An Adaptive CFD Solver for Time-Dependent Environmental Flow Problems

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1 Introduction

This paper will describe the application of the SPRINT2D unstructured mesh finite volume code to time-dependent environmental problems and show that the combination of space and time adaptivity makes it possible to gain greater insight into CFD problems. The code has been written through a joint Shell Research Ltd (Thornton Research Centre) and Leeds University (School of Computer Studies) Research programme. The key feature of the software is that applications codes may be written which are based on a toolkit of robust numerical routines. The paper outlines some of these routines and shows how they have been applied to two example problems. Sections 2 and 3 describe the finite volume discretization scheme and the mesh generation and adaptivity routines for unstructured triangular meshes. Section 4 covers the method of lines time integration approach using a range of explicit and implicit time integration methods for both stiff and nonstiff o.d.e.s. A simple spatial error estimate is used to adapt the mesh, and controlled in conjunction with the time error to balance the two errors. Sections 5 and 6 describe the numerical examples while Section 7 contains a summary and outlines an extension of the approach to three dimensional problems.

2 Finite Volume Method on Triangles

The discretization of two-dimensional p.d.e.s on unstructured triangular meshes necessitates the use of a method which can handle complex flow problems in a stable and accurate manner. For example, the Berzins and Ware [3] method enables accurate solutions to be determined for both smooth and discontinuous flows by making use of local Riemann solver flux techniques (originally developed for the Euler equations) for the convective parts of the fluxes, and centred schemes for the diffusive part. To illustrate this method, consider the equation

$$U_t \;=\; (\,F(u,u_x,u_y)\,)_x + (\,G(u,u_x,u_y)\,)_y + S(u)\quad ,t \in (0,t_e]\,,\;(x,y) \in \Omega \qquad (2.1)$$

with appropriate boundary and initial conditions. A finite volume type approach is adopted in which the solution value at the centroid of triangle i, (x_i, y_i), is U_i and the solutions at the centroids of the triangles surrounding triangle i are U_l, order method and that using a second order method. For time dependent p.d.e.s this estimate shows how the spatial error grows locally over a time step, [1]. A refinement indicator for the jth triangle is defined by an average scaled error ($serr_j$) measurement over all $npde$ p.d.e.s using supplied absolute and relative tolerances

$$serr_j = \sum_{i=1}^{npde} \frac{e_{i,j}(t)}{atol_i/A_j + rtol_i \times u_{i,j}}, \tag{3.1}$$

where $atol$ and $rtol$ are the absolute and relative error tolerances. This formulation for the scaled error provides a flexible way to weight the refinement towards any p.d.e. error. An integer refinement level indicator is calculated from this scaled error to give the number of times the triangle should be refined or derefined.

4 Time Integration

A method of lines approach with the above spatial discretization scheme results in a system of o.d.e.s in time which are integrated using either a Theta method with functional and/or Newton iteration or the DASSL method using Newton Krylov methods [6]. Both codes allow automatic control of the local error. Berzins[1] shows that a Courant stability condition is automatically satisfied if functional iteration converges sufficiently fast.

In most time dependent p.d.e. codes either a CFL stability control is employed or a standard o.d.e. solver is used which controls the local error $\underline{l}_{n+1}(t_{n+1})$ with respect to a user supplied accuracy tolerance. Efficient time integration requires that the spatial and temporal errors are roughly the same order of magnitude. The need for spatial error estimates, unpolluted by temporal error, requires that the spatial error is the larger of the two errors. Berzins [1] has developed a strategy which achieves this by controlling the local time error to be a fraction of the growth in the spatial discretization error over a timestep. The local-in-time spatial error, $\underline{\hat{e}}(t_{n+1})$, for the timestep from t_n to t_{n+1} is defined as the spatial error at time t_{n+1} given the assumption that the spatial error at time t_n is zero. A local-in-time error balancing approach is then given by

$$|| \ \underline{l}_{n+1}(t_{n+1}) \ || < \epsilon \ || \ \underline{\hat{e}}(t_{n+1}) \ ||, \quad 0 < \epsilon < 1. \tag{4.1}$$

In the case of a single p.d.e. the component of $\underline{\hat{e}}(t_{n+1})$ on the j th triangle is estimated by $e_{1,j}(t)$ as defined above.

5 Atmospheric Dispersion

Power station plumes are concentrated sources of NO_x emissions, [7]. The photochemical reaction of this NO_x with polluted air leads to the generation of ozone at large distances downwind from the source. This provides a stringent test of whether adaptive gridding methods can lead to more reliable results for complex multi-scale models. The transport of the plume and the chemical reactions are

A calculation of the area under these curves shows a dramatic 30% difference between the level 0 and the level 3 solutions. The reason is the nonlinearity in the chemical reaction rates. Individual species concentrations on a refined mesh will give rise to very different local production rates than those found from the same concentrations averaged over a coarse mesh.

These preliminary results show key features which cannot be represented by the coarse meshes generally used in regional scale models. Also coarse meshes can also lead to inaccurate estimates of average or integrated concentration levels. Adaptive methods thus appear to be of great importance for these problems.

6 Two-Dimensional Harbour Flow Problem

The environmental problems of harbour and river flooding and pollution dispersion as modelled by the shallow water equations similarly benefit from adaptive meshes when resolving the complex natural geometries of rivers and estuaries. While much work has been carried out on the accurate solution of the these equations in recent years, e.g. Toro, [8] there has been little development in the way of engineering codes. Existing models are usually based on rectangular grids and less sophisticated discretization methods. One exception has been the model presented by Zhao et. al. [9] who have used the Osher Riemann solver in a first order accuracy river model. The method used here is similar, but has second order accuracy and spatial and temporal adaptivity.

A well-known problem is the harbour described by Falconer [4]. This is a physical model of a harbour and the adjacent coastal region: measurements have been taken of the flow and it has also been modelled numerically. Although there is relatively little data in the open literature of the detail of the flow structure, there is sufficient to compare against the results presented here. The initial data for the numerical test was a flat water surface at a depth of 0.38m in the main basin. The flow is driven from the open boundary in Fig.2 (left) by a specified depth to simulate a tidal cycle. This varies sinusoidally from the starting depth, initially increasing, and having an amplitude of 0.1m and a period of 702 seconds.

The two-dimensional shallow water equations, with source terms representing frictional stress and momentum due to a sloping bed, may be written in the form of equation (2.1) with $U = (\phi, \phi u, \phi v)^T$ and

$$E = \begin{pmatrix} \phi u \\ \phi u^2 + \frac{1}{2}\phi^2 \\ \phi uv \end{pmatrix}, G = \begin{pmatrix} \phi v \\ \phi uv \\ \phi v^2 + \frac{1}{2}\phi^2 \end{pmatrix}, S = \begin{pmatrix} 0 \\ g\phi(Sf_x + So_x) \\ g\phi(Sf_y + So_y) \end{pmatrix} \quad (6.1)$$

where u, v are the velocities in the x and y directions respectively, $\phi = gH$, H is the depth of flow, g is the acceleration due to gravity, $So_{x/y}$ are the bed slopes in x and y and $Sf_{x/y}$ are the friction slopes in x and y. The latter can be found using either the Manning or De Chezy formulae (which are equivalent):

$$Sf_x = \frac{n^2 u\sqrt{u^2+v^2}}{(\phi/g)^{4/3}} = \frac{u\sqrt{u^2+v^2}}{C^2(\phi/g)^{4/3}} \quad (6.2)$$

7 Summary and Future Work

The application of time dependent adaptive p.d.e solvers to environmental flow problems has illustrated the potential of such codes to provide a greater degree of detail than may otherwise be possible. The extension of this work to three space dimensions is being addressed by the development of a fast 3D unstructured tetrahedral mesh adaptivity algorithm. An example application is an inviscid shock diffraction problem, modelled by the 3D Euler equations, for which the shock diffracts around the 3D right angled corner formed between the two cuboid mesh regions. Fig.3 shows a projection of the adaptive mesh onto the walls of the structure. Full refinement/derefinement shock propagation tests show a scaling behaviour of $O(N^{1.14})$ in mesh size, with tetrahdera being generated at a rate of 10^4 per second, which is encouraging for future applications.

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