Lagrangian for Navier-Stokes equations of motion: SDPD approach

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The conditions necessary and sufficient for the Smoothed Dissipative Particle Dynamics (SDPD) equations of motion to have a Lagrangian that can be used for deriving these equations of motion, the Helmholtz conditions, are obtained and analysed. They show that for a finite number of SDPD particles the conditions are not satisfied; hence, the SDPD equations of motion can not be obtained using the classical Euler-Lagrange equation approach. However, when the macroscopic limit is considered, that is when the number of particles tends to infinity, the conditions are satisfied, thus providing the conceptual possibility of obtaining the Navier-Stokes equations from the principle of least action.

I. INTRODUCTION

Obtaining hydrodynamic equations of motion from the fundamental Action Principle is a largely unexplored area of research. Even though the generalisation of classical Action Principle for particles to continuous fields is known for some time [1], attempts to take into account energy dissipation are rare and only recently such Lagrangians for fluid dynamics equations of motion are reported [2–4]. An advantage provided by such Lagrangian approach is in natural connection between the dynamics of discrete particles and continuous fields best suitable for describing fluids at macroscale. When particles represent atoms (even at the classical approximation) this connection is the physical foundation of the interaction between the scales representing multiscale, multiphysics description of liquids, which is an active area of research.

To the best of our knowledge Lagrangians that lead to classical Navier-Stokes (NS) equations of hydrodynamics are unknown. Here we take the first step in the direction of finding such Lagrangians, namely we seek to answer the question if such Lagrangians exist. Our approach consists of first considering the discrete approximation of NS equations, the Smoothed Dissipative Particles Dynamics (SDPD) model [5], that converges to continuum NS equations in the limit of infinite number of particles. There are mathematical conditions, attributed to Helmholtz, that if fulfilled guarantee the existence of the Lagrangian. We check these conditions for SDPD equations of motion and then analyse their behaviour for for the macroscopic limit.

Our results show that the conditions are not satisfied for SDPD equations with finite number of particles. However, we show numerically that the discrepancy decreases with increasing the number of particles. Also, in the limit of infinite number of particles the conditions are satisfied, thus providing an approach for obtaining a Lagrangian for the Navier-Stokes equations.

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II. THEORY

Mathematically, finding a Lagrangian for a system of equations of motion amounts to solving the inverse problem of the calculus of variations [6]. It is known that for a system of n given differential equations

$$H_i(t, q_i, \dot{q}_i, \ddot{q}_i) = 0 \tag{1}$$

the necessary and sufficient condition that the system is derivable from a Lagrangian is that the equations of variation of H_i form a self-adjoint system. The conditions under which the system of variations is self-adjoint are attributed to Helmholtz [6]:

$$\frac{\partial H_i}{\partial \ddot{q}_j} = \frac{\partial H_j}{\partial \ddot{q}_i}, \tag{2}$$

$$\frac{\partial H_j}{\partial \dot{q}_i} + \frac{\partial H_i}{\partial \dot{q}_j} = 2\frac{d}{dt}\left(\frac{\partial H_i}{\partial \ddot{q}_j}\right), \tag{3}$$

$$\frac{\partial H_j}{\partial q_i} = \frac{\partial H_i}{\partial q_j} - \frac{d}{dt}\left(\frac{\partial H_i}{\partial \dot{q}_j}\right) + \frac{d^2}{dt^2}\left(\frac{\partial H_i}{\partial \ddot{q}_j}\right), \tag{4}$$

$\forall i, j = 1, \dots, n$. If these conditions are satisfied, H_i must take the form $H_i = M_i + P_{ij}\ddot{q}_j$, where M_i and P_{ij} are functions related to each other with certain conditions (see [6]) and the Lagrangian can be constructed from the functions M_i and P_{ij}. Importantly, a Lagrangian constructed this way does not necessarily have the usual physical meaning of the difference between the kinetic and potential energies. Rather, it is an abstract mathematical function that, when used in Euler-Lagrange equation, produces the required equations of motion.

In SDPD framework the fluid is represented by a set of N particles, each of which is considered as a macroscopic thermodynamic system of constant mass m_i [5]. Particles are described by their positions $\mathbf{r}_i$, velocities $\mathbf{v}_i$, and entropy S_i. The particle's volume ν_i is defined as its inverse number density d_i:

$$\frac{1}{\nu_i} = d_i = \sum_j W(|\mathbf{r}_i - \mathbf{r}_j|), \tag{5}$$

where $W(r,h) = W(|r|,h)$ is a pairwise bell-shaped interpolation function of compact support h (the kernel). Various forms of W exist, we used the Lucy function

$$W(r) = \frac{105}{16\pi h^3}\left(1 + 3\frac{r}{h}\right)\left(1 - \frac{r}{h}\right)^3. \tag{6}$$

The gradient of W defines the function $F(r)$ as $\nabla W(r) = -rF(r), F(r) \geq 0$, which for the Lucy kernel has the form

$$F(r) = \frac{315}{4\pi h^5}\left(1 - \frac{r}{h}\right)^2. \tag{7}$$

Using the auxiliary quantities $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$, $\mathbf{v}_{ij} = \mathbf{v}_i - \mathbf{v}_j$, and $F_{ij} = F(|\mathbf{r}_{ij}|)$ the SDPD equations of motion read

$$\begin{aligned}
\dot{\mathbf{r}}_i &= \mathbf{v}_i, \\
m\dot{\mathbf{v}}_i &= \sum_j \left[\frac{P_i}{d_i^2} + \frac{P_j}{d_j^2}\right] F_{ij}\mathbf{r}_{ij} - \left(\frac{5\eta}{3} - \xi\right)\sum_j \frac{F_{ij}}{d_i d_j}\mathbf{v}_{ij} - \\
&\quad 5\left(\xi + \frac{\eta}{3}\right)\sum_j \frac{F_{ij}}{d_i d_j}\mathbf{e}_{ij}\mathbf{e}_{ij}\cdot\mathbf{v}_{ij}, \\
T_i\dot{S}_i &= \phi_i - 2\kappa\sum_j \frac{F_{ij}}{d_i d_j}(T_i - T_j),
\end{aligned} \tag{8}$$

where

$$\begin{aligned}
\mathbf{e}_{ij} &= \frac{\mathbf{r}_i - \mathbf{r}_j}{|\mathbf{r}_i - \mathbf{r}_j|}, \\
\phi_i &= \left(\frac{5\eta}{6} - \frac{\xi}{2}\right)\sum_j \frac{F_{ij}}{d_i d_j}\mathbf{v}_{ij}^2 + \\
&\quad \frac{5}{2}\left(\xi + \frac{\eta}{3}\right)\sum_j \frac{F_{ij}}{d_i d_j}\left(\mathbf{e}_{ij}\cdot\mathbf{v}_{ij}\right)^2,
\end{aligned}$$

T_i and P_i are particles' temperature and pressure (calculated using phenomenological equations of state), η and ξ are viscosities, κ is the thermal conductivity [5].

We have used the following approximations in our SDPD model: (i) temperature was constant and equal for all particles, (ii) the shear viscosity η was constant and equal for all particles, (iii) the bulk viscosity ξ was negligible, (iv) pressure was calculated using the Tait equation of state

$$P_i = B\left[\left(\frac{d_i}{\rho_0}\right)^\gamma - 1\right],$$

where $\gamma = 7$, $B = \frac{c_0^2\rho_0}{\gamma}$, ρ_0 is the control density, and c_0 is the control speed of sound.

The equation for the entropy in (8) is often considered decoupled from the equations for the position and the velocity to a good approximation, depending on the equations of state for P and T. Therefore, we do not take it into account here as our model equations of state do not depend on S. After substituting $\dot{\mathbf{r}}_i$ for $\mathbf{v}_i$ in the second equation in (8) the system (1) for independent variables $\mathbf{r}_i$, x, y, and z components of which represent variables q_i, become (note, that indexes i refer to different variables here: the particle number for $\mathbf{r}_i$ and the degree of freedom for q_i)

$$\begin{aligned}
H_i &= C\sum_j \left[\left(B\left(\frac{1}{\rho_0}\right)^7 d_i^5 + Bd_i^{-2} + B\left(\frac{1}{\rho_0}\right)^7 d_j^5 + Bd_j^{-2}\right) K_{ij}\mathbf{r}_{ij}\right] - \\
&\quad C\sum_j \left[K_{ij}d_i^{-1}d_j^{-1}\left(A\cdot\dot{\mathbf{r}}_{ij} + D\mathbf{r}_{ij}\left(\mathbf{r}_{ij}\cdot\dot{\mathbf{r}}_{ij}\right)\left(|\mathbf{r}|_{ij}\right)^{-2}\right)\right] - m_i\ddot{\mathbf{r}}_i,
\end{aligned} \tag{9}$$

where $A = \left(\frac{5\eta}{3} - \xi\right)$, $D = \left(\xi + \frac{\eta}{3}\right)$, $C = \frac{315}{4\pi h^5}$ are constants and $K_{ij} = \left(1 - \frac{|\mathbf{r}|_{ij}}{h}\right)^2$, $d_i = \sum_j \frac{105}{16\pi h^3}\left(1 + 3\frac{|\mathbf{r}|_{ij}}{h}\right)\left(1 - \frac{|\mathbf{r}|_{ij}}{h}\right)^3$.

Therefore, checking the Helmholtz conditions for SDPD equations amounts to checking equations (2)-(4) for H_i functions defined by (9).

A. First Helmholtz condition

The first condition (2) is satisfied for all variables as the left and the right hand sides of the equation are 0 for $i \neq j$ since the equation of motion for particle i does not depend on the second time derivative of the coordinate of a different particle j, while the case $i = j$ is trivially satisfied.

As we show below, the second (3) and the third (4) conditions are not satisfied and we analyse the residues as we are interested in the behaviour of these residues when the number of particles tends to infinity.

B. Second Helmholtz condition

In our case, the second Helmholtz condition becomes:

$$\frac{\partial H_j}{\partial \dot{q}_i} + \frac{\partial H_i}{\partial \dot{q}_j} = 0, \tag{10}$$

for $i, j = 1, \ldots, n = 3N$. There are four possibilities for this condition after assigning the particles' coordinates to variables q_i and corresponding functions H_i (again, indexes i have different meaning depending if they refer to the degree of freedom as in (3) and (10) or to the particle number as in (8)):

1. Particle i with respect to itself in the same coordinate x (y, z):

$$\frac{\partial H_{xi}}{\partial \dot{x}_i} + \frac{\partial H_{xi}}{\partial \dot{x}_i} = \sum_j T_{ij} d_i^{-1} d_j^{-1} Q_{ij}^x. \tag{11}$$

2. Particle i with respect to itself in different coordinates x and y (and other pairs of coordinates):

$$\frac{\partial H_{xi}}{\partial \dot{y}_i} + \frac{\partial H_{yi}}{\partial \dot{x}_i} = \sum_j T_{ij} d_i^{-1} d_j^{-1} Q_{ij}^{xy}. \tag{12}$$

3. Particle i with respect to a different particle j in the same coordinate x (y, z):

$$\frac{\partial H_{xi}}{\partial \dot{x}_j} + \frac{\partial H_{xj}}{\partial \dot{x}_i} = T_{ij} d_i^{-1} d_j^{-1} Q_{ij}^x. \tag{13}$$

4. Particle i with respect to a different particle j in different coordinates x and y:

$$\frac{\partial H_{xi}}{\partial \dot{y}_j} + \frac{\partial H_{yj}}{\partial \dot{x}_i} = \frac{\partial H_{xj}}{\partial \dot{y}_i} + \frac{\partial H_{yi}}{\partial \dot{x}_j} = T_{ij} d_i^{-1} d_j^{-1} Q_{ij}^{xy}. \tag{14}$$

The following variables were used:

$$T_{ij} = C K_{ij} m_i m_j, \tag{15}$$

$$Q_{ij}^x = A + D x_{ij} \left(|r|_{ij}\right)^{-2}, \tag{16}$$

$$Q_{ij}^{xy} = D x_{ij} y_{ij} \left(|r|_{ij}\right)^{-2}. \tag{17}$$

C. Third Helmholtz condition

Our functions H_i lead to the following third Helmholtz condition:

$$\frac{\partial H_j}{\partial q_i} - \frac{\partial H_i}{\partial q_j} + \frac{\partial}{\partial t}\left(\frac{\partial H_i}{\partial \dot{q}_j}\right) = 0, \tag{18}$$

for $i, j = 1, \ldots, n = 3N$ with four realisations:

1. Particle i with respect to itself in the same coordinate x (y, z):

$$\frac{\partial H_{xi}}{\partial x_i} - \frac{\partial H_{xi}}{\partial x_i} + \frac{\partial}{\partial t}\left(\frac{\partial H_{xi}}{\partial \dot{x}_i}\right) = R_{ij}^x, \tag{19}$$

variable R_{ij}^x is defined in appendix A.

2. Particle i with respect to itself in different coordinates x and y (and other pairs of coordinates):

$$\begin{aligned}
\frac{\partial H_{xi}}{\partial y_i} - \frac{\partial H_{yi}}{\partial x_i} + \frac{\partial}{\partial t}\left(\frac{\partial H_{yi}}{\partial \dot{x}_i}\right) = \\
= \sum_j \Bigg[T_{ij} \Bigg(\left(L_i y_{ij} + d_i^{-2} d_j^{-1} S_{ij}^y\right) \left(\sum_k C K_{ik} x_{ik}\right) - \\
- \left(L_i x_{ij} + d_i^{-2} d_j^{-1} S_{ij}^x\right) \left(\sum_k C K_{ik} y_{ik}\right) \Bigg) + \\
+ T_{ij} d_i^{-1} d_j^{-1} \left[v_{ij} x_{ij} y_{ij} - v_{ij} y_{ij} x_{ij}\right] \\
\left[\frac{2}{h\,|r|_{ij}\left(1 - \frac{|r|_{ij}}{h}\right)} A - d_j^{-1} K_{ij} A + D \left(|r|_{ij}\right)^{-2} \right] \Bigg] + R_{ij}^{xy}.
\end{aligned} \tag{20}$$

The expression for $\frac{\partial H_{yi}}{\partial x_i} - \frac{\partial H_{xi}}{\partial y_i} + \frac{\partial}{\partial t}\left(\frac{\partial H_{xi}}{\partial \dot{y}_i}\right)$ is almost the same with two signs reverted, see appendix A, equation (A1).

3. Particle i with respect to a different particle p in the same coordinate x (y, z):

$$\frac{\partial H_{xi}}{\partial x_p} - \frac{\partial H_{xp}}{\partial x_i} + \frac{\partial}{\partial t}\left(\frac{\partial H_{xp}}{\partial \dot{x_i}}\right) =$$
$$= C\sum_j \left[T_{ij}\left(K_{ip}x_{ip}\left[L_i x_{ij} + d_i^{-2}d_j^{-1}S_{ij}^x\right] - K_{pj}x_{pj}\left[L_j x_{ij} + d_i^{-1}d_j^{-2}S_{ij}^x\right]\right) + \right.$$
$$\left. + T_{ip}K_{ij}x_{ij}\left(L_i x_{ip} + d_i^{-2}d_p^{-1}S_{ip}^x\right)\right] +$$
$$+ C\sum_l \left(T_{pl}\left[K_{ip}x_{ip}\left(L_p x_{pl} + d_p^{-2}d_l^{-1}S_{pl}^x\right) + K_{il}x_{il}\left(L_l x_{pl} + d_p^{-1}d_l^{-2}S_{pl}^x\right)\right] + \right.$$
$$\left. + T_{ip}K_{pl}x_{pl}\left(L_p x_{ip} + d_i^{-1}d_p^{-2}S_{ip}^x\right)\right) + R_{ip}^x. \quad (21)$$

The expression for $\frac{\partial H_{xp}}{\partial x_i} - \frac{\partial H_{xi}}{\partial x_p} + \frac{\partial}{\partial t}\left(\frac{\partial H_{xi}}{\partial \dot{x_p}}\right)$ is almost the same with two signs at the summations reversed, see appendix A, equation (A2).

4. Particle i with respect to a different particle p in different coordinates x and y:

$$\frac{\partial H_{xi}}{\partial y_p} - \frac{\partial H_{yp}}{\partial x_i} + \frac{\partial}{\partial t}\left(\frac{\partial H_{yp}}{\partial \dot{x_i}}\right) =$$
$$= T_{ip}d_i^{-1}d_p^{-1}\left[v_{ip}y_{ip}x_{ip} - v_{ip}x_{ip}y_{ip}\right]\left[\frac{2}{h\,|r|_{ip}\left(1 - \frac{|r|_{ip}}{h}\right)}A + D\left(|r|_{ip}\right)^{-2}\right] +$$
$$+ C\sum_j \left[T_{ij}\left(K_{ip}y_{ip}\left[L_i x_{ij} + d_i^{-2}d_j^{-1}S_{ij}^x\right] - K_{pj}y_{pj}\left[L_j x_{ij} + d_i^{-1}d_j^{-2}S_{ij}^x\right]\right) - \right.$$
$$\left. - T_{ip}K_{ij}x_{ij}\left(L_i y_{ip} + d_i^{-2}d_p^{-1}S_{ip}^y\right)\right] +$$
$$+ C\sum_l \left[T_{pl}\left(K_{ip}x_{ip}\left[L_p y_{pl} + d_p^{-2}d_l^{-1}S_{pl}^y\right] + K_{il}x_{il}\left[L_l y_{pl} + d_p^{-1}d_l^{-2}S_{pl}^y\right]\right) - \right.$$
$$\left. - T_{ip}K_{pl}y_{pl}\left(L_p x_{ip} + d_i^{-1}d_p^{-2}S_{ip}^x\right)\right] + R_{ip}^{xy}. \quad (22)$$

The analogous expressions for the other combinations of the coordinates as well as definitions of the auxiliary variables are given in appendix A, equations (A3-A11).

As the right hand sides of equations (11-14), (19-22) are clearly not 0, the second and the third Helmholtz conditions are not satisfied for a system of finite number of SDPD particles.

III. THE MACROSCOPIC LIMIT LEADING TO CONTINUOUS NAVIER-STOKES SYSTEM

Even though the second and the third coniditions are not satisfied, it is interesting to investigate how large the discrepancy is. In other words, what is the value of the right hand sides of the conditions, which should be zero if they were satisfied. This is an important question as the SDPD equations are a discrete approximation of the continuous NS equations. It is known, that the SDPD equations converge to NS equation in the limit of infinite number of particles (see below for details).

The original SDPD equations have two parts: deterministic and stochastic [7]. The deterministic part, eq. (3) in [7], defines the macroscopic dynamics and does not depend on the spatial and temporal scales ("scale-free"), that is, it is independent of the volume of particles ν_i. On the contrary, the stochastic part, eq. (4) in [7], defines the scale and it is inversely proportional to the particles' volume. In the large particles limit, the stochastic part is negligible. Therefore, in the macroscopic limit, only the deterministic part of SDPD equations needs to be considered, which are our equations (8).

A. How particles converge to hydrodynamic fields

From the other hand, the SDPD equations are the discrete approximation for continuous Navier-Stokes equations describing the evolution of hydrodynamic fields ρ, $\mathbf{v}$, and S. As explained in [8], in order to obtain the continuous limit of the discrete approximation, the number of particles N should tend to infinity and, at the same time, the width of the kernel's support h should tend to 0. In this limit the set of N SDPD equations tends to three Navier-Stokes equations describing the continuous

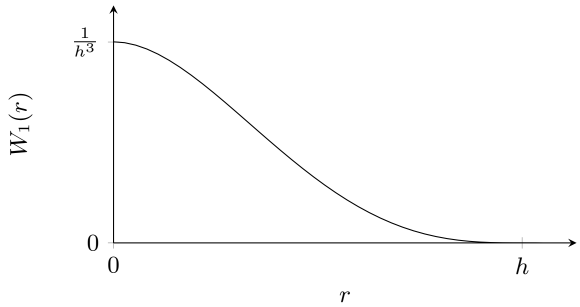

Figure 1. The form of the function W_1

hydrodynamic fields.

We, therefore, need to analyse (or define) how the quantities on the right hand side of equations (10)-(22) depend on N and take the limit $N \to \infty$, making sure that in this limit also $h \to 0$.

B. The Lucy kernel function and particle's number density

The most involved quantity to estimate is the volume of the particles as it is defined through the summation involving the kernel function (5). To analyse its dependence on N let us first consider the Lucy function written in the form

$$W(r;h) = \frac{105}{16\pi} W_1(r;h), \tag{23}$$

where

$$W_1(r;h) = \frac{1}{h^3}\left(1 + 3\frac{r}{h}\right)\left(1 - \frac{r}{h}\right)^3 \tag{24}$$

and $W_1(r) = 0$ for $r < 0$ or $r > h$, Fig. 1.

From (5), the number density d_i of the particle is equal to

$$\frac{1}{\nu_i} = d_i = \frac{105}{16\pi}\sum_{j=1}^{K} W_1(|\mathbf{r}_{ij}|), \tag{25}$$

where K is the number of particles inside the sphere of radius h. K is approximately equal to the fraction of the volume of this sphere in the total volume of the system V_0:

$$K = \frac{\nu_i}{V_0} N = \frac{4\pi}{3V_0} h^3 N. \tag{26}$$

In order to estimate the value of the sum in (25) we need to estimate how the distances $|\mathbf{r}_{ij}|$ are distributed.

In the assumption that the particles are distributed uniformly in 3D space, the *distances* r from the centre of a sphere of radius R are distributed according to the cumulative distribution function (CDF) $F(r) = \left(\frac{r}{R}\right)^3$.

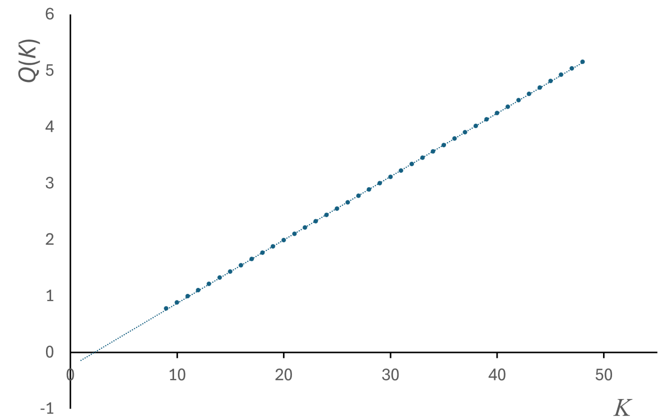

Figure 2. The linear dependence of function Q on K

The distribution of distances r are, then, obtained using inverse transform sampling, where a uniformly distributed values U are transformed by the inverse CDF: $r = F^{-1}(U)$, which in our case is equal to $r = RF^{\frac{1}{3}}$. Taking an equidistant set of points $\frac{j}{K}$ as a set of uniformly distributed points, the value of the distances becomes

$$|\mathbf{r}_{ij}| = \left(\frac{j}{K}\right)^{\frac{1}{3}} h.$$

Substituting this value into the sum of (25) we obtain the following expression

$$\frac{1}{h^3}\sum_{j=1}^{K}\left[1 - 3\left(\frac{j}{K}\right)^{\frac{1}{3}}\right]\left[1 - \left(\frac{j}{K}\right)^{\frac{1}{3}}\right]^3 = \frac{1}{h^3}Q(K).$$

Function Q is very close to a linear function for all $K > 8$, Fig. 2, and can be approximated as $Q(K) \approx 0.11K$.

Substituting this and the value for K from (26), we obtain the estimation for the number density d_i as a function of N:

$$d_i = \frac{105}{16\pi}\frac{1}{h^3}Q(K) \approx \frac{105 \cdot 0.11}{12V_0} N = EN \tag{27}$$

with E constant.

C. The macroscopic limit

In order to estimate the macroscopic limit, what remains is to estimate the distance x_{ij}, which is simply the x-component of the average distance between the particles and, as such, can be assumed to be equal to $\left(\frac{V_0}{N}\right)^{\frac{1}{3}}$ multiplied by j with plus or minus sign depending on the direction of the vector $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$:

$$x_{ij} = \pm\left(\frac{V_0}{N}\right)^{\frac{1}{3}} j.$$

The mass of particles is equal to $m_i = \frac{M_0}{N}$, where M_0 is the total mass of the system.

Finally, we need to define how the kernel support h tends to zero with $N \to \infty$. A reasonable assumption here is to require the radius of the sphere h to be such, that there is always a fixed number of particles K_0 inside the sphere. Hence, from (26), the value of h becomes

$$h = \left(\frac{K_0}{N} \frac{3V_0}{4\pi} \right)^{\frac{1}{3}} = GN^{-\frac{1}{3}}, \tag{28}$$

with G constant.

Putting all together, the right hand side of equation (11) becomes

$$\frac{\partial H_{xi}}{\partial \dot{x}_i} + \frac{\partial H_{xi}}{\partial \dot{x}_i} = \tag{29}$$

$$\frac{315}{4\pi} \sum_j^{K_0} \frac{1}{h^5} \left(1 - \frac{|\mathbf{r}|_{ij}}{h} \right)^2 m_i m_j \frac{1}{d_i} \frac{1}{d_j} \left(A + D x_{ij} \frac{1}{|\mathbf{r}|^2_{ij}} \right) =$$

$$\frac{315}{4\pi} \sum_j^{K_0} \left(GN^{-\frac{1}{3}} \right)^{-5} \left(1 - \left(\frac{j}{K_0} \right)^{\frac{1}{3}} \right)^2 M_0^2 (NE)^{-2} (N)^{-2}$$

$$\left(A \pm D V_0^{\frac{1}{3}} N^{-\frac{1}{3}} j \left(\frac{j}{K_0} \right)^{-\frac{2}{3}} \left(GN^{-\frac{1}{3}} \right)^{-2} \right).$$

In this expression, all terms except N do not grow larger than K_0. Ignoring constants, the dependence on N of the terms under the sum is

$$\frac{\partial H_{xi}}{\partial \dot{x}_i} + \frac{\partial H_{xi}}{\partial \dot{x}_i} \sim \sum_j^{K_0} \left(N^{-\frac{7}{3}} \pm N^{-2} \right), \tag{30}$$

which tends to 0 in the limit $N \to \infty$.

Similar analysis of the other three possibilities for the second Helmholtz condition, section II B, leads to analogous expressions that depend on negative powers of N, thus tending to 0 in the macroscopic limit.

For the third condition, section II C, we also needed to make an additional assumption on how the velocity difference $\mathbf{v}_{ij}$ tends to 0 with the increase of the number of particles N, and, hence, the decrease of the distance between the particles. Assuming the same behaviour as for $\mathbf{r}_{ij}$, that is $\mathbf{v}_{ij} \sim N^{-\frac{1}{3}}$, similar results for the right hand sides of equations (20)-(22) are obtained, that is the dependence on negative powers of N leading to their vanishing in the $N \to \infty$ limit.

IV. SIMULATION DETAILS

To confirm the analysis above, we have also performed numerical estimation of the right hand sides of the conditions by simulating an SDPD system with varying number of particles (keeping all other parameters the same). Our results show that with growing N the right hand sides (the deviation from 0) become smaller, thus confirming the behaviour in the $N \to \infty$ limit.

Table I. Parameters of the simulated system

ν	shear viscosity	1 pg/(μm $\cdot$ μs)
c_0	control sound velocity	10 μm/μs
d_0	control density	1 pg/μm^3
h	cut-off radius	0.18 μm
T	temperature	300 K
m_i	particle mass	0.001 pg
dt	time step	$5 \cdot 10^{-4}$ μs

We used an implementation for SDPD developed as a package for the popular Molecular Dynamics simulator LAMMPS [9]. The package `USER-SDPD` is described in [10]. It simulates water-like liquid with approximations described by (8) at mesoscopic scales where thermal fluctuations are small. The parameters of the simulated system are listed in table I. Cubic simulation box with periodic boundary conditions was used.

An important parameter of simulation was the cut-off radius h that controlled how many neighbour particles were taken into account when calculating the particle summations in SDPD formulas. Clearly, the further a particle from the considered particle i the smaller its contribution to the sum. Therefore, we investigated how the values of calculated quantities changed with increasing h. We have found that in all cases the value of $h = 0.18\mu m$ was sufficiently large for the calculated values to converge.

V. NUMERICAL RESULTS AND DISCUSSION

As the second and the third Helmholtz conditions are not satisfied for SDPD equations of motion we investigated how the residues (the right hand sides of equations (11-14), (19-22)) change with increasing the number of SDPD particles keeping the density of the fluid constant. The limit of infinite number of particles provides the classical continuous Navier-Stokes equations [5].

The second condition in the form of equations (11, 12) demonstrates clear convergence of the residue with increasing the number of particles in the system, Fig. 3,4.

The second condition residues in the form of equations (13) and (14) are functions of the distance between particles i and j. We have summarised their values in Fig. 5,6. The tendency to lower values with increasing the number of particles in the system is evident for both equations.

We found that for the third condition in the form of equations (19,20,A1) the residues values wildly fluctuate between the particles in the system and at different time moments. We are investigating the reasons for this behaviour.

The residues for the third condition in the form of equations (21,22,A3-A5) converge towards 0. All combinations of coordinates produce similar graphs, an example is shown in Fig. 7

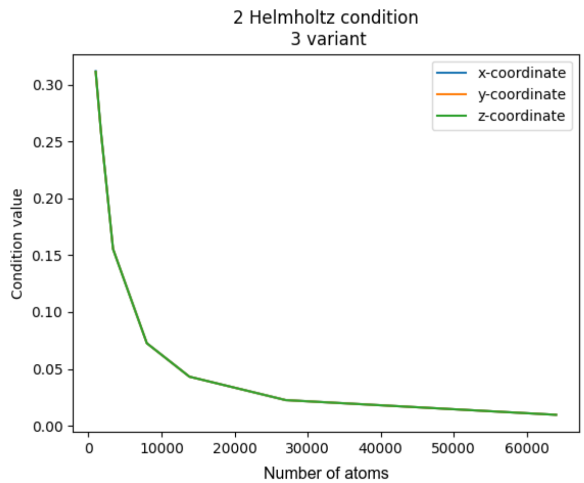

Figure 3. Second Helmholtz condition residue as a function of the number of particles in the system, equation (11); the graphs for x, y, and z coordinates overlap completely

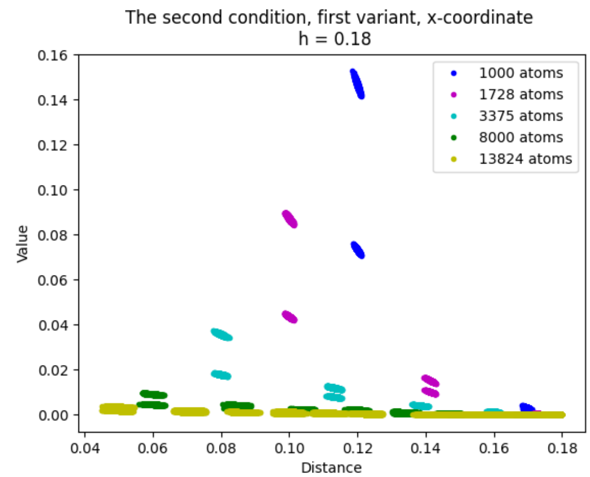

Figure 5. Second Helmholtz condition residue as a function of the distance between two particles, equation (13); the values for different number of particles in the system are shown

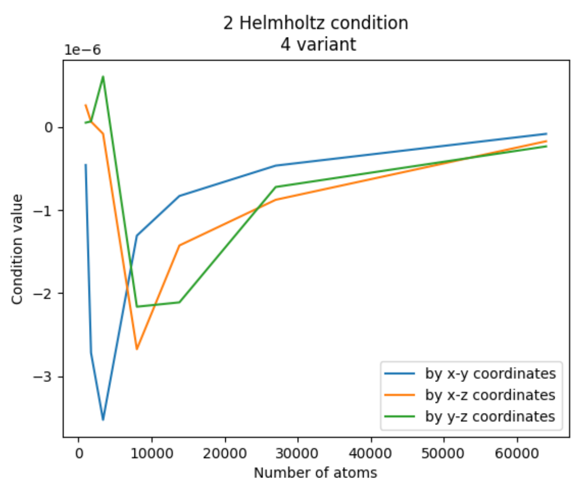

Figure 4. Second Helmholtz condition residue as a function of the number of particles, equation (12); the graphs for x, y (blue), x, z (orange), and y, z (green) combinations of the coordinates are shown

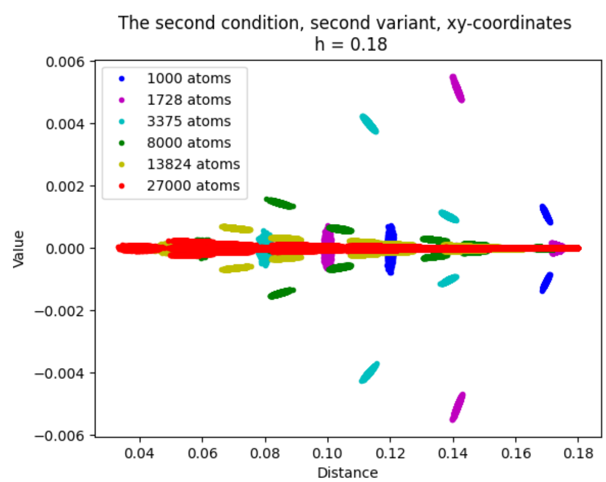

Figure 6. Second Helmholtz condition residue as a function of the distance between two particles, equation (14); the values for different number of particles in the system are shown

VI. CONCLUSIONS

In this paper we investigated if it is possible to derive Navier-Stokes hydrodynamic equations from a Lagrangian using the Euler-Lagrange equation. For this we analysed the three Helmholtz conditions necessary for a dynamical system to be derivable from a Lagrangian function. As the dynamical system we used SDPD equations of motion that are discrete approximations of the Navier-Stokes equations that converge to them in the infinite number of particles and zero kernel function support limit. We have found that the second and the third conditions are not satisfied for a finite number of particles, however the residues tend to zero with increasing number of particles. Also these residues tend to 0 in the analytical limit $N \to \infty$ and $h \to 0$. Thus, the continuous Navier-Stokes equations can be derived from a Lagrangian, at least in principle.

We are currently working on obtaining the explicit form of the Lagrangian in the macroscopic limit when the Helmholtz conditions are satisfied.

Finally, the presented results will be used as the basis for constructing hybrid particles, possessing simultaneously the properties of atoms and mesoscopic hydrodynamic particles, thus opening up the possibility of smooth transformation between physically distinct scales.

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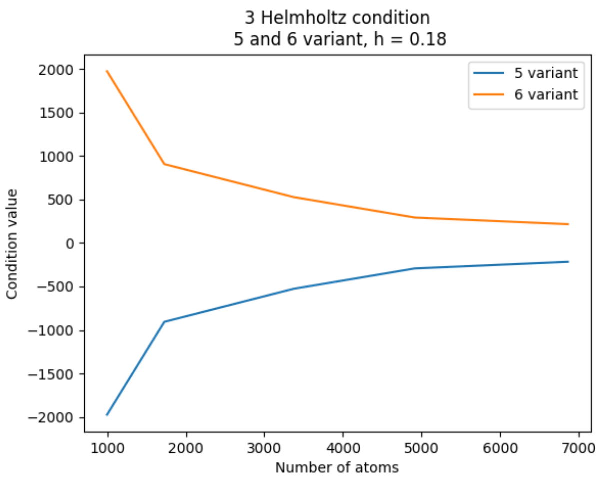

Figure 7. Third Helmholtz condition residues, equations (A4) (blue) and (A5) (orange)

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Appendix A: Expressions for the third Helmholtz condition

The expression for the third Helmholtz condition for particle i with respect to itself in different coordinates x and y, analogous to (20), reads:

$$\frac{\partial H_{yi}}{\partial x_i} - \frac{\partial H_{xi}}{\partial y_i} + \frac{\partial}{\partial t}\left(\frac{\partial H_{xi}}{\partial \dot{y}_i}\right) = \\ = \sum_j \Bigg[-T_{ij} \left(\left(L_i y_{ij} + d_i^{-2} d_j^{-1} S_{ij}^y\right) \left(\sum_k C K_{ik} x_{ik}\right) - \left(L_i x_{ij} + d_i^{-2} d_j^{-1} S_{ij}^x\right) \left(\sum_k C K_{ik} y_{ik}\right)\right) - \\ -T_{ij} d_i^{-1} d_j^{-1} \left[v x_{ij} y_{ij} - v y_{ij} x_{ij}\right] \left[\frac{2}{h\,|r|_{ij}\left(1 - \frac{|r|_{ij}}{h}\right)} A - d_j^{-1} K_{ij} A + D\left(|r|_{ij}\right)^{-2}\right]\Bigg] + R_{ij}^{xy}. \quad \text{(A1)}$$

The expression for the third Helmholtz condition for particle i with respect to a different particle p in the same coordinate x (y, z), analogous to (21), reads:

$$\frac{\partial H_{xp}}{\partial x_i} - \frac{\partial H_{xi}}{\partial x_p} + \frac{\partial}{\partial t}\left(\frac{\partial H_{xi}}{\partial \dot{x}_p}\right) = \\ = -C \sum_j \left[T_{ij}\left(K_{ip} x_{ip}\left[L_i x_{ij} + d_i^{-2} d_j^{-1} S_{ij}^x\right] - K_{pj} x_{pj}\left[L_j x_{ij} + d_i^{-1} d_j^{-2} S_{ij}^x\right]\right) + \right. \\ \left. + T_{ip} K_{ij} x_{ij}\left(L_i x_{ip} + d_i^{-2} d_p^{-1} S_{ip}^x\right)\right] - \\ - C \sum_l \left(T_{pl}\left[K_{ip} x_{ip}\left(L_p x_{pl} + d_p^{-2} d_l^{-1} S_{pl}^x\right) + K_{il} x_{il}\left(L_l x_{pl} + d_p^{-1} d_l^{-2} S_{pl}^x\right)\right] + \right. \\ \left. + T_{ip} K_{pl} x_{pl}\left(L_p x_{ip} + d_i^{-1} d_p^{-2} S_{ip}^x\right)\right) + R_{ip}^x. \quad \text{(A2)}$$

The expressions for the third Helmholtz condition for particle i with respect to a different particle p in different coordinates x and y, analogous to (22) read:

$$\frac{\partial H_{y_p}}{\partial x_i} - \frac{\partial H_{x_i}}{\partial y_p} + \frac{\partial}{\partial t}\left(\frac{\partial H_{x_i}}{\partial \dot{y}_p}\right) = \\ = -T_{ip} d_i^{-1} d_p^{-1}\left[v y_{ip} x_{ip} - v x_{ip} y_{ip}\right]\left[\frac{2}{h\,|r|_{ip}\left(1 - \frac{|r|_{ip}}{h}\right)} A + D\left(|r|_{ip}\right)^{-2}\right] - \\ - C \sum_j \left[T_{ij}\left(K_{ip} y_{ip}\left[L_i x_{ij} + d_i^{-2} d_j^{-1} S_{ij}^x\right] - K_{pj} y_{pj}\left[L_j x_{ij} + d_i^{-1} d_j^{-2} S_{ij}^x\right]\right) - \right. \\ \left. - T_{ip} K_{ij} x_{ij}\left(L_i y_{ip} + d_i^{-2} d_p^{-1} S_{ip}^y\right)\right] - \\ - C \sum_l \left[T_{pl}\left(K_{ip} x_{ip}\left[L_p y_{pl} + d_p^{-2} d_l^{-1} S_{pl}^y\right] + K_{il} x_{il}\left[L_l y_{pl} + d_p^{-1} d_l^{-2} S_{pl}^y\right]\right) - \right. \\ \left. - T_{ip} K_{pl} y_{pl}\left(L_p x_{ip} + d_i^{-1} d_p^{-2} S_{ip}^x\right)\right] + R_{ip}^{xy}, \quad \text{(A3)}$$

$$\frac{\partial H_{xp}}{\partial y_i} - \frac{\partial H_{yi}}{\partial x_p} + \frac{\partial}{\partial t}\left(\frac{\partial H_{yi}}{\partial \dot{x_p}}\right) =$$

$$= T_{ip} d_i^{-1} d_p^{-1} \left[v y_{ip} x_{ip} - v x_{ip} y_{ip} \right] \left[\frac{2}{h \left|r\right|_{ip} \left(1 - \frac{|r|_{ip}}{h}\right)} A + D \left(\left|r\right|_{ip}\right)^{-2} \right] +$$
$$+ C \sum_j \left[T_{ij} \left(K_{pj} x_{pj} \left[L_j y_{ij} + d_i^{-1} d_j^{-2} S_{ij}^y \right] - K_{ip} x_{ip} \left[L_i y_{ij} + d_i^{-2} d_j^{-1} S_{ij}^y \right] \right) \right.$$
$$\left. + T_{ip} K_{ij} y_{ij} \left(L_i x_{ip} + d_i^{-2} d_p^{-1} S_{ip}^x \right) \right] -$$
$$- C \sum_l \left[T_{pl} \left(K_{ip} y_{ip} \left[L_p x_{pl} + d_p^{-2} d_l^{-1} S_{pl}^x \right] \right) - K_{il} y_{il} \left[L_l x_{pl} + d_p^{-1} d_l^{-2} S_{pl}^x \right] - \right.$$
$$\left. - T_{ip} K_{pl} x_{pl} \left(L_p y_{ip} + d_i^{-1} d_p^{-2} S_{ip}^y \right) \right] + R_{ip}^{xy}, \quad \text{(A4)}$$

$$\frac{\partial H_{y_i}}{\partial x_p} - \frac{\partial H_{x_p}}{\partial y_i} + \frac{\partial}{\partial t}\left(\frac{\partial H_{x_p}}{\partial \dot{y_i}}\right) =$$

$$= -T_{ip} d_i^{-1} d_p^{-1} \left[v y_{ip} x_{ip} - v x_{ip} y_{ip} \right] \left[\frac{2}{h \left|r\right|_{ip} \left(1 - \frac{|r|_{ip}}{h}\right)} A + D \left(\left|r\right|_{ip}\right)^{-2} \right] -$$
$$- C \sum_j \left[T_{ij} \left(K_{pj} x_{pj} \left[L_j y_{ij} + d_i^{-1} d_j^{-2} S_{ij}^y \right] - K_{ip} x_{ip} \left[L_i y_{ij} + d_i^{-2} d_j^{-1} S_{ij}^y \right] \right) \right.$$
$$\left. + T_{ip} K_{ij} y_{ij} \left(L_i x_{ip} + d_i^{-2} d_p^{-1} S_{ip}^x \right) \right] +$$
$$+ C \sum_l \left[T_{pl} \left(K_{ip} y_{ip} \left[L_p x_{pl} + d_p^{-2} d_l^{-1} S_{pl}^x \right] \right) - K_{il} y_{il} \left[L_l x_{pl} + d_p^{-1} d_l^{-2} S_{pl}^x \right] - \right.$$
$$\left. - T_{ip} K_{pl} x_{pl} \left(L_p y_{ip} + d_i^{-1} d_p^{-2} S_{ip}^y \right) \right] + R_{ip}^{xy}, \quad \text{(A5)}$$

where $A = \left(\frac{5\eta}{3} - \xi\right)$, $D = \left(\xi + \frac{\eta}{3}\right)$, $C = \frac{315}{4\pi h^5}$ are constants and the following auxiliary variables were introduced:

$$L_i = 5B \left(\frac{1}{\rho_0}\right)^7 d_i^4 + 2B d_i^{-3}, \quad \text{(A6)}$$

$$S_{ij}^x = A v x_{ij} + D x_{ij} \left(r_{ij} \cdot v_{ij} \right) \left(\left|r\right|_{ij}\right)^{-2}, \quad \text{(A7)}$$

$$R_{ij}^x = \sum_j T_{ij} \left[Q_{ij}^x \left(- \frac{2}{h \left|r\right|_{ij} d_i d_j \left(1 - \frac{|r|_{ij}}{h}\right)} \left(r_{ij} \cdot v_{ij} \right) + \right. \right.$$
$$\left. + d_i^{-1} d_j^{-2} \left(\sum_k C K_{jk} \left(r_{jk} \cdot v_{jk} \right) \right) + d_i^{-2} d_j^{-1} \left(\sum_k C K_{ik} \left(r_{ik} \cdot v_{ik} \right) \right) \right) +$$
$$\left. + 2 d_i^{-1} d_j^{-1} D \left(\left|r\right|_{ij}\right)^{-2} \left[v x_{ij} x_{ij} - \left(r_{ij} \cdot v_{ij} \right) x_{ij}^2 \left(\left|r\right|_{ij}\right)^{-2} \right] \right], \quad \text{(A8)}$$

$$R_{ij}^{xy} = \sum_j T_{ij} \left[Q_{ij}^{xy} \left(- \frac{2}{h \left|r\right|_{ij} d_i d_j \left(1 - \frac{|r|_{ij}}{h}\right)} \left(r_{ij} \cdot v_{ij} \right) + \right. \right.$$
$$\left. + d_i^{-2} d_j^{-1} \left(\sum_k C K_{ik} \left(r_{ik} \cdot v_{ik} \right) \right) + d_i^{-1} d_j^{-2} \left(\sum_k C K_{jk} \left(r_{jk} \cdot v_{jk} \right) \right) \right) +$$
$$\left. + d_i^{-1} d_j^{-1} D \left(\left|r\right|_{ij}\right)^{-2} \left[v x_{ij} y_{ij} + v y_{ij} x_{ij} - 2 \left(\left|r\right|_{ij}\right)^{-2} \left(r_{ij} \cdot v_{ij} \right) x_{ij} y_{ij} \right] \right], \quad \text{(A9)}$$

$$R_{ip}^{x} = T_{ip}\left[Q_{ip}^{x}\left(\frac{2}{h\left|r\right|_{ip}d_{i}d_{p}\left(1-\frac{\left|r\right|_{ip}}{h}\right)}\left(r_{ip}\cdot v_{ip}\right)- -d_{i}^{-1}d_{p}^{-2}\left(\sum_{j}CK_{pj}\left(r_{pj}\cdot v_{pj}\right)\right)-d_{i}^{-2}d_{p}^{-1}\left(\sum_{j}CK_{ij}\left(r_{ij}\cdot v_{ij}\right)\right)\right)+ +d_{i}^{-1}d_{p}^{-1}2Dx_{ip}\left(\left|r\right|_{ip}\right)^{-2}\left[x_{ip}\left(\left|r\right|_{ip}\right)^{-2}\left(r_{ip}\cdot v_{ip}\right)-vx_{ip}\right]\right], \quad \text{(A10)}$$

$$R_{ip}^{xy} = T_{ip}\left[Q_{ip}^{xy}\left(-\frac{2}{h\left|r\right|_{ip}d_{i}d_{p}\left(1-\frac{\left|r\right|_{ip}}{h}\right)}\left(r_{ip}\cdot v_{ip}\right)+ +d_{i}^{-1}d_{p}^{-2}\left(\sum_{j}CK_{pj}\left(r_{pj}\cdot v_{pj}\right)\right)+d_{i}^{-2}d_{p}^{-1}\left(\sum_{j}CK_{ij}\left(r_{ij}\cdot v_{ij}\right)\right)\right)+ +d_{i}^{-1}d_{p}^{-1}D\left(\left|r\right|_{ip}\right)^{-2}\left[vx_{ip}y_{ip}+x_{ip}vy_{ip}-2\left(r_{ip}\cdot v_{ip}\right)x_{ip}y_{ip}\left(\left|r\right|_{ip}\right)^{-2}\right]\right]. \quad \text{(A11)}$$