Multi-Material Flows

Flows with two or more materials are very important in applications and create a number of difficulties for numerical simulation. Examples of such flows include Rayleigh-Taylor and Richtmyer-Meshkov instability in which one fluid is accelerated into another by either a body force or shock wave respectively. These instabilities occur in such applications as inertial confinement fusion and supernova explosions. At an opposite end of the spectrum are diffusive type flows such as the motion of a hot fluid in a cold fluid, or the diffusion of a dye. These two extremes illustrate a general division of flow regimes, non-diffusion regimes where the interface between the two materials remains sharp, and diffusive regimes where the materials mix at the molecular level. Of course in reality all flows contain some mixture of the two regimes, but in practice the choice of the relevant length and time scales of interest dictate the appropriate flow regime. Compressible flows are usually associated with time scales that are short relative to the rate of molecular diffusion and so are often in the non-diffusive regime. Indeed the applications such as inertial confinement fusion and supernova explosions, the time scales are on the order of nanoseconds and are as much 6-9 orders of magnitude smaller than the time scale for significant molecular mixing. In this course we will focus on the sharp interface flow regime, and will discuss numerical methods that attempt to maintain relatively sharp material interfaces.
Numerical methods for the solution of a multi-material flow are generally one of several types, although it is possible to develop algorithms that combine features of any or all of these methods.

- **Mixed cell methods** in which the fractional volume and fractional mass of each species is computed and the material is assumed to be well mixed at the cell level. Such methods are extremely diffusive, but when combined with adaptive mesh refinement that keeps the size of the mixed cells small this method can be quite effective. One important question that arises in mixed cell methods is how to specify the thermodynamic properties of the mixed material. If the mixing is molecular one generally has that the multiple materials are in thermal and mechanical equilibrium (equal temperature and pressure). This provides a method for computing an effective multi-material equation of state for the mixture. However for the applications considered in this course the mixing is very far from molecular and the question of an appropriate mixed material equation of state is quite open and indeed is problem dependent.
• **Volume of fluid and interface reconstruction methods.** Like the mixed cell method, fractional volumes and masses of the individual species are computed. However this information is used to reconstruct interfaces between the materials so that they become effectively demixed at a subcell level. These interfaces are then used to compute the numerical fluxes at the cell boundaries to that mass for a given species can only flow into and out of the boundary through regions occupied by that material. This method eliminates the need for mixed material equations of state since the interfaces separate the materials into separate regions inside of which each material is pure. At the end of each time step the interfaces are discarded and recomputed during the next time step using only the fractional volume and mass information. Care is taken during the reconstruction so that the interfaces created in each cell are as consistent as possible with those in the next cell. This method is much less diffusive than the mixed cell method but is still much more diffusive than the real physical process.
Level set methods. In this method the interface between separate materials is modeled as the level set \( t = \phi(x) \), and the numerical calculations seek first to compute the level set as a solution to a Hamilton-Jacobi equation and then to update the physical flow variables using the computed interface. A nice feature of this method is that interface interactions are handled automatically. A major problem is that the level set function is not a true physical variable and as such the interface interactions may be handled in an unphysical manner. Depending on the implementation, the equation of state may be misapplied to materials due to the artificial location of the interface. Also this method has difficulty in treating triple points where three or more material meet at a point. Another problem is the topological restriction that the interface be the level set of a global function. This problem can be addressed by using a local level set approach in which the level set function only applies to a local region. Most of these difficulties are being addressed in current implementations of level set methods by applying front tracking type approaches to the algorithm.
Front Tracking. The numerical method that comes closest to modeling the physical behavior of a non-diffusive flow is front tracking. In this method the material interfaces become part of the numerical representation of the flow. These fronts are propagated using the mathematically correct Rankine-Hugoniot conditions at the front together with a method of characteristics (see the next slide) computation for coupling the front states to the flow adjacent to the front. For the update of the non-front (cell centered) states, the fronts provide moving space-time boundary conditions. The problem of mixed material equations of state does not occur since the fronts provide a sharp division between pure material regions. The physically correct balance conditions are maintained at material fronts so that the pressure is continuous (in the absence of surface tension) at the front, but temperature is maintained independently in the adjacent two materials. (Recall that the Euler equations models adiabatic flow.) Mathematically, front tracking eliminates numerical diffusion at the interfaces since the flow variables are allowed to jump discontinuously across tracked fronts. The remainder of this lecture will discuss front tracking algorithms for one dimensional flows. The following lecture will discuss extensions of this method to higher dimensional flows.
Front Tracking Representation of a Flow (1)

For simplicity we consider a one space dimensional gas dynamical flow with a single material discontinuity. Let the two materials be labeled by the indices \( l \) and \( r \), where \( l \) indicated the material to the left of the material boundary and \( r \) indicates the material to the right. The flow is modeled by the Euler equations in which it is understood that at any position in space only one of the two materials is present. The two materials may have separate equations of state. Again for simplicity let us assume both materials are perfect gases with gammas and specific heats \( \gamma_i \) and \( c_i \), \( i = l, r \) that are possibly different for the two materials. Suppose the position of the material interface is given by \( x_c(t) \). The discrete representation of the flow consists of a set of cell centers and mesh sizes, \( x_i, \Delta x_i, i = 1, \ldots, N \), where \( x_i + \Delta x_i/2 = x_{i+1} - \Delta x_{i+1}/2 \), together with a density \( \rho_i \), a momentum density \( m_i = \rho_i u_i \), and a total energy density \( E_i = \rho_i \left( \frac{1}{2} u_i^2 + e_i \right) \) associated with each cell. Except for the cell containing the tracked point \( x_c(t) \) these values can be regarded as the cell averages of the corresponding flow variable over the indicated cell. Quantities derived from these primitive flow variables will also be indicated by the appropriate index. Associated with the tracked point \( x_c(t) \) we have two sets of flow variables, \( \rho_l, m_l, \) and \( E_l \) corresponding to the flow on the left of \( x_c(t) \), and \( \rho_r, m_r, \) and \( E_r \) corresponding to the flow on the right of this point.
The states at the front can be interpreted as the limit of the flow as the discontinuity front is approached from the appropriate side. The state associated with the cell center in the grid block containing the front is not the average of the flow across that cell, since such an interpretation would involve smearing the flow variables across the front, rather it should be regarded as a quantity associated with the side of the front on which the cell center lies. For example this value might be thought of as an approximation of the pointwise value of the flow variables at the given position. For simplicity we assume the mesh size $\Delta x_i = \Delta x$ is constant, so that $x_{i+1} = x_i + \Delta x$. The diagram below shows a schematic representation of the density.
Propagating the Front Tracking Solution

The time step propagation consists of advancing the flow states at each cell center, computing the new position of the tracked front and updating the left and right states at the tracked points. As implemented in the front tracking code FronTier, this consists of the following steps.

- Use Riemann problem solutions and method of characteristics computations to compute the time updated position and states at the propagated fronts.
- Use finite differences to time advance the interior states using the old and new front states and positions (i.e. the states and positions of the fronts at the beginning and end of the time step) as interior boundary conditions for the cell centered states. The critical operation here is to avoid taking finite differences across a tracked front, so that all difference quantities are taken from the same side of a discontinuity.
The Method of Characteristics (1)

The method of characteristics has now been mentioned at least twice without any explanation. Let us take a minute to review this important concept. Recall that for smooth flow the Euler equations can be written:

\[
\frac{\partial P}{\partial t} + \rho c^2 u_x = 0 \\
\rho \frac{\partial u}{\partial t} + P_x = 0 \\
\frac{\partial S}{\partial t} = 0
\]

Adding and subtracting the first equation and \(c\) times the second we obtain:

\[
\left( \frac{\partial}{\partial t} + c \frac{\partial}{\partial x} \right) P + \rho c \left( \frac{\partial}{\partial t} + c \frac{\partial}{\partial x} \right) u = 0 \\
\left( \frac{\partial}{\partial t} - c \frac{\partial}{\partial x} \right) P - \rho c \left( \frac{\partial}{\partial t} - c \frac{\partial}{\partial x} \right) u = 0 \\
\frac{\partial}{\partial t} \frac{\partial S}{\partial x} = 0
\]

or

\[
\left( \frac{\partial}{\partial t} + (u + c) \frac{\partial}{\partial x} \right) P + \rho c \left( \frac{\partial}{\partial t} + (u + c) \frac{\partial}{\partial x} \right) u = 0 \\
\left( \frac{\partial}{\partial t} + (u - c) \frac{\partial}{\partial x} \right) P - \rho c \left( \frac{\partial}{\partial t} + (u - c) \frac{\partial}{\partial x} \right) u = 0
\]
The Method of Characteristics (2)

The important feature of the characteristic equations is that all of the derivatives in each equation appear in the same directional form. More precisely we define the characteristic curves through each point in our domain by the formulas:

\[
\frac{d}{dt} x_f(t, x_0, t_0) = u + c, \quad x_f(t_0, x_0, t_0) = x_0
\]

\[
\frac{d}{dt} x_p(t, x_0, t_0) = u, \quad x_f(t_0, x_0, t_0) = x_0
\]

\[
\frac{d}{dt} x_b(t, x_0, t_0) = u - c, \quad x_f(t_0, x_0, t_0) = x_0.
\]

These three curves are referred to as the forward, particle, and backward characteristics through the given point. From the characteristic form of the Euler equations we see that the evolution of the state variables along the characteristics are related by the formulas:

\[
\frac{dP}{dt} + \rho c \frac{du}{dt} = 0, \quad \text{along} \quad \frac{dx}{dt} = u + c
\]

\[
\frac{dS}{dt} = 0, \quad \text{along} \quad \frac{dx}{dt} = u
\]

\[
\frac{dP}{dt} - \rho c \frac{du}{dt} = 0, \quad \text{along} \quad \frac{dx}{dt} = u - c
\]
The algorithm for propagating a contact discontinuity point (most commonly corresponding to a material interface) uses what is called a three point wave speed calculation. The data for the propagation consists of the position of the contact $x_c(t)$, the states on the left and right of wave, $s_l$ and $s_r$, and two states $s_{ll}$ and $s_{rr}$ obtained by sampling the solution a distance $\Delta x$ to the left and right of the contact point. Here by a “state” we mean the flow variables describing the flow at a given location, so for example $s_l$ represents the density, velocity, and internal energy (and any other derived flow variable) at the left side of the contact. The off front states $s_{ll}$ and $s_{rr}$ are obtained by sampling a reconstructed interpolant of the solution. One possible choice for such an interpolant is the piecewise linear curve obtained by connecting the cell centered data and the front data with line segments, while allowing a jump in the variables across tracked fronts. The graph on slide 7 shows such an interpolant for density. Generally we only interpolate a minimal set of flow variables (such as density, momentum density, and total energy density or density, velocity, and specific internal energy) and compute the other flow variables using their formulas in terms of the minimal set.
The chart below illustrates the choice of initial data.

Contact Discontinuity Propagation (2)
(Method of Characteristics Version)
The first step in the propagation algorithm is to solve a Riemann problem with data $s_l$ and $s_r$. The mid state speed $u_m$ from the solution is used as a predictor for the updated contact position, $x_p(t_0+\Delta t) \approx x_c(t_0) + u_m \Delta t$. 
Contact Discontinuity Propagation (4)
(Method of Characteristics Version)

Using the forward characteristic speed on the left side of the interface and the backward characteristic speed on the right, trace back a linear approximation to the incoming characteristics at the propagated point from time $t_0 + \Delta t$ back to time $t_0$, obtaining positions $x_{lf}(t_0) = x_c(t_0) - c_{ml}\Delta t$, and $x_{rb}(t_0) = x_c(t_0) + c_{mr}\Delta t$ together with interpolated state values $s_{lf}$ and $s_{rb}$ at these locations.
Contact Discontinuity Propagation (5)  
(Method of Characteristics Version)

Solve for the updated states on both sides of the contact using an implicit Euler integration:

\[ u^+ - u_{lf} + \frac{1}{2} \left( \frac{1}{\rho_{lf} c_{lf}} + \frac{1}{\rho_i c_i^+} \right) (P^+ - P_{lf}) = 0, \quad u_{rb} - u^+ + \frac{1}{2} \left( \frac{1}{\rho_{rb} c_{rb}} + \frac{1}{\rho_r c_r^+} \right) (P^+ - P_{lf}) = 0 \]

\[ e_i^+ - e_i + \frac{1}{2} (P^+ + P_0) \left( \frac{1}{\rho_i^+} - \frac{1}{\rho_i} \right) = 0, \quad e_r^+ - e_r + \frac{1}{2} (P^+ + P_0) \left( \frac{1}{\rho_r} - \frac{1}{\rho_r} \right) = 0 \]

\[ P^+ = P_i(e_i^+, \rho_i^+), \quad c_i^+ = c_i(e_i^+, \rho_i^+), \quad P^+ = P_r(e_r^+, \rho_r^+), \quad c_r^+ = c_r(e_r^+, \rho_r^+). \]

Note that we use the separate equations of state on either side of the interface to relate the pressures, densities, specific internal energies, and sound speeds on either side of the interface. Finally we use central differences in time to determine the net interface speed and updated contact position.

\[ v_{\text{interface}} = \frac{1}{2} (u^+ + u_m), \quad x_c(t_0 + \Delta t) = x_c(t_0) + v_{\text{interface}} \Delta t. \]
The algorithm just described makes an implicit assumption that the main discontinuity is at the tracked contact and that all other waves, either incoming or outgoing are relatively weak. This assumption is used to validate the use of the method of characteristics on either side of the interface, since this method is based on the smooth flow Euler equations. An alternative algorithm that replaces the method of characteristics calculations with the solution of Riemann problems has proven to be more useful in practice, especially for flows with strong captured waves. This variation proceeds identically to the previous version up until the point where the two states $s_{lf}$ and $s_{rb}$ have been found at the feet of the traced backed characteristics from the predicted new position of the contact. Then instead of applying the method of characteristics we solve a Riemann problem with data $s_{lf}$ and $s_{rb}$ and use the mid state solutions from this Riemann problem to replace the method of characteristic solutions found from the equations on the previous slide. The remainder of the algorithm proceeds as before. Variations of this algorithm may replace $s_{lf}$ by $s_{ll}$ and $s_{rb}$ by $s_{rr}$ to provide more upwinding for the incoming waves.
The final step in the time step update of the solution is to use finite differences to advance the cell centered states. For cells whose discrete domain of dependency stencil (i.e. the set of states used in the finite difference formula to update the solution at a given position) does not overlap the fronts, this is done using standard finite differences as described in the previous lecture. At points whose stencil overlaps the front we wish to use front information as local boundary conditions for the finite difference method. This can be done in a variety of different ways, but in practice a very simple method has proven adequate for many problems. We call this method extrapolation by constant state. We simply replace any state in the finite difference stencil that lies on a different side of the point being updated (with respect to the propagated interface) by the state on the interface nearest that point. This of course introduces some error in the computation near the front, but this is compensated by the removal of the differencing across the front and the more accurate computation of the front position and states. Several authors have proposed alternative methods that use more complicated algorithms, but the above method has proven to be surprisingly successful in practice.
1. Show that for a perfect gas, with \( e = c_v T \), \( PV = RT \) (\( V = 1/\rho \)):

\[
\gamma = 1 + \frac{R}{c_v}, \quad e = \rho^{\gamma-1} \exp \left( \frac{S - S_{\text{ref}}}{c_v} \right), \quad P = \rho^\gamma \exp \left( \frac{S - S_{\text{ref}}}{c_v} \right),
\]

where \( S_{\text{ref}} \) is some reference entropy. (Note only changes in entropy have physical meaning for a perfect gas.)

2. Show that for a perfect gas,

\[
\int_{P_0}^P \frac{dP}{\rho c} \bigg|_S = \frac{2}{\gamma - 1} (c - c_0).
\]

3. For fixed \( P_0 \), define

\[
\rho(P, S) = \int_{P_0}^P \frac{dp}{\rho c(p, S)}.
\]

Show that the forward and backward characteristic equations can be written:

\[
\frac{d}{dt} (u + r) = \left( \frac{\partial}{\partial S} \int_{P_0}^P \frac{dp}{\rho c(p, S)} \right) c \frac{\partial S}{\partial x}, \quad \text{along } \frac{dx}{dt} = u + c
\]

\[
\frac{d}{dt} (u - r) = \left( \frac{\partial}{\partial S} \int_{P_0}^P \frac{dp}{\rho c(p, S)} \right) c \frac{\partial S}{\partial x}, \quad \text{along } \frac{dx}{dt} = u - c
\]
Further Reading

