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Analysis of the convergence properties for a non-linear implicit Equilibrium Flux Method using Quasi Newton–Raphson and BiCGStab techniques

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ABSTRACT

In this work, an investigation is carried out into the implicit formulation of the Equilibrium Flux Method (EFM) applied to the numerical solution of the Euler Equations for an ideal inviscid gas. The discretization employs a non-linear Finite Volume Method (FVM) approach which requires the solution to a system of non-linear equations, which is solved using various modifications to the Quasi-Newton–Raphson method. The core of the analysis presented here lies in the investigation of the convergence properties of the BiConjugate Stabilized (BiCGStab) method used to solve the $J\Delta x = R$ where R is our vector of residuals computed directly using the Euler Equations, Δx is the increment to our estimated solution x for our system and J is the Jacobian of the residual functions. The increment to our solution Δx is modified to ensure the solution remains bound and finite. Results are shown for multiple one dimensional and two dimensional benchmark problems, with convergence properties of both the Newton–Raphson and BiCGStab procedures shown. Several conclusions may be drawn from the results shown: (a) increasing CFL numbers result in increasing dispersion errors, (b) higher order treatment of temporal derivatives results in lower condition numbers, resulting in fewer BiCGstab iterations per Newton–Raphson iteration, (c) higher order treatment of spatial derivatives results in higher condition numbers, hence requiring additional BiCGstab iterations, and (d) preconditioning using a simple Jacobi preconditioner significantly reduces the number of BiCGstab iterations required to obtain a solution.
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1. Introduction

The Finite Volume Method (FVM) is one of the cornerstone techniques for numerical simulation of compressible fluid flows. In such approaches, the multidimensional flow equations are solved through the computation of one-dimensional fluxes of mass, momentum and energy across the surfaces separating cells. These fluxes are a non-linear function of the states on each side of said surfaces which may be approximated using a large number of approaches. For the transient motion of a compressible ideal gas, the partial differential equations governing the behavior of the gas are the Euler Equations. The Euler Equations are non-linear—the flux vector cannot be written in terms of conserved quantities without undergoing a linearization process, which we will not consider here. For the classical Finite Volume Method, the above equation is discretized using the divergence theorem to provide an expression for the evolution of a discrete volume in terms of the fluxes across all surfaces of the said volume, which is referred to as a "cell". The state in each cell is evolved, with large

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numbers of cells making up the simulation domain, until a desired simulation time has been reached or, in the case of steady flows, until a steady solution has been obtained.

The computation of fluxes across each cell may be performed using a variety of methods—one such family of methods belonging to that arising from a kinetic theory description of the gas. In such an approach, fluxes are computed by taking moments around the particle velocity probability distribution function at cell surfaces. Perhaps the first method published based on this approach was Pullin's Equilibrium Flux Method [1], or the Kinetic where the particle velocity probability distribution at cell interfaces was taken to be the Maxwell–Boltzmann equilibrium probability distribution function. Recent, more advanced approaches examine situations where the fluxes are computed by taking moments around near-equilibrium distribution functions [2,3] for solutions to the Navier–Stokes equations.

The EFM has been applied extensively to the explicit computation of multidimensional flows [4,5] using an explicit finite volume scheme—where the spatial derivatives are treated at time level k in order to compute the evolved state at time level $k+1$. Such explicit treatments are ideal for application to parallel architectures as they are usually highly local—however, depending on the treatment of the temporal derivative, the size of the discrete time step between time levels is restricted to ensure stability of the scheme. If the CFL number is too large – typically larger than 1 – then the mass, momentum or energy taken out of a cell during a time step may exceed the amount stored in the cell, resulting in unphysical solutions.

The investigation of EFM applied to an implicit approach has been investigated previously [6] for the self-similar Euler Equations, with promising results. The self-similar formulation of the Euler equations – which is possible since the Euler Equations are non-dissipative – allows for simple application of a non-linear solver to the self-similar equations as opposed to the standard multidimensional (x, t) formulation. However, in the work contained in [6], there is little emphasis on the influence of time or spatial accuracy on the difficulties of inverting the Jacobian/Residual system of equations or on the numerical dispersion relating to the size of time step taken—as these problems were essentially avoided through the use of the self-similar equations.

This work focuses on the analysis of the non-linear implicit solution to the Euler Equations without the application of a self-similar form. Specifically, we primarily investigate the influence that temporal and spatial accuracy on the convergence property of the Bi-Conjugate Stabilized (BiCGstab) iterative solver required as part of a Newton–Raphson solver. This is relevant to large scale parallel computation using heterogeneous devices such as Graphics Processing Units (GPU's), as the direct inversion of the Jacobian system is not well suited to GPU devices and the BiCGstab is a commonly used alternative for non-symmetric systems. This paper first reviews the Equilibrium Flux Method (EFM) and its application to an implicit form for the determination of the residual function. After this, computation of the Jacobian, its inversion using BiCGstab and required modifications to the Quasi-Newton–Raphson scheme are presented and discussed. Results are shown for several popular benchmarks and the influence on temporal and spatial accuracy on both the physical results and convergence properties of the scheme discussed.

2. Equilibrium Flux Method

The Equilibrium Flux Method (EFM) [1] was one of the earliest attempts at using the Kinetic Theory of Gases as part of a numerical solution to the Euler Equations, which can be written in two dimensional form as:

$$\frac{d}{dt}[U] + \frac{d}{dx}[F] = \frac{d}{dt}\begin{bmatrix}\rho\\ \rho u\\ \rho v\\ E\end{bmatrix} + \frac{d}{dx}\begin{bmatrix}\rho u\\ \rho u^2 + P\\ \rho uv\\ u\,(E+P)\end{bmatrix} + \frac{d}{dy}\begin{bmatrix}\rho v\\ \rho uv\\ \rho v^2 + P\\ v\,(E+P)\end{bmatrix} = 0 \tag{1}$$

where U is the vector of conserved quantities, F is the fluxes of conserved quantities, E is the total energy $E = \rho(C_V T + 0.5V^2)$ and P is the pressure, which for an ideal gas is $P = \rho RT$. Analysis of the Boltzmann equation reveals a gas in thermal equilibrium reproduces the Euler Equations. The velocity of particles in a gas in thermal equilibrium are dictated by the Maxwell–Boltzmann particle velocity probability distribution function, which can be written in one dimensional form as:

$$f(v) = \frac{1}{\sqrt{2\pi}s}\exp\left[\frac{-(v-\bar{v})^2}{2s^2}\right]. \tag{2}$$

In Eq. (2), v is the particle velocity, s is the deviation of the distribution ($s = RT^{1/2}$) and the bulk velocity of the particles is represented by the overbar. In the Equilibrium Flux Method, the fluxes across a surface are split into contributions from the left (F^+) and right (F^-) hand side of the interface such that the total flux F_{tot} is the sum of these split fluxes, which can be written as:

$$F^+ = \int_0^\infty f(v_n)\, v_n Q(U_L)\, dv_n \qquad F^- = \int_\infty^0 f(v_n)\, v_n Q(U_R)\, dv_n \tag{3}$$

where v_n is the particle velocity normal to the cell interface, and U_L and U_R represent the states on the left and right hand side and the vector Q can be written as:

$$Q = \left\{\rho, \rho v_n, v_p, \rho(0.5V^2 + E_{in})\right\} \tag{4}$$

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