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Three–Dimensional Fully Adaptive Solution of Thermo–Diffusive Flame Propagation Problems

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Abstract. In this paper we present a self–adaptive finite element method to solve flame propagation problems in 3D. An implicit time integrator of Rosenbrock type is coupled with a multilevel approach in space. The proposed method is applied to an unsteady thermo–diffusive combustion model to demonstrate its potential for the solution of complicated problems.

1 Introduction

Many combustion phenomena are set up by time–dependent systems of PDEs which have to be solved in three–dimensional domains. The solution of such complex problems is still a grand challenge and requires the development of highly efficient numerical methods. Adaptivity is an important and essential means to drastically reduce the amount of work.

Adaptive finite element methods have been developed by the authors over several years to solve problems with highly non–uniform solutions. The reliability of the algorithm has been demonstrated for a variety of real–life chemical problems [8]. In [9] and [11] the application and implementation of reaction–diffusion problems has been dealt. Various combustion systems are solved in [10, 5].

To include more practically relevant problems we extended our approach to the three–dimensional case. In this paper we demonstrate the flexibility of the algorithm for a thermo–diffusive combustion problem governed by different time scales and spatial non–uniformity. In all these cases adaptivity both in time and space allows us to automatically adjust the time step and the local spatial resolution in order to keep the numerical error below a prescribed tolerance.

2 The Thermo–Diffusive Model

In order to develop efficient adaptive techniques for 3D combustion simulations it is of interest to consider flame propagation models which decouple the reaction–diffusion process from the hydrodynamical flow. The thermal reaction process is formulated for nondeformable materials of constant density. This leads to the well–known thermo–diffusive model which consists of two nonlinear equations

$$Le\, T_t - \Delta T = \alpha D Y exp\left(-\frac{\delta}{T}\right) , \qquad (1)$$

$$Y_t - \Delta Y = -D Y exp\left(-\frac{\delta}{T}\right) . \qquad (2)$$

Here, T is the dimensionless temperature, Y the concentration of a reactant and Le is the Lewis number, the ratio of diffusivity of heat and diffusivity of mass. The positive constants α (chemical heat release), δ (activation energy) and $D = Re^{\delta}/(\alpha\delta)$ (Damkohler number) with R being the reaction rate, are special combustion numbers. This system describes a one–step reaction in the presence of Arrhenius chemistry. The one–dimensional version of this problem was investigated via activation–energy asymptotics in [7].
The above reaction–diffusion system allows us to study a whole ignition process and the propagation of a reaction wave. Initially, the temperature increases slowly during an induction period with relatively weak reaction. Induction is followed by an extremely rapid development and growth of a localized hot spot. A sharply focused temperature region appears in which the concentration of the reactant is rapidly depleted. Then the reaction front propagates through the system.

3 Numerical Algorithm

We present a time–space adaptive algorithm implemented in the programming package KARDOS. For high values of δ, the problem is stiff and involves additional non–uniformity in time (ignition) and space (wave propagation). An accurate simulation of the combustion process therefore requires an implicit time integrator with automatic adjustment of time steps and a dense moving computational mesh in the propagating flame region to resolve the high gradients as well.

In contrast to the widely used method of lines approach, we first discretize in time and then in space. This discretization sequence has the advantage that the task of spatial adaptivity can be directly attacked by an efficient elliptic solver [1, 3, 4].

For the time discretization we use one–step methods of Rosenbrock type that are accepted to integrate stiff equations efficiently for moderate accuracy requirements. 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

$$u_{k+1} = u_k + \sum_{j=1}^{s} b_j l_j \,, \tag{3}$$

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 (3) 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

$$\tau_{k+1} = \frac{\tau_k}{\tau_{k-1}} \left(\frac{TOL_t \; \varepsilon_{k-1}}{\varepsilon_k \; \varepsilon_k} \right)^{1/(p+1)} \tau_k \,. \tag{4}$$

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 [6].

The elliptic subproblems for the l_j are discretized by an adaptive multilevel finite element method. We consider conforming partitions of the computational domain Ω into 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. Each tetrahedron where the solution is not accurate enough, is refined into eight tetrahedra in such a way that the ratio of the diameter and the radius of the largest interior ball of the new tetrahedra remains uniformly bounded. Special closures are utilized to obtain a regular triangulation after refinement [2].

The necessary estimation process is based on local quantities computed as approximate residuals on small subdomains employing quadratic finite elements. Each of these domains is the union of all 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 $G_k^0,\ G_k^1, ...,\ G_k^n$ 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 [11].
The arising linear equations are solved iteratively by the BICGSTAB algorithm [12] with ILU–preconditioning.

4 Numerical Results

We solved (1,2) on the domain $\Omega = \{x = (x_1, x_2, x_3) \in R^3, 0 < x_1, x_2, x_3 < 1\}$ for $t > 0$ with $Le = 0.9$, $\delta = 20$, $\alpha = 1$ and $R = 5$. The initial conditions read

$$Y(x, 0) \ = \ T(x, 0) \ = \ 1.0\ ,\ x \in \Omega\ .$$

Homogeneous Neumann conditions are applied for all points x on boundaries with $x_1 = 0$ or $x_2 = 0$ or $x_3 = 0$. Otherwise we use Dirichlet boundary conditions, i.e.

$$Y(x, t) \ = \ T(x, t) \ = \ 1.0 \qquad \text{for } x_1 = 1 \text{ or } x_2 = 1 \text{ or } x_3 = 1,\ t > 0\ .$$

The hot spot is formed at $(0, 0, 0)$ where the temperature jumps from 1 to approximately $1+\alpha$.

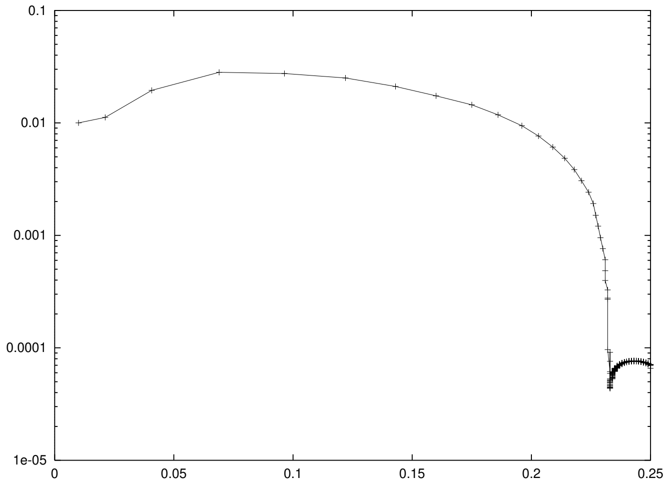

Fig.1: Time steps used by KARDOS

Fig.1 shows the evolution of the time steps used by KARDOS with a three–stage Rosenbrock method of order three. The two different phases of the integration process are clearly visible. During ignition $t = 0, \ldots, 0.23$ the time steps decreases. Afterwards the high speed of the flame forces a time step not larger as $8\mathrm{E} - 5$.

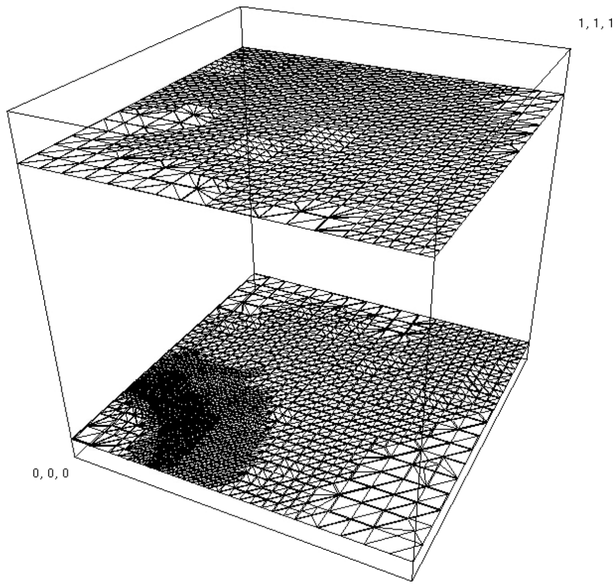

Fig.2: Adaptive grids applied in the planes $z = 0.05$, $z = 0.85$ at $t = 0.235$

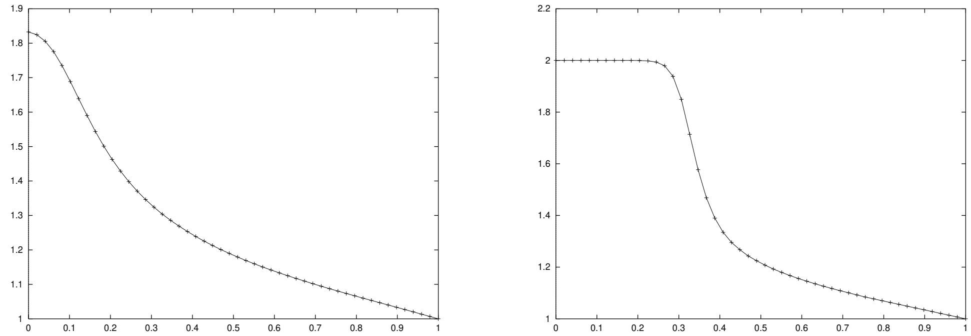

Fig.3: Cuts through the temperature (left: $t\!=\!0.233$, right: $t\!=\!0.235$)

Fig.2 shows the adaptivity in space: two adaptive grids are plotted with respect to the planes $z = 0.05$ and $z = 0.85$ at $t = 0.235$. Due to the hot spot at the origin the computational mesh is more refined in this region. A sharp reaction front subsequently forms and propagates rapidly towards the Dirichlet boundaries. Fig.3 reports cuts through the temperature along the x–axis at two different times $t\!=\!0.233$ and $t\!=\!0.235$. They illustrate the good spatial resolution of the reaction front.

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