Mesh Quality and Moving Meshes for 2D and 3D Unstructured Mesh Flow Solvers.

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Abstract

The issue of mesh quality for the solution of problems with anisotropic solutions on unstructured triangular and tetrahedral meshes is considered. A three dimensional time-dependent problem from atmospheric dispersion is described and used to motivate a discussion of mesh quality. A survey of recent research in the development of finite element methods describes work on moving mesh methods, on anisotropic meshing algorithms and on the provision of appropriate error estimates. As such error estimates are presently not always available, one option is to use local error estimates for transient problems. One such approach is described and is used to decide how to adapt the mesh. A visualization system for identifying poor quality elements is described and used to find the poor quality elements in the atmospheric dispersion problem.

1 Introduction

The issue of what is an appropriate spatial mesh is as old as the finite element method itself, but the increasingly complex nature of 3D applications may involve dealing with multicomponent problems with time dependence, turbulence and anisotropy to name but some of many possible complications.

A relatively simple example which is useful to illustrate the difficulties is the following 3D advection-reaction problem. The example is a model of atmospheric dispersion from a power station plume which is a concentrated source of NOx emissions, [31]. The photo-chemical reaction of this NOx with polluted air leads to the generation of ozone at large distances downwind from the source. An accurate description of the distribution of pollutant concentrations is needed over large spatial regions in order to compare with field measurement calculations. The present trend is to use models incorporating an ever larger number of reactions and chemical species in the atmospheric chemistry model. The complex chemical kinetics in the atmospheric model gives rise to abrupt and sudden changes in the concentration of the chemical species in both space and time. These changes must be matched by changes in the spatial mesh and the timesteps if high resolution is required, [31]. This application is modelled by the atmospheric diffusion equation in three space dimensions given by:

$$\frac{\partial c_s}{\partial t} + u\frac{\partial c_s}{\partial x} + v\frac{\partial c_s}{\partial y} + w\frac{\partial c_s}{\partial z} = D + R_s + E_s - \kappa_s c_s, \qquad (1)$$

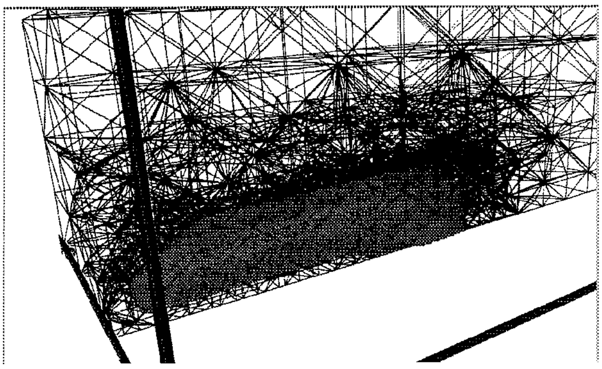

Figure 1: Tetrahedral Mesh for Reacting Flow P.D.E.

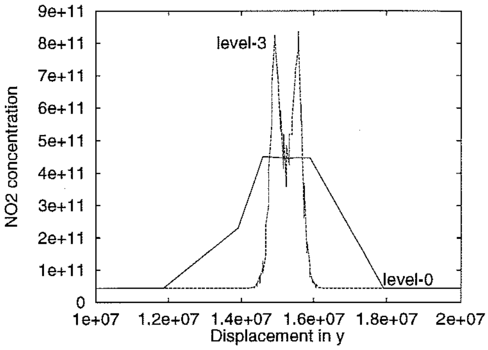

Figure 2: Cross section of plume

where c_s is the concentration of compound s , u, v and w, are constant wind velocities and κ_s is the sum of the wet and dry deposition velocities. E_s describes the distribution of emission sources for compound s and R_s is the chemical reaction term which may contain nonlinear terms in c_s. D is the diffusion term which is set to zero here. For n chemical species a set of n partial differential equations (p.d.e's) is formed where each is coupled to the others through the nonlinear chemical reaction terms.

The test case model covers a region of 300 km x 500 km and is a three-dimensional form of that used by [31] and although far from detailed, does represent the main features which would commonly be found in an atmospheric model including slow and fast nonlinear chemistry, concentrated source terms and advection. Although the chemical reaction terms involve only 7 species they still represent the main features of a tropospheric mechanism, namely the competition of the fast inorganic reactions given by $NO_2 \xrightarrow{O_2} O_3 + NO$ and $NO + O_3 \rightarrow NO_2 + O_2$ with the chemistry of volatile organic compounds (VOC's), which occurs on a much slower time-scale. This separation in time-scales generates stiffness in the resulting equations. The reaction rate constants and the background concentrations that form the initial conditions for the model are given by Tomlin et al. [31]. These concentrations will then change diurnally as the chemical transformations take place. The power station is taken to be the only source of NOx and this source is treated by setting the concentration in the chimney set as an internal boundary condition. In terms of the mesh generation this ensures that the initial grid will contain more elements close to the concentrated emission source. The concentration in the chimney corresponds to an emission rate of NOx of 400kghr^{-1} with only 10% of the NOx being emitted as NO_2. A constant wind speed of 5ms^{-1} in the x-direction with y and z components of one tenth of this value is assumed.

Spatial discretisation of the model atmospheric diffusion equation on unstructured tetrahedral meshes reduces the set of p.d.e's in four independent variables to a system of ordinary differential equations (o.d.e's) in one independent variable: time. This system of o.d.e's can then be solved as an initial value problem. For advection-dominated problems it is important to choose a discretisation scheme which preserves the physical range of the solution [30]. The method used here is the cell-centered finite volume discretisation scheme used by [30] which enables accurate solutions to be determined for both smooth and discontinuous flows by making use of upwind techniques for the advective parts of the fluxes.

Figure 1 shows the plume developing with the adaptive mesh clustered around the