Smoothed particle hydrodynamics: checking a tensor approach to calculating gradients

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Abstract

We describe and check a novel formulation of Smoothed Particle Hydrodynamics (SPH) based on an Integral Approach to the Derivatives, called IAD_0 , that can be applied to simulate astrophysical systems. The method relies in a tensor approach to calculating gradients, which is more accurate than the standard procedure (STD), due to its better renormalization properties. The proposed scheme fully conserves momentum and energy in isentropic flows, and is less susceptible to the pairing instability. The resulting algorithm is verified using two tests: a two-dimensional simulation of the Kelvin-Helmholtz instability and the three-dimensional simulation of the merging of two polytropes. The analysis of these test cases suggests that the method is able to improve the results of the standard technique with only a moderate computational overload.

1 Introduction

Nowadays, multidimensional numerical hydrodynamics is one of the most powerful tools to approach astrophysical problems. Among them, the Smoothed Particle Hydrodynamics (SPH) is one of the preferred techniques because of its ability to describe the evolution of fluids with complicated geometries and diversity of length scales. Formulated more than thirty years ago, by [4] and [5], it has largely evolved during the last decade, making it an interesting alternative to grid based methods of Eulerian type. Details of the modern mathematical formulation can be found in the recent review by [6].

It has been recently suggested by [3] and [1] that the use of matrix methods [2] in Astrophysics could improve the simulations with the SPH technique, and with an affordable computational cost. The good behavior of IAD_0 to describe hydrodynamic instabilities is first highlighted in connection to the growth of the Kelvin-Helmholtz instability (KHI) in a parallel shear flow subjected to a small perturbation in the transverse velocity field. We also check the ability of IAD₀ to describe a very dynamical situation by simulating the coalescence of two polytropes. In this case, a catastrophic merging of the stars ensues after a few orbital periods. For this test, the tensor method gives results of comparable quality as those obtained using the standard SPH scheme, but displaying a more homogeneous mixing of the material of both stars.

2 Mathematical foundations of the IAD_0 approach

As stated in [3] and [1], the new scheme relies in the integral,

$$I(\mathbf{r}) = \int_{V} \left[f(\mathbf{r}') - f(\mathbf{r}) \right] (\mathbf{r}' - \mathbf{r}) W(|\mathbf{r}' - \mathbf{r}|, h) dr'^{3}, \qquad (1)$$

where $W(|\mathbf{r'} - \mathbf{r}|, h)$ is a spherically symmetric interpolating function and h is called the smoothing length. The IAD₀ interpretation of SPH is the consequence of approaching Eq. (1) with summations along with two reasonable simplifications,

$$f(\mathbf{r_b}) - f(\mathbf{r_a}) \simeq \nabla \mathbf{f_a} \cdot (\mathbf{r_b} - \mathbf{r_a}),$$
 (2)

where a and b refer to neighbor particles with masses m_a and m_b respectively, and

$$I(\mathbf{r}_{\mathbf{a}}) \simeq \sum_{b} \frac{m_{b}}{\rho_{b}} f(\mathbf{r}_{\mathbf{b}})(\mathbf{r}_{\mathbf{b}} - \mathbf{r}_{\mathbf{a}}) W(|\mathbf{r}_{\mathbf{b}} - \mathbf{r}_{\mathbf{a}}|, h_{a}), \qquad (3)$$

is the corresponding discrete expression for Eq. (1). Direct application of Eqs. (1), (2) and (3) to calculating the gradient of density, leads to a matrix equation,

$$\begin{bmatrix} \partial \rho / \partial x_1 \\ \partial \rho / \partial x_2 \\ \partial \rho / \partial x_3 \end{bmatrix}_a = \begin{bmatrix} \tau_{11} & \tau_{12} & \tau_{13} \\ \tau_{21} & \tau_{22} & \tau_{23} \\ \tau_{31} & \tau_{32} & \tau_{33} \end{bmatrix}^{-1} \begin{bmatrix} I_1 \\ I_2 \\ I_3 \end{bmatrix},$$
(4)

where

$$\tau_{ij,a} = \sum_{b} \frac{m_b}{\rho_b} (x_{i,b} - x_{i,a}) (x_{j,b} - x_{j,a}) W_{ab}(h_a) \, ; \, i, j = 1, 3 \, , \tag{5}$$

and

$$I_{k,a} = \sum_{b} m_b \, (x_{k,b} - x_{k,a}) W_{ab}(h_a) \, ; \, k = 1, 3 \, . \tag{6}$$

It was shown in [3] that Eq. (4) leads to a formulation of the SPH Euler equations compatible with the variational principle,

$$\rho_a = \sum_{b=1}^{n_b} m_b W_{ab}(|\mathbf{r_b} - \mathbf{r_a}|, h_a), \qquad (7)$$

$$\ddot{x}_{i,a} = -\sum_{b=1}^{n_b} m_b \left(\frac{P_a}{\Omega_a \rho_a^2} \mathcal{A}_{i,ab}(h_a) + \frac{P_b}{\Omega_b \rho_b^2} \mathcal{A}'_{i,ab}(h_b) + \Pi_{ab} \ \tilde{\mathcal{A}}_{i,ab} \right) , \tag{8}$$

$$\left(\frac{du}{dt}\right)_a = \sum_{b=1}^{n_b} \sum_{i=1}^d m_b(v_{i,a} - v_{i,b}) \left(\frac{P_a}{\Omega_a \ \rho_a^2} \ \mathcal{A}_{i,ab}(h_a) + \frac{\Pi_{ab}}{2} \ \widetilde{\mathcal{A}}_{i,ab}\right) , \tag{9}$$

where $\mathcal{A}_{i,ab}$ is

$$\mathcal{A}_{i,ab}(h_a) = \sum_{j=1}^d c_{ij,a}(h_a)(x_{j,b} - x_{j,a})W_{ab}(h_a), \qquad (10)$$

being c_{ij} the coefficients of the inverse matrix defined in Eq. (4), d the dimension of the space and $\widetilde{\mathcal{A}}$ is the arithmetic mean of \mathcal{A} and \mathcal{A}' . As usual, Π_{ab} gives the viscous pressure due to the artificial viscosity (AV) and Ω accounts for the gradient of the the smoothing length [6]. Therefore, Eqs. (7), (8) and (9) summarize the basis of the IAD₀ formalism. Any expression of standard SPH can be made compatible with IAD₀ just taking the kernel derivative as,

$$\frac{\partial W_{ab}(h_a)}{\partial x_{i,a}} = \mathcal{A}_{i,ab}(h_a); i = 1, 3.$$
(11)

If the matrix coefficients in Eq. (4) are calculated analytically, the matrix \mathcal{T} becomes diagonal. In that case, it can be shown that for Gaussian kernels the standard and *IAD* descriptions are equivalent.

3 Simulating the Kelvin-Helmhotz instability

The ability of any hydrocode to simulate the growth of the KHI has become one of the most popular test in computational fluid dynamics. This instability appears when there is a sufficient velocity shear in the interface layer between two fluids with different densities. Small perturbations of the velocity field in the orthogonal direction to the interface grow up, leading to a mixing of both fluids. This is usually simulated in a box with periodic boundary conditions, where two fluid regions are defined with densities ρ_1 and ρ_2 respectively. Both layers have opposite parallel velocities leading to a shear discontinuity in the contact interface. In order to develop the instability a small perturbation is seeded in the interface as a sinusoidal mode of length scale λ .

We have simulated a central band of high density fluid (ρ_1) moving in a low-density medium (ρ_2) in a squared lattice of 1 cm side in the XY plane using N = 62500 particles. The mass of the particles was arranged in order to obtain the correct density profile following a ramp function [3]. In this way we smoothed the interface density jump to make it comparable to the SPH resolution using

$$f(y) = \frac{1}{A} \frac{1}{1 + \exp\frac{2(y - 0.25)}{\Delta y}} \frac{1}{1 + \exp\frac{2(0.75 - y)}{\Delta y}},$$
(12)



Figure 1: Evolution of the KHI (see the text for the explanation of the meaning of each row).

where A is a normalization constant and $\Delta y = 0.05$ cm. The density profile is given by

$$\rho(y) = \rho_2 + (\rho_1 - \rho_2) f(y), \qquad (13)$$

where $\rho_1 = 2 \text{ g cm}^{-3}$ and $\rho_2 = 1 \text{ g cm}^{-3}$. The seed of the perturbation is obtained using a sinusoidal function for the v_y component of the velocity field,

$$v_x(y) = v_2 + (v_1 - v_2) f(y), \qquad v_y(x) = \Delta v_y \sin(n\pi x),$$
(14)

where we took n = 2, $\Delta v_y = 0.1$ cm s⁻¹, $v_1 = 0.5$ cm s⁻¹ and $v_2 = -0.5$ cm s⁻¹, which corresponds to the high and low density bands respectively. Fig. 1 shows four snapshots of the growth of the Kelvin-Helmholtz instability at different times (t = 0, 0.1, 1, 2 and 3 s) for the calculation using IAD₀ (first row) and the standard SPH implementation (second row). As it can be seen the standard formulation does a poor job resolving the structure of the instability. In the case of the tensor calculation the instability grows cleanly and at good rate, and the definition of the extremes of the billows, where the finest structure appears, is clearly enhanced. To achieve similar results to those obtained with the IAD₀ technique, different methods have been proposed to maintain the standard description, mainly based on including an artificial thermal conductivity [6]. In order to test the tensor approach in a harder scenario, we diminished the amplitude of the initial perturbation an order of magnitude (i.e. $\Delta v_y = 0.01$ cm s⁻¹). In third and fourth rows of Fig. 1 we show the results of the simulations using the schemes IAD₀ and STD, for times t = 0, 1, 3, 4 and 5 s. It is clear that in the standard formulation the instability was unable to grow, while it does using IAD₀.



Figure 2: Density color map of the merging process of two stars as calculated with IAD₀ (upper row) at times t = 0.31P, t = 2.8P and t = 4.3P (P = 29.3 s), and STD at t = 0.23P, t = 2.15P and t = 3.3P (lower row).

Changing the geometry of the initial particle setting from square to an hexagonal lattice or reducing the size of h taking less neighbors, did not appreciably alter the results.

4 Merging of two polytropes

We have simulated the merging of two twin polytropes with index n = 3/2 and mass 0.6 M_{\odot} with both, the IAD₀ and STD schemes. Both stars were put in a circular rigid rotation orbit in the plane XY with radius $r_{orb}^0 = 1.5 R_s$ (being $R_s = 8000$ km, the theoretical surface radius of the polytrope) from the center of mass of the system. To enforce the coalescence, a braking force proportional to the velocity was imposed during the first revolution period, P = 29.3 s. In Fig. 2 it is shown the density color map of both stars in the orbital plane as obtained with IAD₀ and STD schemes respectively. On the whole, the behavior is rather similar, although the coalescence evolves at slower pace for the matrix method.

An important challenge for the hydrocodes is to adequately represent the mix of the advected material during the coalescence process. In our system the initial conditions are fully symmetric. Therefore, one would expect that few minutes after the merging the core is homogeneously composed with material of both stars. Fig. 3 (center and right) depicts the approximate distribution of the gas belonging to each star one minute after the catastrophic stage of the coalescence process. As we can see, material of both stars is much better mixed in the IAD₀ calculation than in the standard one. We want to stress that the recipe to handle with the AV is exactly the same in both calculations. Therefore, the larger mixing in the IAD₀ calculation is due to the enhanced treatment of the gradients. Fig. 3 (left) shows the angular velocity profile of the particles in the orbital plane as a function of their mass coordinate.



Figure 3: Angular velocity profiles at $t \simeq 220$ s (left). Mixing of material of both stars in the core of the remnant for IAD₀ (center), and standard SPH (right).

As we can see, the standard calculation predicts rigid rotation for $M_r < 0.8 \,\mathrm{M_{\odot}}$, followed by a Keplerian velocity distribution beyond that point. At distances $M_r > 1 \,\mathrm{M_{\odot}}$ the velocity profile obtained with IAD₀ is also Keplerian, but below that point rigid rotation is never attained. In the standard calculation, the high amount of viscosity, which prevents the mix of the core, is coupling the different layers of the fluid so that the system rapidly approaches rigid rotation. However, the time delay for core synchronization in nature is a function of the real physical viscosity. In the simulations the synchronization time is artificially shortened by the much larger numerical viscosity of the codes.

5 Conclusions

A novel scheme to calculating gradients in SPH has been proposed and checked. The results of the simulations suggest that the method provides a better description of hydrodynamic instabilities and a better mixing of gas during the merging process of stellar objects.

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