technische universiteit eindhoven

Numerical modelling of laminar flames

M. Graziadei, J.H.M. ten Thije Boonkkamp, R.M.M. Mattheij

Introduction

The equations that describe laminar flames are characterized by the presence of **high activity regions**, where most of the activity is concentrated. There, gradients are quite large compared to those in the rest of the domain. When solving such problems numerically, this solution behaviour requires a much finer grid in the **high activity region**, or flame front, than in the zones where the solution is fairly smooth.

Laminar reacting flow equations

Laminar recting flows can be described by the following equations

Continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0,$$

Momentum equation

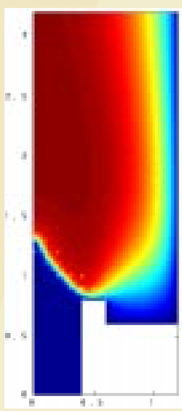
$$\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v}) = \rho \mathbf{g} - \nabla p + \nabla \cdot (\mu(\nabla \mathbf{v} + (\nabla \mathbf{v})^T - \tfrac{2}{3}\mathbf{I}(\nabla \cdot \mathbf{v}))),$$

Energy equation

$$c_p \frac{\partial \rho T}{\partial t} + c_p \nabla \cdot (\rho \mathbf{v} T) = \nabla \cdot (\lambda \nabla T) + \sum_{i=1}^{N_s - 1} (c_{pi} - c_{pN_s}) \rho D_{im} \nabla Y_i \cdot \nabla T + s_T,$$

Species equation

$$\frac{\partial \rho Y_i}{\partial t} + \nabla \cdot (\rho \mathbf{v} Y_i) = \nabla \cdot (\rho D_{im} \nabla Y_i) + s_i.$$



Bunsen flame: graphical representation of the temperature.

- Discretization: finite difference or finite volume method.
- A coarse grid covers the entire domain.
- In the high activity region a finer grid is required to get the desired accuracy.

Local Defect Correction (LDC) method

The LDC method uses the solution computed on the fine grid to improve the coarse grid solution. It works as follows:

- Compute the coarse grid solution.
- Define a fine grid BVP by interpolating the BCs on the interface between the fine and the coarse grid from the coarse grid solution.
- Compute the solution of the fine grid problem
- The fine grid solution is then used to estimate the defect of discretization on the coarse grid.
- Finally, to correct the coarse grid problem, add the defect of discretization to its right-hand side.

The method is used in an iterative way. It converges very fast: tipically one iteration suffices.

Test problem

LDC thecnique has been implemented with several fine grid types. The following test problem is described by the two-dimensional convection-diffusion-reaction equation

$$-\nabla^2 u + \frac{\partial u}{\partial x} + \frac{\partial u}{\partial y} = f(\mathbf{x}) \qquad \mathbf{x} \in \Omega := (0, l_1) \times (0, l_2),$$

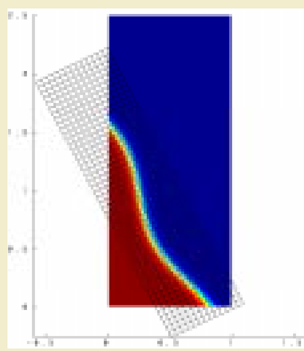
$$u = g(\mathbf{x}) := \mathbf{1} - \tanh[\beta \mathbf{s}(\mathbf{x})] \qquad \mathbf{x} \in \partial\Omega,$$

where f is such that the exact solution is given by

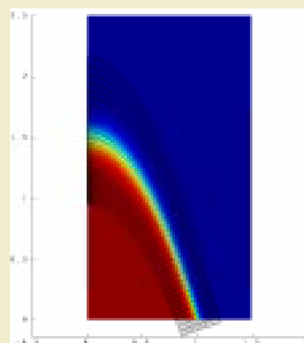
$$u(\mathbf{x}) = 1 - \tanh[\beta s(\mathbf{x})].$$

- $s(\mathbf{x})$ describes the **flame front** shape;
- β determines the steepness of $u(\mathbf{x})$ in the vicinity of the **flame front**.

It can be solved either with a slanting or with a curvilinear fine grid.



Slanting grid



Curvilinear grid

Slanting grid

- Advantage: the system of equations maintains the same level of complexity; it needs only to be rotated.
- Drawback: The number of fine grid points is redundant.

Curvilinear orthogonal grid

They are made such that a set of coordinate lines follows the level curves.

- Advantage: the number of fine grid points can be reduced. In fact, the step size along the coordinate lines tracing the level curves can be bigger than the step size in the orthogonal direction. Furthermore, the lines can be more dense just close to the high activity region and less dense far away from it.
- Drawback: the system of equations becomes more complex. In fact, we want to solve our system in a rectangular domain, which has thus to be mapped into the curvilinear grid.

Future developments

Application of LDC in combination with slanting and curvilinear fine grids to real flame problems.