Numerical Simulation of Reacting Mixing Layer with a Parallel Implementation

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Abstract. This work concerns the parallelization of an explicit algorithm for the simulation of compressible reacting gas flows, applied to supersonic mixing layers. The reacting Navier-Stokes equations are characterized by three tightly coupled physical phenomena, i.e. the convection, diffusion and chemical source terms. To compute the chemical source terms, full complex chemistry is used. By considering the elapsed time for solving the problem, the numerical treatment of the chemical source terms takes about 75% of the total execution time. The main goal of the present work is to reduce the relative cost of chemical source terms calculation and also to optimize the global cost of the procedure resolution by the use of parallel computation.

1 Choice of Parallel Approach

On parallel architectures, independent computations are executed simultaneously. To achieve this goal, the algorithm is divided into several independent tasks. All tasks can be executed simultaneously and communicate with each other during the execution.

Two different types of parallel methodologies exist: data-parallelism and control parallelism [14]. The first approach relies on the fact that each processor performs at a given time the same instruction on different data. This approach exploits the great potential of massively-parallel computers, SIMD (Single Instruction Multiple Data) architectures [11].

In the control-parallelism approach, the computational problem is divided into a number of more-or-less independent tasks, with different processors performing different tasks in parallel. This approach is adapted to multi-processor computers, MIMD (Multiple Instruction Multiple Data) architectures [1].

In order to use MIMD computers very efficiently, the granularity of tasks should be as large as possible. In CFD the space decomposition of the computational domain is the most efficient technique in order to increase the granularity of tasks for MIMD architectures [5]. This technique (the so-called multi-domain

* This work took a large benefit of discussions with Yves Escaig (Mechanical Engineering Laboratory, INSA of Rouen)
technique) consists in partitioning the computational domain into a number of blocks, and to distribute blocks onto different processors [4]. However, there is still a problem to maintain a well balanced decomposition.

The choice of the adopted parallel approach is influenced by the numerical algorithm. However, one can notice that data-parallel and control-parallel approaches can both be combined [12]. By considering that in most reacting flows, reacting and non-reacting zones occur simultaneously, the computation of chemical source terms can be restricted to the main reactive region. Thus a decomposition efficient for pure hydrodynamical problem becomes inefficient when the reacting zones dimension differ greatly between blocks. In such a way the standard multi-block technique is no longer well suited for the reacting flow. In this paper, a classical multi-block technique is used for convective and diffusive terms, whereas SPMD (Single Program Multiple Data) approach is employed for chemical source terms.

2 Flow configuration, physical, chemical and mathematical model

Figure 1 shows the physical model considered in the present study. It consists of two chemically active hydrogen and air streams with different streamwise velocities. In this work the spatial mixing of reacting streams has been simulated in a two-dimensional domain. The static pressure at the inlet side is the same for both streams. To prescribe the inlet conditions the self similar solution of the compressible mixing layer [9] is used at the inlet with a vorticity thickness equal to 0.05 of the transverse length.

![Fig. 1. Flow configuration](image)

The flow evolution is governed by the unsteady compressible Navier-Stokes equations coupled with the energy and species transport equations. These equations are written in two-dimensional form as:

\[
\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} + \frac{\partial G(U)}{\partial y} = S(U)
\] (1)