Simulating a 1D Sod Shock Tube with SPH

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In this report, the Euler's equations for a one dimensional shock tube is solved by means of Smoothed Particle Hydrodynamics. First, an overview of the theory and model is presented and then the results. The results are in agreeance to what is predicted by theory as all major components of the shock are seen. Although they agree, there are discrepancies that arise from the particle-based approximation.

I. INTRODUCTION

Computational Fluid Dynamics (CFD) is a robust field with varying techniques that seeks to solve the Navier-Stokes or Euler equations. There currently seems to be two paradigms of solvers in this field. The first being Eulerian based solvers, in which the mesh used is stationary. The ladder being Lagrangian codes. Some such solvers are a combination of boths such as the particle-in-cell method. A popular Lagrangian based solver is known as Smoothed Particle Hydrodynamics (SPH).

SPH was first introduced by Gingold and Monaghan to study non-spherical stars that have a polytropic equation of state. [1] This first paper sets the ground work to be able to extend such a formulation to other physical phenomena. To begin, a discretized Euler's equations state that for a fluid with no external forces the equation of motion for a segment i is given as:

$$\frac{d^2 r_i}{dt^2} = -\frac{1}{\rho_i}\nabla P, \tag{1}$$

where ρ_i is the density of the segment and ∇P is the pressure gradient. The fluid segments are commonly referred to as particles.

In SPH, the density is approximated (smoothed) with the use of kernel function, $W(r)$. A kernel smoother is a function that estimates the value of a real valued function as the weighted average of neighboring data points. Such a function must also follow a normalisation condition:

$$\int dr\, W(r) = 1 \tag{2}$$

Our smoothed density, $\rho_s(r)$, can then be expressed as:

$$\rho_s(r) = \int dr'\, W(r - r')\rho(r') \tag{3}$$

$\rho(r')$ is an unknown function. This means that eq. (3) can not be solved in its current form. In order to arrive at a solution, we must make use of Monte Carlo integration. With this, we can write the density for a particle i as:

$$\rho_i = \sum_j m_j W(r_i - r_j), \tag{4}$$

where j notates some other particle in the system. It is important to note that the particles have a self-contribution to their density.

With our particle discretization of our fluid and kernel estimation, we can express eq. (1) as:

$$\frac{d^2 r_i}{dt^2} = -\sum_j m_j \left(\frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2}\right)\nabla W(r_i - r_j), \tag{5}$$

where $\nabla W(r_i - r_j)$ is the gradient of our chosen kernel and P_i is given by a chosen equation of state. The chosen equation of state for our model is that of the Ideal Gas. This equation of state is given as:

$$P = e\rho(\gamma - 1), \tag{6}$$

where e is the internal energy and γ is set to 1.4 to model an adiabatic ideal gas. Euler's equations states that energy conservation is given as:

$$\frac{de}{dt} = -\frac{P}{\rho}\frac{\partial v}{\partial x}, \tag{7}$$

In our particle based representation, we can express the previous equation as:

$$\frac{de}{dt} = -\sum_j m_j \left(\frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2}\right)(v_i - v_j)\nabla W(r_i - r_j) \tag{8}$$

For our simulation, these are the only two quantities that are necessary for time-evolution as they both relate to energy and momentum conservation. In fact after initial condition are set, these quantities are integrated using the sympletic leap-frog integration method with a time-step of $\Delta t = 0.005$.

The dynamics of the system is not invariant under kernel choice. This makes it important to understand which kernel you are working with. A function that fits all requirements for a good kernel would be the Gaussian distribution, but this is in fact problematic. This is due to the fact that the Gaussian distribution only converges to zero after an infinite distance from the origin making the computation more expensive. Although this is not an issue for the systems we consider, the chosen kernel for our system is the cubic spline kernel:

$$W(r) = \begin{cases} \sigma_3\left[1 - \frac{3}{2}q^2(1 - \frac{q}{2})\right] & \text{if } 0 \le q \le 1 \\ \frac{\sigma_3}{4}(2 - q)^3 & \text{if } 1 < q \le 2 \\ 0 & \text{if } 2 < q \end{cases} \tag{9}$$

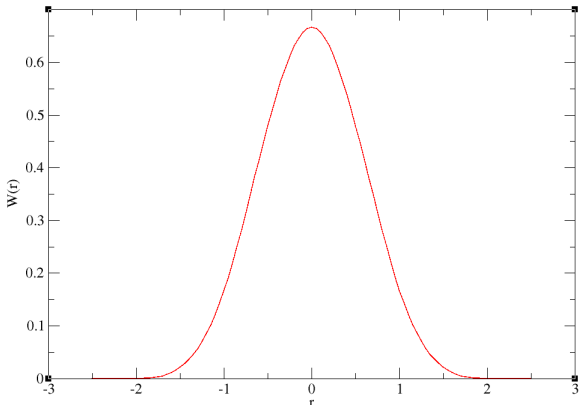

FIG. 1. A plot of the kernel function.

In eq. (9), σ_3 is a normalization constant that equals $(2/3)h$ and $q = \frac{r}{h}$, where h is the smoothing length.

Although the previous results are all that is needed to run a simulation, some issues persist with this method alone. For contact discontinuities, one will see noticeable ringing along the shock wave. This ringing can be curbed by adding artificial viscosity. The addition of this also allows for additional entropy generation in our system. Previously, the system could only generate conformational entropy. This viscosity also prevents the non-physical penetration of neighboring particles. One simple and effective artificial viscosity is the Monaghan viscosity given in his 1983 paper. [2] It starts by perturbing the pressure terms in eq. (5) and (8):

$$\frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2} + \Pi_{ij}, \tag{10}$$

where Π_{ij} is our artificial viscosity. It is given as:

$$\Pi_{ij} = \begin{cases} \frac{-\alpha_\Pi \bar{c_{ij}} \phi_{ij} + \beta_\Pi \phi_{ij}^2}{\bar{\rho_{ij}}} & \text{if} 0 > v_{ij} x_{ij} \\ 0 & \text{if} 0 \leq v_{ij} x_{ij}, \end{cases} \tag{11}$$

where α_Π and β_Π are constants that are normally set to be 1. The additional factors are given as:

$$\bar{c_{ij}} = \frac{1}{2}(c_i + c_j), \tag{12}$$

where $c_i = \sqrt{\gamma \frac{P_i}{\rho_i}}$.

$$\bar{\rho_{ij}} = \frac{1}{2}(\rho_i + \rho_j) \tag{13}$$

$$\phi_{ij} = \frac{h v_{ij} x_{ij}}{|x_{ij}|^2 + \phi^2}, \tag{14}$$

where $v_{ij} = v_i - v_j$, $x_{ij} = x_i - x_j$, and $\phi = 0.1h$. The term ϕ is used to prevent divergences in the case of closely separated particles.

For this report, we consider one system. That system being a classic test for SPH solvers: the Sod shock tube. The Sod shock tube was heavily considered by Gary A. Sod in 1978. This shock tube has an analytical solution for one dimension which makes it a great test for solvers.

II. MODEL AND PARAMETERS

Our parameters were obtained from Liu and Liu in their book for SPH. [3] For our simulation, we consider a one dimensional tube with dimensionless length 1.2. The fluid in this tube is then split into 400 particles. In order to get the desired contact discontinuity, we partition particle i as:

$$x_i = \begin{cases} i(\Delta x/4) - x_0 + \Delta x/4 & \text{if } 0 \leq i \leq 319, \\ (i - 320)\Delta x + 0.5\Delta x & \text{if } 320 \leq i \leq 399, \end{cases} \tag{15}$$

where $x_0 = 0.6$ and $\Delta = x_0/80$. This partition gives the particles on the left side a density of 1 and on the right side a density of 0.25. We then assign initial internal energy as:

$$e_i = \begin{cases} 2.5 & \text{if } 0 \leq i \leq 319, \\ 1.795 & \text{if } 320 \leq i \leq 399, \end{cases} \tag{16}$$

The smoothing length is chosen to be $h = 0.016$ unless stated otherwise. Due to the small timescales we consider, we do not employ any sort of boundary conditions on our system.

III. RESULTS

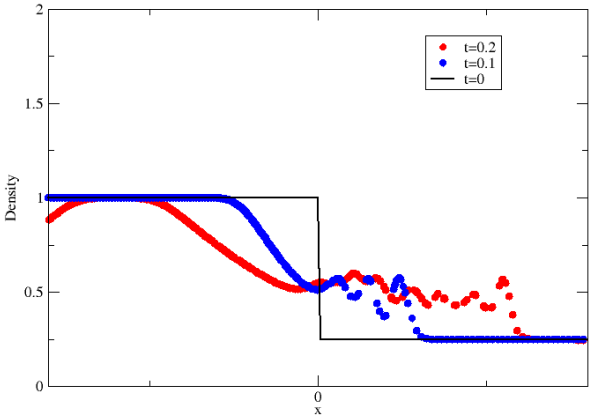

FIG. 2. A plot of the density of the sod shock tube at various times with no artificial viscosity.

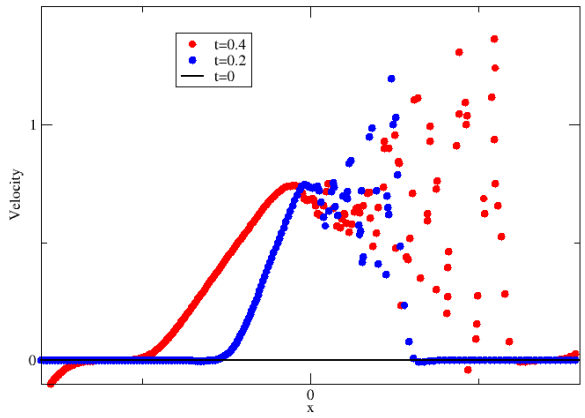

FIG. 3. A plot of the velocity of the sod shock tube at various times with no artificial viscosity.

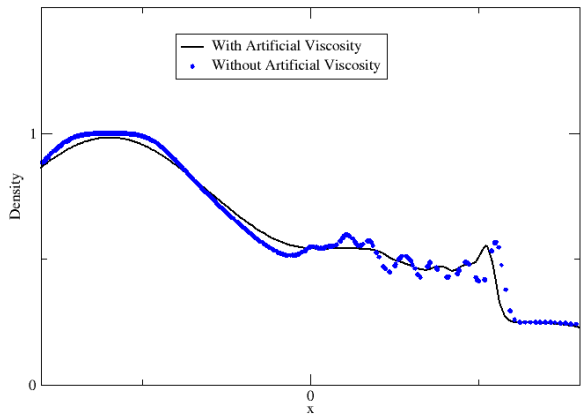

FIG. 4. A comparison of the density at the final time with and without artificial viscosity.

By plotting the density distribution as in fig. 1, we can get a nice qualitative sense that our code is working. At the beginning of the simulation, there is a contact discontinuity between the left and right sides of our tube. As the system is evolved, the shock begins to move throughout. One can see that the rarefaction wave progresses quite nicely. In fig. 2, the velocity distribution is plotted. This plot also agrees with the analytical solution. It is noticeable that the shock wave not only progress towards the right side of the tube, but also perturbs the pre-shock region on the left. The shock appears to progress slower in this region.

In both fig. 1 and fig. 2, there is a highly apparent ringing along the path of the shock-wave. In fact with a cursory view, it appears to be tantamount to as if the function was a convolution with a simple sine function. The ringing is even more apparent in fig. 2. This ringing is highly influenced by the nonphysical penetration of approaching particles. This is one of the issues discussed in the introduction. We can curb this effect with the addition of artificial viscosity.

Fig. 3 plots the final density of the simulation with and without perturbing the pressure terms with Π_{ij}. With the addition, the final resolved system is much smoother. Although this is a nicer result, there an issue at the precipice of the shock-wave. The result with artificial viscosity has a rarefaction wave that does not extend fully to the predicted position which disagrees with theory. This brings in mind a phrase: "there's no such thing as a free lunch." If one tries to entirely eliminate the ringing in the simulation, the higher the error becomes at the rarefaction wave.

IV. SUMMARY AND CONCLUSION

Overall, the SPH solver written for this report follows the analytical solution with some discrepancies. Following the normal SPH mechanisms provides a solution that qualitatively follows theory, but it introduces a ringing along the shock-wave. An artificial viscosity can be introduced to prevent the nonphysical penetration of near particles which leads to the reduction of the noted ringing phenomenon. Although this addition serves its intended effect of curbing the ringing, it also introduces an additional error at the rarefaction wave. The more one tries to curb the ringing the more the error at this region is introduced.

[1] R. A. Gingold and J. J. Monaghan, Monthly Notices of the Royal Astronomical Society **181**, 375 (1977), https://academic.oup.com/mnras/article-pdf/181/3/375/3104055/mnras181-0375.pdf.

[2] J. Monaghan and R. Gingold, Journal of Computational Physics **52**, 374 (1983).

[3] G. R. Liu and M. B. Liu, *Smoothed Particle Hydrodynamics* (WORLD SCIENTIFIC, 2003) https://www.worldscientific.com/doi/pdf/10.1142/5340.