UNSTRUCTURED MESH SOLVERS FOR HYPERBOLIC PDES WITH SOURCE TERMS: ERROR ESTIMATES AND MESH QUALITY

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Abstract. The solution of hyperbolic systems with stiff source terms is of great importance in areas such as atmospheric dispersion. The finite-volume approach used here for such problems employs Godunov-type methods, a sophisticated splitting approach for efficiency and adaptive tetrahedral meshes to provide the necessary resolution for physically meaningful solutions. This raises the issues of how to estimate the error for Godunov type methods and what is an appropriate mesh for such applications. A new mesh visualization and haptic-interface tool will be shown to help clarify this and its use illustrated for a model problem in three space dimensions.

1. Introduction

Unstructured triangular and tetrahedral meshes are widely used in engineering and scientific computing for solving problems via finite element and finite volume methods. At the same time Godunov methods are widely used in the solution of problems with hyperbolic parts (Godlewski and Raviart, 1996; Kröner, 1997; Toro, 1999). The intention here is to consider some of the issues that arise from combining these approaches when solving
problems such as the 3D advection reaction problem, taken from a model of atmospheric dispersion from a power station plume - a concentrated source of NOx emissions, (Tomlin, 1999). 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 complex chemical kinetics in the atmospheric model gives rise to 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, (Tomlin, 1999). The effects of the plume interestingly causes levels of ozone to rise above the background levels at quite large distances downwind from the source of NOx. This application is modelled by the atmospheric diffusion equation in three space dimensions given by:

$$\frac{\partial c_s}{\partial t} + \frac{\partial uc_s}{\partial x} + \frac{\partial vc_s}{\partial y} + \frac{\partial wc_s}{\partial z} = D + R_s + E_s - \kappa_s c_s,$$

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

The solution techniques employed consist of time integration methods specially designed for explicit convection and implicit source terms handled by using a very efficient Gauss-Seidel iteration. Finite volume cell-vertex and cell-centred Godunov-type schemes (Godunov, 1959; Van Leer, 1984) are both used for space discretization. For this atmospheric diffusion model, the meshes and means of obtaining them are described in (Johnson, 1998; Speares, 1997). The advantage of the Godunov-type methods based on upwinding and approximate Riemann problems is that it is possible to preserve positivity of the solution - a key requirement for reacting flow problems. Mesh adaptation using h refinement, even based on simple gradient information gives dramatically improved solutions, see (Tomlin, 1999) but raises the issue of whether or not the mesh is appropriate for all the species.

The only sure way of knowing whether or not the mesh is appropriate is to use error indicators and to understand how the error depends on both the solution and on element shape, preferably by visualization. It is hard to visualize all the mesh elements in a full 3D mesh display and it is difficult to comprehend fully the myriad of element shapes and sizes, see Figure 1. The combined haptic and visual interface of (Durbeck, 1999) has been designed to overcome the daunting task of finding "bad" tetrahedra in a