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Effects of direction decoupling in flux calculation in finite volume solvers

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Abstract

In a finite volume CFD method for unsteady flow fluxes of mass, momentum and energy are exchanged between cells over a series of small time steps. The conventional approach, which we will refer to as direction decoupling, is to estimate fluxes across interfaces in a regular array of cells by using a one-dimensional flux expression based on the component of flow velocity normal to the interface between cells. This means that fluxes cannot be exchanged between diagonally adjacent cells since they share no cell interface, even if the local flow conditions dictate that the fluxes should flow diagonally. The direction decoupling imposed by the numerical method requires that the fluxes reach a diagonally adjacent cell in two time-steps.

To evaluate the effects of this direction decoupling, we examine two numerical methods which differ only in that one uses direction decoupling while the other does not. We examine a generalized form of Pullin's equilibrium flux method (EFM) [D.I. Pullin, Direct simulation methods for compressible ideal gas flow, J. Comput. Phys. 34 (1980) 231–244] which we have called the true direction equilibrium flux method (TDEFM). The TDEFM fluxes, derived from kinetic theory, flow not only between cells sharing an interface, but ultimately to any cell in the grid. TDEFM is used here to simulate a blast wave and an imploding flow problem on a structured rectangular mesh and is compared with results from direction decoupled EFM. Since both EFM and TDEFM are identical in the low CFL number limit, differences between the results demonstrate the detrimental effect of direction decoupling. Differences resulting from direction decoupling are also shown in the simulation of hypersonic flow over a rectangular body. The computational cost of allowing the EFM fluxes to flow in the correct directions on the grid is minimal.

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1. Introduction

Bird's Direct Simulation Monte Carlo (DSMC) method [5] simulates a rarefied flow by following the motion and collisions of a large number of simulator particles as they move through the flow. DSMC in the high collision rate limit has been used as an Euler solver [1,6–8] and as the 'continuum' part of a hybrid DSMC/continuum solver. DSMC is generally more robust than a conventional Euler solver but suffers from statistical scatter which requires large amounts of CPU power to reduce to acceptable limits. One reason for DSMC's stability is that the fluxes of mass, momentum and energy are carried by particles which move in the physically correct directions; in any time step fluxes may flow from any cell to any other cell in the computational domain.

In continuum solvers the fluxes are typically 'direction decoupled'; one dimensional flux calculations are performed in the direction normal to the interface between two cells, and the fluxes are only exchanged with cells that share an interface. For example, on a 2D structured grid the fluxes flow in two coordinate directions and never flow in one time step between cells which are diagonally contiguous (share a vertex in common) but do not have a common interface. Cook [9] shows that when the cell structure is not well aligned with the physical structures in the flow, direction decoupled methods may produce non-physical results such as negative temperatures or densities where strong shocks occur or interact. These solvers may also produce asymmetrical results where symmetrical results are theoretically required.

This phenomenon can be demonstrated through the solutions of radially imploding or exploding flows on rectangular meshes. Fig. 1 shows the computational domain and the initial condition in which there is a low pressure cylindrical region surrounded by a high pressure region with a sharp discontinuity between the two. A cylindrically symmetric shock wave will propagate toward the center, causing an increase in temperature and density as the shock travels inwards. The figure also shows density contours found using three existing direction decoupled methods. It can be seen that the direction decoupled methods give asymmetrical results.

Pullin [1] proposed the equilibrium flux method (EFM) in which the fluxes carried by particles having velocities conforming to the local Maxwell–Boltzmann distribution were calculated analytically for the limit of an infinite number of particles. EFM eliminates the statistical scatter associated with the effectively equivalent particle flux methods. When EFM was used in 2D and 3D flows [10–13] the conventional direction decoupling approach described above was used. A 1D solution using EFM to calculate fluxes between cells is presented in Fig. 2. Viscous effects are ignored, although the numerical viscosity inherent to EFM is present. Fig. 2 also shows the radially symmetric density contours as constructed from the 1D solution corresponding to the conditions and elapsed time used in the direction decoupled results shown in Fig. 1.

Since the EFM fluxes are just the amounts of mass, momentum and energy transported by molecules in free-molecular flight there is no need, other than for simplicity, to use direction decoupling when EFM is applied in two or three dimensions. The true direction equilibrium flux method [3,4] represent the analytical expressions for the fluxes carried by molecules originating in a rectangular cell with velocities selected from the Maxwell–Boltzmann distribution and moved in free-flight in a specified time of flight to any rectangular region. One-dimensional TDEFM fluxes are equivalent to EFM fluxes when the CFL number approaches zero. In this limit, the only difference between TDEFM and EFM exists in higher dimensions when EFM is direction decoupled while TDEFM is not. The TDEFM flux expressions are the analytical equivalent to Macrossan et al.'s particle flux method (PFM) [15] applied to rectangular cells.

Here we compare TDEFM results to those obtained from direction decoupled EFM for a 2D implosion problem and a 2D blast wave problem. These differences are then further demonstrated in the simulation of hypersonic flow over a rectangular body. The aim of the paper is to examine the effects of direction coupling alone, thus both methods are restricted to first order accuracy in space and time, using identical grids with identical time steps. Since both solvers share the same underlying principles and differ only in the direction decoupling aspect, results show the detrimental effects due to direction decoupling.

2. Derivation of TDEFM flux expressions

Below are the expressions for the mass, momentum and energy carried by molecules in free-molecular flight for time Δt, starting from a rectangular region (in 2D) to any other rectangular region. All forces acting on