Introduction to Computational Multiphysics
Practical 6: Diffuse interface methods, the Allaire formulation.

In this practical we will implement a first-order accurate one-dimensional diffuse interface method using the Allaire formulation. It is best to approach this practical by altering one of your single-material codes, moving from three variables to five variables. The flux functions and the variable conversion will need to be modified to achieve this. In this practical, only ideal and stiffened gases are being used, which means that all variable calculation is analytic. Some calculations are a little bit more challenging though, for example, computing pressure. For these materials, this requires mixture quantities for the equation of state quantities and is given in equations (32)-(34) in the original Allaire *et al.* paper,

$$\xi = \frac{1}{\gamma - 1} = \sum_i \frac{z_i}{\gamma_i - 1}, \tag{32}$$

$$\frac{\pi\gamma}{\gamma - 1} = \sum_i z_i \frac{\pi_i \gamma_i}{\gamma_i - 1}, \tag{33}$$

$$P(z, \rho\varepsilon) = (\gamma - 1)\rho\varepsilon - \gamma\pi. \tag{34}$$

For the numerical method, a first-order accurate Godunov scheme should be used, with the HLLC approximate Riemann solver. We have not covered the exact form of this solver, though it can be derived using the techniques described in CCM1. The momentum and energy HLLC states are entirely unchanged (they simply use mixture rules), and the other variables have only small changes (here, $i = (1, 2)$):

$$\alpha_K^{\text{HLLC}} = \alpha_K$$
$$(\alpha\rho)_{i,K}^{\text{HLLC}} = (\alpha\rho)_{i,K} \left(\frac{S_K - v_K}{S_K - S^*} \right)$$

For the volume fraction, we note that this formulation actually reduces the update to an upwind update (which, given the form of the equations, is not surprising). Though this does also require the source term update to be implemented as described on slide 47 of the lectures.

Exercises:

The tests used for the ghost fluid method can also be used here. For these tests, the each material has an individual density, and the pressure and velocity of the real material should be used. The volume fraction will determine

which material exists initially in a given discontinuity. One challenge here is that if the volume fraction is set to 0 for one of the materials (and 1 for the other), then computing variables, e.g. rho from $\alpha\rho$, will cause the code to crash. Instead, it is standard for diffuse interface methods to define a volume fraction to have a small, non-zero number in regions a material doesn't exist, e.g.:

$$\alpha_1 = \begin{cases} 10^{-6} & x > x_0 \\ 1 - 10^{-6} & \text{otherwise} \end{cases}$$

All tests previously used should run, though focus should be given to:

1. The moving contact discontinuity, one-material and two-material - this is an important debugging case
2. Toro's first test, again important debugging
3. Fedkiw's test B, the air-helium shock
4. The air-helium slab
5. Chinnayya's water-air test