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Comparison of the Computational Performance of Traditional Hydrodynamics and Smoothed Particle Hydrodynamics for Strong Shock Test Problems

Conner Myers, Camille Palmer, and Todd Palmer

School of Nuclear Science and Engineering, Oregon State University, Corvallis, OR

INTRODUCTION

The accurate modeling of strong shocks is vital for many applications in astronomy, aerospace, and defense. Strong shocks are characterized by near instantaneous spikes in fluid values such as pressure and density and are difficult to model in an accurate and efficient way. Capturing the profile and behavior of a traveling shock requires the use of small spatial discretization in computational modeling. Given that the timestep of a simulation with spatial discretization is dependent on the size of the smallest spatial grid for stability, a small timestep is required to evolve strong shock simulations accurately. Adaptive mesh refinement can be used to decrease the number of cells by only including small spatial grids where needed, but the timestep size is still dependent on the wave crossing time of the smallest grid and therefore the simulations require significant computational resources to run. To further increase performance, alternative computational methods must be explored.

An unconventional yet promising method for strong shock problems is the smoothed particle hydrodynamics method. Smoothed particle hydrodynamics (SPH) is a meshfree approach to hydrodynamics where the fluid is represented by freely moving, simulated particles [2]. The field functions representing the fluid are approximated at the location of the simulated particles or nodes. As the field functions are approximately only at particle locations, the fluid is entirely represented by node particles and the interactions between nodes determines fluid behavior. A distinct advantage of this approach when applied to shock problems is the lack of a spatial grid which leads to a maximum timestep size to preserve accuracy and stability. The timestep is still limited by similar conditions in SPH, but the characteristic resolution can be larger than mesh-based approaches for the same problem, leading to a larger allowable timestep.

Smoothed Particle Hydrodynamics Formulation

The representation of the fluid equations in SPH is done using two approximations. The first approximates a function using a smoothing kernel approximation or kernel [2]. Starting from the identity:

$$f(x) = \int_{\Omega} f(x')\delta(x - x')dx' \tag{1a}$$

Where f is any function, $\delta(x - x')$ is the dirac delta function and Ω is a volume over which the kernel is valid. Replacing the delta function with a smoothing function, $W(x - x', h)$, yields the kernel approximation:

$$< f(x) >= \int_{\Omega} f(x')W(x - x', h)dx' \tag{1b}$$

The brackets around f denote the approximation operator and the h in the smoothing function defines the region of influence for the function $W(x - x', h)$. This formulation allows for the representation of any arbitrary function f in the above integral form. Similarly, the kernel approximation of the derivative of an arbitrary function can be derived to be:

$$< \nabla \cdot f(x) >= -\int_{\Omega} f(x') \cdot \nabla W(x - x', h)dx' \tag{1c}$$

This expression is only valid for smoothing functions that are entirely contained within the domain of interest. For smoothing functions that extend beyond the domain, for example points near a boundary, special treatment must be taken.

To use the kernel approximation for a numerical simulation of a problem, the system must be represented by a finite number of particles. A second approximation, the particle approximation, is used to express the integral representation with discretized sums of all the particles that fall within a given point in space's influence region, defined by the smoothing function. For a given particle in space with mass, volume, and density:

$$m_j = \Delta V_j \rho_j \tag{2a}$$

Equation 1b can then be written in discretized particle form:

$$f(x) \approx \sum_{j=1}^{N} f(x_j)W(x - x_j, h)\Delta V j \tag{2b}$$

Substituting equation 2a:

$$f(x) \approx \sum_{j=1}^{N} f(x_j)W(x - x_j, h)\frac{\rho_j \Delta V j}{\rho_j} \tag{2c}$$

Finally we arrive at the particle representation of an arbitrary function f:

$$< f(x_i) >= \sum_{j=1}^{N} \frac{m_j}{\rho_j} f(x_j) \cdot W_{ij} \tag{2d}$$

Where

$$W_{ij} = W(x_i - x_j, h) \tag{2e}$$

Similarly, for the spatial derivative:

$$< \nabla \cdot f(x_i) >= -\sum_{j=1}^{N} \frac{m_j}{\rho_j} f(x_j) \cdot \nabla_i W_{ij} \tag{2f}$$

Where

$$\nabla_i W i j = \frac{x_i - x_j}{r_{ij}} \frac{\partial W_{ij}}{\partial r_{ij}} \tag{2g}$$

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With this basic formulation, the fluid equations can be approximated through a finite number of particles. It is necessary for the fluid properties to be approximated at each particle location to determine the behavior of the fluid. However, the fluid properties can be approximated at any point using the described formulation without a particle. This allows for the arbitrary sampling of fluid properties for a given system with a finite number of simulated particles.

DESCRIPTION

The Smoothed Particle Hydrodynamics method poses several distinct advantages and disadvantages when compared to traditional hydrodynamics methods for simulating strong shocks. Many advantages of SPH simulations are laid out by Price in [3]: An exact, time-independent, solution to the continuity equation; Zero intrinsic dissipation (note that dissipation can be included by adding artificial viscosity terms); Exact and simultaneous conservation of mass, momentum, angular momentum, energy and entropy; A guaranteed minimum energy state for the particles; and Resolution that follows mass. The exact conserving of quantities and mass following resolution make SPH a promising method for improving performance of strong shock simulations. It is important to note, however, that the implementation of a dissipation scheme beyond basic SPH is required to accurately capture the evolution of a shockwave in time.

One key disadvantage for this method is that SPH particles interact with all other SPH particles within their smoothing distance, or the range over which particles can interact. The number of interactions increases with the density of SPH particles linearly in each dimension- increasing quadratically and two dimensions and cubically in three. The scaling of interactions in SPH can quickly increase the number of interactions per particle to well above the number of interactions required between nodes in a finite difference or finite volume scheme, where communication is only between close neighbors. It can be expected that a SPH scheme alone will have a worse performance than traditional mesh-based hydrodynamics methods. However, a hybrid scheme can take advantage of the strengths of both SPH and traditional hydrodynamics methods to improve performance.

The python packages Pyro2 [4] and PySPH [5] are open-source implementations of the finite volume and smoothed particle hydrodynamics methods respectively. Both python libraries are commonly used and well documented. In preparation for the implementation of a hybrid-SPH method for simulating strong shocks using parts of both codes, each code is tested in several test problems as a baseline evaluation of performance. The tests examined include the Sod Shocktube problem, the Woodward-Collela Blast problem, and the Sedov explosion problem. The accuracy and performance of each scheme is analyzed for future use as benchmarks for the hybrid implementation.

RESULTS

The Sod Shocktube problem was run in both Pyro2 and PySPH and compared against both the analytical solution and results from the hydrodynamics code CTH [6]. The plot of pressure at time t=0.2 is displayed in figure 1. In the Woodward-Collela Blast and Sedov explosion problems, the cases we ran in a high and medium resolution configuration and compared against results from CTH in figures 2 and 3. Table I shows the timing for each of the test cases in Pyro2, PySPH and CTH.

A comparison of the resolution levels between Pyro2 and PySPH is difficult as the units used to characterize the resolution are different in each case. Pyro2 utilizes a mesh made of gridpoints while the fluid in PySPH is composed of simulated particles. In each code, the high resolution case for the problem was taken to be the level of gridpoints or particles required to closely approximate the exact solution. For the medium resolution case, the solution deviates by at least five percent in critical areas such as peaks and troughs while retaining the overall shape of the exact solution. In the Sedov problem, the solution leads slightly in the PySPH solution and with less amplitude. In the medium resolution solutions for both Pyro2 and PySPH, the peaks and troughs are less resolved and appear with a smoothed or filtered shape. The Sod Shocktube problem, being a computationally inexpensive test, is accurately modeled by all the codes examined with runtimes of 10 seconds or less.

The runtimes for each test case are shown in table I. In all cases, the Fortran code CTH is exceedingly faster than either Pyro2 or PySPH. Additionally, in all cases Pyro2 is faster than PySPH, however the timing is relatively close in the one dimensional cases. Since particles in PySPH must interact with any nearby particles, which in many cases can reach over 100, PySPH performance suffers more than Pyro2 when the dimensions are increased from one to two.

This investigation serves as a comparison between the finite volume hydrodynamics and smoothed particle hydrodynamics for three test problems. While the tests ran significantly faster in Pyro2 than PySPH in two dimensions, in all cases the timing was within an order of magnitude. In a hybrid scheme utilizing both methods, the SPH method would be applied at the shock front where high resolution is needed using traditional hydrodynamic methods and these methods suffer from a small timestep. Regions outside of the shock front can be modeled using larger grids with correspondingly larger timesteps, while the SPH particles are less constrained by timestep limitations due to the lack of a spatial grid. This investigation will serve as a comparitive baseline for the implementation of a hybrid scheme as this project continues.

ACKNOWLEDGMENTS

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REFERENCES

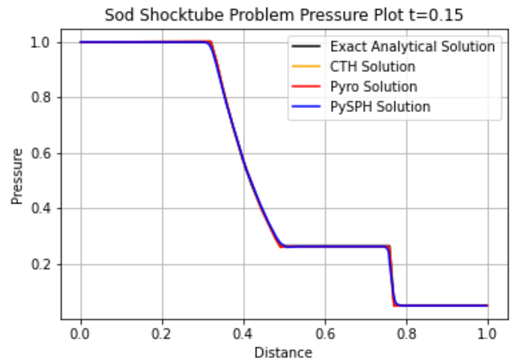

Fig. 1. Comparison of the results of the Sod Shocktube problem in Pyro2, PySPH, and CTH against an analytical solution

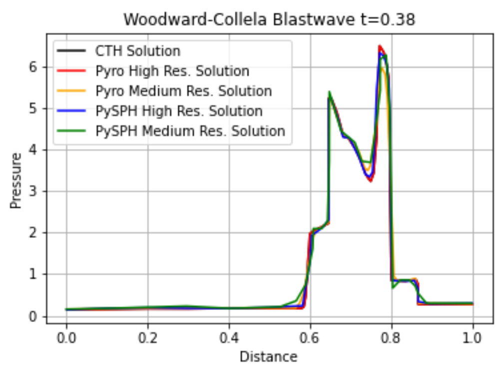

Fig. 2. Comparison of the results of the Woodward-Collela Blast in Pyro2, PySPH, and CTH for high and medium resolutions

	CTH	Pyro2	PySPH
Sod Shocktube	0.1s	3.71s	10.3
Woodward-Collela Blast High Resolution	18.0s	121s	96.2s
Woodward-Collela Blast Low Resolution		34.6s	63.3s
Sedov Explosion High Resolution	66.1s	339s	1210s
Sedov Explosion Low Resolution		45.5s	353s

TABLE I. Timing comparison for test problems in CTH, Pyro2, and PySPH

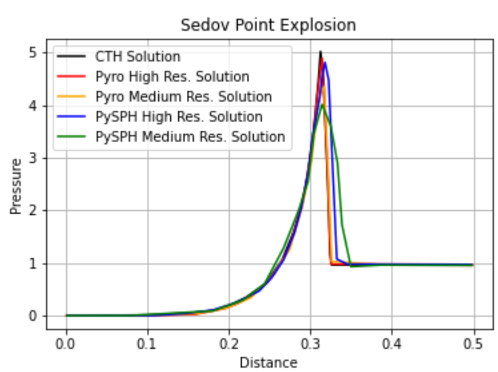

Fig. 3. Comparison of the results of the Sedov explosion problem in Pyro2, PySPH, and CTH for high and medium resolutions