APiE Exercise – SPH

Exercise: Sod Shock (1D) using SPH (1EC)

Hint: The algorithm for SPH and MD is very similar and thus re-visit the MD-exercises, in particular the pseudo-code in MD1D/2D, which contains the general formulation. Note that in 1D systems, this method can be simplified avoiding the vectors - but this is only possible in 1D and can lead to confusion.

The Sod Shock is a common test case for CFD codes. It involves the simulation of a 1D Riemann problem for an ideal gas. To the left of a discontinuity at $x = 0$ the parameters of the gas are $(v_l, \rho_l, P_l) = (0.0, 1.0, 1.0)$. To the right the parameters are $(v_r, \rho_r, P_r) = (0.0, 0.125, 0.1)$. Use
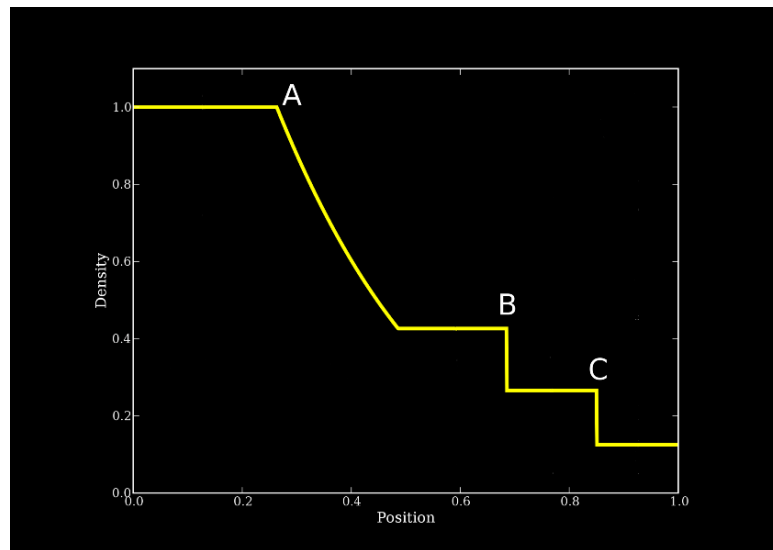

Figure 4: Plot of density at $t = 0.2\,\mathrm{s}$ for the given Sod Shock parameters.

SPH to calculate the evolution of a Sod Shock over the spatial domain $-0.5 < x < 0.5$. Write a report on your solution at $t = 0.2s$. Include plots of the density and the thermal energy and discuss the solution near the front of the rarefaction wave (see label 'A' in Figure 1), the contact discontinuity (label 'B') and the shock (label 'C'). As a guide, Figure 1 shows the analytical solution for the density at $t = 0.2s$. Compare your solution against this plot.

Use the equation of state for an ideal gas in terms of the density ρ and thermal energy u

$$P = (\gamma - 1)u\rho, \tag{1}$$

with an adiabatic index of $\gamma = 1.4$. This parameter choice is due to the test case specifications. For a more detailed explanation of the Sod Shock parameters and the equation of state used, please see the paper by Sod [G. A. Sod, A survey of several finite difference methods for systems of nonlinear hyperbolic conservation laws, J. Comp. Phys. 27(1):1-31, 1978].

Implement the following SPH equations for density, acceleration and rate of change of thermal

energy for particle a:

$$\rho_a = \sum_b m_b W_{ab} \tag{2}$$

$$\frac{dv_a}{dt} = -\sum_b m_b \left(\frac{P_a}{\rho_a^2} + \frac{P_b}{\rho_b^2} + \Phi_{ab} \right) \nabla_a W_{ab} \tag{3}$$

$$\frac{du_a}{dt} = \frac{P_a}{\rho_a^2} \sum_b m_b v_{ab} \cdot \nabla_a W_{ab} \tag{4}$$

where $v_{ab} = v_a - v_b$. Note that the signs of the relative velocity v_{ab} and the gradient of the Kernel function cancel each other in 1D cases, so that the vector notation is dropped here.

Use the the artificial viscosity in order to stabilise the shock

$$\Phi_{ab} = -\frac{K v_{sig}(v_{ab} \cdot x_{ab})}{\overline{\rho}_{ab} |x_{ab}|} \tag{5}$$

with $K = 1.0$ and signal velocity $v_{sig} = 0.5(c_a + c_b - 4 v_{ab} \cdot \hat{x}_{ab})$. Only apply the viscosity for particle pairs that are approaching each other ($v_{ab} \cdot x_{ab} < 0$).

Integrate the particle variables using the timestep

$$\Delta t = 0.3 \min \left(\frac{h_a}{v_{sig}} \right) \tag{6}$$

where the function 'min' calculates the minimum value over all the SPH particles.

Use the kernel function:

$$W(r, h) = \frac{2}{3h} \begin{cases} 1 - \frac{3}{2}(r/h)^2 + \frac{3}{4}(r/h)^3 & \text{for } 0 \le r/h < 1 \\ \frac{1}{4}\left[2 - (r/h)\right]^3 & \text{for } 1 \le r/h < 2 \\ 0 & \text{for } r/h \ge 2 \end{cases} \tag{7}$$

and use a symmetric kernel between particle pairs (e.g. $W_{ab} = W(r, 0.5(h_a + h_b))$) with $r = |x_a - x_b|$.

Use a smoothing length that varies with the density so that:

$$h_a = 1.3 \frac{m_a}{\rho_a} \tag{8}$$

It might be easier to modify one of your old MD codes to an SPH code rather than write it from scratch. Compute the SPH-hydrodynamic acceleration using Eq. (3) and use it instead of f_i/m_i in the MD program for integration. Integrate the thermal energy u in the same manner as the particle velocity using Eq. (4). At the beginning of each acceleration computation make sure to update the density using Eq. (2) and the pressure P using the given equation of state in Eq. (1).

Hint: In order to model the initial density discontinuity, you either use different masses and equal spacing or you can use different particle spacings to the left and right of $x = 0$ with equal masses. Aim to use approximately 450 particles, but feel free to experiment.

Hint: Do not evolve the variables for the first and last 4 particles in the line. These particles will model the boundary condition.

Hint: For radially symmetric kernels the following applies:

$$\nabla_a W_{ab} = \frac{\mathbf{r}_{ab}}{|\mathbf{r}_{ab}|} \frac{\partial W_{ab}(r)}{\partial r}.$$ (9)