Enhancing SPH using Moving Least-Squares and Radial Basis Functions*

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Summary. In this paper we consider two sources of enhancement for the meshfree Lagrangian particle method *smoothed particle hydrodynamics* (SPH) by improving the accuracy of the particle approximation. Namely, we will consider *shape functions* constructed using: moving least-squares approximation (MLS); radial basis functions (RBF). Using MLS approximation is appealing because polynomial consistency of the particle approximation can be enforced. RBFs further appeal as they allow one to dispense with the *smoothing-length* – the parameter in the SPH method which governs the number of particles within the support of the shape function. Currently, only ad hoc methods for choosing the smoothing-length exist. We ensure that any enhancement retains the conservative and meshfree nature of SPH. In doing so, we derive a new set of variationally-consistent hydrodynamic equations. Finally, we demonstrate the performance of the new equations on the Sod shock tube problem.

1 Introduction

Smoothed particle hydrodynamics (SPH) is a meshfree Lagrangian particle method primarily used for solving problems in solid and fluid mechanics (see [10] for a recent comprehensive review). Just some of the attractive characteristics that SPH possesses include: the ability to handle problems with large deformation, free surfaces and complex geometries; truly meshfree nature (no background mesh required); exact conservation of momenta and total energy. On the other hand, SPH suffers from several drawbacks: an instability in tension; difficulty in enforcing essential boundary conditions; fundamentally based on inaccurate kernel approximation techniques. This paper addresses the last of these deficiencies by suggesting improved particle

approximation procedures. Previous contributions in this direction (reviewed in [2]) have focused on corrections of the existing SPH particle approximation (or its derivatives) by enforcing polynomial consistency. As a consequence, the conservation of relevant physical quantities by the discrete equations is usually lost.

The outline of the paper is as follows. In the next section we review how the SPH equations for the non-dissipative motion of a fluid can be derived. In essence this amounts to a discretization of the Euler equations:

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = -\rho \nabla \cdot v, \qquad \frac{\mathrm{d}v}{\mathrm{d}t} = -\frac{1}{\rho}\nabla P, \qquad \frac{\mathrm{d}e}{\mathrm{d}t} = -\frac{P}{\rho}\nabla \cdot v, \qquad (1)$$

where $\frac{\mathrm{d}}{\mathrm{d}t}$ is the total derivative, ρ, v, e and P are the density, velocity, thermal energy per unit mass and pressure, respectively. The derivation is such that important conservation properties are automatically satisfied by the discrete equations. Within the same section we derive a new set of variationally-consistent hydrodynamic equations based on improved particle approximation. In Sect. 3 we construct specific examples – based on moving least-squares approximation and radial basis functions – to complete the newly derived equations. The paper finishes with Sect. 4 where we demonstrate the performance of the new methods on the Sod shock tube problem [12] and make some concluding remarks.

To close this section, we briefly review the SPH particle approximation technique on which the SPH method is fundamentally based and which we purport to be requiring improvement. From a set of scattered particles $\{x_1, \ldots, x_N\} \subset \mathbb{R}^d$, SPH particle approximation is achieved using

$$Sf(x) = \sum_{j=1}^{N} f(x_j)\frac{m_j}{\rho_j}W(|x - x_j|, h), \qquad (2)$$

where m_j and ρ_j denotes the mass and density of the jth particle, respectively. The function W is a normalised kernel function which approximates the δ-distribution as the *smoothing-length*, h, tends to zero. The function $\frac{m_j}{\rho_j}W(|x - x_j|, h)$ is called an SPH *shape function* and the most popular choice for W is a compactly supported cubic spline kernel with support $2h$. The parameter h governs the extent to which contributions from neighbouring particles are allowed to smooth the approximation to the underlying function f. Allowing a spatiotemporally varying smoothing-length increases the accuracy of an SPH simulation considerably. There are a selection of ad hoc techniques available to accomplish this, although often terms arising from the variation in h are neglected in the SPH method. The approximating power of the SPH particle approximation is perceived to be poor. The SPH shape functions fail to provide a partition of unity so that even the constant function is not represented exactly. There is currently no approximation theory available for SPH particle approximation when the particles are in general positions. The result of a

shock tube simulation using the SPH equations derived in Sect. 2 is shown in Fig. 1 (see Sect. 4 for the precise details of the simulation). The difficulty
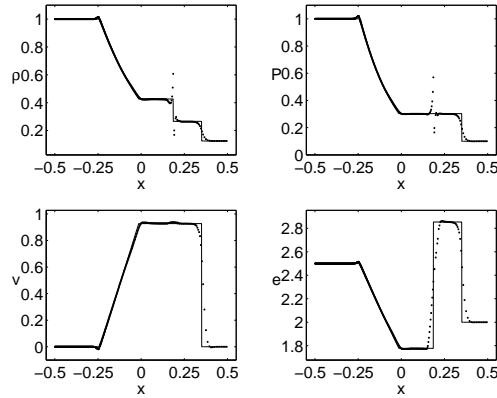
Fig. 1. Shock tube simulation (t=0.2) using SPH.

that SPH has at the contact discontinuity ($x \approx 0.2$) and at the head of the rarefaction wave ($x \approx -0.25$) is attributed to a combination of the approximation (2) and the smoothing-length not being self-consistently incorporated.

2 Variationally-Consistent Hydrodynamic Equations

It is well known (see [10] and the references cited therein) that the most common SPH equations for the non-dissipative motion of a fluid can be derived using the Lagrangian for hydrodynamics and a variational principle. In this section we review this procedure for a particular formulation of SPH before deriving a general set of variationally-consistent hydrodynamic equations.

The aforementioned Lagrangian is a particular functional of the dynamical coordinates: $L(x, v) = \int \rho(v^2/2 - e)\,\mathrm{d}x$, where x is the position, v is the velocity, ρ is the density, e is the thermal energy per unit mass and the integral is over the volume being discretized. Given N particles $\{x_1 \ldots, x_N\} \subset \mathbb{R}^d$, the SPH discretization of the Lagrangian, also denoted by L, is given by

$$L = \sum_{j=1}^{N} m_j \left(\frac{v_j^2}{2} - e_j \right), \tag{3}$$

where m_j has replaced $\rho_j V_j$ to denote particle mass (assumed to be constant), and V_j is a volume associated with each particle. Self-evidently, the notation f_j is used to denote the function f evaluated at the jth particle.

To obtain the SPH equations of motion, one can appeal to a variational principle – the principle of stationary action, the *action* being the time integral

of L. To do this we require a constraint on density which we obtain by discretizing the first equation of (1) using (2). By assuming that the SPH shape functions form a partition of unity we commit error but are able to artificially provide the discretization with invariance to a constant shift in velocity (Galilean invariance):

$$\frac{\mathrm{d}\rho_i}{\mathrm{d}t} = -\rho_i \sum_{j=1}^{N} \frac{m_j}{\rho_j}(v_j - v_i) \cdot \nabla_i W(|x_i - x_j|, h_i), \qquad i = 1, \ldots, N, \quad (4)$$

where ∇_i is the gradient with respect to the coordinates of the ith particle.

Omitting the detail, see [10] for example, the equations of motion that are variationally-consistent with (4) is

$$\frac{\mathrm{d}v_i}{\mathrm{d}t} = -\frac{1}{\rho_i} \sum_{j=1}^{N} \frac{m_j}{\rho_j}\Big(P_i \nabla_i W(|x_i - x_j|, h_i) + P_j \nabla_i W(|x_i - x_j|, h_j)\Big), \quad (5)$$

for $i = 1, \ldots, N$, where P_i denotes the pressure of the ith particle (provided via a given equation of state). Using the first law of thermodynamics, the equation for the rate of change of thermal energy is given by

$$\frac{\mathrm{d}e_i}{\mathrm{d}t} = \frac{P_i}{\rho_i^2} \frac{\mathrm{d}\rho_i}{\mathrm{d}t}, \qquad i = 1, \ldots, N. \tag{6}$$

A beneficial consequence of the Lagrangian approach to SPH is that one automatically preserves, in the discrete equations (4)–(6), fundamental properties of the original system (1). Indeed, by virtue of (4) being Galilean invariant, one is guaranteed to conserve linear momentum and total energy (assuming perfect time integration). Angular momentum is also a conserved quantity.

Now, we propose to enhance SPH by improving the particle approximation (2). Suppose we have constructed shape functions ϕ_j that provide at least a partition of unity. With these shape functions we form a quasi-interpolant:

$$Sf = \sum_{j=1}^{N} f(x_j)\phi_j, \tag{7}$$

which we implicitly assume provides superior approximation quality than that provided by (2). We defer particular choices for ϕ_j until the next section. The discretization of the continuity equation now reads

$$\frac{\mathrm{d}\rho_i}{\mathrm{d}t} = -\rho_i \sum_{j=1}^{N}(v_j - v_i) \cdot \nabla\phi_j(x_i), \qquad i = 1, \ldots, N, \tag{8}$$

where, this time, we have supplied genuine Galilean invariance, without committing an error, using the partition of unity property of ϕ_j. As before, the principle of stationary action provides the equations of motion and

conservation properties of the resultant equations reflect symmetries present in the constraint equation (8).

To obtain (3), two assumptions were made. Firstly, the SPH shape functions were assumed to form a sufficiently good partition of unity. Secondly, it was assumed that the kernel approximation $\int f W(|\cdot - x_j|, h)\, \mathrm{d}x \approx f(x_j)$, was valid. For our general shape functions the first of these assumptions is manifestly true. The analogous assumption we make to replace the second is that the error induced by the approximations

$$\int f \phi_j \, \mathrm{d}x \approx f_j \int \phi_j \, \mathrm{d}x \approx f_j V_j, \qquad j = 1, \ldots, N, \tag{9}$$

is negligible. With the assumption (9), the approximate Lagrangian associated with ϕ_j is identical in form to (3). Neglecting the details once again, which can be recovered from [10], the variationally-consistent equations of motion are

$$\frac{\mathrm{d}v_i}{\mathrm{d}t} = \frac{1}{m_i} \sum_{j=1}^{N} \frac{m_j}{\rho_j} P_j \nabla \phi_i(x_j), \qquad i = 1, \ldots, N, \tag{10}$$

with the thermal energy equation obtained in the same manner as before (6).

Linear momentum and total energy are automatically conserved by the new equations, and this can be verified immediately using the partition of unity property of ϕ_j. If it is also assumed that the shape functions reproduce linear polynomials, namely, $\sum x_j \phi_j(x) = x$, then it is simple to verify that angular momentum is also conserved.

The equations (6), (8) and (10) constitute a new set of variationally-consistent hydrodynamic equations. These equations give rise to the formulation of SPH derived earlier under the transformation $\phi_j(x_i) \mapsto \frac{m_j}{\rho_j} W(|x_i - x_j|, h_i)$. The equations of motion (10) appear in [8] but along side variationally-inconsistent companion equations. The authors advocate using a variationally-consistent set of equation because evidence from the SPH literature [3, 9] and suggests that not doing so can lead to poor numerical results.

3 Moving Least-Squares and Radial Basis Functions

In this section we construct quasi-interpolants of the form (7). In doing so we furnish our newly derived hydrodynamic equations (6), (8) and (10) with several examples.

Moving least-squares (MLS). The preferred construction for MLS shape functions, the so-called Backus–Gilbert approach [4], seeks a quasi-interpolant of the form (7) such that:

- $Sp = p$ for all polynomials p of some fixed degree;
- $\phi_j(x)$, $j = 1, \ldots, N$, minimise the quadratic form $\sum \phi_j^2(x) \left[w\left(\frac{|x - x_j|}{h} \right) \right]^{-1}$,

where w is a fixed *weight function*. If w is continuous, compactly supported and positive on its support, this quadratic minimisation problem admits a unique solution. Assuming f has sufficient smoothness, the order of convergence of the MLS approximation (7) directly reflects the degree of polynomial reproduced [14].

The use of MLS approximation in an SPH context has been considered before. Indeed, Belytschko et al. [2] have shown that correcting the SPH particle approximation up to linear polynomials is equivalent to an MLS approximation with $w(|\cdot - x_j|/h) = W(|\cdot - x_j|, h)$. There is no particular reason to base the MLS approximation on an SPH kernel. We find that MLS approximations based on Wendland functions [13], which have half the natural support of a typical SPH kernel, produce results which are less noisy. Dilts [7, 8] employs MLS approximation too. Indeed, in [7], Dilts makes an astute observation that addresses an inconsistency that arises due to (9) – we have the equations

$$\frac{\mathrm{d}V_i}{\mathrm{d}t} = V_i \sum_{j=1}^{N} (v_j - v_i) \cdot \nabla \phi_j(x_i, h_i) \qquad \text{and} \qquad \frac{\mathrm{d}V_i}{\mathrm{d}t} \approx \frac{\mathrm{d}}{\mathrm{d}t}\left(\int \phi_i(x, h)\,\mathrm{d}x \right).$$

Dilts shows that if h_i is evolved according to $h_i \propto V_i^{1/d}$ then there is agreement between the right-hand sides of these equations when a one-point quadrature of $\int \phi_i\,\mathrm{d}x$ is employed. Thus, providing some theoretical justification for choosing this particular variable smoothing-length over other possible choices.

Radial basis functions (RBFs). To construct an RBF interpolant to an unknown function f on $x_1, \ldots, x_N$, one produces a function of the form

$$If = \sum_{j=1}^{N} \lambda_j \psi(|\cdot - x_j|), \tag{11}$$

where the λ_j are found by solving the linear system $(If)(x_i) = f(x_i)$, $i = 1, \ldots, N$. The *radial basis function*, ψ, is a pre-specified univariate function chosen to guarantee the solvability of this system. Depending on the choice of ψ, a low degree polynomial is sometimes added to (11) to ensure solvability, with the additional degrees of freedom taken up in a natural way. This is the case with the *polyharmonic splines*, for which

$$\psi(r) \doteq \begin{cases} r^{2m-d} \log r & \text{if } d \text{ is even,} \\ r^{2m-d} & \text{otherwise,} \end{cases} \qquad r \geq 0, \ m > \frac{d}{2},$$

and a polynomial of degree $m-1$ is added. The choice $m \geq 2$ ensures the RBF interpolant reproduces linear polynomials as required for angular momentum to be conserved by the equations of motion. As with MLS approximation, one has certain strong assurances regarding the quality of the approximation induced by the RBF interpolant (e.g. [6] for the case of polyharmonic splines).

In its present form (11), the RBF interpolant is not directly amenable. One possibility is to rewrite the interpolant in *cardinal form* so that it coincides with (7). This naively constitutes much greater computational effort. However, there are several strategies for constructing approximate cardinal RBF shape functions (e.g. [5]) and fast evaluation techniques (e.g. [1]) which reduce this work significantly. The perception of large computational effort is an attributing factor as to why RBFs have not been considered within an SPH context previously. Specifically for polyharmonic splines, another possibility is to construct shape functions based on discrete m-iterated Laplacians of ψ. This is sensible because the continuous iterated Laplacian, when applied ψ, results in the δ-distribution (up to a constant). This is precisely the approach we take in Sect. 4 where we employ cubic B-spline shape functions for one of our numerical examples. The cubic B-splines are discrete bi-Laplacians of the shifts of $|\cdot|^3$, and they gladly reproduce linear polynomials.

In addition to superior approximation properties, using globally supported RBF shape functions has a distinct advantage. One has dispensed with the smoothing-length entirely. Duely, issues regarding how to correctly vary and self-consistently incorporate the smoothing-length vanish. Instead, a natural 'support' is generated related to the relative clustering of particles.

4 Numerical Results

In this section we demonstrate the performance of the scheme (6), (8) and (10) using both MLS and RBF shape functions. The test we have selected has become a standard one-dimensional numerical test in compressible fluid flow – the Sod shock tube [12]. The problem consists of two regions of ideal gas, one with a higher pressure and density than the other, initially at rest and separated by a diaphragm. The diaphragm is instantaneously removed and the gases allowed to flow resulting in a rarefaction wave, contact discontinuity and shock. We set up 450 equal mass particles in $[-0.5, 0.5]$. The gas occupying the left-hand and right-hand sides of the domain are given initial conditions $(P_L, \rho_L, v_L) = (1.0, 1.0, 0.0)$ and $(P_R, \rho_R, v_R) = (0.1, 0.125, 0.0)$, respectively. The initial condition is not smoothed.

With regards to implementation, artificial viscosity is included to prevent the development of unphysical oscillations. The form of the artificial viscosity mimics that of the most popular SPH artificial viscosity and is applied with a switch which reduces the magnitude of the viscosity by a half away from the shock. A switch is also used to administer an artificial thermal conductivity term, also modelled in SPH. Details of both dissipative terms and their respective switches can be accessed through [10]. Finally, we integrate, using a predictor–corrector method, the equivalent hydrodynamic equations

$$\frac{\mathrm{d}V_i}{\mathrm{d}t} = V_i \sum_{j=1}^{N} (v_j - v_i) \cdot \nabla \phi_j(x_i), \tag{12}$$

$$\frac{\mathrm{d}v_i}{\mathrm{d}t} = \frac{1}{m_i} \sum_{j=1}^{N} V_j P_j \nabla \phi_i(x_j), \qquad \frac{\mathrm{d}e_i}{\mathrm{d}t} = -\frac{P_i}{m_i} \frac{\mathrm{d}V_i}{\mathrm{d}t},$$

together with $\frac{\mathrm{d}x_i}{\mathrm{d}t} = v_i$, to move the particles. To address the consistency issue regarding particle volume mentioned earlier – which is partially resolved by evolving h in a particular way when using MLS approximation – we periodically update the particle volume predicted by (12) with $\int \phi_i \, \mathrm{d}x$ if there is significant difference between these two quantities. To be more specific, the particle volume V_i is updated if $|V_i - \int \phi_i \, \mathrm{d}x|/V_i \geq 1.0 \times 10^{-3}$.

We first ran a simulation with linearly complete MLS shape functions. The underlying univariate function, w, was selected to be a Wendland function with C^4-smoothness. The smoothing-length was evolved by taking a time derivative of the relationship $h_i \propto V_i$ and integrating it alongside the other equations, the constant of proportionality was chosen to be 2.0. The result is shown in Fig. 2. The agreement with the analytical solution (solid line)
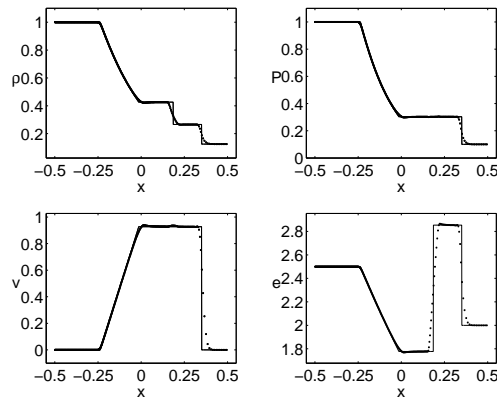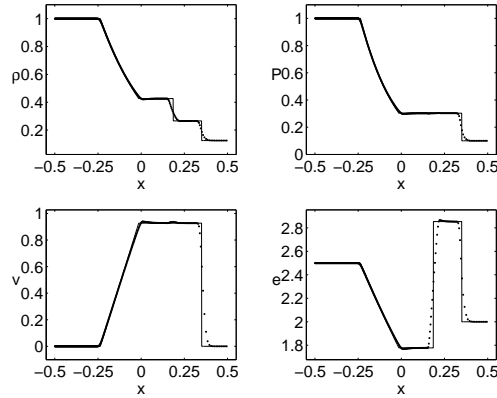

Fig. 2. Shock tube simulation (t=0.2) using linearly complete MLS shape functions.

is excellent, especially around the contact discontinuity and the head of the rarefaction wave. Next, we constructed RBF shape functions. As we mentioned in Sect. 3, for this one-dimensional problem we employ cubic B-spline because they constitute discrete bi-Laplacians of the shifts of the globally supported basis function, $\psi = |\cdot|^3$. The result of this simulation is shown in Fig. 3. Again, the agreement with the analytical solution is excellent.

In the introduction an SPH simulation of the shock tube was displayed (Fig. 1). There, we integrated (4)–(6) and h was updated by taking a time derivative of the relationship $h_i = 2.0 m_i/\rho_i$. To keep the comparison fair, the same initial condition, particle setup and dissipative terms were used. As previously noted, this formulation of SPH performs poorly on this problem, especially around the contact discontinuity. Furthermore, we find that this formulation of SPH does not converge in the L_∞-norm for this problem. In

Fig. 3. Shock tube simulation (t=0.2) using cubic B-spline shape functions.

Fig. 4 we have, at a fixed time ($t = 0.2$), plotted number of particles, N, versus L_∞-error in pressure, in the region of the computational domain where the solution is smooth, for the described MLS, RBF and SPH simulations. An approximation order of around 2/3, attributed to the low regularity of the
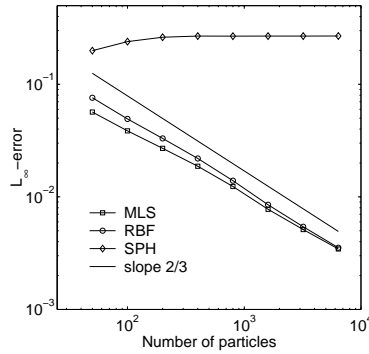
Fig. 4. N versus L_∞-error in pressure away from the shock ($t = 0.2$).

analytical solution, is observed for the MLS and RBF methods, whereas our SPH simulations show no convergence. This is not to say that SPH can not perform well on this problem. Indeed, Price [11] shows that, for a formulation of SPH where density is calculated via summation and variable smoothing-length terms correctly incorporated, the simulation does exhibit convergence in pressure. The SPH formulation we have used is fair for comparison with the MLS and RBF methods since they all share a common derivation. In particular, we are integrating the continuity equation in each case.

To conclude, this paper has proposed a new set of discrete conservative variationally-consistent hydrodynamic equations based on a partition of unity.

These equations, when actualised with MLS and RBF shape functions, outperform the SPH method on the Sod shock tube problem. Further experimentation and numerical analysis of the new methods is a goal for the future work of the authors.

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