Addendum to “On the consistency of MPS”

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Abstract
The analogies between the Moving Particle Semi-implicit method (MPS) and Incompressible Smoothed Particle Hydrodynamics method (ISPH) are established in this note, as an extension of the MPS consistency analysis conducted in Souto-Iglesias et al., Computer Physics Communications, 184(3), 2013.

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1. Introduction
Smoothed Particle Hydrodynamics (SPH) method started in the seventies [1] and was applied in the early nineties to free-surface flows using an explicit approach with a weakly compressible fluid model to numerically simulate liquid behavior [2]. In the mid nineties, the Moving Particle Semi-implicit method (MPS) appeared [3, 4] imposing incompressibility with a projection scheme [5]. Slightly later, 1999, a similar approach was followed by Cummins and Rudman to obtain the first incompressible SPH (ISPH) model [6, 7]. Although two MPS references were cited, no clear connections between ISPH and MPS were established. A similar treatment was given to MPS in the posterior ISPH literature (e.g. [8, 9, 10]). In our opinion such MPS-SPH connections are clear after the equivalence between SPH and MPS approximation to first and second order differential operators was established in [11]. Because these operators are

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the ones that play a major role in projection schemes, this addendum to [11] aims at clarifying the relationship between ISPH and MPS methods. With this main goal set, this note is organized as follows: first the projection scheme is reviewed, second, the MPS and ISPH implementations are discussed and finally links between them are established.

2. Projection fundamentals

This section introduces the notation and reviews the fundamentals of the pressure projection schemes.

In a projection, or fractional step, method [5] for solving incompressible flows, the pressure needed to enforce incompressibility is calculated by projecting an estimate of the velocity field onto a divergence-free space.

The incompressible Navier-Stokes equations in Lagrangian formalism are the field equations:

\[
\frac{D\mathbf{r}}{Dt} = \mathbf{u}, \\
\nabla \cdot \mathbf{u} = 0, \\
\frac{D\mathbf{u}}{Dt} = \mathbf{g} + \frac{\nabla \cdot \mathbf{T}}{\rho}. \tag{3}
\]

where \( \rho \) stands for the fluid density and \( \mathbf{g} \) is a generic external volumetric force field. The flow velocity \( \mathbf{u} \) is defined as the material derivative of a fluid particle with position \( \mathbf{r} \). \( \mathbf{T} \) denotes the stress tensor of a Newtonian incompressible fluid:

\[
\mathbf{T} = -P \mathbf{I} + 2\mu \mathbf{D}, \tag{4}
\]

in which \( P \) is the pressure, \( \mathbf{D} \) is the rate of deformation tensor (\( \mathbf{D} = (\nabla \mathbf{u} + \nabla \mathbf{u}^T)/2 \)) and \( \mu \) is the dynamic viscosity. With this notation, the divergence of the stress tensor \( \mathbf{T} \) is computed as:

\[
\nabla \cdot \mathbf{T} = -\nabla P + \mu \nabla^2 \mathbf{u}. \tag{5}
\]

In order to numerically integrate these equations, the fluid domain is discretized in a set of particles whose positions are \( \mathbf{r}_a \). For the fractional step method, in a generic time step \( n \), first, the particle positions are advected with the available velocity, \( \mathbf{u}_a^n \), considering a time step \( \Delta t \):

\[
\mathbf{r}_a^* = \mathbf{r}_a^n + \Delta t (\mathbf{u}_a^n). \tag{6}
\]
Second, considering the advected positions to evaluate the viscous interactions, an intermediate velocity field $u^*$ is explicitly computed using the momentum equation but ignoring the pressure term:

$$u^*_a = u^n_a + \Delta t \left( \mu \nabla^2 u^*_a + \Delta t \mathbf{g} \right).$$  \hfill (7)

Third, the zero divergence condition is imposed on the velocity field at the next time step, thus obtaining the Poisson equation for the pressure:

$$\left( \nabla^2 P \right)^{n+1}_a = \frac{\rho}{\Delta t} \left( \nabla \cdot u^*_a \right).$$ \hfill (8)

Once the pressure is found, pressure gradients are computed, the velocity is updated:

$$u^{n+1}_a = u^*_a - \frac{1}{\rho} \Delta t \left( \nabla P \right)^{n+1}_a,$$ \hfill (9)

and the particle positions are modified, usually with an implicit scheme:

$$\mathbf{r}^{n+1}_a = \mathbf{r}^n_a + \Delta t \left( u^{n+1}_a \right),$$ \hfill (10)

or a Crank-Nicholson one, yielding:

$$\mathbf{r}^{n+1}_a = \mathbf{r}^n_a + \Delta t \left( \frac{u^{n+1}_a + u^n_a}{2} \right).$$ \hfill (11)

Let us see how this scheme is applied in MPS and in ISPH.

3. Moving Particle Semi-implicit method (MPS)

Let us focus on the MPS time integration scheme [12], in which the Poisson problem for the pressure is written as:

$$\langle \nabla^2 P^{n+1} \rangle^{MPS}_a = \frac{\rho}{\Delta t} \langle \nabla \cdot u^* \rangle^{MPS}_a,$$ \hfill (12)

$$\frac{u^{n+1}_a - u^*_a}{\Delta t} = -\frac{1}{\rho} \langle \nabla P^{n+1} \rangle^{MPS}_a.$$ \hfill (13)

The problem setup therefore respects the formalism described in section [2] but referred to the smoothed operators. The positions are in the MPS literature mostly advected with the first order implicit scheme (10).
If the operators \([12,13]\) are written in their MPS integral form \([11]\), equations \((12), (13)\) become:

\[
\frac{2A_0}{(r_e)^2} A_2 \int_{\mathbb{R}^d} \left[ P(x') - P(x_a) \right] w \left( \frac{|x_a - x'|}{r_e} \right) dx' = \frac{\rho}{\Delta t} \int_{\mathbb{R}^d} \frac{(u' - u_a) \cdot (x' - x_a)}{|x' - x_a|^2} W \left( \frac{|x_a - x'|}{r_e} \right) dx',
\]

\((14)\)

\[
\frac{u_{a+1}^* - u_a^*}{\Delta t} = -\frac{d}{\rho (r_e)^d} A_0 \int_{\mathbb{R}^d} \frac{P(x') - P(x_a)}{|x' - x_a|^2} (x' - x_a) W \left( \frac{|x_a - x'|}{r_e} \right) dx',
\]

\((15)\)

where \(d\) is the dimensionality of the problem, \(w\) is the MPS weighting function, \(r_e\) is the cut-off radius of \(w\) and \(A_0, A_2\) are constants which depend on the specific form of the weighting function \([11]\).

4. Incompressible SPH (ISPH)

The system solved in ISPH is the same as in MPS \([8]\):

\[
\langle \nabla^2 P_{a+1}^{SPH} \rangle_a = \frac{\rho}{\Delta t} \langle \nabla \cdot u_a^{SPH} \rangle_a,
\]

\((16)\)

\[
\frac{u_{a+1}^* - u_a^*}{\Delta t} = -\frac{1}{\rho} \langle \nabla P_{a+1}^{SPH} \rangle_a,
\]

\((17)\)

where the previously mentioned operators can be written in the integral SPH formalism according to the consistency analysis of \([13,14,15]\).

\[
-\frac{2}{h^{d+1}} \int_{\mathbb{R}^d} \frac{P(x') - P(x_a)}{|x' - x|} \tilde{W}' \left( \frac{|x' - x|}{h} \right) dx' = \frac{\rho}{\Delta t} \frac{1}{h^{d+1}} \int_{\mathbb{R}^d} \frac{(u' - u_a) \cdot (x - x')}{|x - x'|} \tilde{W}' \left( \frac{|x - x'|}{h} \right) dx',
\]

\((18)\)

\[
\frac{u_{a+1}^* - u_a^*}{\Delta t} = -\frac{1}{\rho} \frac{1}{h^{d+1}} \int_{\mathbb{R}^d} \frac{P(x') - P(x_a)}{|x_a - x'|} (x_a - x') \tilde{W}' \left( \frac{|x_a - x'|}{h} \right) dx',
\]

\((19)\)

where \(\tilde{W} : \mathbb{R} \to \mathbb{R}\) is a nonnegative differentiable function such that:

\[
\int_{\mathbb{R}^d} \tilde{W}(|x|) dx = 1.
\]

\((20)\)
and the SPH kernel $W$ is defined on the basis of $\tilde{W}$ as:

$$W(x; h) = \frac{1}{h^d} \tilde{W}\left(\frac{|x|}{h}\right). \quad (21)$$

with $h$ being proportional to the cut-off radius of the kernel.

Although different options are available for the gradient formula, such as Monaghan’s symmetrized one \cite{2} commonly used in SPH, their order is $h^2$ regardless of the formula.

5. Passing from MPS to ISPH and the other way around

Equations (14)-(15) and (18)-(19) corresponding to MPS and ISPH respectively, present at the formal level some structural similarities. Hence it is only natural to explore deeper relations between these two methods.

Using the results of Souto-Iglesias et al.\cite{11} to establish the MPS consistency, it is possible to obtain equivalent operators in SPH from MPS ones and vice versa. As a matter of fact, these equivalences at the integral level are based on formulae that relate the MPS weighting function with the SPH kernel.

More precisely, the MPS scheme (14)-(15) can be written using the ISPH formalism as:

$$-\frac{2}{h^{d+1}} \int_{\mathbb{R}^d} P(x') - P(x_a) \tilde{W}_\Delta\left(\frac{|x'| - x}{h}\right) dx' =$$

$$\frac{\rho}{\Delta t} \frac{1}{h^{d+1}} \int_{\mathbb{R}^d} \frac{(u' - u_a) \cdot (x - x')}{|x - x'|} \tilde{W}_\nabla\left(\frac{|x - x'|}{h}\right) dx', \quad (22)$$

$$\frac{u^{n+1}_a - u^*_a}{\Delta t} = -\frac{1}{\rho} \frac{1}{h^{d+1}} \int_{\mathbb{R}^d} P(x') - P(x_a) \tilde{W}_\nabla\left(\frac{|x' - x_a|}{h}\right) dx', \quad (23)$$

using different kernels for first and second order differential operators:

$$\tilde{W}_\nabla(q) = -\frac{d}{A_0} \int_0^q \frac{1}{s} w(s) ds + C_1, \quad (24)$$

$$\tilde{W}_\Delta(q) = -\frac{d}{A_2} \int_0^q s w(s) ds + C_2. \quad (25)$$

with $q = |x/h|$. Constants $C_1, C_2$ are obtained by imposing $\tilde{W}_\nabla(1) = \tilde{W}_\Delta(1) = 0$ \cite{11}.
On the other hand, the ISPH integral formulation of the problem as expressed in equations (18)-(19) can be seen from the MPS point of view provided different weighting functions are used to approximate first and second order differential operators, respectively:

\[
\frac{2A_0}{(r_e)^2 A_2} \int_{\mathbb{R}^d} [P(x') - P(x_a)] w^A \left( \frac{|x_a - x'|}{r_e} \right) dx' = \\
\frac{\rho}{\Delta t} \int_{\mathbb{R}^d} \frac{(u' - u_a) \cdot (x' - x_a)}{|x' - x_a|^2} w^\nabla \left( \frac{|x_a - x'|}{r_e} \right) dx'
\]

(26)

\[
\frac{u_{n+1}^a - u_n^a}{\Delta t} = -\frac{d}{\rho (r_e)^d A_0} \int_{\mathbb{R}^d} \frac{P(x') - P(x_a)}{|x' - x|^2} (x' - x_a) w^\nabla \left( \frac{|x_a - x'|}{r_e} \right) dx',
\]

(27)

with

\[
w^\nabla (q) := -\frac{q}{d} \tilde{W}'(q),
\]

(28)

\[
w^A (q) := -\frac{d}{q} \tilde{W}'(q).
\]

(29)

The equivalences established so far do not depend neither on the time integration scheme used nor on the implementation of boundary conditions. Most importantly, these equivalences are not affected by the discretization of the smoothed operators, where mass-carrying particles are used to represent the integrals in both methods [16, 4]. Summarizing, any MPS formulation can be equivalently reformulated as an ISPH scheme and reciprocally.

At this point, it becomes clear that the question of comparing the solution obtained through an MPS based method to one obtained by an ISPH implementation reduces to that of understanding the sensitivity of MPS to the weighting function used (or equivalently that of ISPH to the kernel considered). This remark is relevant since the choice of the kernel may have a significant influence on several properties of the numerical scheme, namely: stability (see e.g. [17, 18, 19]), accuracy [20, 21] and thermodynamic consistency [22].

6. Alternative RHS formulation

6.1. General

The corrective term on the right hand side of the Poisson equation (12) can be reformulated using the continuity equation to estimate the divergence of the
velocity field:

\[
\nabla \cdot \mathbf{u}^* = -\frac{1}{\rho} \frac{d\rho}{dt}.
\]

(30)

This leads to an alternative way to write equation (12), namely:

\[
\nabla^2 P_{n+1} = -\frac{\rho_0}{A t^2} \left( \rho^* - \rho_0 \right),
\]

(31)

in which \(\rho_0\) is the reference density and \(\rho^*\) is the intermediate time step, which is obtained at the discrete level by summations across neighboring particles either using a MPS weight function or an SPH kernel. These summations may reflect an excess or defect of local mass, a consequence of the fact that the intermediate velocity field \(\mathbf{u}^*\) may not satisfy the divergence free constraint.

6.2. MPS approximation

This alternative formulation has been used in a large proportion of the MPS literature [23, 24, 25] including the seminal papers by Koshizuka and collaborators [3, 4].

The intermediate density \(\rho^*\) is obtained in MPS for each particle \(a\) as [12]:

\[
\langle \rho^* \rangle_{MPS}^a = \int_{\mathbb{R}^d} \frac{m}{W(r_e)} dx = \frac{m}{A_0 r_e^d} \sum_{b \in J_a} w\left( \frac{|\mathbf{x}_a - \mathbf{x}_b|}{r_e} \right).
\]

(32)

In this formula \(m\) is the mass of each individual particle and \(\langle n \rangle_a\) is a particle number density defined as:

\[
\langle n \rangle_a := \sum_{b \in J_a} w\left( \frac{|\mathbf{x}_a - \mathbf{x}_b|}{r_e} \right),
\]

(33)

where \(J_a\) is the set of indexes corresponding to neighboring particles. When \(w\) is singular for argument zero (e.g. [4, 25]) this index set does not include the particle \(a\) itself.

Since the MPS weight function \(w\) is positive, isotropic and with compact support, an SPH kernel can be constructed from \(w\) as:

\[
W(\mathbf{x}; r_e) = \frac{1}{A_0 r_e^d} w\left( \frac{|\mathbf{x}|}{r_e} \right),
\]

(34)

It is straightforward to see that the volume integral of this function equals one, a necessary condition for \(W\) to be a well defined kernel. Let us denote this kernel as \(W_\Sigma\).
Considering this new kernel, one can write:

\[
\langle \rho^* \rangle_{a}^{MPS} = m \sum_{b \in J_a} W_{\Sigma}(x_b - x_a; r_e) = \langle \rho^* \rangle_{a}^{SPH},
\] (35)

and this summation becomes the canonic SPH approximation to the local value of the density, \( \langle \rho^* \rangle_{a}^{SPH} \), where, as in [11], the cut-off radius \( r_e \) is identified to the SPH smoothing length.

Therefore, for each MPS weight function \( w \) a well defined SPH kernel \( W_{\Sigma} \) exists, providing an equivalent local estimation of the density field. Note that in the cases when \( w \) is singular at the origin, the SPH kernel \( W_{\Sigma} \) cannot be used to approximate differential operators.

6.3. ISPH approximation

The idea of using a corrective term based on density variations with respect to the reference density can also be found in the ISPH literature [23, 26], although, originally, in the works of Cummins and Rudman [6], such a term was based on the velocity divergence. We should also mention Zhou [27] who even used a mixed formulation, computing the Poisson equation RHS by weight averaging the velocity divergence and the density correction terms.

Analogously to section 6.2, from equations (34-35) it follows that given an SPH kernel it is possible to find an infinite number of MPS weight functions which provide the same local estimation of the density field. However, all these MPS weight functions are proportional.

6.4. Summary

If the corrective source term is based on the density variation, establishing the equivalence between SPH and MPS requires defining a new SPH kernel from the MPS weight function. This kernel adds to the ones that are necessary for MPS operators to consistently represent first and second order differential operators [11]. Therefore, three SPH kernels need to be defined from each MPS function in order to pass from MPS to SPH:

\[
\tilde{W}_{\Sigma}(q) = \frac{1}{A_0} w(q),
\]

\[
\tilde{W}_{\nabla}(q) = -\frac{d}{A_0} \int_0^q \frac{1}{s} w(s) ds + C_1,
\]

\[
\tilde{W}_{\Delta}(q) = -\frac{d}{A_2} \int_0^q s w(s) ds + C_2.
\]
Each kernel is re-scaled by introducing the cut-off radius:

\[ W_\Box (\mathbf{x}; r_\epsilon) = \frac{1}{r_\epsilon} \tilde{W}_\Box \left( \frac{\| \mathbf{x} \|}{r_\epsilon} \right). \]  

(36)

It is also possible to build equivalent MPS weight functions from a given SPH kernel. For details we refer the reader to [11].

A final outcome of the present analysis is to provide MPS with a consistent interpolation formula for any flow field which allows to compute it at any point in space regardless of whether a particle exists there:

\[ \langle f \rangle_{MPS}^{a} = \sum_{b \in J_a} \frac{m}{\rho_b} f_b W_{\Sigma} (\mathbf{x}_b - \mathbf{x}_a; r_\epsilon). \]  

(37)

Due to its equivalence with SPH, the order of this formula is \( O(r_\epsilon^2) \).

7. Conclusions

Analogies between the Moving Particle Semi-implicit method (MPS) and Incompressible Smoothed Particle Hydrodynamics method (ISPH) have been discussed in the present paper, showing that any MPS scheme can be reformulated as an ISPH one and vice versa.

This equivalence is based on reformulating the MPS density interpolation formula and the first and second order differential operators within the ISPH framework by defining different SPH kernels for each of these operators.

The numerical analysis of meshless methods presents unsettled issues concerning stability, conservation properties, computational efficiency, etc., that are still unresolved today. We think that the present note could be useful in providing the framework needed to view the significant amount of work on SPH and MPS on these topics from a new perspective and help the progress of meshless methods.

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References

[1] R. Gingold, J. Monaghan, Mon. Not. Roy. Astron. Soc. (MNRAS) 181 (1977) 375–389.

[2] J. Monaghan, J. Comp. Phys. 110 (1994) 39–406.

[3] S. Koshizuka, Y. Oka, H. Tamako, in: International Conference, Mathematics and Computations, Reactor Physics, and Environmental Analyses, volume 2, pp. 1514–1521.

[4] S. Koshizuka, Y. Oka, Nuclear Science and Engineering 123 (1996) 421–434.

[5] A. J. Chorin, Mathematics of Computation 22 (1968) 745–762. URL: http://dx.doi.org/10.2307/2004575 doi:10.2307/2004575

[6] S. Cummins, M. Rudman, J. Comp. Phys. 152 (1999) 584–607.

[7] S. Cummins, Applications of Projection Techniques for incompressible flows, Ph.D. thesis, Monash University, 2000.

[8] E. S. Lee, C. Moulinec, R. Xu, D. Violeau, D. Laurence, P. Stansby, Journal of Computational Physics 227 (2008) 8417–8436.

[9] A. Rafiee, S. Cummins, M. Rudman, K. Thiagarajan, European Journal of Mechanics - B/Fluids 36 (2012) 1 – 16. URL: http://www.sciencedirect.com/science/article/pii/S0997754612000714 doi:10.1016/j.euromechflu.2012.05.001

[10] R. Xu, P. Stansby, D. Laurence, Journal of Computational Physics 228 (2009) 6703 – 6725. URL: http://www.sciencedirect.com/science/article/pii/S0021999109002885 doi:10.1016/j.jcp.2009.05.032

[11] A. Souto-Iglesias, F. Macià, L. M. González, J. L. Cercos-Pita, Computer Physics Communications 184 (2013) 732–745. URL: http://www.sciencedirect.com/science/article/pii/S0010465512003852?v=s5 doi:10.1016/j.cpc.2012.11.009

[12] H.-Y. Yoon, S. Koshizuka, Y. Oka, International Journal for Numerical Methods in Fluids 30 (1999) 407–424.
[13] P. Español, M. Revenga, Phys. Rev. E 67 (2003) 026705. doi:10.1103/PhysRevE.67.026705

[14] J. J. Monaghan, Reports on Progress in Physics 68 (2005) 1703–1759.

[15] F. Macià, M. Antuono, L. M. González, A. Colagrossi, Progress of Theoretical Physics 125 (2011) 1091–1121. URL: http://ptp.ipap.jp/link?PTP/125/1091/ doi:10.1143/PTP.125.1091

[16] J. Monaghan, Annual Review of Astronomy and Astrophysics 30 (1992) 543–574.

[17] J. W. Swegle, D. L. Hicks, S. W. Attaway, Journal of Computational Physics 116 (1995) 123–134.

[18] W. Dehnen, H. Aly, Monthly Notices of the Royal Astronomical Society 425 (2012) 1068–1082. URL: http://dx.doi.org/10.1111/j.1365-2966.2012.21439.x doi:10.1111/j.1365-2966.2012.21439.x

[19] A. Colagrossi, A. Souto-Iglesias, M. Antuono, S. Marrone, Phys. Rev. E 87 (2013) 023302. URL: http://link.aps.org/doi/10.1103/PhysRevE.87.023302 doi:10.1103/PhysRevE.87.023302

[20] N. J. Quinlan, M. Lastiwka, M. Basa, International Journal for Numerical Methods in Engineering 66 (2006) 2064–2085. URL: http://dx.doi.org/10.1002/nme.1617

[21] A. Amicarelli, J.-C. Marongiu, F. Leboeuf, J. Leduc, J. Caro, Computers & Fluids 44 (2011) 279 – 296. URL: http://www.sciencedirect.com/science/article/B6V26-52079TP-1/2/28aecd9efa85d5499c04f8974f4f0fdd doi:DOI:10.1016/j.compfluid.2011.01.018

[22] D. Violeau, Phys. Rev. E 80 (2009) 036705. URL: http://link.aps.org/doi/10.1103/PhysRevE.80.036705 doi:10.1103/PhysRevE.80.036705

[23] S. Shao, E. Y. Lo, Advances in Water Resources 26 (2003) 787 – 800. URL: http://www.sciencedirect.com/science/article/pii/S0309170803000307 doi:10.1016/S0309-1708(03)00030-7
[24] M. M. Tsukamoto, L.-Y. Cheng, K. Nishimoto, Computers & Fluids 49 (2011) 1 – 21. URL: http://www.sciencedirect.com/science/article/pii/S0045793011001423. doi:10.1016/j.compfluid.2011.04.008.

[25] A. Khayyer, H. Gotoh, Applied Ocean Research 32 (2010) 124 – 131. URL: http://www.sciencedirect.com/science/article/pii/S014111871000027. doi:10.1016/j.apor.2010.01.001.

[26] S. Shao, Journal of Hydraulic Research 43 (2005) 366–375. URL: http://www.tandfonline.com/doi/abs/10.1080/00221680509500132. doi:10.1080/00221680509500132. arXiv:http://www.tandfonline.com/doi/pdf/10.108

[27] J. Zhou, Numerical investigation of breaking waves and their interactions with structures using MLPG_R method, Ph.D. thesis, City University London, 2010.