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A ghost fluid, moving finite volume plus remap method for compressible Euler flows.

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27^{th} April 2004

Numerical Analysis Report 7/04

Presented at the ICFD conference on Numerical Methods for Fluid Dynamics, Oxford, UK, 29 March - 1 April 2004

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Abstract

A numerical solution method for accurately capturing material interfaces in unsteady compressible Euler flows is presented. The method consists of a finite volume scheme on a moving computational mesh and employs the HLLC approximate Riemann solver to evaluate intercell numerical fluxes. The mesh is moved in a Lagrangian fashion with the material, and to avoid the associated grid distortion scenarios, the finite volume scheme is augmented with an algorithm to rezone the solution variables to a tangle free mesh. The focus of the work is multimaterial flows consisting of two immiscible materials separated by an interface. The interface position is tracked using a volume of fluid technique, and the flow solution at the interface is resolved using a conservative ghost fluid method.

Governing Equations

The Euler equations for one dimensional (1D), unsteady compressible flow, in the reference frame of a moving control volume, can be expressed in integral form as

$$\frac{\partial}{\partial \mathrm{t}} \int_{\Omega(t)} \mathbf{q}(x,t)\ \mathrm{d}\Omega + \oint_{\Gamma(t)} \mathbf{f}(\mathbf{q}(x,t)) \cdot \hat{n}\ \mathrm{d}\Gamma\ =\ 0\,. \tag{1}$$

The moving control volume $\Omega(t)$ is enclosed by its boundary $\Gamma(t)$, and $\hat{n}$ denotes the outward unit normal to $\Gamma(t)$. The vector of conserved variables is given by $\mathbf{q} = (\rho, \rho u, \rho E)^T$, and the flux vector is $\mathbf{f}(\mathbf{q}) = (u - \dot{x})\mathbf{q} + (0, p, up)^T$, where ρ is density, u is flow velocity, $\dot{x}$ is the velocity of $\Gamma(t)$, E is specific total energy, and p is pressure. The system of equations (1) represents conservation of mass, momentum and energy. The system is completed by the ideal gas equation of state (EOS), $p = (\gamma - 1)\rho e$, where $e = E - \frac{1}{2}u$ is the specific internal energy and γ ($1 < \gamma < \frac{5}{3}$) is a constant representing the ratio of specific heat capacities of the material.
It is assumed that the flow consists of two immiscible components separated by a material interface. Both flow components can be described by a single velocity and pressure function, and each component is uniquely characterised by the value of γ in the EOS.

The finite volume scheme

The spatial domain is discretised into N non-overlapping computational cells, I_i, initially of a uniform size. The average value of $\mathbf{q}$ over each cell is approximated and stored at the cell centre (node). The governing equations (1) are discretised according to the conservative finite volume formula

$$\frac{\mathbf{Q}_i^{n+1}\Delta x_i^{n+1} - \mathbf{Q}_i^n \Delta x_i^n}{\Delta t} = -\left(\mathbf{F}_{i+\frac{1}{2}} - \mathbf{F}_{i-\frac{1}{2}}\right) \qquad i = 0, \ldots, N; \tag{2}$$

where

$$\mathbf{Q}_i^n \approx \frac{1}{\Delta x_i^n} \int_{x^n_{i-\frac{1}{2}}}^{x^n_{i+\frac{1}{2}}} \mathbf{q}(x, t^n)\, \mathrm{d}x \quad \text{and} \quad \mathbf{F}_{i-\frac{1}{2}} \approx \frac{1}{\Delta t} \int_{t^n}^{t^{n+1}} \mathbf{f}(\mathbf{q}(x_{i-\frac{1}{2}}(t), t))\, \mathrm{d}t\ . \tag{3}$$

Here, Δt is the variable time interval from time t^n to time t^{n+1}, Δx_i^n is the cell volume at time t^n, and $x^n_{i\pm\frac{1}{2}}$ are the cell boundaries. In 1D cell boundaries coincide with mesh vertices. To evaluate $\mathbf{F}_{i-\frac{1}{2}}$ the cell average values are used to reconstruct a polynomial data distribution function in each cell of the computational domain, and the resulting Riemann problems that arise at the cell boundaries are solved approximately.
The mesh movement is determined by the evolution of the vertex positions. It is assumed that the vertex velocity $\dot{x}_{i-\frac{1}{2}}$ is constant in magnitude and direction during the time interval, and $\dot{x}_{i-\frac{1}{2}}$ is evaluated from the values of the flow velocity at the beginning of a time interval using linear interpolation.
Control of the time step size is achieved, prior to each time interval, by selecting Δt to satisfy two constraints. The first constraint is that Δt should be chosen so that during a time interval none of the waves resulting from a Riemann problem travel more than half a cell width of the initial uniform mesh. The second constraint is that Δt is chosen so that the mesh vertices are not displaced during the time interval by more than half a cell width of the initial uniform mesh.

The HLLC Riemann solver

The principle behind the HLLC Riemann solver is to reduce the full Riemann problem to an approximate solution which consists of a wave structure involving four constant states separated by three discontinuous waves. If the wave speeds of the three discontinuities are known, then application of the integral form of the conservation laws over an appropriate control volume, produces a closed-form expression for the intercell numerical flux. The original derivation [7] was with respect to fixed reference frame. The expression below accounts for the movement of the mesh.

$$\mathbf{F}_{i-\frac{1}{2}} = \begin{cases} \mathbf{F}_L = (u_L - \dot{x}^n_{i-\frac{1}{2}})\mathbf{Q}_L - \mathbf{F}^{lag}_L & \dot{x}^n_{i-\frac{1}{2}} \leq S_L \\ \mathbf{F}^*_L = (u_L - \dot{x}^n_{i-1})\mathbf{Q}_L + \mathbf{F}^{lag}_L - (S_L - \dot{x}^n_{i-1})\mathbf{Q}_L + (S_L - \dot{x}^n_{i-\frac{1}{2}})\mathbf{Q}^*_L & S_L < \dot{x}^n_{i-\frac{1}{2}} \leq S^* \\ \mathbf{F}^*_{LR} = \frac{1}{2}(\mathbf{F}^*_L + \mathbf{F}^*_R) & \dot{x}^n_{i-\frac{1}{2}} = S^* \\ \mathbf{F}^*_R = (u_R - \dot{x}^n_i)\mathbf{Q}_R + \mathbf{F}^{lag}_R - (S_R - \dot{x}^n_i)\mathbf{Q}_R + (S_R - \dot{x}^n_{i-\frac{1}{2}})\mathbf{Q}^*_R & S^* < \dot{x}^n_{i-\frac{1}{2}} < S_R \\ \mathbf{F}_R = (u_R - \dot{x}^n_{i-\frac{1}{2}})\mathbf{Q}_R - \mathbf{F}^{lag}_R & \dot{x}^n_{i-\frac{1}{2}} \geq S_L \end{cases} .$$

Here, $\dot{x}^n_i = (x^{n+1}_i - x^n_i)/\Delta t$, $\mathbf{Q}_L$ and $\mathbf{Q}_R$ are respectively the left and right data states at the boundary $\dot{x}^n_{i-\frac{1}{2}}$, $\mathbf{F}^{lag}_K = (0, p_K, u_K p_K)^T$, and $\mathbf{Q}^*_K = (\rho^*_K, \rho^*_K u^*_K, \rho^*_K E^*_K)^T$ where $\rho^*_K = \rho_K(S_K - u_K)/(S_K - S^*)$, $u^*_K = S^*$, $p^*_K = p_K + \rho_K(u_K - S_K)(u_K - S^*)$ and $K = L, R$. The wave speed estimates S_L, S^* and S_R are acquired following an approach suggested in [7].
A MUSCL-Hancock technique, involving characteristic slope limiting, is applied in order to obtain a high-resolution flux [7].

Evolution of the volume fractions

The fractional volume, $\phi^{(M)}_i$, of each cell occupied by each material is stored. They are evolved in time independently of the flow solution according to a predictor-corrector discretisation [4] of the equation

$$\frac{\partial \psi^{(M)}}{\partial t} + \frac{\partial}{\partial x}\left(\psi^{(M)}\dot{u}\right) = \frac{\psi^{(M)}\overline{K}_S}{\overline{\rho} K^{(M)}_S} \cdot \frac{\partial \dot{u}}{\partial x} \ , \tag{4}$$

where $K_S = \gamma^{(M)} p^{(M)}$, $\overline{\rho} = \sum_{M=1}^{2} \phi^{(M)} \rho^{(M)}$, $\overline{K}_S = \left(\sum_{M=1}^{2} \frac{\psi^{(M)}}{K^{(M)}_S} \right)^{-1}$ and $\dot{u}$ is the flow velocity relative to the moving reference frame. Equation (4) ensures adherence to the constraint $\sum_{M=1}^{2} \phi^{(M)}_i = 1$.

The Ghost Fluid Method (GFM)

The central idea behind the GFM [2] is to create two separate computational regions, one for each of the materials that resides either side of the interface. Both these regions are to contain the interface and their creation is achieved using ghost solution values (GSV) within the existing computational mesh. GSV are defined in every cell in the domain so that at each node there is a cell average value of mass, momentum and energy for the real fluid that exists in that cell, and a ghost cell average value of mass, momentum and energy for the material that exists on the 'other side' of the interface. Once the

two regions are defined, the single material flow solver can be employed to evolve both sets of solution variables separately. GSV are defined and discarded respectively at the beginning and end of each moving mesh phase, with the exception of the interface cell. GSV in the interface cell are retained until the mesh is remapped, and then the magnitude of the updated volume fractions are used to determine which of the two materials is valid. An important feature of the GFM is that there is no requirement to solve a multi-material Riemann problem at the interface. The process can be optimised for implementation by applying the method only in a band of cells on either side of the interface.

The success of the GFM relies on capturing the appropriate interface conditions when defining GSV. It is fundamental that their creation should not interfere with the behaviour of the real material solution away from the interface. The simplest approach is to define the GSV to be identically equal to the real solution values, then the flow solver determines a solution to a single material version of the two material problem. However, a failing of the finite volume Riemann solver scheme is that it suffers from numerical diffusion at contact discontinuities which degrades the results of the discontinuous variables. Following the methodology of [2] it is proposed to reduce the diffusive effect by accepting the real values of the continuous variables (pressure and velocity) but to alter the values of the discontinuous variables in the ghost material. This is achieved through one-sided extrapolation of one of the discontinuous variables across the interface from a reference state. Constant extrapolation is used in order to create a continuous variable profile and to minimise the variation from the reference state. Based on work in [3] and confirmed by numerical experiment, entropy is taken to be the extrapolated value. Figure 1 shows a schematic outlining the details involved in defining the GSV. An isobaric fix is imposed by using the extrapolation technique to alter the entropy values of the real material values [2].

To obtain a fully conservative GFM, a post processing correction algorithm following on from work in [5] is implemented in conjunction with the moving finite volume scheme.

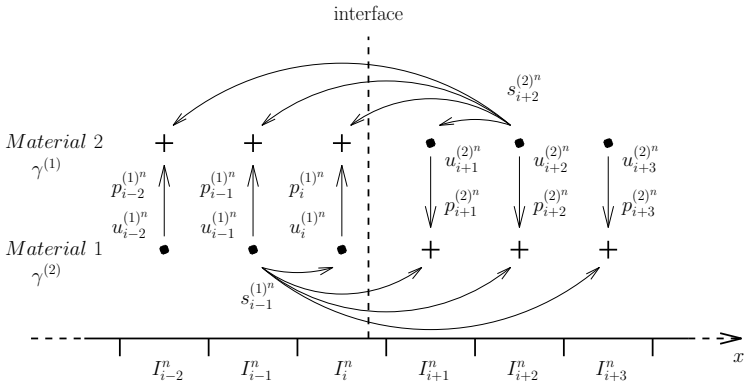

Figure 1: Defining GSV using an isobaric fix. p is pressure, u is flow velocity and s is entropy.

Remapping/Rezoning

The remap procedure may be regarded as integrating the known solution variables on the old distorted grid over the cell of a new predetermined mesh. In this work rezoning is performed at the end of each time step and the mesh is remapped to the grid that was

generated at the initial time level. The actual quantities remapped are the conserved variables. In multi-material flows each material is rezoned separately and the values of the volume fractions are modified in accordance with the transfer of data from the old mesh to the new. The remap procedure for material M in cell I_i can be expressed in integral form as

$$\overline{\mathbf{Q}}_i^{(M)} = \frac{1}{\Delta \overline{x}_i} \int_{\overline{x}_{i-\frac{1}{2}}}^{\overline{x}_{i+\frac{1}{2}}} \tilde{\mathbf{Q}}^{(M)}(x, t^{n+1})\, \mathrm{d}x \ . \tag{5}$$

The overbar denotes rezoned values and $\tilde{\mathbf{Q}}(x, t^{n+1})$ is a piecewise polynomial function reconstructed from the cell average values $\mathbf{Q}_i^{n+1}$. Equation (5) can be written as a sum of integrals over the overlap regions between cell I_i and the cells on the old distorted mesh. The accuracy of the remap procedure is determined by the degree of the piecewise polynomial function $\tilde{\mathbf{Q}}$. In this work a piecewise linear function is reconstructed using characteristic slope limiting. Mesh vertices and nodes are remapped by simply returning them to the positions they held at the begininng of the time interval. The remapping process is conservative.

2D - Preliminary discussion

Current work is proposing to extend the presented numerical method to two dimensional, unsteady multimaterial compressible Euler flows. The governing equations can be written in integral form as

$$\frac{\partial}{\partial \mathrm{t}} \int_{\Omega(t)} \mathbf{q}(x, y, t)\ \mathrm{d}\Omega + \oint_{\Gamma(t)} (\mathbf{f}(\mathbf{q}(x, y, t)), \mathbf{g}(\mathbf{q}(x, y, t))) \cdot \hat{n}\ \mathrm{d}\Gamma \ = \ 0 \ , \tag{6}$$

where $\Omega(t)$ is the moving control volume enclosed by its boundary $\Gamma(t)$, $\mathbf{q} = (\rho, \rho u, \rho v, \rho E)$, $\mathbf{f}(\mathbf{q}) = (u - \dot{x})\mathbf{q} + (0, p, 0, up)$, $\mathbf{g}(\mathbf{q}) = (v - \dot{y})\mathbf{q} + (0, 0, p, vp)$, and $\hat{n}$ denotes the outward unit normal to $\Gamma(t)$. The system of equations (6) is discretised through the following dimensional splitting

$$\mathbf{Q}_{i,j}^{n+1'} = \frac{\Omega_{i,j}^n}{\Omega_{i,j}^{n+1'}} \left(\mathbf{Q}_{i,j}^n - \frac{\Delta t}{\Omega_{i,j}^n} \left[s_{i+\frac{1}{2},j}^n \mathbf{F}_{i+\frac{1}{2},j} - s_{i-\frac{1}{2},j}^n \mathbf{F}_{i-\frac{1}{2},j} \right] \right) \ ; \ \mathbf{F}_{i-\frac{1}{2},j} \left(\mathbf{Q}_{i-1,j}^n, \mathbf{Q}_{i,j}^n, \overline{u} \right) \tag{7}$$

$$\mathbf{Q}_{i,j}^{n+1} = \frac{\Omega_{i,j}^{n+1'}}{\Omega_{i,j}^{n+1}} \left(\mathbf{Q}_{i,j}^{n+1'} - \frac{\Delta t}{\Omega_{i,j}^{n+1'}} \left[s_{i,j+\frac{1}{2}}^{n+1'} \mathbf{G}_{i,j+\frac{1}{2}} - s_{i,j-\frac{1}{2}}^{n+1'} \mathbf{G}_{i,j-\frac{1}{2}} \right] \right) \ ; \ \mathbf{G}_{i,j-\frac{1}{2}} \left(\mathbf{Q}_{i,j-1}^{n+1'}, \mathbf{Q}_{i,j}^{n+1'}, \overline{v} \right) \tag{8}$$

where $\Omega_{i,j}^n$ is the volume of cell $I_{i,j}$ at time t^n, $\overline{u}$, $\overline{v}$, and $s_{i-\frac{1}{2},j}$, $s_{i,j-\frac{1}{2}}$ are respectively facial velocities and lengths calculated in accordance with a geometric conservation law [8]. $\mathbf{F}_{i-\frac{1}{2},j}$ and $\mathbf{G}_{i,j-\frac{1}{2}}$ are numerical approximations to the time average flux across faces $\Gamma_{i-\frac{1}{2},j}$ and $\Gamma_{i,j-\frac{1}{2}}$ respectively. They are evaluated by solving the x and y split one dimensional Riemann problem using the HLLC Riemann solver in conjuction with the GFM. Evaluation of Δt takes into account wave speeds and mesh dimensions in both spatial directions.

The principle of the GFM in 2D is the same as in 1D. However, in 2D defining the GSV is more involved since there is more than one velocity component and a choice for the direction of extrapolation must be made. The GSV for the pressure and velocity components are defined by setting them equal to the real material values in each cell in the computational domain. Constant extrapolation of entropy into cells containing

and bordering the interface is performed in the direction of the normal to the interface. The normal value is extracted from a piecewise linear interface reconstructed from the fractional volume data.

The interface reconstruction algorithm is based on an approach developed in [1]. Reconstruction of a linear interface in an interface cell is transformed to a problem that analyses a 'local central dual' mesh of the interface cell in question and its eight surrounding cells. Each vertex in the dual mesh has associated with it the volume fraction of the cell within which it is centred. Material boundaries on the dual mesh are found by considering the volume fractions in 'material space' and evaluating intersections with Voronoi cells that represent the regions where one material dominates. These intersections are used to calculate interface points on the dual mesh. With a complete set of interface points on the dual mesh the interface line, created through connection of the interface points, is transformed into a linear approximation to the interface within the original interface cell. The position of the interface line is adjusted to ensure the correct volume fraction is captured.

In 2D the remap procedure remains an integration problem, with each material being rezoned separately through integration over polygonal mesh overlap regions.

At present a conservative correction algorithm has not been implemented with the 2D scheme.

Numerical Results

In 1D, the selected test problem is a two material shock tube problem based on [6]. The initial conditions of the test consist of two constant states separated by a discontinuity. The two states are given by $(\rho_L, u_L, p_L)^T = (1.0, 0.0, 1.0)^T$ and $(\rho_R, u_R, p_R)^T = (0.125, 0.0, 0.1)^T$ with $\gamma_L = 1.6$ and $\gamma_R = 1.2$. The discontinuity was initially situated at $x = 0.505$. The numerical (dotted line) and exact (solid line) solutions are computed in the spatial domain $[0, 1]$ and the output time is $t = 0.2$ seconds. The numerical solution is computed with 100 cells and transmissive boundary conditions are applied. Figure 2(a) shows good agreement between the numerical and analytical solutions. The test problem

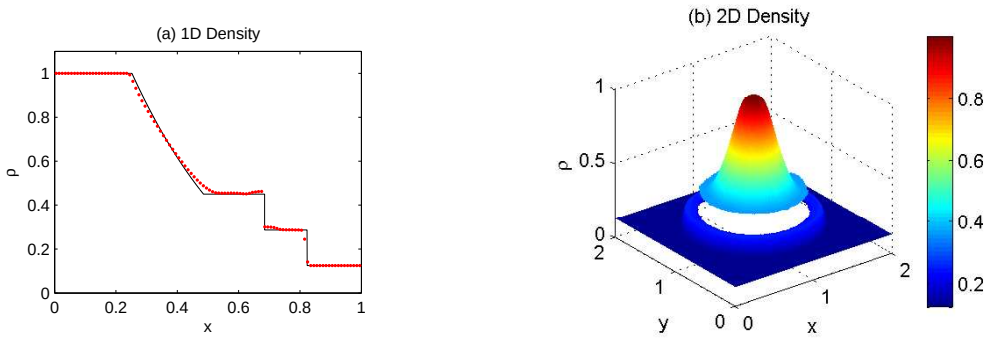

Figure 2: Solution plots for Density in the (a) 1D and (b) 2D tests problems.

is extended to 2D using a cylindrical explosion problem [7]. The governing equations are solved in the spatial domain $[0, 2] \times [0, 2]$. Initial conditions consist of a region inside a circle of radius 0.4 centred at (1,1), and the region outside of this circle. Initially, the flow variables take constant values in each of these regions, and are joined by a circular discontinuity. The two states are given by $(\rho_{in}, u_{in}, v_{in}, p_{in})^T = (1.0, 0.0, 0.0, 1.0)^T$ and $(\rho_{out}, u_{out}, v_{out}, p_{out})^T = (0.125, 0.0, 0.0, 0.1)^T$ with $\gamma_L = 1.6$ and $\gamma_R = 1.2$. The output

time is $t = 0.2$ seconds. Results are shown in Figure 2(b).

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