Application of the Modified Reactive SPH Method for Simulating Explosions

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ABSTRACT

Smoothed Particle Hydrodynamics (SPH) is a Lagrangian method widely used for the modeling fluid flows. Simulations of explosions require, besides the hydrodynamic equations, a realistic equation of state, an energy source term, and a set of chemical kinetic equations to follow the composition changes of the gas during the explosion. The performance of the hydrodynamic equations is investigated in the framework of the Sedov-Taylor blast-wave. The implementation of chemical kinetic equations and equation of state is studied with 1D detonation of TNT slab. Our results are compared to those from analytical and experimental studies.

Key words: SPH, Particle Method, Simulations, High Explosive

1. Introduction

The SPH method is a grid free Lagrangian based method in which the fluid flow is represented by fluid pseudo-particles. These individual particles interact with one other, moving with the flow and carrying with them all of the computational information about the fluid. Fluid properties are then interpolated between the particles. Although this technique was introduced by Lucy[1] and Monaghan[2] in the context of Astrophysical modeling, it was applied successfully applied for many engineering problems including simulations of high explosive (HE) detonation. The detonation speed is extremely high and the gaseous products can be assumed to be inviscid and the explosion process is adiabatic, In such case the Eulerian equations together with suitable equation of state (EOS) can be used

$$\begin{cases} \frac{D\rho}{Dt} = -\rho\nabla\cdot\vec{v} \\ \frac{D\vec{v}}{Dt} = -\frac{1}{\rho}\nabla p \\ \frac{De}{Dt} = -\frac{p}{\rho}\nabla\cdot\vec{v} \\ p = p(\rho, e) \end{cases} \quad (1)$$

where ρ e, $p, \vec{v}$ and t are density, internal energy, pressure, velocity and time, respectively.

Kernel interpolation is the basis of the SPH method. Any function $f(x)$ can be defined through its convolution with a kernel function , W, as follows

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$$f(x) = \sum_{j=1}^{N} \frac{m_j}{\rho_j} f(\vec{x}_j) W(\vec{x} - \vec{x}_j, h), \tag{2}$$

where h is the smoothing length defining the kernel influence domain, m is the mass associated with the interpolation point $\overrightarrow{x_j}$. The kernel satisfies the following conditions

$$\int W(x - x', h) dx' = 1$$
$$\lim_{h \to 0} W(x - x', h) = \delta(x - x') \tag{3}$$

In our work we use the spike kernel function defined as follows

$$W = \alpha_d \begin{cases} \left[1 - \frac{|\vec{x}_i - \vec{x}_j|}{3h}\right]^3, & \frac{|\vec{x}_i - \vec{x}_j|}{h} < 3 \\ 0, & \frac{|\vec{x}_i - \vec{x}_j|}{h} \geq 3 \end{cases} \tag{4}$$

where α_d is $2/3h$, $10/9\pi h^2$ in one- and two-case, respectively.

According to the SPH approximation, the equations (1) can be written as follows:

$$\begin{cases} \frac{D\rho_i}{Dt} = \sum_{j=1}^{N} m_j (\vec{v}_i - \vec{v}_j) \cdot \nabla_i W \\ \frac{D\vec{v}_i}{Dt} = -\sum_{j=1}^{N} m_j \left(\frac{p_i + p_j}{\rho_i \rho_j} + \Pi\right) \nabla_i W \\ \frac{De_i}{Dt} = \sum_{j=1}^{N} \frac{m_j}{2} \left(\frac{p_i + p_j}{\rho_i \rho_j} + \Pi\right) (\vec{v}_i - \vec{v}_j) \cdot \nabla_i W \\ \frac{D\vec{x}_i}{Dt} = \vec{v}_i \\ p = p(\rho, e) \end{cases} \tag{5}$$

where Π_{ij} accounts for the dissipation rate of internal energy due to the artificial viscosity. We used a form of the viscosity based on an analogy to the Riemann problem, which can be written as

$$\begin{gathered} \Pi = -\frac{\alpha}{2} \frac{\omega v^{sig}}{\bar{\rho}}, \\ v^{sig} = c_i + c_j - 3\omega, \quad \bar{\rho} = (\rho_i + \rho_j)/2, \\ \omega = (\vec{v}_i - \vec{v}_j) \cdot (\vec{x}_i - \vec{x}_j)/|\vec{x}_i - \vec{x}_j|, \end{gathered} \tag{6}$$

where c_i is the speed of the sound for particle i, α is the parameter order of unity.

In order to keep the resolution of the method nearly constant, the smoothing length is updating in accordance with the requirement that the mass influence domain should be constant

$$\rho_i h_i^{\,d} \approx const \tag{7}$$

where d is the number of dimensions. The initial value of h is typically set to $1.3\Delta x$ where Δx is the initial particle spacing.

Equations (5-6) guarantee the preservation of the linear and angular momentum which is obvious advantage of the SPH.

2. Sedov blast wave

This test demonstrates that the method can handle the steep temperature and density gradients created by an explosion.

A settled, uniform-density glass-liked distribution of 72000 SPH particles is created. Then the particles located within small area at the origin are given a net impulse of thermal energy $E_0 = 1000$. The remaining particles have an internal energy 10 ^{6} times smaller than the particle with the maximum internal energy.

We have deliberately chosen a large energy jump for our Sedov blast in order to make this test challenging. The impulse of thermal energy results in an outward propagating shock front which sweeps the surrounding gas into a dense layer.

In this particular case we can assume that the gas is ideal, and so the pressure and specific internal energy are related by

$$p = (\gamma - 1)\rho\epsilon \tag{8}$$

where $\gamma = 1.4$ is the ratio of specific heats. Sedov [5] provides an analytic similarity solution for the subsequent evolution of this system. Fig. 1 shows the results from the Sedov blast test at $t = 0.1$ for SPH and the analytical solution. The lower SPH peak density is not a surprise as the inherent smoothing of the SPH method broadens the shock front and lowers the maximum recoverable density. The small oscillations of the particle velocities around the theoretically predicted is the consequence of the artificial viscosity implementation and perhaps unavoidable for particle based codes.

3. Detonation of TNT slab

The detonation of HE is the propagation of the reactive wave that advances through the explosive with constant detonation velocity related to the particular explosive concerned. For TNT the detonation velocity is $6930\, m/s$. Once initiated the intense heat and the pressure developed are sufficient to maintain the detonation process. In a steady state detonation process, the reaction rate is essentially infinite and the chemical equilibrium is attained.

For the explosive gas, the standard Jones-Wilkins-Lee EOS is employed. The pressure of the explosive gas is

$$P = A(1 - \psi\eta/R_1)e^{-\frac{R_1}{\eta}} + B(1 - \psi\eta/R_2)e^{-\frac{R_2}{\eta}} + \psi\eta\rho_0\epsilon \qquad (9)$$

where $\eta = \rho/\rho_0$, $A, B, R_1, R_2, \omega, \epsilon$ are coefficients obtained by fitting the experimental data. The values of these coefficients are listed in Table 1.

One important benchmark in HE simulation is a 1D TNT slab detonation [4], in which a $0.1\, m$ long TNT slab detonates at one end of the TNT slab. In this case, a symmetric setup can be employed when the detonation of the $0.1\, m$ long slab from one end to the other end is equivalent to the detonation of a $0.2\, m$ long slab from the middle point to both ends. According to the detonation velocity, it takes around $14.4\, \mu s$ to complete the detonation to the end of the slab.

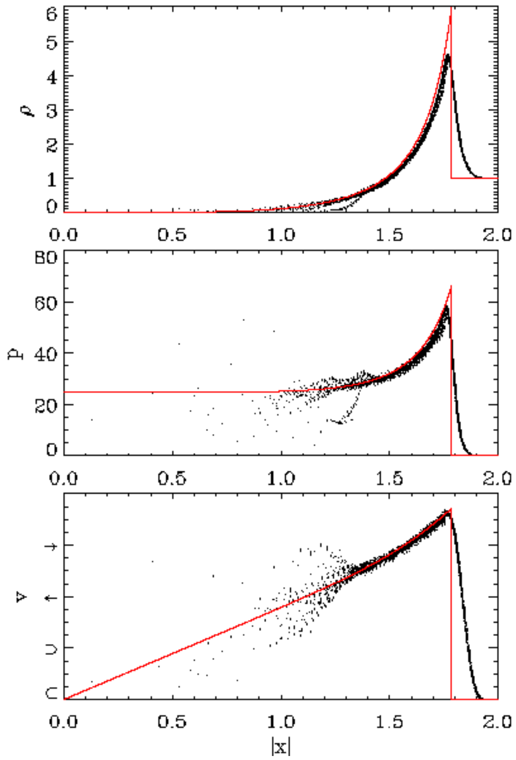

Fig.1 Results of the Sedov blast wave test at a time $t = 0.1$. The black dots represent the SPH result and the red lines show the semi analytic solution provided by Sedov

Table 1. EOS coefficients

Symbol	Meaning	Value
ρ_0	Initial density	1630 Kg/m^3
A	Coefficient	$3.7 \cdot 10^{11}$ N/m^2
B	Coefficient	$3.2 \cdot 10^{9}$ N/m^2
R_1	Coefficient	4.15
R_2	Coefficient	0.95
ψ	Coefficient	0.3
ϵ	Detonation energy	$4.29 \cdot 10^{6}$ J/Kg

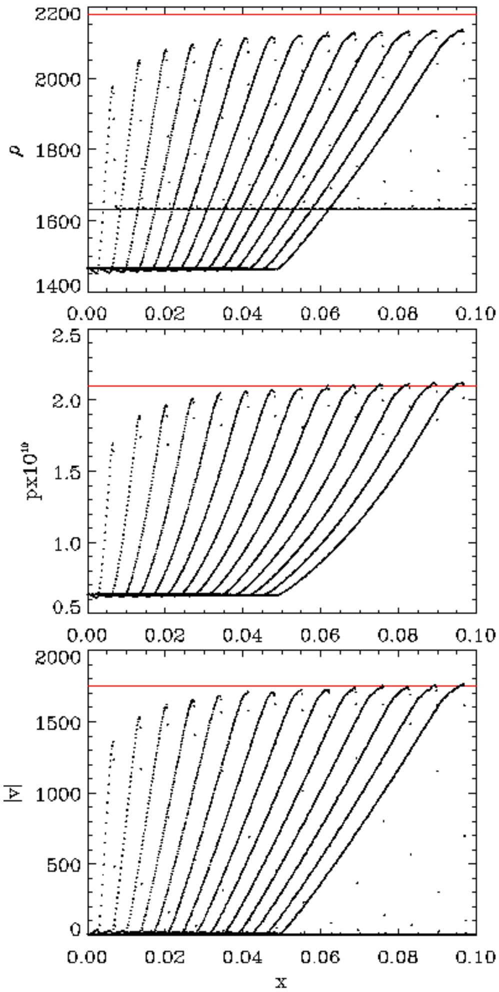

Fig. 2 Density, pressure and velocity profiles along the one dimensional TNT slab. The red lines indicate the experimental values for the peak values of the density, pressure and velocity at the trailing edge of the thin reaction zone

Figure 2 show the density, velocity and the pressure profiles along the slab at $1\mu s$ interval from 1 to $14\mu s$ obtained using 2000 particles. The solid red lines illustrate the experimental pressure, density, and the velocity at the trailing edge of the thin reaction zone.

It can be seen from Fig. 2 that with the process of detonation the pressure and the particle velocity converges to the experimental values, while density is slightly underestimated for the same reason discussed in the previous section. However, the peak value of the density tends to the experimental when the number of particles increases. Our results are in a good agreement with those of other authors and experimental data suggesting that the SPH can be applied for the simulations of HE detonation.

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