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PARTICLE MESH HYDRODYNAMICS FOR ASTROPHYSICS SIMULATIONS

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We present a particle method for the simulation of three dimensional compressible hydrodynamics based on a hybrid Particle-Mesh discretization of the governing equations. The method is rooted on the regularization of particle locations as in remeshed Smoothed Particle Hydrodynamics (rSPH).

The rSPH method was recently introduced to remedy problems associated with the distortion of computational elements in SPH, by periodically re-initializing the particle positions and by using high order interpolation kernels.

In the PMH formulation, the particles solely handle the convective part of the compressible Euler equations. The particle quantities are then interpolated onto a mesh, where the pressure terms are computed. PMH, like SPH, is free of the convection CFL condition while at the same time it is more efficient as derivatives are computed on a mesh rather than particle-particle interactions. PMH does not detract from the adaptive character of SPH and allows for control of its accuracy. We present simulations of a benchmark astrophysics problem demonstrating the capabilities of this approach.

Keywords: Particle methods; SPH; Euler equations; compressible flow.

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1. Introduction

Particle methods are distinguished by their robustness and adaptivity when they are applied to convection dominated flows. A prime example of particle methods applied to compressible hydrodynamics is the method of Smoothed Particle Hydrodynamics (SPH). Introduced in the 70's [1,2] SPH has been applied to a wide variety of problems ranging from incompressible flows to gas dynamics in astrophysics (see Ref. 3 and references therein).

SPH is based on the discretization of the extensive flow quantities of the governing equations by a set of Lagrangian particles. The method employs smooth kernels to evaluate explicitly the differential operators at the particle locations. As a consequence, in SPH one has to carry out neighbor searches and summations. The Lagrangian character of SPH allows its elements to track flow features but at the same time this results in non-uniform particle distributions that may be associated with areas of particle clustering and depletion. The non-uniform particle distribution may affect the computational efficiency and the accuracy of the method. Particle accretion and adaptivity control has motivated the development of repulsion models (see Ref. 4 and references therein). The particle repulsion forces introduce however spurious bulk and shear viscosity in particular for inviscid flows. Another remedy for the non-uniform particle distribution was introduced by periodically remeshing the particle locations. In remeshed SPH (rSPH)[5] a mesh is employed to periodically re-initialize the particle locations onto undistorted locations while particle strengths are determined via a particle-mesh interpolation. In rSPH besides the re-initialisation all differential operators are evaluated at the particle locations. Recent work[6,7] presented two dimensional simulations of compressible flows by using particles and an underlying mesh. A remeshing procedure remedies particle distortion and the mesh is utilized to discretize the differential operators. The present work extends this PMH technique to three dimensional compressible flows. The method does not detract from the adaptive character of SPH and allows for control of its accuracy. The accuracy of the method is demonstrated on an astrophysics benchmark problem.

This paper is organized as follows. In Section 2, we cover the governing equations and the related particle-based numerical methods. The hybrid particle-mesh method is presented in Section 3; its performance on an astrophysical test case is discussed in Section 4.

2. Hydrodynamics

2.1. *Governing equations*

We consider the Euler equations for a compressible, inviscid and adiabatic flow in conservative form

$$\begin{aligned} \frac{\mathcal{D}\rho}{\mathcal{D}t} &= 0 \\ \frac{\mathcal{D}\rho\mathbf{u}}{\mathcal{D}t} &= \rho\mathbf{f} - \nabla p \\ \frac{\mathcal{D}\rho E}{\mathcal{D}t} &= \rho\mathbf{f}\cdot\mathbf{u} - \nabla\cdot(p\mathbf{u}) \end{aligned} \tag{1}$$

where we defined

$$\frac{\mathcal{D}q}{\mathcal{D}t} = \frac{\partial q}{\partial t} + \nabla\cdot(q\mathbf{u}) \,, \tag{2}$$

and ρ, $\mathbf{u}$, E and $\mathbf{f}$ denote respectively the density, the velocity, the energy and body force fields. The conservation laws are completed with an equation of state, in this case the ideal gas model.

2.2. *Smoothed Particle Hydrodynamics*

In SPH, the particles weights do not involve the particle volume. The flow variables can be evaluated at any point through the evaluation of smooth interpolation kernels, here denoted by W, centered at the particle locations. This evaluation technique is extended to the derivatives of the flow variables, thus allowing the evaluation of the right-hand side of Eq. (1). This yields the following evolution equations for the particles

$$\frac{d\mathbf{x}_i}{dt} = \mathbf{u}_i \tag{3}$$

$$\frac{d\rho_i}{dt} = \sum_j m_j \mathbf{u}_{ij} \cdot \nabla_i W(\mathbf{r}_{ij}, h_{ij}) \tag{4}$$

$$\frac{d\mathbf{u}_i}{dt} = -\sum_j m_j \left(\frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2} + \Pi_{ij} \right) \nabla_i W(\mathbf{r}_{ij}, h_{ij}) \tag{5}$$

$$\frac{dU_i}{dt} = -\sum_j m_j \left(\frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2} + \Pi_{ij} \right) \mathbf{u}_{ij} \cdot \nabla_i W(\mathbf{r}_{ij}, h_{ij}) \tag{6}$$

where U is the internal energy, $\mathbf{r}_{ij} = \mathbf{x}_i - \mathbf{x}_j$, $\mathbf{u}_{ij} = \mathbf{u}_i - \mathbf{u}_j$, and h_{ij} is an average of the kernel radii h_i and h_j.

It is important to note that the kernel evaluations require a relatively costly neighbor search or neighbor list management for every particle. The artificial repulsion term Π_{ij} is introduced to reduce particle collisions. The Π_{ij} introduces artificial bulk and shear viscosities that are difficult to control. We refer to SPH reviews[8,4] for a detailed discussion of Π_{ij}. At the same time the repulsion forces, have a limited effect on the overall distortion of the elements. The resulting loss of smooth particle overlap greatly affects the accuracy of the method[9,10,11].

2.3. *Remeshed Smoothed Particle Hydrodynamics*

The adaptivity of computational elements in SPH has an important effect on the numerical dissipation of the method. Inspired by related work on Vortex Methods, recent works[5,12] have proposed remeshing to maintain adaptivity while reducing the artificial dissipation of SPH. Remeshing consists in the periodic regularization onto a grid of the particle set via high order interpolation. The relationship between the old and new particle weights, q_i and q_i', is then

$$q_i' = \sum_j q_j W(\mathbf{x}_j - \mathbf{x}_i, h) \tag{7}$$

where W is the interpolation kernel and h is the grid spacing. One popular scheme uses the tensor product of the so-called M_4' function

$$M_4'(x,h) = \begin{cases} 1 - \frac{5s^2}{2} + \frac{3s^3}{2} & 0 \le s < 1, \\ \frac{(1-s)(2-s)^2}{2} & 1 \le s < 2, \\ 0 & s \ge 2. \end{cases} \quad s = \frac{|x|}{h} \quad . \tag{8}$$

The rSPH constitutes a clear departure from the purely Lagrangian character of SPH. Adaptivity is not lost in rSPH however; it is more controlled, in a fashion consistent with AMR approaches or multilevel particle methods[13].

3. Particle Mesh Hydrodynamics

We consider a limiting case of rSPH where one carries out remeshing at every time-step. The particles then lie on a grid and the differential operators of the governing equations are computed by differentiating the particle kernels. In PMH this differentiation however can be performed more efficiently by using finite differences. In turn PMH is reminiscent of particle-in-cell (PIC) methods[14]. One key difference is that in PIC the particles are not re-initialized at each time step.

The system of Eq. (1) is split into an advection problem and an acoustic problem (indicated by *)

$$\frac{\mathcal{D}}{\mathcal{D}t}\begin{pmatrix}\rho\\ \rho\mathbf{u}\\ \rho E\end{pmatrix} = 0 \tag{9}$$

$$\frac{\partial}{\partial t}\begin{pmatrix}\rho^*\\ \rho^*\mathbf{u}^*\\ \rho^* E^*\end{pmatrix} = \begin{pmatrix}0\\ -\nabla p^*\\ -\nabla\cdot(p^*\mathbf{u}^*)\end{pmatrix} . \tag{10}$$

The advection step of Eq. (9) is carried out with particles, which do not need to interact. Over the substeps of a time integration scheme, the velocity field needs to be evaluated at the particle locations. This is achieved through mesh-to-particle interpolation, using $M_4'(8)$. At the end of the advection step, the initial condition to Eq. (10) is generated by a particle-to-mesh interpolation and the flow variables, now represented on the mesh can be advanced with finite differences for the pressure terms.

We note that the mesh controls the adaptivity of the method and provides the support for the fast evaluation of the pressure terms. PMH maintains a key feature of particle methods, namely unconditional linear stability. The non-linear stability condition requires that particles trajectories do not cross

$$\Delta t \leq C_1 \|\nabla\mathbf{u}\|_\infty^{-1} , \tag{11}$$

and there remains a CFL condition on the pressure terms

$$\Delta t \leq C_2 h c^{-1} \tag{12}$$

where $c = \sqrt{\gamma p/\rho}$ is the speed of sound. C_1 and C_2 are $\mathcal{O}(1)$ constants which depend on the time integration scheme. The numerical dissipation and dispersion of the method is determined by the type of particle-mesh interpolation. The presence of the grid allows for the incorporation of existing Eulerian models for artificial viscosity.

4. Results

We consider an astrophysics test-case which has been the subject of recent work[15] benchmarking SPH and Finite Volumes methods. The test case consists of a three-dimensional periodic flow of hot gas past a colder and denser cloud. The box size is $(2000, 2000, 8000)$kpc (1kpc = 1kiloparsec = $3.08568025\,10^{19}m$); the initial cloud is spherical, $r = 197\,\text{kpc}$, and centered in (x, y). The cloud has uniform temperature $T = 10^6 K$ and density $\rho = 3.13\,10^{-7} M_\odot\,\text{kpc}^{-3}$ ($M_\odot$ = mass of the sun $= 1.98892\,10^{30} kg$) while the surrounding medium is at $T = 10^7 K$, $\rho = 3.13\,10^{-8} M_\odot\,\text{kpc}^{-3}$ and a velocity of $10^3\,km\,s^{-1}$. We assume that it is an ideal gas, making these two media in pressure equilibrium. The gas is assumed to be atomic hydrogen with a heat capacity ratio $\gamma = 5/3$; the incoming flow is thus hypersonic at $M = 2.7$. We note that the initial condition is sampled from a slightly perturbed set of SPH particles, thus introducing noise.

Simulations were performed on a $256 \times 256 \times 1024$ mesh. The code is a client of the parallel particle mesh library (PPM)[a] [16]; it was run on 64 processors of a CRAY XT-3 at CSCS, Switzerland.

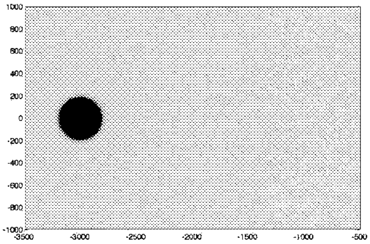
We present the evolution of the density field in Fig. 1. A bow shock forms rapidly upstream of the blob, while a system of expansions and shock waves develop downstream. The blob is accelerated and deformed to eventually mix with the main flow. Two instability mechanisms drive this mixing. In the early stages, the front of the blob is an accelerated density discontinuity with its density gradient aligned with the acceleration vector. It is thus subject to the Rayleigh-Taylor instability.Simultaneously, this geometry develops strong shear flows, which evolve into Kelvin-Helmholtz instabilities. The head-on view of Fig. 2 confirms the complexity and three-dimensionality of the instabilities.

In Fig. 3, we consider the evolutions of the cold cloud mass for simulations with PMH, SPH and an Adaptive Mesh Refinement (AMR)-capable, Finite Volume method with AMR disabled (we refer the reader to Ref. 15 for the descriptions of these last two codes). The cloud is defined as the region where $T < 9\,10^6 K$ and $\rho > 2\,10^{-7} M_\odot\,\text{kpc}^{-3}$. The results indicate that SPH has difficulties in controlling its dissipation and accuracy. While for SPH, the cloud remains cohesive, the FV and PMH results indicate a faster destruction and mixing with the free-stream. At the same time, we observe differences between PMH and FV. In the early stages, before the instabilities grow ($t < 2.0\,\text{Gyr}$), the cloud loses more mass in PMH than for the other methods. The FV method also allows higher instability modes leading to the faster destruction of the cloud.

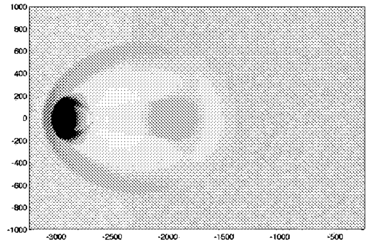
5. Conclusion

We have presented a hybrid particle-mesh method for simulations of compressible hydrodynamics. The method exploits the performance of Lagrangian methods to

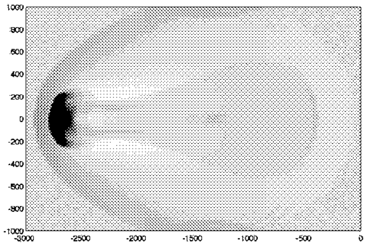
[a]the PPM library is available at www.cse-lab.ethz.ch



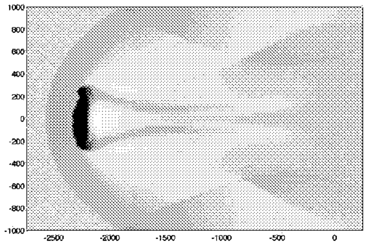
(a) $t = 0.0$



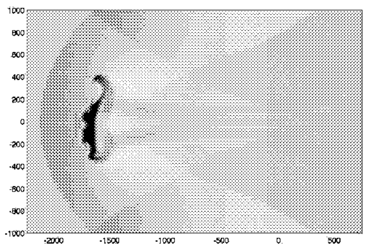
(b) $t = 1.0$



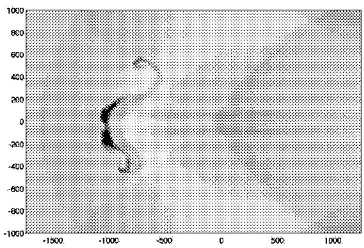
(c) $t = 2.0$



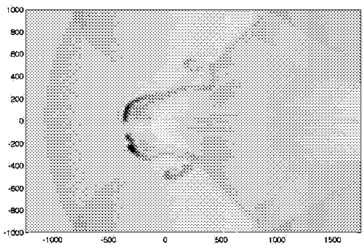
(d) $t = 3.0$



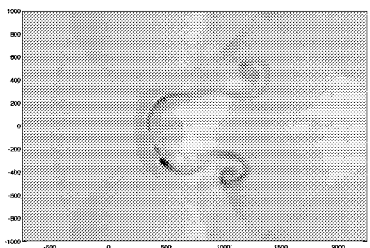
(e) $t = 4.0$



(f) $t = 5.0$

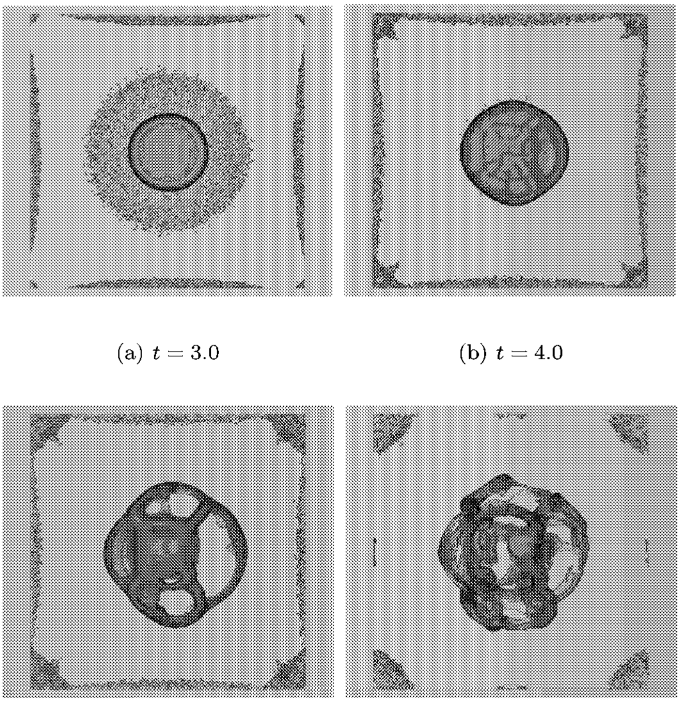


(g) $t = 6.0$



(h) $t = 7.0$

Fig. 1. Astrophysics test-case: density in the symmetry plane; color range: white $\rho = 0$, black $\rho = 2e^{-7}\, M_{\odot}\, \mathrm{kpc}^{-3}$; free-stream coming from the left.



(a) $t = 3.0$ (b) $t = 4.0$

(c) $t = 5.0$ (d) $t = 6.0$

Fig. 2. Astrophysics test-case: iso-density surfaces, view from upstrea.m

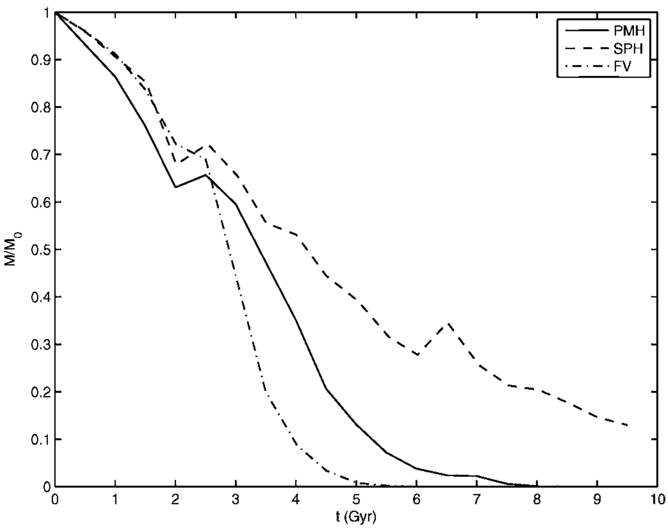


Fig. 3. Astrophysics test-case: time evolution of the cloud mass for three methods, PMH, SPH and Eulerian.

tackle advection and the efficiency of finite differences for the evaluation of Eulerian differential operators.

The results on an astrophysics benchmark problem reveal the dissipation and dispersion of the method. PMH is found to be superior to SPH in both aspects as SPH can not indeed capture the instabilities. Additional tests[15] showed that in SPH, a decreased numerical viscosity destabilizes the cloud only marginally and generates unphysical noise and structures.

Present work involves the extension of PMH to multiresolution and adaptive mesh refinement methods[17]. Future work will include investigation of remeshing schemes with TVD properties and the translation of artificial dissipation and flux limiters to the PMH framework.

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