIME AND SPACE DISCRETIZATION

Many combustion phenomena are set up by time-dependent systems of PDEs of the following type

$$\begin{aligned} H(x, t, u)u_t - \nabla \cdot (D(x, t, u)\nabla u) &= F(x, t, u, \nabla u) \\ x \in \Omega \subset \mathfrak{R}^n, t > 0, n &= 1, 2, 3 \end{aligned} \quad (1)$$

with additional boundary and initial conditions. The heat capacity matrix H and the diffusion matrix D may be singular, the right-hand side vector F describes some coupling of the components.

In the following we shortly outline the time-space adaptive algorithm implemented in the programming package KARDOS.

We first discretize in time using one-step methods of Rosenbrock type that are accepted to integrate stiff equations efficiently for moderate accuracy requirements [2, 13]. Starting with the solution u_k at time t_k , the solution u_{k+1} at the advanced time $t_{k+1} = t_k + \tau_k$ is computed by the following linear combination of u_k and different intermediate stage values l_j

$$u_{k+1} = u_k + \sum_{j=1}^s b_j l_j, \quad (2)$$

with suitable chosen real values for the coefficients b_j . Each of these functions l_j is the solution of a linear elliptic problem. Replacing the coefficients b_j in (2) by different coefficients \hat{b}_j a second solution \hat{u}_{k+1} of inferior order can be obtained. The difference $\|u_{k+1} - \hat{u}_{k+1}\| =: \varepsilon_k$ satisfactorily estimates the error introduced by the temporal discretization, and can be utilized to propose a new time step

$$\tau_{k+1} = \frac{\tau_k}{\tau_{k-1}} \left(\frac{TOL_t \varepsilon_{k-1}}{\varepsilon_k \varepsilon_k} \right)^{1/(p+1)} \tau_k. \quad (3)$$

Here, p is the local order of the solution \hat{u}_{k+1} . This step size selection guarantees an error control with respect to a desired tolerance TOL_t [9].

The elliptic subproblems for the l_j are discretized by an adaptive multilevel finite element method [3, 5, 6]. We consider conforming partitions of the computational domain Ω into intervals, triangles, or tetrahedra. The weak solutions of the elliptic problems are approximated in the finite dimensional space of piecewise linear continuous functions. Starting with an initial mesh G_k^0 at time t_k , we successively improve the spatial discretization by local refinement until a prescribed tolerance TOL_x is reached.

The necessary estimation process is based on local quantities computed as approximate residuals on small subdomains employing quadratic finite elements.

In the one–dimensional case one estimates the error within each element, in the two– and three–dimensional case each of those subdomains is the union of all triangles or tetrahedra having one common edge. Imposing homogeneous Dirichlet boundary conditions, the local spatial error can be represented by only one degree of freedom at the midpoint of the corresponding edge.

We end up with a nested sequence $G_k^0, G_k^1, \dots, G_k^n$ of triangulations. To compute the solution u_{k+1} at time t_{k+1} we choose a new initial mesh G_{k+1}^0 derived from G_k^n by coarsening. Degrees of freedom are only removed in such regions where the local errors are small enough. If necessary this mesh is again improved analyzing the new solution u_{k+1} . For a more detailed description see [13].

SELECTED PROBLEMS

1D–Example: Bubble Reactor [12].

We consider a gas–fluid system where the phase boundaries change their shapes and sizes in time. Fig. 1 (left) shows a vertical and cylindrical bubble reactor in section. Different gaseous chemicals stream in at the lower end of the reactor filled with a fluid. The bubbles rise to the top dissolving and reacting with each other. Bubble reactors are used in practice to form a synthesis process of different chemicals.

The reaction takes place in the outer shell of each bubble. In an 1D–model it is assumed that the width of this shell stays equal although the radius of the bubble decreases. Fig. 1 (right) shows the temporal grid evolution taking the height in the reactor as time axis.

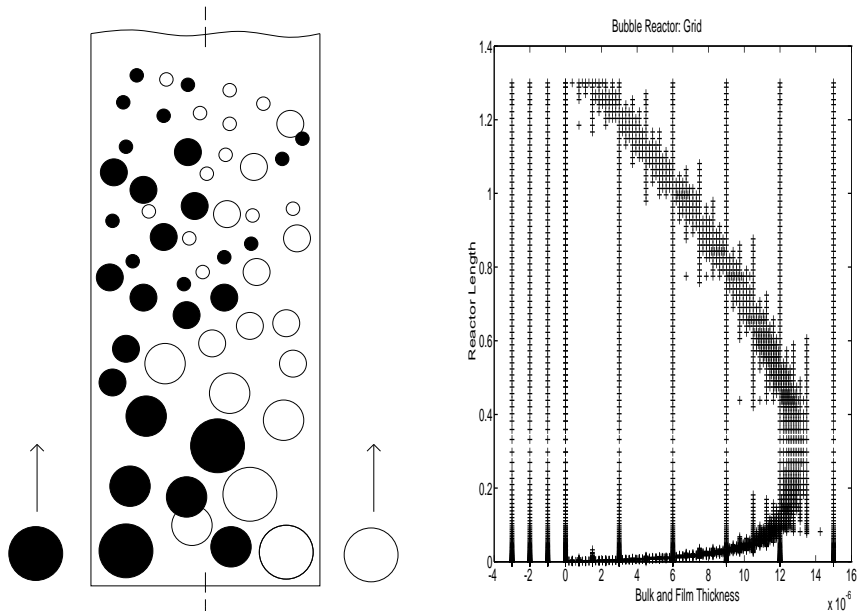


Fig. 1: Bubble reactor (left: cut through reactor, right: mesh evolution)

Initially, the reaction front finds its way into the bubble shell with a high speed forcing small time steps. After that the concentration of the reactant decreases

and the front propagates in the other direction. Finally, the reaction stops when the top of the reactor is reached. This simulation is used to determine the right dimension of such a reactor.

2D–Example: Non–Uniformly Packed Solid Reactor [8].

This application is constituted by solid–solid alloying reactions. The particularity of such a process is that convection is impossible and that the macroscopic diffusion for the species in solids is in general negligible with respect to heat conductivity. The ignition takes place at the left boundary in a small domain. The reactor is non–uniformly packed with solid forcing a strongly increased flame velocity close to the outer border. This is illustrated for the concentration of the reactant in Fig. 2 where the light color corresponds to intermediate stages of combustion. The corresponding adaptive mesh is well fitted to this solution state.

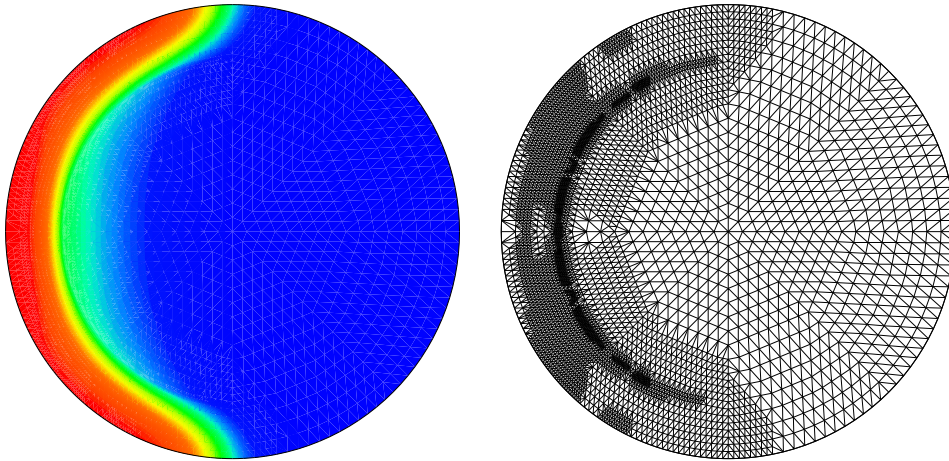


Fig. 2: Non–uniformly packed reactor (left: concentration of reactant, right: adaptive mesh)

3D–Example: Thermo–Diffusive Flame Propagation [11].

This problem describes the propagation of a three–dimensional premixed flame in a gaseous mixture with non adiabatic walls. The thermo–diffusive model is used to decouple the reaction–diffusion process from the hydrodynamical flow. The thermal reaction is formulated for nondeformable materials of constant density. The flame extinguishes if the heat loss at the wall is too strong. Otherwise, the time–dependent flame eventually converges to a steady non adiabatic curved flame. Fig. 3 shows two snapshots from an adaptive 3D–mesh at different times. They illustrate the high resolution of the flame inside the tube and show special refinement regions at the boundary where the flame is cooled. This picture gives an impression of saving in terms of computational work in 3D with respect to uniform methods.

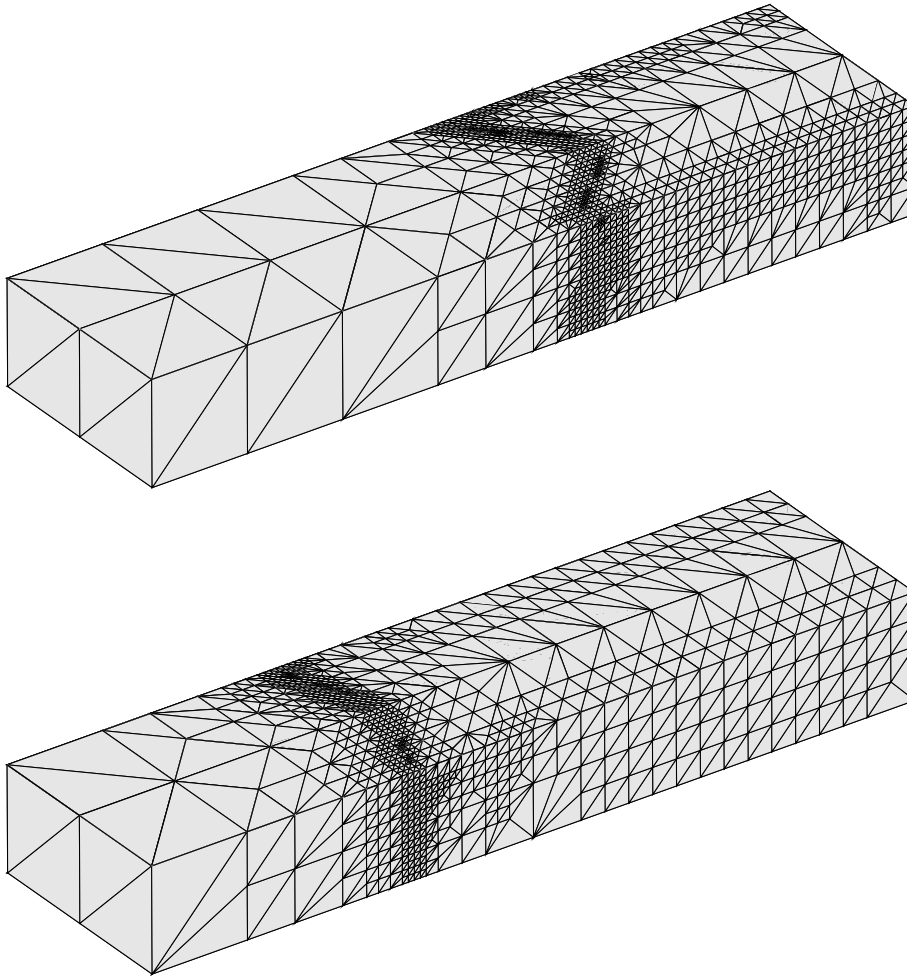


Fig. 3: Adaptive grids for a propagating flame front

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