

From continuum mechanics to SPH particle systems and back: Systematic derivation and convergence

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In this paper, we derive from the principle of least action the equation of motion for a continuous medium with regularized density field in the context of measures. The eventual equation of motion depends on the order in which regularization and the principle of least action are applied. We obtain two different equations, whose discrete counterparts coincide with the scheme used traditionally in the Smoothed Particle Hydrodynamics (SPH) numerical method [27], and with the equation treated by Di Lisio *et al.* in [9], respectively. Additionally, we prove the convergence in the Wasserstein distance of the corresponding measure-valued evolutions, moreover providing the order of convergence of the SPH method. The convergence holds for a general class of force fields, including external and internal conservative forces, friction and non-local interactions. The proof of convergence is illustrated numerically by means of one and two-dimensional examples.

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1 Introduction

The Smoothed Particle Hydrodynamics (SPH) numerical method was initially introduced to solve the equations of astrophysical flows. In the course of time it found application to equations describing a plethora of physical processes (for its diverse applications, see [28]). These processes predominantly involve continua and the equations refer to systems with infinite degrees of freedom. The central idea of the SPH method is to set up a relation between the continuum and a particle system, in which the continuum is loosely considered to be the limit case in which the number of particles tends to infinity. Here, a ‘particle’ should *not* be interpreted as a physical object of any scale (like an atom, molecule or grain) but rather as a numerical entity attributed with mass, position, velocity and other properties of the medium it represents.

It is well-established that the classical SPH scheme can be derived formally by applying the *principle of least action* to the particle system, where the SPH density approximation acts as a constraint; see e.g. [27, 30, 39]. The importance of the particle system’s Lagrangian function was already recognized in the first articles describing SPH; cf. [21]. A subtlety lies in the fact that in the derivation of the SPH equations, the action of the particle system is minimized rather than the action of the continuum. The minimization of the action at the continuum level and the subsequent discretization of the motion equation in terms of particles do not necessarily yield the same equation (at the discrete level).

The main achievement of this paper is twofold:

- We introduce a systematic procedure for deriving measure-valued and particle formulations of continuum mechanics equations. We obtain two different schemes depending on the stage at which a regularization of the density is introduced. See Sect. 2.
- We prove the convergence of both schemes using the Wasserstein distance on the space of probability measures; cf. Sect. 3.

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We now describe the two parts of our paper in more detail.

In the first part (Sect. 2), we aim at clarifying the exact difference in outcome between minimizing the action of the particle system and minimizing the action at the continuum level. To achieve this, we introduce a systematic procedure consisting of the following three steps:

- A** formulation in terms of measures and, simultaneously, the regularization¹ of the density;
- B** introduction of a particle formulation;
- C** application of the principle of least action.

These three steps are introduced in more detail in Sect. 2.2. It turns out that the order in which these steps are executed determines what the resulting equation is. To be more precise, the classical SPH scheme (as described e.g. in [27]) is obtained, whenever the regularization of the density takes place before applying the principle of least action. That is, whenever the steps are executed in the order **A-B-C** or **A-C-B**. Both procedures are presented here; see Sect. 2.3 and 2.4. If we apply the principle of least action (to the action at the continuum mechanics level) before regularizing the density then we obtain a scheme that appears in Di Lisio *et al.* [9] and in the recent paper [7]. However, this variant of the scheme is studied far less in literature. The procedure to obtain this scheme follows the order **C-A-B**. Its distinct characteristic is that it requires the gradient of the pressure field to be expressed analytically, while the pressure itself does not appear in the numerical scheme, in contrast to the commonly used SPH schemes. We emphasize that although both schemes arrive from the principle of least action, the latter can also be derived directly from Newtonian mechanics and introduction of the density regularization. The details of our rational derivation and the mutual relation between the two schemes have, to our knowledge, not been described in literature before.

In any case, regularization of the density practically means that the original problem is deliberately turned into a regularized one, which is afterwards solved by means of some variant of an SPH scheme. Hence, by choosing SPH as the solution method one is automatically bound to studying a different problem than the original one at the continuum level. Thus, two questions naturally arise:

- Does the solution of the regularized problem converge to the solution of the original problem?
- Does the particle solution of the regularized problem converge (in a certain sense) to the solution of the regularized continuum problem?

The former is out of the scope of the present study ([10] has dealt with it), while the latter is the topic of the current work's second part.

Measure theory provides a framework to study the limiting behaviour as the number of particles goes to infinity (cf. also e.g. [26]). Both the particle system, and the limiting continuum setting can be formulated in terms of measures. Hence, a distance between measures is a natural tool to characterize convergence; in this work we take the Wasserstein distance on the space of probability measures. This particular distance has the advantage that it can be formulated as the *infimum* over a set of joint representations (more details follow in Definitions 3.2 and 3.3). This is convenient, since one can thus obtain an upper bound (needed to prove convergence!) by choosing any admissible joint representation. See also [36], Chapter 6, for more discussion.

We prove the convergence of measure-valued solutions, as the initial measure is approximated; cf. Sect. 3. The line of arguments is similar to the one followed by Di Lisio *et al.* in [9], who first employed measures in combination with the Wasserstein distance to prove the convergence of the SPH method, but the result obtained in the present work is more general. It should be mentioned that in the earlier work [29] convergence of the *empirical measure* representing the particle system was proven, but using a different technique. Moreover, the only forces considered were mutual interactions between particles. Other approaches to obtain convergence are given e.g. by [2] using maximum local entropy estimates, [31] employing estimates for the truncation error, and [23, 32]. In [37, 38] the author establishes (weak) convergence for continuum models in fluid dynamics.

Nonetheless, the scheme treated in [9] is not the aforementioned traditional scheme. Our proof applies both to traditional SPH and to the scheme covered by [9]. Moreover, we allow for a much more general class of force fields. Apart from

¹ The regularization of equations is an old concept, introduced by Friedrichs in 1944 [19]. Additionally, notice that the regularization kernels used in SPH are a special subclass of the mollifier functions used by Friedrichs [19]; the SPH kernels are symmetric positive mollifiers.

external and internal conservative forces, we can deal with nonconservative forces such as viscosity of fluids and plasticity of solids; cf. [3, 14]. Finally, our results are valid in the presence of certain non-local interactions, that may arise in applications such as surface tension [34], defects in metal crystals (dislocations) [20, 26], pedestrian dynamics [8, 18] and swarming [5].

Previous work in the framework of measures by the authors of the current paper can be found in [13], where apart from the aforementioned force terms also random noise is treated. In [16, 17] measure-valued evolutions are treated in the scope of equations of motion that are first-order in time. The link between first-order and second-order models is discussed in [15].

The theoretical result of this paper regarding the order of convergence is supported numerically in Sect. 3.6 for one and two-dimensional illustrative examples, which involve different force fields.

In Sect. 4 concluding remarks are given about Sect. 2 and 3. Also, some attention is given to possible future research directions.

2 Systematic derivation of the equations of motion

In this section we derive equations of motion from Hamilton's principle of least action, which involves the Lagrangian function posed in a continuum mechanics setting. We describe an explicit 'recipe', hence avoiding the need to introduce approximations in an *ad hoc* manner. This 'recipe' consists of three building blocks (coined **A**, **B** and **C**; see Sect. 2.2). The order in which these blocks are executed, influences the final outcome. As such, the systematic procedure we describe here also shows exactly how different formulations/schemes arise from the same basic principles.

2.1 Derivation of the action in a continuous setting

Assume that for fixed time t a mass density ρ_t on a spatial domain Ω_t is given. We define the *Lagrangian density* of our system as

$$\mathcal{L}(\rho; y, u) := \left(\frac{1}{2} |u|^2 - e(\rho(y), y) \right) \rho(y),$$

where y and u are independent Eulerian coordinates, and e denotes the internal energy density. To obtain the *Lagrangian* L , we integrate \mathcal{L} over the spatial domain Ω_t :

$$L(t) := \int_{\Omega_t} \mathcal{L}(\rho_t; y, u) dy. \quad (1)$$

For this integration to make sense, we assume now that u is actually a velocity field, defined as a function of t and y : $u := u(t, y)$. Let there be a coordinate transform Φ_t such that $\Omega_t = \Phi_t(\Omega_0)$ for some initial domain Ω_0 . We call the family of transformations $(\Phi_t)_{t \geq 0}$ a *motion mapping* and transform the integral above according to $y = \Phi_t(x)$ with $x \in \Omega_0$:

$$L[\Phi](t) = \int_{\Omega_0} \left(\frac{1}{2} |u(t, \Phi_t(x))|^2 - e(\rho_t(\Phi_t(x)), \Phi_t(x)) \right) \rho_t(\Phi_t(x)) |J\Phi_t(x)| dx. \quad (2)$$

The *functional dependence* of L on the motion mapping is indicated by explicitly including Φ in square brackets. The expression $|J\Phi_t|$ denotes the determinant of the Jacobian matrix of the transformation, consisting of the derivatives of the components of Φ_t with respect to the components of x . Now we assume that the density ρ_t relates to the density ρ_0 defined on the original domain Ω_0 by the same transformation Φ_t , which is mathematically described by a *push-forward*, $\rho_t = \Phi_t \# \rho_0$ (cf. Definition 3.1). In particular, the densities relate in the following way (see e.g. [6], p. 90):

$$\rho_0(x) = \rho_t(\Phi_t(x)) |J\Phi_t(x)|. \quad (3)$$

Combined, (2) and (3) yield

$$L[\Phi](t) = \int_{\Omega_0} \left(\frac{1}{2} |u(t, \Phi_t(x))|^2 - e(\rho_t(\Phi_t(x)), \Phi_t(x)) \right) \rho_0(x) dx.$$

In the above we fixed t , but obviously all arguments can be repeated for every t in some interval $[0, T]$. In particular, we are interested in those motion mappings that are continuous and differentiable in time, and we wish to obtain their equation

of motion. The introduction of the motion mapping $(\Phi_t)_{t \in [0, T]}$ has taken us from pure Eulerian coordinates in (1) towards Lagrangian (material) coordinates in (2). The crucial and final step to complete this procedure is now to specify what the velocity field u is. In order to remain consistent with the motion mapping we introduced, we postulate the relation:

$$u(t, \Phi_t(x)) = \dot{\Phi}_t(x) \quad \text{for all } x \in \Omega_0. \quad (4)$$

The velocity $u(t, \Phi_t(x))$ is the velocity at time t of a material point that started in x at time 0, and – in words – (4) means that this velocity is equal to the time derivative at time t of the position $\Phi_t(x)$ of that particular material point. By connecting the Eulerian velocity u to the Lagrangian velocity $\dot{\Phi}_t$, we obtain the Lagrangian functional

$$L[\Phi](t) = \int_{\Omega_0} \left(\frac{1}{2} |\dot{\Phi}_t(x)|^2 - e(\rho_t(\Phi_t(x)), \Phi_t(x)) \right) \rho_0(x) dx. \quad (5)$$

We define the *action* of our system by

$$S[\Phi] := \int_0^T L[\Phi](t) dt. \quad (6)$$

2.2 Three procedures

The aim of this part of our paper is to derive equations of motion from the action (6), by means of the Euler-Lagrange equations (we will see that these appear in different shapes). Moreover, we wish to derive these equations of motion for a particle system, which naturally induces a numerical scheme. A methodological way to go from the continuum (Sect. 2.1) to a particle system, is via a measure-valued formulation. Our motivation to do so is the fact that we need a framework that incorporates the ‘real physics’, i.e. the density ρ_t , and an approximating particle system to establish the convergence of the particle scheme to the continuum.

To get the transition from the continuous action (6) to equations of motion for the particle positions, three steps are necessary:

- A** introduction of measures: replace $\rho_t(x)dx$ by $\mu_t(dx)$ and, wherever necessary, approximate ρ_t by some $\tilde{\rho}_t$ that depends on μ_t ;
- B** substituting for μ_t a discrete measure $\bar{\mu}_t^n = \sum_i m_i \delta_{x_i(t)}$;
- C** Derive the Euler-Lagrange equations (either classically or in variational sense).

The steps are here described in a somewhat simplistic and unprecise way; their true meaning will become clear in Sect. 2.3, 2.4 and 2.5. Step **A** takes us to a regularized version of the problem, which is a problem different from the original one. Step **B** cannot happen before **A**, but we have the freedom to choose the further ordering. This gives rise to three different derivations:

ABC : this procedure discretizes the Lagrangian and derives the corresponding equations of motion afterwards; see Sect. 2.3.

ACB : this procedure derives the equations of motion from the measure-valued Lagrangian and discretizes these equations afterwards; see Sect. 2.4.

CAB : this procedure derives the equations of motion from the continuum Lagrangian, writes them in measure-valued form and discretizes afterwards; see Sect. 2.5.

Procedures **ABC** and **ACB** eventually yield the same particle scheme. This is the scheme traditionally used in the SPH community (cf. [27]). Procedure **CAB** is the one that yields the equations used in [9] and [7].

2.2.1 Preview of the resulting particle schemes

We anticipate here concisely the resulting schemes and the crucial difference between them. To facilitate the exposition here, we assume that e depends only on the density and not explicitly on the spatial coordinate (we assume *here* also that no

nonconservative forces are present); the essence of the difference between the schemes lies in the remaining contributions. The ODEs governing the particle positions $x_k = x_k(t)$, with $k \in \{1, \dots, n\}$, turn out to be

$$\frac{d^2 x_k}{dt^2} = \begin{cases} - \sum_{i=1}^n m_i \nabla W_h(x_k - x_i) \left[\frac{\partial e}{\partial \rho}(\tilde{\rho}_t(x_k)) + \frac{\partial e}{\partial \rho}(\tilde{\rho}_t(x_i)) \right] & \text{for route ABC and ACB;} \\ - \left[2 \frac{\partial e}{\partial \rho}(\tilde{\rho}_t(x_k)) + \tilde{\rho}_t(x_k) \frac{\partial^2 e}{\partial \rho^2}(\tilde{\rho}_t(x_k)) \right] \sum_{i=1}^n m_i \nabla W_h(x_k - x_i) & \text{for route CAB,} \end{cases}$$

where $\tilde{\rho}_t$ is the aforementioned particle-based approximation of the density.

The full ODEs (including spatial dependence of e and nonconservative forces) are given in (13) and (24), and we present the details of the derivations in the sequel of this section; see Sect. 2.3, 2.4 and 2.5. The precise connection between the two schemes is elaborated on in Sect. 2.6.

2.3 Equations of motion via the route ABC

2.3.1 Step A

In Sect. 2.1 we introduced (for each t) the density ρ_t as the push-forward of the initial density ρ_0 under the mapping Φ_t . In this section we lift the evolution of ρ_t to the space of (time-dependent) measures. Let μ_0 and μ_t be the measures associated to the densities ρ_0 and ρ_t . Hence, $\mu_t = \Phi_t \# \mu_0$. In (5)–(6) we can substitute $\rho_0(x)dx$ by $\mu_0(dx)$. Afterwards, there is one more aspect that we need to ‘repair’ before we are completely in a measure formulation. The internal energy density e depends on ρ_t itself, via pointwise evaluation at $\Phi_t(x)$. An approximation of ρ_t is needed to obtain a general expression that is even well-defined for measures that have no density (w.r.t. the Lebesgue measure). We propose to introduce a regularization via convolution

$$\tilde{\rho}_t(\xi) := (W_h * \mu_t)(\xi) = \int_{\Omega_t} W_h(\xi - y) \mu_t(dy), \quad (7)$$

for all $\xi \in \mathbb{R}^d$. Here, the smoothing function W_h is nonnegative and even (so that it has an odd gradient, a property which is used later in the derivation of the equations), h is a small parameter, and $W_h \rightarrow \delta_0$ in the narrow topology as $h \rightarrow 0$ (i.e. tested against bounded continuous functions). A typical example is the Gaussian with zero mean and variance $h^2/2$. If μ_t has a density ρ_t then the convergence $\tilde{\rho}_t \rightarrow \rho_t$ holds *in some sense and under certain mathematical conditions*. E.g. if ρ_t is continuous and bounded, then by definition of $W_h \rightarrow \delta_0$, $\tilde{\rho}_t(\xi)$ converges to $\rho_t(\xi)$ for all ξ . In any case, the convolution regularizes the solution, introducing an artificial ‘density’ $\tilde{\rho}_t$, such that pointwise evaluation and the gradient are defined even when ρ_t does not exist or is not differentiable. Note that, $\tilde{\rho}_t$ also depends on h , but in this work we do not consider the limit $h \rightarrow 0$, therefore for simplicity of notation, we leave out h in $\tilde{\rho}_t$. However, we stick to the subscript h in W_h in agreement with the common notation in SPH literature.

Note that $\tilde{\rho}_t$ can also be written as

$$\tilde{\rho}_t(\xi) = \int_{\Omega_0} W_h(\xi - \Phi_t(x)) \mu_0(dx), \quad (8)$$

by definition of the push-forward. Hence, we should keep in mind that $\tilde{\rho}$ has either a functional dependence on μ_t , or an extra dependence on $\Phi_t(\cdot)$, depending on which formulation we choose, but we do not write this dependence explicitly.

In e , we substitute $\tilde{\rho}_t$ for ρ_t in the sequel and redefine the Lagrangian (in a measure-formulation) such that the action becomes

$$S[\Phi] = \int_0^T L[\Phi](t) dt = \int_0^T \int_{\Omega_0} \left(\frac{1}{2} |\dot{\Phi}_t(x)|^2 - e(\tilde{\rho}_t(\Phi_t(x)), \Phi_t(x)) \right) \mu_0(dx) dt. \quad (9)$$

The new, generalized formulation in terms of measures allows us to consider more types of solutions, simply by allowing for more general initial conditions. This is exactly what we exploit in the following step via a particle approximation.

2.3.2 Step B

In this step, we substitute for μ_0 a discrete measure of the form $\bar{\mu}_0^n = \sum_{i=1}^n m_i \delta_{x_{i,0}}$. Under push-forward, the measure remains a discrete measure with positions of the Diracs $\{x_i(t)\}$ evolving under the motion mapping: $x_i(t) = \Phi_t(x_{i,0})$. We emphasize that the equation for Φ_t is yet unknown and is to be derived in the next step.

The Lagrangian takes the form

$$L(t) = \sum_{i=1}^n m_i \left(\frac{1}{2} |\dot{x}_i(t)|^2 - e(\tilde{\rho}_t(x_i(t)), x_i(t)) \right), \quad (10)$$

with

$$\tilde{\rho}_t(x_i(t)) = \sum_{j=1}^n m_j W_h(x_i(t) - x_j(t)).$$

In the literature of SPH, particles of the same mass are employed for the modeling of the flow of a single fluid. In that case, the term m_i corresponds to $1/n$. On the other hand, multiphase media of piecewise continuous mass density can be modeled with the use of particles of different masses [27, 39]. For that reason, we adopt the general case of (in principle) unequal masses m_i .

2.3.3 Step C

The equations of motion are obtained via the ‘classical’ Euler-Lagrange equations, see (1.57) in [22], applied to the Lagrangian

$$L(t) = \sum_{i=1}^n m_i \left(\frac{1}{2} |u_i|^2 - e \left(\sum_{j=1}^n m_j W_h(y_i - y_j), y_i \right) \right),$$

cf. (10). In the presence of nonconservative forces (cf. p. 23 in [22]) the corresponding Euler-Lagrange equations are

$$\frac{d}{dt} \left(\nabla_{u_k} L \Big|_{(y_i, u_i) = (\Phi_t(x_{i,0}), \dot{\Phi}_t(x_{i,0}))} \right) - \nabla_{y_k} L \Big|_{(y_i, u_i) = (\Phi_t(x_{i,0}), \dot{\Phi}_t(x_{i,0}))} = m_k q[\bar{\mu}_t^n](\Phi_t(x_{k,0}), \dot{\Phi}_t(x_{k,0})), \quad (11)$$

for each $k \in \{1, \dots, n\}$, where q is the force density (per unit mass) of nonconservative forces. The functional dependence in square brackets denotes that q incorporates a nonlocal interaction term. More details will follow later; cf. (28). The subscript “ $(y_i, u_i) = (\Phi_t(x_{i,0}), \dot{\Phi}_t(x_{i,0}))$ ” should be read as performing this substitution for all $i \in \{1, \dots, n\}$.

After calculating the derivatives ∇_{u_k} and ∇_{y_k} in (11), we obtain

$$\begin{aligned} m_k \frac{d}{dt} \dot{\Phi}_t(x_{k,0}) &= \\ &- m_k \frac{\partial e}{\partial \rho} \left(\sum_{j=1}^n m_j W_h(\Phi_t(x_{k,0}) - \Phi_t(x_{j,0})), \Phi_t(x_{k,0}) \right) \sum_{j=1}^n m_j \nabla W_h(\Phi_t(x_{k,0}) - \Phi_t(x_{j,0})) \\ &+ \sum_{i=1}^n m_i \frac{\partial e}{\partial \rho} \left(\sum_{j=1}^n m_j W_h(\Phi_t(x_{i,0}) - \Phi_t(x_{j,0})), \Phi_t(x_{i,0}) \right) m_k \nabla W_h(\Phi_t(x_{i,0}) - \Phi_t(x_{k,0})) \\ &- m_k \nabla_y e \left(\sum_{j=1}^n m_j W_h(\Phi_t(x_{k,0}) - \Phi_t(x_{j,0})), \Phi_t(x_{k,0}) \right) + m_k q[\bar{\mu}_t^n](\Phi_t(x_{k,0}), \dot{\Phi}_t(x_{k,0})). \end{aligned} \quad (12)$$

We denote by $\nabla_y e$ the gradient of e only in the explicit spatial coordinate; that is, the second variable of e . We divide all terms by m_k (which is nonzero without loss of generality). If in the second line we take $\partial e / \partial \rho$ inside the sum and we use

in the third line that ∇W_h is an odd function, then the corresponding terms in (12) can be combined, and we obtain

$$\begin{aligned} \ddot{\Phi}_t(x_{k,0}) = & \\ & - \sum_{i=1}^n m_i \nabla W_h(\Phi_t(x_{k,0}) - \Phi_t(x_{i,0})) \left[\frac{\partial e}{\partial \rho}(\tilde{\rho}_t(\Phi_t(x_{k,0})), \Phi_t(x_{k,0})) + \frac{\partial e}{\partial \rho}(\tilde{\rho}_t(\Phi_t(x_{i,0})), \Phi_t(x_{i,0})) \right] \\ & - \nabla_y e(\tilde{\rho}_t(\Phi_t(x_{k,0})), \Phi_t(x_{k,0})) + q[\bar{\mu}_t^n](\Phi_t(x_{k,0}), \dot{\Phi}_t(x_{k,0})), \end{aligned} \quad (13)$$

for each $k \in \{1, \dots, n\}$. For brevity of notation, we use $\tilde{\rho}$ again in the argument of e .

2.4 Equations of motion via the route ACB

2.4.1 Step A

This step is exactly the same as in Sect. 2.3.1.

2.4.2 Step C

We start from the action given in (6). Instead of using the classical Euler-Lagrange equations, we employ here a generalized form of the principle of least action (see p. 127 and Sect. 4.4 of [3]):

$$S'[\Phi](\Psi) = -Q[\Phi](\Psi), \quad (14)$$

for all test functions $\Psi \in C_c^\infty((0, T); C_c^\infty(\Omega_0; \mathbb{R}^d))$. Here, $S'[\Phi](\Psi)$ denotes the variational derivative of S in the direction of Ψ , and $Q[\Phi](\Psi)$ is the work done along Ψ . It is defined as

$$Q[\Phi](\Psi) := \int_0^T \int_{\Omega_0} q[\mu_t](\Phi_t(x), \dot{\Phi}_t(x)) \cdot \Psi_t(x) \mu_0(dx) dt, \quad (15)$$

where q is the force density as in (11). For S' we have:

$$S'[\Phi](\Psi) := \left. \frac{d}{d\varepsilon} S[\Phi + \varepsilon\Psi] \right|_{\varepsilon=0}. \quad (16)$$

Note that

$$\begin{aligned} & \left. \frac{d}{d\varepsilon} \left[e \left(\int_{\Omega_0} W_h(\Phi_t(x) + \varepsilon\Psi_t(x) - \Phi_t(y) - \varepsilon\Psi_t(y)) \mu_0(dy), \Phi_t(x) + \varepsilon\Psi_t(x) \right) \right] \right|_{\varepsilon=0} \\ & = \frac{\partial e}{\partial \rho} \left(\int_{\Omega_0} W_h(\Phi_t(x) - \Phi_t(y)) \mu_0(dy), \Phi_t(x) \right) \int_{\Omega_0} \nabla W_h(\Phi_t(x) - \Phi_t(y)) \cdot (\Psi_t(x) - \Psi_t(y)) \mu_0(dy) \\ & \quad + \nabla_y e \left(\int_{\Omega_0} W_h(\Phi_t(x) - \Phi_t(y)) \mu_0(dy), \Phi_t(x) \right) \cdot \Psi_t(x). \end{aligned} \quad (17)$$

To avoid lengthy notation, we denote here by $e'[\Phi](\Psi)(x)$ the expression in (17). The variational derivative of S can be expressed as:

$$\begin{aligned} S'[\Phi](\Psi) & = \int_0^T \int_{\Omega_0} \left(\dot{\Phi}_t(x) \cdot \dot{\Psi}_t(x) - e'[\Phi](\Psi)(x) \right) \mu_0(dx) dt \\ & = \int_0^T \int_{\Omega_0} \left(-\ddot{\Phi}_t(x) \cdot \Psi_t(x) - e'[\Phi](\Psi)(x) \right) \mu_0(dx) dt, \end{aligned} \quad (18)$$

where the last step follows from integration by parts with respect to the time variable. The boundary terms disappear because Ψ has compact support within $(0, T)$.

We rewrite the part involving $\Psi_t(y)$ in (17) as follows:

$$\begin{aligned} & \int_0^T \int_{\Omega_0} -\frac{\partial e}{\partial \rho}(\tilde{\rho}_t(\Phi_t(x)), \Phi_t(x)) \int_{\Omega_0} \nabla W_h(\Phi_t(x) - \Phi_t(y)) \cdot \Psi_t(y) \mu_0(dy) \mu_0(dx) dt \\ & = \int_0^T \int_{\Omega_0} \int_{\Omega_0} \frac{\partial e}{\partial \rho}(\tilde{\rho}_t(\Phi_t(y)), \Phi_t(y)) \nabla W_h(\Phi_t(x) - \Phi_t(y)) \mu_0(dy) \cdot \Psi_t(x) \mu_0(dx) dt, \end{aligned} \quad (19)$$

by subsequently interchanging the order of integration, using that the function ∇W is odd, and replacing x by y and *vice versa*. A combination of (14), (15), (17), (18) and (19) yields for $S'[\Phi](\Psi) + Q[\Phi](\Psi)$ an integral of the form

$$\int_0^T \int_{\Omega_0} [\dots] \cdot \Psi_t(x) \mu_0(dx) dt,$$

where we deliberately do not explicitly write the integrand in square brackets. Since this integral equals 0 for all $\Psi \in C_c^\infty((0, T); C_c^\infty(\Omega_0; \mathbb{R}^d))$ – cf. (14) – the theorem of du Bois-Reymond yields that the integrand should vanish for almost all $t \in [0, T]$ and for μ_0 -almost every x . Hence, we obtain

$$\begin{aligned} \ddot{\Phi}_t(x) = & - \int_{\Omega_0} \nabla W_h(\Phi_t(x) - \Phi_t(y)) \left[\frac{\partial e}{\partial \rho}(\tilde{\rho}_t(\Phi_t(x)), \Phi_t(x)) + \frac{\partial e}{\partial \rho}(\tilde{\rho}_t(\Phi_t(y)), \Phi_t(y)) \right] \mu_0(dy) \\ & - \nabla_y e(\tilde{\rho}_t(\Phi_t(x)), \Phi_t(x)) + q[\mu_t](\Phi_t(x), \dot{\Phi}_t(x)). \end{aligned} \quad (20)$$

2.4.3 Step B

The transition to a particle system takes place by substitution of $\bar{\mu}_0^n = \sum_{i=1}^n m_i \delta_{x_{i,0}}$ for μ_0 in (20). Moreover, in $\tilde{\rho}_t$ and q we replace μ_t by $\bar{\mu}_t^n := \Phi_t \# \bar{\mu}_0^n$. Note that, after substitution, (20) holds $\bar{\mu}_0^n$ -a.e. and should therefore (only) be evaluated at $x = x_{k,0}$ for all $k \in \{1, \dots, n\}$. We obtain exactly (13).

2.5 Equations of motion via the route CAB

2.5.1 Step C

At the continuum level, deriving the Euler-Lagrange equations resembles considerably what was done in Sect. 2.4.2. Note however that the action as defined in (5)–(6) is used. In (5) $\rho_t(\Phi_t(x))$ occurs. The dependence on Φ_t that is explicitly written down, corresponds to the position at which ρ_t is evaluated. In addition however, if Φ_t is varied, also the function ρ_t itself changes. This is somewhat confusing, as this is an implicit, ‘hidden’ dependence of ρ_t on the motion mapping Φ_t . However, the exact relation is given by (3), which we therefore substitute in (5). The variational derivative becomes

$$\begin{aligned} S'[\Phi](\Psi) = & \frac{d}{d\varepsilon} \left(\int_0^T \int_{\Omega_0} \left(\frac{1}{2} |\dot{\Phi}_t(x) + \varepsilon \dot{\Psi}_t(x)|^2 - e \left(\frac{\rho_0(x)}{|J(\Phi_t + \varepsilon \Psi_t)(x)|}, \Phi_t(x) + \varepsilon \Psi_t(x) \right) \right) \rho_0(x) dx dt \right) \Bigg|_{\varepsilon=0}, \end{aligned}$$

cf. (16). Some effort is needed to deal with the ε -dependence in the Jacobian matrix. We refer here to Sect. 2 of [33], where the equation of motion is derived from the action, for the case where e has no explicit dependence on the spatial coordinate; i.e. $e = e(\rho)$. The determinant of the Jacobian matrix is a polynomial of the entries of that matrix. The basic idea in [33] is that the chain rule has to be applied with respect to every element of the Jacobian matrix. To avoid having to introduce a considerable amount of extra notation, we only state the result of [33] here:

$$\ddot{\Phi}_t(x) = - \frac{1}{\rho_t} \nabla \left(\rho_t^2 \frac{\partial e}{\partial \rho} \right) \Bigg|_{\Phi_t(x)} = - \left(2 \frac{\partial e}{\partial \rho}(\rho_t(\Phi_t(x))) + \rho_t(\Phi_t(x)) \frac{\partial^2 e}{\partial \rho^2}(\rho_t(\Phi_t(x))) \right) \nabla \rho_t(\Phi_t(x)). \quad (21)$$

On the right-hand side the gradient of the pressure P appears, due to the thermodynamic relation $\partial e / \partial \rho = P / \rho^2$. The reader should note that the notation used in [33] differs substantially from ours, but that the philosophy of deriving the equations of motion is the same.²

If $e = e(\rho, y)$, and moreover, we include nonconservative forces, then instead of (21) we obtain

$$\begin{aligned} \ddot{\Phi}_t(x) = & - \left(2 \frac{\partial e}{\partial \rho}(\rho_t(\Phi_t(x)), \Phi_t(x)) + \rho_t(\Phi_t(x)) \frac{\partial^2 e}{\partial \rho^2}(\rho_t(\Phi_t(x)), \Phi_t(x)) \right) \nabla \rho_t(\Phi_t(x)) \\ & - \nabla_y e(\rho_t(\Phi_t(x)), \Phi_t(x)) + q[\rho_t](\Phi_t(x), \dot{\Phi}_t(x)). \end{aligned} \quad (22)$$

The additional terms follow from similar steps as the ones leading to (20). We omit further details. Note that, in correspondence with q as introduced before, the dependence on ρ_t in square brackets indicates the presence of a nonlocal term; cf. (28). In the next step, this will become a dependence on the measure μ_t like before.

² Another interesting observation in [33] is that the Lagrangian density – when formulated in terms of Eulerian coordinates – is just the pressure P .

2.5.2 Step A

In this step, we formulate (22) in terms of measures. The only place where the measure μ_t can be incorporated directly, is in the nonconservative force density. We write $q[\mu_t](\Phi_t(x), \dot{\Phi}_t(x))$ instead of $q[\rho_t](\Phi_t(x), \dot{\Phi}_t(x))$. All the other occurrences of ρ_t in (22) we approximate by $\tilde{\rho}_t$ as defined in (7). We obtain

$$\ddot{\Phi}_t(x) = - \left(2 \frac{\partial e}{\partial \rho}(\tilde{\rho}_t(\Phi_t(x)), \Phi_t(x)) + \tilde{\rho}_t(\Phi_t(x)) \frac{\partial^2 e}{\partial \rho^2}(\tilde{\rho}_t(\Phi_t(x)), \Phi_t(x)) \right) \nabla \tilde{\rho}_t(\Phi_t(x)) - \nabla_y e(\tilde{\rho}_t(\Phi_t(x)), \Phi_t(x)) + q[\mu_t](\Phi_t(x), \dot{\Phi}_t(x)). \quad (23)$$

2.5.3 Step B

We take $\bar{\mu}_0^n := \sum_{i=1}^n m_i \delta_{x_{i,0}}$ and replace μ_t by $\bar{\mu}_t^n := \Phi_t \# \bar{\mu}_0^n$ in $\tilde{\rho}_t$ and q that appear in (23). We evaluate the resulting equation at $x = x_{k,0}$ for all $k \in \{1, \dots, n\}$ to obtain

$$\ddot{\Phi}_t(x_{k,0}) = - \left(2 \frac{\partial e}{\partial \rho}(\tilde{\rho}_t(\Phi_t(x_{k,0})), \Phi_t(x_{k,0})) + \tilde{\rho}_t(\Phi_t(x_{k,0})) \frac{\partial^2 e}{\partial \rho^2}(\tilde{\rho}_t(\Phi_t(x_{k,0})), \Phi_t(x_{k,0})) \right) \nabla \tilde{\rho}_t(\Phi_t(x_{k,0})) - \nabla_y e(\tilde{\rho}_t(\Phi_t(x_{k,0})), \Phi_t(x_{k,0})) + q[\bar{\mu}_t^n](\Phi_t(x_{k,0}), \dot{\Phi}_t(x_{k,0})), \quad (24)$$

where each appearance of $\tilde{\rho}_t$ denotes a sum over all particle positions. Namely,

$$\tilde{\rho}_t(\Phi_t(x_{k,0})) = \sum_{j=1}^n m_j W_h(\Phi_t(x_{k,0}) - \Phi_t(x_{j,0})), \quad \text{and}$$

$$\nabla \tilde{\rho}_t(\Phi_t(x_{k,0})) = \sum_{j=1}^n m_j \nabla W_h(\Phi_t(x_{k,0}) - \Phi_t(x_{j,0})).$$

2.6 Comparison of the resulting equations (13) and (24)

Procedures **ABC** and **ACB** yield the same equations of motion, namely (13). As anticipated already in Sect. 2.2, the equation resulting from Procedure **CAB** is different; see (24). This difference between the two final equations arose because we introduced the regularization via $\tilde{\rho}$ at different stages. In fact, (13) contains an extra regularization in space, as we will show now.

Note that only the term involving $\partial e / \partial \rho$ and $\partial^2 e / \partial \rho^2$ is different. In (13), we have

$$- \sum_{i=1}^n m_i \nabla W_h(\Phi_t(x_{k,0}) - \Phi_t(x_{i,0})) \left[\frac{\partial e}{\partial \rho}(\tilde{\rho}_t(\Phi_t(x_{k,0})), \Phi_t(x_{k,0})) + \frac{\partial e}{\partial \rho}(\tilde{\rho}_t(\Phi_t(x_{i,0})), \Phi_t(x_{i,0})) \right],$$

while the corresponding part in (24) is

$$- \left(2 \frac{\partial e}{\partial \rho}(\tilde{\rho}_t(\Phi_t(x_{k,0})), \Phi_t(x_{k,0})) + \tilde{\rho}_t(\Phi_t(x_{k,0})) \frac{\partial^2 e}{\partial \rho^2}(\tilde{\rho}_t(\Phi_t(x_{k,0})), \Phi_t(x_{k,0})) \right) \nabla \tilde{\rho}_t(\Phi_t(x_{k,0})).$$

Note that both of them contain a part $-\frac{\partial e}{\partial \rho}(\tilde{\rho}_t(\Phi_t(x_{k,0})), \Phi_t(x_{k,0})) \nabla \tilde{\rho}_t(\Phi_t(x_{k,0}))$, hence let us consider in (24) only

$$- \left(\frac{\partial e}{\partial \rho}(\tilde{\rho}_t(\Phi_t(x_{k,0})), \Phi_t(x_{k,0})) + \tilde{\rho}_t(\Phi_t(x_{k,0})) \frac{\partial^2 e}{\partial \rho^2}(\tilde{\rho}_t(\Phi_t(x_{k,0})), \Phi_t(x_{k,0})) \right) \nabla \tilde{\rho}_t(\Phi_t(x_{k,0})) = - \nabla \left(\tilde{\rho}_t(\Phi_t(x_{k,0})) \frac{\partial e}{\partial \rho}(\tilde{\rho}_t(\Phi_t(x_{k,0})), \Phi_t(x_{k,0})) \right). \quad (25)$$

To obtain this equality, we have assumed that $\nabla_y \partial e / \partial \rho \equiv 0$; this assumption anticipates the choice we make in (26). Let us even go back one more step and consider this term before the introduction of $\tilde{\rho}$, i.e. as in (22). To see how this term

relates to the corresponding one in (13), we take the convolution with W_h , and proceed as follows:

$$\begin{aligned} - \int_{\Omega_t} W_h(\xi - y) \nabla_y \left(\rho_t(y) \frac{\partial e}{\partial \rho}(\rho_t(y), y) \right) dy &= \int_{\Omega_t} \nabla_y W_h(\xi - y) \rho_t(y) \frac{\partial e}{\partial \rho}(\rho_t(y), y) dy \\ &= - \int_{\Omega_0} \nabla W_h(\xi - \Phi_t(y)) \frac{\partial e}{\partial \rho}(\rho_t(\Phi_t(y)), \Phi_t(y)) \rho_t(\Phi_t(y)) |J\Phi_t(y)| dy \\ &= - \int_{\Omega_0} \nabla W_h(\xi - \Phi_t(y)) \frac{\partial e}{\partial \rho}(\rho_t(\Phi_t(y)), \Phi_t(y)) \rho_0(y) dy. \end{aligned}$$

In the first step, we performed integration by parts, with vanishing boundary terms on $\partial\Omega_t$. This is because $\Omega_t = \text{supp } \rho_t$ and hence ρ_t vanishes on its boundary. Now replace $\rho_0(y)dy$ by $\mu_0(dy)$ and approximate ρ_t by $\tilde{\rho}_t$. Take $\mu_0 := \sum_{i=1}^n m_i \delta_{x_{i,0}}$ and evaluate at $\xi = \Phi_t(x_{k,0})$ and obtain

$$- \sum_{i=1}^n m_i \nabla W_h(\Phi_t(x_{k,0}) - \Phi_t(x_{i,0})) \frac{\partial e}{\partial \rho}(\tilde{\rho}_t(\Phi_t(x_{i,0})), \Phi_t(x_{i,0})).$$

This expression exactly appears in (13). To summarize: the connection between (13) and (24) is that in the former during the derivation procedure an extra regularization in space was introduced for *a part of* the right-hand side.

Note that, if we only consider the part involving $\partial e/\partial \rho$, (13) is the same as Eq. (3.8) in [27]. The notation used therein shows the direct dependence on the pressure. In Eq. (3.5) of [27], the equivalent of (24) is given. The reason why (13) is the one traditionally used in the SPH community is given in [27]: it does conserve linear and angular momentum exactly, as opposed to (24). Having derived the schemes, we are now able also to elaborate on the remark already made in the introduction: (24) ‘‘requires the gradient of the pressure field to be expressed analytically, while the pressure itself does not appear in the numerical scheme’’. The first part on the right-hand side of (24) is – anticipating (27) – of the form $-\frac{1}{\tilde{\rho}} \frac{d}{d\tilde{\rho}} (\tilde{\rho}^2 \bar{F}'(\tilde{\rho})) \nabla \tilde{\rho} = -\frac{1}{\tilde{\rho}} \frac{d}{d\tilde{\rho}} (P(\tilde{\rho})) \nabla \tilde{\rho}$. Hence we need an analytical expression for $\frac{d}{d\tilde{\rho}} (P(\tilde{\rho}))$.

2.7 Measure-valued formulation

In Sect. 2.3, 2.4 and 2.5 we derived particle-based schemes. To establish their convergence (as $n \rightarrow \infty$) we use a measure-valued formulation. Such formulation incorporates both the limit and the approximating sequence. Hence, we focus on the measure-formulations (20) and (23), without the specific choice $\mu_0 = \bar{\mu}_0^n$. Our convergence proof is applicable to a class of approximating measures that is much broader than just sums of Dirac deltas. The SPH-inspired particle approach is a special case; see Remark 3.13.

Although (20) and (23) are different (cf. Sect. 2.6), we wish to establish the convergence proof for both formulations simultaneously. Hence, we introduce a switching parameter $\theta \in \{0, 1\}$ to unify both variants in a single equation of motion. First, we assume that e is of the form

$$e(\rho, y) := V(y) + \bar{F}(\rho), \tag{26}$$

in agreement with the remark we already made underneath (25). Note that $\partial e/\partial \rho = \bar{F}'$ and $\nabla_y e = \nabla V$. Here, $V \in C_b^2(\mathbb{R}^d; \mathbb{R})$ describes the portion of potential energy which is due to a gravitational or magnetic field and $\bar{F} \in C^2(\mathbb{R}^+; \mathbb{R})$, where $\mathbb{R}^+ := (0, \infty)$ the potential energy due to the thermodynamics of the medium under consideration. This decomposition of e is typical for an ideal medium, such as a compressible inviscid fluid. Note moreover that this is a common modeling assumption in the derivation of the SPH equations for a system of particles [27]. We introduce two auxiliary functions defined by

$$F_0(\rho) := \frac{1}{\rho} \frac{d}{d\rho} (\rho^2 \bar{F}'(\rho)), \quad \text{and} \quad F_1(\rho) := \bar{F}'(\rho). \tag{27}$$

In the sequel, we use the generic notation F_θ , with $\theta \in \{0, 1\}$, to denote these functions.

We choose q to be of the form

$$q[\mu](y, u) := -\eta(y) u + (K * \mu)(y), \tag{28}$$

with $\eta \in C_b^1(\mathbb{R}^d; \mathbb{R}^+)$ and $K \in C_b^1(\mathbb{R}^d; \mathbb{R}^d)$. The K -term describes non-local interactions within the system, while the η -term is a viscous term. We use $-\eta \cdot u$, which is a simplified version of the usual viscous term in SPH that (also) involves

Definition 3.2 (Joint representation) A *joint representation* of two measures $\mu_1, \mu_2 \in \mathcal{P}(\mathbb{R}^d)$ is a measure π on $\mathbb{R}^d \times \mathbb{R}^d$ such that

$$\pi(A \times \mathbb{R}^d) = \mu_1(A), \quad \text{and} \quad \pi(\mathbb{R}^d \times B) = \mu_2(B),$$

for all A and B in the Borel σ -algebra of \mathbb{R}^d . We denote by $\Pi(\mu_1, \mu_2)$ the set of all joint representations of μ_1 and μ_2 . Joint representations are also called *couplings*.

A useful property of a joint representation $\pi \in \Pi(\mu_1, \mu_2)$ is that for each $i \in \{1, 2\}$

$$\int_{\mathbb{R}^d \times \mathbb{R}^d} f(x_i) \pi(dx_1, dx_2) = \int_{\mathbb{R}^d} f(x) \mu_i(dx) \quad (32)$$

for all measurable, bounded functions f on \mathbb{R}^d . In fact, this is an alternative definition.

Definition 3.3 (Wasserstein distance) The *Wasserstein distance* between two probability measures $\mu_1, \mu_2 \in \mathcal{P}(\mathbb{R}^d)$ is defined as

$$\mathcal{W}(\mu_1, \mu_2) := \inf_{\pi \in \Pi(\mu_1, \mu_2)} \int_{\mathbb{R}^d \times \mathbb{R}^d} |x - y| \pi(dx, dy).$$

Note that, to be more precise, we should call this the *1-Wasserstein distance*, as a special case of the *p-Wasserstein distance* for which the cost function $|x - y|^p$ is used in the integral. The 1-Wasserstein distance is usually written as W_1 , but we will stick to \mathcal{W} to avoid confusion with the smoothing function W_h . The particular choice $p = 1$ is made because it is compatible with the Lipschitz properties of the functions and the motion mapping that we use. This is what Sect. 3 hinges on. For an exposition on the Wasserstein distance and the related concept of *optimal transport*, we refer to [35] and [36].

3.2 Assumptions

Throughout the paper, we assume the following:

Assumption 3.4 The functions V, η and K satisfy $V \in C_b^2(\mathbb{R}^d; \mathbb{R})$, $\eta \in C_b^1(\mathbb{R}^d; \mathbb{R}^+)$ and $K \in C_b^1(\mathbb{R}^d; \mathbb{R}^d)$.

Remark 3.5 Note in particular that the above assumption implies that ∇V and K are Lipschitz continuous. We denote their Lipschitz constants by $\|\nabla V\|_{\text{Lip}}$ and $\|K\|_{\text{Lip}}$, respectively.

For F_θ and W_h we have requirements that depend on the value of θ . Recall that

$$\mathbb{R}^+ := (0, \infty) \quad \text{and define} \quad \mathbb{R}_0^+ := [0, \infty).$$

Assumption 3.6 The function $W_h \in C_b^2(\mathbb{R}^d; \mathbb{R}_0^+)$ is even and satisfies $\int_{\mathbb{R}^d} W_h(x) dx = 1$.

Assumption 3.7 (The case $\theta = 0$) We require that $F_0 \in C^1(\mathbb{R}^+; \mathbb{R})$. Moreover, we assume that there is a constant $M_1 > 0$ such that for all $\mu \in \mathcal{P}(\mathbb{R}^d)$

$$\sup_{x \in \mathbb{R}^d} |F_0((W_h * \mu)(x)) \nabla(W_h * \mu)(x)| \leq M_1. \quad (33)$$

Define the quantity $r(T) := r_0 + T\|v_0\|_\infty + \frac{1}{2}T^2(\|\nabla V\|_\infty + M_1 + \|K\|_\infty)$, cf. (43), and the set

$$U_{T, W_h} := \left\{ u \in \mathbb{R}_0^+ : \left(\inf_{B(2r(T))} W_h \right) \leq u \leq \|W_h\|_\infty \right\}.$$

Ultimately, we assume that there are constants $M_2, M_3 > 0$ such that

$$\sup_{u \in U_{T, W_h}} |F_0(u)| \leq M_2, \quad \text{and} \quad \sup_{u \in U_{T, W_h}} |F_0'(u)| \leq M_3. \quad (34)$$

Remark 3.8 The upper bound in (33) is needed to get an *a priori* bound on the propagation speed in Lemma 3.14. Consequently, we can restrict ourselves to measures with bounded support afterwards; cf. Corollary 3.15.

For all $t \in [0, T]$, the measure μ_t that solves (31) has its support contained in $B(r(T))$. Since μ_t is a probability measure, and $\tilde{\rho}_t = W_h * \mu_t$, on $[0, T]$ the function $\tilde{\rho}_t$ can only take values in U_{T, W_h} , cf. (51)–(52). Consequently, to bound $|F_0(\tilde{\rho}_t)|$ and $|F_0'(\tilde{\rho}_t)|$ we only need to take the supremum over values in U_{T, W_h} . This is what we do in (34). Due to this technicality, an F_0 that satisfies Assumption 3.7 may still have singularities at the origin, but *only* if W_h is strictly positive everywhere in $B(2r(T))$. Such F_0 and W_h are used in [9]. See also Sect. 3.5 for further discussion.

If $\theta = 1$ we need the following assumption:

Assumption 3.9 (The case $\theta = 1$) We assume that $F_1 \in C^1(\mathbb{R}_0^+; \mathbb{R})$.

Under Assumption 3.9, there are constants $M_2, M_3 > 0$ such that

$$\sup_{u \in [0, \|W_h\|_\infty]} |F_1(u)| \leq M_2, \quad \text{and} \quad \sup_{u \in [0, \|W_h\|_\infty]} |F_1'(u)| \leq M_3.$$

Subsequently, define $M_1 := 2 M_2 \|\nabla W_h\|_\infty$.

In both cases $\theta = 0$ and $\theta = 1$, we use the same letters M_1, M_2 and M_3 for the constants, to ease notation in the sequel.

Remark 3.10 We need Assumption 3.9 to achieve the *a priori* bound in Lemma 3.14 for $\theta = 1$. However, Assumption 3.9 does not allow for singularities in F_1 around zero. We demonstrate now why a weaker assumption for F_1 , resembling (33) is not feasible. Assume that $F_1(\rho) := \rho^\alpha$ with $\alpha \in (-1, 0)$. This is the case also considered in [9]. To bound the first term on the right-hand side of (29), in [9] it is assumed that $|\nabla W_h(\xi)| \leq c|W_h(\xi)|^{-\alpha}$ for some $c > 0$. We would need an estimate on

$$\sup_{x \in \text{supp } \mu} |(\nabla W_h * [(F_1 \circ (W_h * \mu)) \cdot \mu])(x)|, \quad (35)$$

for fixed $h > 0$ and uniformly with respect to $\mu \in \mathcal{P}(\mathbb{R}^d)$. Let W_h be strictly positive everywhere. Since $W_h \in L^1(\mathbb{R}^d)$, $\lim_{\xi \rightarrow \infty} W_h(\xi) = 0$. Let W_h satisfy the aforementioned condition $|\nabla W_h(\xi)| \leq c|W_h(\xi)|^{-\alpha}$. Then also $\lim_{\xi \rightarrow \infty} |\nabla W_h(\xi)| = 0$. Under these (not very strict) conditions one can show that (35) is unbounded; to see this, use e.g. the sequence of measures $(\mu^\kappa)_{\kappa \in \mathbb{N}^+}$ defined by $\mu^\kappa := (\delta_{-\kappa \underline{e}_1} + \delta_{\kappa \underline{e}_1} + \delta_{(\kappa+1) \underline{e}_1})/3$, where \underline{e}_1 is the first unit vector in \mathbb{R}^d . Note in particular that (35) is unbounded for a Gaussian W_h . The Gaussian however is one of the standard choices for W_h that we do want to allow for.

3.3 Main convergence result

Before we can prove the convergence of SPH particle systems, we need to establish the well-posedness of (31); that is, the existence and uniqueness of solutions, and in particular the continuous dependence on the initial conditions.

For any $r > 0$, define $\mathcal{P}_r(\mathbb{R}^d) := \{\mu \in \mathcal{P}(\mathbb{R}^d) : \text{supp } \mu \subset B(r)\}$. We also define \mathcal{A} as

$$\mathcal{A} := \left\{ \Psi : B(r_0) \rightarrow C^2([0, T]; \mathbb{R}^d) : \Psi_t(\cdot) \in C(B(r_0); \mathbb{R}^d) \text{ for all } t \in [0, T] \right\}.$$

Hence, each element of \mathcal{A} is a mapping $(x, t) \mapsto \Psi_t(x)$ that for each fixed x is twice continuously differentiable in time, and for each fixed t is continuous in the spatial variable x .

Theorem 3.11 (Well-posedness of solutions) *Let $h > 0$ be fixed and let $\theta \in \{0, 1\}$. Assume that $v_0 \in C_b^1(\mathbb{R}^d; \mathbb{R}^d)$, and that Assumptions 3.4 and 3.6 hold. Let moreover (depending on the value of θ) Assumption 3.7 or 3.9 be satisfied.*

Then we have the following results:

1. *For each $\mu_0 \in \mathcal{P}_{r_0}(\mathbb{R}^d)$ there exists a unique pair $(\mu, \Phi) \in C([0, T]; \mathcal{P}_{r(T)}(\mathbb{R}^d)) \times \mathcal{A}$ that satisfies (31);*
2. *Solutions to (31) are continuous with respect to their initial conditions. In particular that is, if for $i \in \{1, 2\}$ the pairs $(\mu^i, \Phi^i) \in C([0, T]; \mathcal{P}_{r(T)}(\mathbb{R}^d)) \times \mathcal{A}$ are the (unique) solutions of (31) corresponding to initial conditions $\mu_0^i \in \mathcal{P}_{r_0}(\mathbb{R}^d)$, then*

$$\sup_{t \in [0, T]} \mathcal{W}(\mu_t^1, \mu_t^2) \leq (1 + T (\|\nabla v_0\|_\infty + \|\eta\|_\infty)) \exp\left(\|\eta\|_\infty T + \frac{1}{2} (M_4 + M_5) T^2\right) \mathcal{W}(\mu_0^1, \mu_0^2), \quad (36)$$

for some constants $M_4, M_5 > 0$ that are independent of μ_0^1 and μ_0^2 .

The proof is given in Sect. 3.4. The main result of the present paper is a direct consequence of the previous theorem that roughly reads: if we have a converging sequence of initial conditions (e.g. particle approximations) then the sequence of corresponding solutions converges. This statement is made precise in the following corollary.

Corollary 3.12 (Convergence of approximate solutions) *Fix $\theta \in \{0, 1\}$. Consider a family of initial conditions $\{\mu_0^n\}_{n \in \mathbb{N}} \subset \mathcal{P}_{r_0}(\mathbb{R}^d)$ such that*

$$\mathcal{W}(\mu_0^n, \mu_0) \xrightarrow{n \rightarrow \infty} 0, \quad (37)$$

for some $\mu_0 \in \mathcal{P}_{r_0}(\mathbb{R}^d)$. Let (μ^n, Φ^n) be the solution of (31) with initial distribution μ_0^n and the same initial velocity v_0 for all n . Let (μ, Φ) be the solution corresponding to the initial distribution μ_0 and the initial velocity v_0 . Then μ^n converges to μ in the following sense:

$$\sup_{t \in [0, T]} \mathcal{W}(\mu_t^n, \mu_t) \xrightarrow{n \rightarrow \infty} 0.$$

Remark 3.13 (Convergence of SPH particle approximations) In particular, Corollary 3.12 implies the convergence of SPH particle approximations. These are the (time-dependent) discrete measures $\bar{\mu}_t^n = \sum_{k=1}^n m_k \delta_{\Phi_t(x_{k,0})}$ associated to the particle schemes:

$$\begin{aligned} \ddot{\Phi}_t(x_{k,0}) = & - \sum_{i=1}^n m_i \nabla W_h(\Phi_t(x_{k,0}) - \Phi_t(x_{i,0})) [F_\theta(\tilde{\rho}_t(\Phi_t(x_{k,0}))) + \theta F_\theta(\tilde{\rho}_t(\Phi_t(x_{i,0})))] \\ & - \nabla V(\Phi_t(x_{k,0})) - \eta(\Phi_t(x_{k,0})) \dot{\Phi}_t(x_{k,0}) + (K * \bar{\mu}_t^n)(\Phi_t(x_{k,0})), \end{aligned} \quad (38)$$

where the initial measures are of the form $\bar{\mu}_0^n := \sum_{j=1}^n m_j \delta_{x_{j,0}} \in \mathcal{P}_{r_0}(\mathbb{R}^d)$ for some $\{m_j\}_{j=1}^n \subset \mathbb{R}^+$ such that $\sum_{j=1}^n m_j = 1$, and for some $\{x_{j,0}\}_{j=1}^n \subset B(r_0)$. The measure-valued trajectories $(\bar{\mu}_t^n)_{0 \leq t \leq T}$ converge, provided that the initial measures converge.

3.4 Proof of the main convergence theorem

Before proving Theorem 3.11, we need two auxiliary lemmas concerning the properties of the motion mapping Φ_t . The first lemma is an upper estimate for Φ_t .

Lemma 3.14 *Let Assumptions 3.4, 3.6 and 3.7 or 3.9 (depending on the value of θ) be satisfied. For any given $\mu \in \mathcal{C}([0, T]; \mathcal{P}(\mathbb{R}^d))$ and for any $x \in \mathbb{R}^d$ assume that the mapping $t \mapsto \Phi_t$ is a solution to (29) completed with $\tilde{\rho}_t := W_h * \mu_t$, $\Phi_0(x) = x$ and $\dot{\Phi}_0(x) = v_0(x)$. Then for all $t \in [0, T]$ it holds that*

$$|\Phi_t(x)| \leq |x| + t \|v_0\|_\infty + \frac{1}{2} t^2 (M_1 + \|\nabla V\|_\infty + \|K\|_\infty). \quad (39)$$

Proof. Using an integrating factor $H(t) := \exp\left(\int_0^t \eta(\Phi_\tau(x)) d\tau\right) \geq 1$, we deduce from (29) that

$$\begin{aligned} |\Phi_t(x)| & \leq |\Phi_0(x)| + \left| \int_0^t \frac{v_0(x)}{H(s)} ds \right| + \left| \int_0^t \frac{1}{H(s)} \int_0^s H(r) \left(\ddot{\Phi}_r(x) + \eta(\Phi_r(x)) \dot{\Phi}_r(x) \right) dr ds \right| \\ & \leq |x| + t \|v_0\|_\infty + \int_0^t \int_0^s \frac{H(r)}{H(s)} \left| \ddot{\Phi}_r(x) + \eta(\Phi_r(x)) \dot{\Phi}_r(x) \right| dr ds. \end{aligned}$$

Since η is a positive function and hence $0 \leq H(r)/H(s) \leq 1$ in the inner integral, it follows that

$$\begin{aligned} |\Phi_t(x)| & \leq |x| + t \|v_0\|_\infty + \int_0^t \int_0^s \left| -\nabla V(\Phi_r(x)) + (K * \mu_r)(\Phi_r(x)) \right. \\ & \quad \left. - F_\theta((W_h * \mu_r)(\Phi_r(x))) \nabla(W_h * \mu_r)(\Phi_r(x)) - \theta (\nabla W_h * [(F_\theta \circ (W_h * \mu_r))\mu_r])(\Phi_r(x)) \right| dr ds. \end{aligned} \quad (40)$$

In the case $\theta = 0$, the following estimate holds for all $x \in \mathbb{R}^d$ due to Assumption 3.7:

$$\begin{aligned} |F_\theta((W_h * \mu_r)(\Phi_r(x))) \nabla(W_h * \mu_r)(\Phi_r(x)) + \theta (\nabla W_h * [(F_\theta \circ (W_h * \mu_r))\mu_r])(\Phi_r(x))| \\ = |F_0((W_h * \mu_r)(\Phi_r(x))) \nabla(W_h * \mu_r)(\Phi_r(x))| \leq M_1. \end{aligned} \quad (41)$$

Note that for any $\mu \in \mathcal{P}(\mathbb{R}^d)$ it holds that $\|W_h * \mu\|_\infty \leq \|W_h\|_\infty$. Hence, in the case $\theta = 1$:

$$\begin{aligned} & |F_\theta((W_h * \mu_r)(\Phi_r(x))) \nabla(W_h * \mu_r)(\Phi_r(x)) + \theta (\nabla W_h * [(F_\theta \circ (W_h * \mu_r))\mu_r])(\Phi_r(x))| \\ & \leq M_2 \|\nabla W_h\|_\infty + \|\nabla W_h\|_\infty M_2 = M_1, \end{aligned} \quad (42)$$

where the bounds of Assumption 3.9 are used.

A combination of (40), (41) and (42) yields that for each $\theta \in \{0, 1\}$

$$|\Phi_t(x)| \leq |x| + t \|v_0\|_\infty + \int_0^t \int_0^s (\|\nabla V\|_\infty + \|K\|_\infty + M_1) dr ds$$

holds for all $x \in \mathbb{R}^d$ and $t \in [0, T]$, from which the statement of the lemma follows. \square

Corollary 3.15 *Let $\mu_0 \in \mathcal{P}_{r_0}(\mathbb{R}^d)$, and let Assumptions 3.4, 3.6 and 3.7 or 3.9 (depending on the value of θ) be satisfied. Then any solution of (31) must satisfy*

$$\text{supp } \mu_t \subset B(r(t)),$$

for each $t \in [0, T]$, where

$$r(t) := r_0 + t \|v_0\|_\infty + \frac{1}{2} t^2 (M_1 + \|\nabla V\|_\infty + \|K\|_\infty). \quad (43)$$

The next lemma provides a Lipschitz-like estimate on Φ_t .

Lemma 3.16 *Let $\nu^1, \nu^2 \in C([0, T]; \mathcal{P}_{r(T)}(\mathbb{R}^d))$ be given, with $\text{supp } \nu_0^i \subset B(r_0)$ for each $i \in \{1, 2\}$. Consider the motion mappings corresponding to ν^i defined by:*

$$\begin{aligned} \ddot{\Phi}_t^{\nu^i}(\xi) &= -F_\theta \left((W_h * \nu_t^i)(\Phi_t^{\nu^i}(\xi)) \right) \nabla(W_h * \nu_t^i)(\Phi_t^{\nu^i}(\xi)) - \theta (\nabla W_h * [(F_\theta \circ (W_h * \nu_t^i))\nu_t^i])(\Phi_t^{\nu^i}(\xi)) \\ &\quad - \nabla V(\Phi_t^{\nu^i}(\xi)) - \eta(\Phi_t^{\nu^i}(\xi)) \dot{\Phi}_t^{\nu^i}(\xi) + (K * \nu_t^i)(\Phi_t^{\nu^i}(\xi)) \end{aligned} \quad (44)$$

for all $\xi \in B(r_0)$ and all $t \in [0, T]$, with initial conditions $\Phi_0^{\nu^i}(\xi) = \xi$, $\dot{\Phi}_0^{\nu^i}(\xi) = v_0(\xi)$. Then, for all $t \in [0, T]$ and $x, y \in B(r_0)$ it holds that

$$\begin{aligned} |\Phi_t^{\nu^1}(x) - \Phi_t^{\nu^2}(y)| &\leq (1 + t \|\eta\|_\infty) |x - y| + t |v_0(x) - v_0(y)| \\ &\quad + \int_0^t [M_4(t-s) + \|\eta\|_\infty] |\Phi_s^{\nu^1}(x) - \Phi_s^{\nu^2}(y)| ds + M_5 \int_0^t (t-s) \mathcal{W}(\nu_s^1, \nu_s^2) ds, \end{aligned} \quad (45)$$

where

$$\begin{aligned} M_4 &:= \|\nabla V\|_{\text{Lip}} + (1 + \theta) M_2 \|D^2 W_h\|_\infty + M_3 \|\nabla W_h\|_\infty^2 + \|K\|_{\text{Lip}}, \quad \text{and} \\ M_5 &:= (1 + \theta) M_2 \|D^2 W_h\|_\infty + (1 + \theta) M_3 \|\nabla W_h\|_\infty^2 + \|K\|_{\text{Lip}}. \end{aligned}$$

Proof. Note that, by the Fubini's theorem, for any integrable function f , we have

$$\int_0^t \int_0^r f(s) ds dr = \int_0^t \int_s^t f(s) dr ds = \int_0^t (t-s) f(s) ds. \quad (46)$$

Integration of (44) in time together with (46) yields that

$$\begin{aligned}
|\Phi_t^{\nu^1}(x) - \Phi_t^{\nu^2}(y)| &\leq |x - y| + t |v_0(x) - v_0(y)| + \int_0^t (t - s) |\nabla V(\Phi_s^{\nu^1}(x)) - \nabla V(\Phi_s^{\nu^2}(y))| ds \\
&\quad + \left| \int_0^t \int_0^r \eta(\Phi_s^{\nu^1}(x)) \dot{\Phi}_s^{\nu^1}(x) - \eta(\Phi_s^{\nu^2}(y)) \dot{\Phi}_s^{\nu^2}(y) ds dr \right| \\
&\quad + \int_0^t (t - s) \left| F_\theta \left((W_h * \nu_s^1)(\Phi_s^{\nu^1}(x)) \right) \nabla (W_h * \nu_s^1)(\Phi_s^{\nu^1}(x)) \right. \\
&\quad \quad \left. - F_\theta \left((W_h * \nu_s^2)(\Phi_s^{\nu^2}(y)) \right) \nabla (W_h * \nu_s^2)(\Phi_s^{\nu^2}(y)) \right| ds \\
&\quad + \theta \int_0^t (t - s) \left| (\nabla W_h * [(F_\theta \circ (W_h * \nu_s^1)) \nu_s^1])(\Phi_s^{\nu^1}(x)) \right. \\
&\quad \quad \left. - (\nabla W_h * [(F_\theta \circ (W_h * \nu_s^2)) \nu_s^2])(\Phi_s^{\nu^2}(y)) \right| ds \\
&\quad + \int_0^t (t - s) \left| (K * \nu_s^1)(\Phi_s^{\nu^1}(x)) - (K * \nu_s^2)(\Phi_s^{\nu^2}(y)) \right| ds. \tag{47}
\end{aligned}$$

Furthermore, we have

$$\int_0^t (t - s) |\nabla V(\Phi_s^{\nu^1}(x)) - \nabla V(\Phi_s^{\nu^2}(y))| ds \leq \|\nabla V\|_{\text{Lip}} \int_0^t (t - s) |\Phi_s^{\nu^1}(x) - \Phi_s^{\nu^2}(y)| ds, \tag{48}$$

and

$$\begin{aligned}
\left| \int_0^t \int_0^r \eta(\Phi_s^{\nu^1}(x)) \dot{\Phi}_s^{\nu^1}(x) - \eta(\Phi_s^{\nu^2}(y)) \dot{\Phi}_s^{\nu^2}(y) ds dr \right| &= \left| \int_0^t \int_0^r \frac{d}{ds} \left[\int_{\Phi_s^{\nu^2}(y)}^{\Phi_s^{\nu^1}(x)} \eta(z) dz \right] ds dr \right| \\
&= \left| \int_0^t \left[\int_{\Phi_r^{\nu^2}(y)}^{\Phi_r^{\nu^1}(x)} \eta(z) dz - \int_y^x \eta(z) dz \right] dr \right| \leq \|\eta\|_\infty \int_0^t |\Phi_r^{\nu^1}(x) - \Phi_r^{\nu^2}(y)| dr + \|\eta\|_\infty t |x - y|. \tag{49}
\end{aligned}$$

Regarding the term involving F_θ on the third and fourth line of (47), we proceed as follows

$$\begin{aligned}
&|F_\theta((W_h * \nu_s^1)(\xi_1)) \nabla(W_h * \nu_s^1)(\xi_1) - F_\theta((W_h * \nu_s^2)(\xi_2)) \nabla(W_h * \nu_s^2)(\xi_2)| \\
&\leq |F_\theta((W_h * \nu_s^1)(\xi_1))| |\nabla(W_h * \nu_s^1)(\xi_1) - \nabla(W_h * \nu_s^1)(\xi_2)| \\
&\quad + |F_\theta((W_h * \nu_s^1)(\xi_1))| |\nabla(W_h * \nu_s^1)(\xi_2) - \nabla(W_h * \nu_s^2)(\xi_2)| \\
&\quad + |F_\theta((W_h * \nu_s^1)(\xi_1)) - F_\theta((W_h * \nu_s^1)(\xi_2))| |\nabla(W_h * \nu_s^2)(\xi_2)| \\
&\quad + |F_\theta((W_h * \nu_s^1)(\xi_2)) - F_\theta((W_h * \nu_s^2)(\xi_2))| |\nabla(W_h * \nu_s^2)(\xi_2)|. \tag{50}
\end{aligned}$$

We only consider $\xi_1, \xi_2 \in B(r(T))$. For each $i, j \in \{1, 2\}$, we have the following estimates:

$$(W_h * \nu_s^i)(\xi_j) \leq \|W_h\|_\infty, \tag{51}$$

(since ν_s^i is a probability measure), and

$$(W_h * \nu_s^i)(\xi_j) \geq \inf_{\xi_j, z \in B(r(T))} W_h(\xi_j - z) = \inf_{B(2r(T))} W_h. \tag{52}$$

Thus we get $(W_h * \nu_s^i)(\xi_j) \in U_{T, W_h}$. We proceed with the estimation of (50):

$$\begin{aligned}
&|F_\theta((W_h * \nu_s^1)(\xi_1)) \nabla(W_h * \nu_s^1)(\xi_1) - F_\theta((W_h * \nu_s^2)(\xi_2)) \nabla(W_h * \nu_s^2)(\xi_2)| \\
&\leq M_2 \|D^2 W_h\|_\infty |\xi_1 - \xi_2| + M_2 |\nabla(W_h * \nu_s^1)(\xi_2) - \nabla(W_h * \nu_s^2)(\xi_2)| \\
&\quad + M_3 \|\nabla W_h\|_\infty^2 |\xi_1 - \xi_2| + M_3 \|\nabla W_h\|_\infty |(W_h * \nu_s^1)(\xi_2) - (W_h * \nu_s^2)(\xi_2)|, \tag{53}
\end{aligned}$$

where we used that $\|\nabla(W_h * \nu_s^2)\|_\infty \leq \|\nabla W_h\|_\infty$, $\|D^2(W_h * \nu_s^2)\|_\infty \leq \|D^2 W_h\|_\infty$ and the fact that $\|\psi\|_{\text{Lip}} = \|\nabla\psi\|_\infty$ for any differentiable function ψ . Note that:

$$\begin{aligned} |(W_h * \nu_s^1)(\xi_2) - (W_h * \nu_s^2)(\xi_2)| &= \left| \int W_h(\xi_2 - z) \nu_s^1(dz) - \int W_h(\xi_2 - w) \nu_s^2(dw) \right| \\ &= \left| \int (W_h(\xi_2 - z) - W_h(\xi_2 - w)) \tilde{\pi}_s(dz, dw) \right| \\ &\leq \int |W_h(\xi_2 - z) - W_h(\xi_2 - w)| \tilde{\pi}_s(dz, dw) \\ &\leq \|\nabla W_h\|_\infty \int |z - w| \tilde{\pi}_s(dz, dw), \end{aligned}$$

where $\tilde{\pi}_s \in \Pi(\nu_s^1, \nu_s^2)$ is arbitrary and the second equality follows from (32). By minimizing over all couplings in $\Pi(\nu_s^1, \nu_s^2)$, we obtain

$$|(W_h * \nu_s^1)(\xi_2) - (W_h * \nu_s^2)(\xi_2)| \leq \|\nabla W_h\|_\infty \mathcal{W}(\nu_s^1, \nu_s^2). \quad (54)$$

We stress that the bound (54) is independent of the choice of ξ_1, ξ_2 . Analogously, we have

$$|\nabla(W_h * \nu_s^1)(\xi_2) - \nabla(W_h * \nu_s^2)(\xi_2)| \leq \|D^2 W_h\|_\infty \mathcal{W}(\nu_s^1, \nu_s^2). \quad (55)$$

It follows that

$$\begin{aligned} |F_\theta((W_h * \nu_s^1)(\xi_1)) \nabla(W_h * \nu_s^1)(\xi_1) - F_\theta((W_h * \nu_s^2)(\xi_2)) \nabla(W_h * \nu_s^2)(\xi_2)| \\ \leq (M_2 \|D^2 W_h\|_\infty + M_3 \|\nabla W_h\|_\infty^2) (|\xi_1 - \xi_2| + \mathcal{W}(\nu_s^1, \nu_s^2)). \end{aligned} \quad (56)$$

If $\theta = 1$, similar estimates as in the first term on the right-hand side of (53), and as in (54) and (55) yield

$$\begin{aligned} |(\nabla W_h * [(F_\theta \circ (W_h * \nu_s^1))\nu_s^1])(\xi_1) - (\nabla W_h * [(F_\theta \circ (W_h * \nu_s^2))\nu_s^2])(\xi_2)| \\ \leq M_2 \|D^2 W_h\|_\infty |\xi_1 - \xi_2| + (M_2 \|D^2 W_h\|_\infty + M_3 \|\nabla W_h\|_\infty^2) \mathcal{W}(\nu_s^1, \nu_s^2). \end{aligned} \quad (57)$$

The last term in (47) we treat as follows:

$$\begin{aligned} |(K * \nu_s^1)(\xi_1) - (K * \nu_s^2)(\xi_2)| &\leq |(K * \nu_s^1)(\xi_1) - (K * \nu_s^1)(\xi_2)| + |(K * \nu_s^1)(\xi_2) - (K * \nu_s^2)(\xi_2)| \\ &\leq \|K\|_{\text{Lip}} (|\xi_1 - \xi_2| + \mathcal{W}(\nu_s^1, \nu_s^2)). \end{aligned} \quad (58)$$

The estimate of the second term is obtained like in (54).

We combine (47), (48), (49), (56), (57) and (58) to get

$$\begin{aligned} |\Phi_t^{\nu^1}(x) - \Phi_t^{\nu^2}(y)| &\leq (1 + t \|\eta\|_\infty) |x - y| + t |v_0(x) - v_0(y)| \\ &\quad + \int_0^t [M_4(t-s) + \|\eta\|_\infty] |\Phi_s^{\nu^1}(x) - \Phi_s^{\nu^2}(y)| ds + M_5 \int_0^t (t-s) \mathcal{W}(\nu_s^1, \nu_s^2) ds, \end{aligned}$$

with M_4 and M_5 as defined in the statement of the lemma. \square

Now we have all ingredients to prove Theorem 3.11.

Proof of Part 1 of Theorem 3.11.

If $M_5 = 0$ then the well-posedness of (31) is straightforward. In that case, $F_\theta \circ (W_h * \mu_t) = 0$ on $B(r(T))$ for all t and moreover K must be constant, so the first equation in (31) is independent of μ_t . The Picard-Lindelöf Theorem guarantees, for each $x \in B(r_0)$, the existence and uniqueness of a solution to (31). Moreover, the solution to the ODE depends continuously on the initial data, which implies that $x \mapsto \Phi_t(x)$ is continuous for every $t \in [0, T]$ and hence $\Phi_t : B(r_0) \rightarrow \mathbb{R}^d$ is measurable. The push-forward of μ_0 by Φ_t is therefore well-defined for all t . The solution $(\mu_t)_{0 \leq t \leq T}$ is uniquely defined by $\mu_t = \Phi_t \# \mu_0$.

If $M_5 \neq 0$, the well-posedness proof is based on a fixed-point argument (Banach's Fixed Point Theorem). Let $T > 0$ be fixed. Choose $N \in \mathbb{N}^+$ large enough, such that $T^* := T/N$ satisfies

$$\kappa_{T^*} := \frac{1}{2} (T^*)^2 M_5 \exp \left(\|\eta\|_\infty T^* + \frac{1}{2} M_4 (T^*)^2 \right) < 1. \quad (59)$$

Let $j \in \{1, \dots, N\}$ be fixed. Suppose that $\mu_0^{(j)} \in \mathcal{P}(\mathbb{R}^d)$ and $v_0^{(j)} \in C_b^1(\Omega^{(j)}; \mathbb{R}^d)$ are given, with $\Omega^{(j)}$ such that $\text{supp } \mu_0^{(j)} \subset \Omega^{(j)}$. Consider a mapping $\mathcal{F}^{(j)} : \nu \mapsto \mu := \mathcal{F}^{(j)}(\nu)$ from

$$\mathcal{C}_j := \left\{ \nu \in C([0, T^*]; \mathcal{P}_{r(jT^*)}(\mathbb{R}^d)) : \nu|_{t=0} = \mu_0^{(j)} \right\} \quad (60)$$

to itself, defined by

$$\mu_t = [\Phi_t^{(j)}]^\nu \# \mu_0^{(j)}, \text{ for all } t \in [0, T^*],$$

where the motion mapping $[\Phi_t^{(j)}]^\nu : \Omega^{(j)} \rightarrow C^2([0, T^*]; \mathbb{R}^d)$ is the solution to the following ODE

$$\begin{cases} [\dot{\Phi}_t^{(j)}]^\nu(x) = -F_\theta \left(\tilde{\rho}_t([\Phi_t^{(j)}]^\nu(x)) \right) \nabla \tilde{\rho}_t([\Phi_t^{(j)}]^\nu(x)) - \theta (\nabla W_h * [(F_\theta \circ \tilde{\rho}_t)\nu_t])([\Phi_t^{(j)}]^\nu(x)) \\ \quad - \nabla V \left([\Phi_t^{(j)}]^\nu(x) \right) - \eta \left([\Phi_t^{(j)}]^\nu(x) \right) [\Phi_t^{(j)}]^\nu(x) + (K * \nu_t)([\Phi_t^{(j)}]^\nu(x)); \\ \tilde{\rho}_t := W_h * \nu_t; \\ [\Phi_0^{(j)}]^\nu(x) = x, \quad [\dot{\Phi}_0^{(j)}]^\nu(x) = v_0^{(j)}(x). \end{cases} \quad (61)$$

Endowed with the metric

$$\sup_{\tau \in [0, T^*]} \mathcal{W}(\mu_1(\tau), \mu_2(\tau)),$$

\mathcal{C}_j is a complete metric space for arbitrary $j \in \{1, \dots, N\}$. This is because the space of continuous functions on a complete metric space (in this case: $\mathcal{P}_{r(jT^*)}(\mathbb{R}^d)$ endowed with \mathcal{W}) is complete. Moreover, by fixing the initial condition, we select a closed subspace, while any closed subspace of a complete space is complete itself. Further details are left to the reader. A full proof can be found in Appendix A of [18].

Note that a fixed point $\mu^{(j)}$ of this mapping together with the corresponding motion mapping $\Phi^{(j)}$ is a solution of (31) on $[0, T^*]$ with initial data $\mu_0^{(j)}$ and $v_0^{(j)}$. We create a hierarchy of the mappings $\mathcal{F}^{(j)}$ for $j \in \{1, \dots, N\}$ by defining

$$\begin{array}{lll} \mu_0^{(1)} := \mu_0 & v_0^{(1)} := v_0 & \Omega^{(1)} := B(r_0) \\ \mu_0^{(j+1)} := \mu_{T^*}^{(j)} & v_0^{(j+1)} := \dot{\Phi}_{T^*}^{(j)} & \Omega^{(j+1)} := \Phi_{T^*}^{(j)}(\Omega^{(j)}) \end{array}$$

Such definition only makes sense if mapping j actually has a unique fixed point and thus $\mu_{T^*}^{(j)}$, $\Phi_{T^*}^{(j)}$ and $\dot{\Phi}_{T^*}^{(j)}$ are well-defined. In view of the to be constructed hierarchy, $\text{supp } \mu_0^{(j)} \subset B(r((j-1)T^*))$ should be satisfied for each j .

For any $\nu \in \mathcal{C}_j$ the image $\mu = \mathcal{F}^{(j)}(\nu)$ exists, and it is an element of \mathcal{C}_j . This is the case, because well-posedness of the motion mapping (for given ν and for each $x \in \Omega^{(j)}$) follows from Picard-Lindelöf (see before) and guarantees the existence and uniqueness of μ . Moreover, the support of the image measure, $\text{supp } \mu_t$, is contained in a ball of radius

$$r(jT^*) = r_0 + jT^* \|v_0\|_\infty + \frac{1}{2} (jT^*)^2 (M_1 + \|\nabla V\|_\infty + \|K\|_\infty).$$

This is easily checked by use of (39) and a recursive relation involving $\|[\dot{\Phi}_{T^*}^{(j)}]^\nu\|_\infty = \|v_0^{(j+1)}\|_\infty$ for each $j \in \{1, \dots, N-1\}$. Thus, the image μ of our mapping $\mathcal{F}^{(j)}$ is an element of \mathcal{C}_j .

Consider two measures $\nu^1, \nu^2 \in \mathcal{C}_j$ and their corresponding images $\mu^1 := \mathcal{F}^{(j)}(\nu^1)$ and $\mu^2 := \mathcal{F}^{(j)}(\nu^2)$. Let $\pi_0 \in \Pi(\mu_0^{(j)}, \mu_0^{(j)})$ be arbitrary. For an arbitrary fixed $t \in [0, T^*]$ define $\pi_t \in \Pi(\mu_t^1, \mu_t^2)$ by

$$\pi_t := \left([\Phi_t^{(j)}]^\nu{}^1, [\Phi_t^{(j)}]^\nu{}^2 \right) \# \pi_0.$$

Note that this π_t is indeed a joint representation of μ_t^1 and μ_t^2 for each t . We drop the dependence on j of π_0, μ^1, μ^2 and π_t since no ambiguity appears. By definition of the push-forward and of the Wasserstein distance (see Definitions 3.1 and 3.3), we have

$$\mathcal{W}(\mu_t^1, \mu_t^2) \leq \int |z - w| \pi_t(dz, dw) = \int \left| [\Phi_t^{(j)}]^{v^1}(x) - [\Phi_t^{(j)}]^{v^2}(y) \right| \pi_0(dx, dy) \quad (62)$$

holds for each $t \in [0, T^*]$. Applied to (45), a version of Gronwall's Lemma yields that for each $x, y \in \text{supp } \mu_0^{(j)}$

$$\begin{aligned} \left| [\Phi_t^{(j)}]^{v^1}(x) - [\Phi_t^{(j)}]^{v^2}(y) \right| \leq & \left[(1 + t \|\eta\|_\infty) |x - y| + t |v_0^{(j)}(x) - v_0^{(j)}(y)| \right. \\ & \left. + M_5 \int_0^t (t - s) \mathcal{W}(\nu_s^1, \nu_s^2) ds \right] \exp \left(\|\eta\|_\infty t + \frac{1}{2} M_4 t^2 \right). \quad (63) \end{aligned}$$

We remark that Gronwall's Lemma may be applied because the term $|v_0^{(j)}(x) - v_0^{(j)}(y)|$ is bounded and $s \mapsto (t - s) \mathcal{W}(\nu_s^1, \nu_s^2)$ is bounded and continuous. The former can be shown by using estimates similar to those in the proof of Lemma 3.14. The continuity of $s \mapsto \mathcal{W}(\nu_s^1, \nu_s^2)$ follows from the triangle inequality. Indeed, since

$$|\mathcal{W}(\nu_s^1, \nu_s^2) - \mathcal{W}(\nu_{s_0}^1, \nu_{s_0}^2)| \leq \mathcal{W}(\nu_s^1, \nu_{s_0}^1) + \mathcal{W}(\nu_{s_0}^2, \nu_s^2),$$

we have that $\lim_{s \rightarrow s_0} \mathcal{W}(\nu_s^1, \nu_s^2) = \mathcal{W}(\nu_{s_0}^1, \nu_{s_0}^2)$ because $\mathcal{W}(\nu_s^1, \nu_{s_0}^1) \rightarrow 0$ and $\mathcal{W}(\nu_{s_0}^2, \nu_s^2) \rightarrow 0$. The estimate $(t - s) \mathcal{W}(\nu_s^1, \nu_s^2) \leq T^* \max_{s \in [0, T^*]} \mathcal{W}(\nu_s^1, \nu_s^2)$ then implies that the (continuous) left-hand side is bounded.

Now we combine (62) and (63), and obtain

$$\begin{aligned} \mathcal{W}(\mu_t^1, \mu_t^2) \leq & \left[(1 + t \|\eta\|_\infty) \int |x - y| \pi_0(dx, dy) + t \int |v_0^{(j)}(x) - v_0^{(j)}(y)| \pi_0(dx, dy) \right. \\ & \left. + M_5 \int_0^t (t - s) \mathcal{W}(\nu_s^1, \nu_s^2) ds \right] \exp \left(\|\eta\|_\infty t + \frac{1}{2} M_4 t^2 \right). \quad (64) \end{aligned}$$

The integral with respect to $\pi_0(dx, dy)$ disappeared for the third term inside the square brackets, since this term is independent of x and y , and moreover $\int \pi_0(dx, dy) = 1$. Now we take

$$\pi_0 := (I \otimes I) \# \mu_0^{(j)},$$

which is the measure concentrated on the diagonal $x = y$ with marginals both $\mu_0^{(j)}$. With some abuse of notation it can also be written as

$$\pi_0(dx, dy) := \delta(x - y) \mu_0^{(j)}(dy).$$

For this choice of π_0 , we have that

$$\int |x - y| \pi_0(dx, dy) = 0, \quad \text{and} \quad \int |v_0^{(j)}(x) - v_0^{(j)}(y)| \pi_0(dx, dy) = 0.$$

Therefore, only the third term in square brackets on the right-hand side of (64) remains. Since

$$\int_0^t (t - s) \mathcal{W}(\nu_s^1, \nu_s^2) ds \leq \sup_{s \in [0, t]} \mathcal{W}(\nu_s^1, \nu_s^2) \int_0^t (t - s) ds = \frac{1}{2} t^2 \sup_{s \in [0, t]} \mathcal{W}(\nu_s^1, \nu_s^2),$$

we obtain

$$\mathcal{W}(\mu_t^1, \mu_t^2) \leq \frac{1}{2} t^2 M_5 \exp \left(\|\eta\|_\infty t + \frac{1}{2} M_4 t^2 \right) \sup_{s \in [0, t]} \mathcal{W}(\nu_s^1, \nu_s^2).$$

Finally, we take the supremum over $t \in [0, T^*]$:

$$\sup_{t \in [0, T^*]} \mathcal{W}(\mu_t^1, \mu_t^2) \leq \frac{1}{2} (T^*)^2 M_5 \exp \left(\|\eta\|_\infty T^* + \frac{1}{2} M_4 (T^*)^2 \right) \sup_{t \in [0, T^*]} \mathcal{W}(\nu_t^1, \nu_t^2).$$

By the specific choice of T^* , $\mathcal{F}^{(j)}$ is a contraction mapping for each j , since

$$\sup_{t \in [0, T^*]} \mathcal{W}(\mu_t^1, \mu_t^2) \leq \kappa_{T^*} \sup_{t \in [0, T^*]} \mathcal{W}(\nu_t^1, \nu_t^2),$$

where $\kappa_{T^*} < 1$ by assumption; cf. (59). As argued before, the space \mathcal{C}_j is complete for each j . Banach's Fixed Point Theorem then guarantees the existence of a unique fixed point $\mu^{(j)}$ of $\mathcal{F}^{(j)}$ for each j . The corresponding mapping $\Phi^{(j)}$ then follows from (61) with $\nu = \mu^{(j)}$. The pair $(\mu^{(j)}, \Phi^{(j)})$ satisfies $\mu_t^{(j)} = \Phi_t^{(j)} \# \mu_0^{(j)}$ for all $t \in [0, T^*]$.

Having the construction of $(\mu^{(j)}, \Phi^{(j)})$ for $j \in \{1, \dots, N\}$, we 'glue' these pieces together to define a couple (μ, Φ) of a measure and a motion mapping as follows:

$$\text{if } t \in ((j-1)T^*, jT^*] \text{ then } \mu_t := \mu_{t-(j-1)T^*}^{(j)} \text{ and } \Phi_t := \Phi_{t-(j-1)T^*}^{(j)} \circ \Phi_{T^*}^{(j-1)} \circ \dots \circ \Phi_{T^*}^{(1)}$$

for $j \in \{1, \dots, N\}$. By our construction $(\mu, \Phi) \in C([0, T]; \mathcal{P}_{r(T)}(\mathbb{R}^d)) \times \mathcal{A}$ and it uniquely satisfies (31) with initial data μ_0 and v_0 .

Proof of Part 2 of Theorem 3.11.

Note that Part 1 implies that for both initial measures μ_0^1 and μ_0^2 there is a corresponding unique solution (μ^1, Φ^1) , (μ^2, Φ^2) , respectively. Let $\pi_0 \in \Pi(\mu_0^1, \mu_0^2)$ be arbitrary. We use (45), substituting $\nu^1 = \mu^1$ and $\nu^2 = \mu^2$. Thus $\Phi^{\nu^1} = \Phi^1$ and $\Phi^{\nu^2} = \Phi^2$. First of all, we estimate

$$|v_0(x) - v_0(y)| \leq \|\nabla v_0\|_\infty |x - y|,$$

for all $x, y \in B(r_0)$. This is possible, since $v_0 \in C_b^1(\mathbb{R}^d; \mathbb{R}^d)$ is given, is defined on the whole of \mathbb{R}^d and has bounded derivative. Using this Lipschitz estimate and integrating (45) against $\pi_0(dx, dy)$, we obtain

$$\begin{aligned} \int |\Phi_t^1(x) - \Phi_t^2(y)| \pi_0(dx, dy) &\leq (1 + t (\|\nabla v_0\|_\infty + \|\eta\|_\infty)) \int |x - y| \pi_0(dx, dy) \\ &+ \int_0^t [M_4(t-s) + \|\eta\|_\infty] \int |\Phi_s^1(x) - \Phi_s^2(y)| \pi_0(dx, dy) ds + M_5 \int_0^t (t-s) \mathcal{W}(\mu_s^1, \mu_s^2) ds, \end{aligned} \quad (65)$$

where we used that the last term is independent of x and y , and the fact that π_0 is a probability measure on $\mathbb{R}^d \times \mathbb{R}^d$. If we define $\tilde{\pi}_s \in \Pi(\mu_s^1, \mu_s^2)$ as

$$\tilde{\pi}_s := (\Phi_s^1, \Phi_s^2) \# \pi_0$$

for each $s \in [0, T]$, then we have, analogously to (62), the following:

$$\mathcal{W}(\mu_s^1, \mu_s^2) \leq \int |z - w| \tilde{\pi}_s(dz, dw) = \int |\Phi_s^1(x) - \Phi_s^2(y)| \pi_0(dx, dy). \quad (66)$$

We substitute this estimate for $\mathcal{W}(\mu_s^1, \mu_s^2)$ in the right-hand side of (65) and apply Gronwall's Lemma to obtain

$$\begin{aligned} \int |\Phi_t^1(x) - \Phi_t^2(y)| \pi_0(dx, dy) \\ \leq \left[(1 + t (\|\nabla v_0\|_\infty + \|\eta\|_\infty)) \int |x - y| \pi_0(dx, dy) \right] \exp \left(\|\eta\|_\infty t + \frac{1}{2} (M_4 + M_5) t^2 \right). \end{aligned} \quad (67)$$

Together, (66) and (67) yield

$$\mathcal{W}(\mu_t^1, \mu_t^2) \leq \left[(1 + t (\|\nabla v_0\|_\infty + \|\eta\|_\infty)) \int |x - y| \pi_0(dx, dy) \right] \exp \left(\|\eta\|_\infty t + \frac{1}{2} (M_4 + M_5) t^2 \right).$$

We take the infimum over $\pi_0 \in \Pi(\mu_0^1, \mu_0^2)$ on the right-hand side:

$$\mathcal{W}(\mu_t^1, \mu_t^2) \leq (1 + t (\|\nabla v_0\|_\infty + \|\eta\|_\infty)) \exp \left(\|\eta\|_\infty t + \frac{1}{2} (M_4 + M_5) t^2 \right) \mathcal{W}(\mu_0^1, \mu_0^2).$$

Finally, we take the supremum over $t \in [0, T]$ on both sides of the inequality and obtain

$$\sup_{t \in [0, T]} \mathcal{W}(\mu_t^1, \mu_t^2) \leq (1 + T (\|\nabla v_0\|_\infty + \|\eta\|_\infty)) \exp \left(\|\eta\|_\infty T + \frac{1}{2} (M_4 + M_5) T^2 \right) \mathcal{W}(\mu_0^1, \mu_0^2).$$

This finishes the proof. \square

3.5 Discussion on Assumptions 3.7 and 3.9, and the condition (37)

We comment here on the assumptions needed for the results presented in Sect. 3.3. That is, Theorem 3.11, Corollary 3.12 and Remark 3.13.

Assumptions on F_θ and W_h : We remark here that in [9] only $\theta = 0$ is used, and furthermore $\nabla V \equiv 0$, $\eta \equiv 0$ and $K \equiv 0$. All possible F_0 and W_h treated in [9] satisfy Assumption 3.7:

1. $F_0(u) = u^\alpha$, for $\alpha \geq 0$, satisfies the assumptions for all choices of $W_h \in C_b^2(\mathbb{R}^d; \mathbb{R}_0^+)$;
2. $F_0(u) = u^\alpha$, for $-1 < \alpha < 0$, satisfies the assumptions if W_h is an element of $C_b^2(\mathbb{R}^d; \mathbb{R}^+)$ and satisfies the extra condition $|\nabla W_h(x)| \leq c|W_h(x)|^{-\alpha}$ for all x , for some constant $c > 0$.

We remark that the class of admissible pairs (F_0, W_h) covered by Assumption 3.7 is more general than in [9], where only F_0 of the form $F_0(u) = u^\alpha$ is treated. For instance, in our work any $F_0 \in C_b^1(\mathbb{R}^+; \mathbb{R}^+)$ (bounded and with bounded derivative) is allowed in combination with an arbitrary $W_h \in C_b^2(\mathbb{R}^d; \mathbb{R}_0^+)$.

Assumption (37) on convergence of initial data: Given the initial probability measure μ_0 supported in the ball $B(r_0)$, we demonstrate here two ways of constructing an approximating sequence of measures $(\mu_0^n)_{n \in \mathbb{N}^+}$.

The first way of constructing μ_0^n is deterministic and has been used in [4]. For simplicity of presentation, we assume $d = 1$ and $\text{supp } \mu_0 \subset [0, 1]$. For each $n \in \mathbb{N}^+$, define

$$\mu_0^n := \sum_{i=1}^n m_i \delta_{\frac{i}{n} - \frac{1}{2n}}, \tag{68}$$

where $m_i := \int_{[\frac{i-1}{n}, \frac{i}{n})} \mu_0(dx)$, for each $i = 1, \dots, n-1$, and $m_n := \int_{[1-\frac{1}{n}, 1]} \mu_0(dx)$.

It follows that $\sum_i m_i = \int \mu_0(dx) = 1$ and $\mu_0^n \in \mathcal{P}(\mathbb{R})$. Define a map $\Psi : [0, 1] \rightarrow \{\frac{i}{n} - \frac{1}{2n} : 1 \leq i \leq n\}$ by $\Psi(x) := \frac{i}{n} - \frac{1}{2n}$ if $\frac{i-1}{n} \leq x < \frac{i}{n}$ and $\Psi(1) := 1 - \frac{1}{2n}$. For every measurable and bounded function f , defined on $[0, 1]$ it holds that

$$\begin{aligned} \int_{[0,1]} f(x) \mu_0^n(dx) &= \sum_{i=1}^n m_i f\left(\frac{i}{n} - \frac{1}{2n}\right) \\ &= \sum_{i=1}^{n-1} \int_{[\frac{i-1}{n}, \frac{i}{n})} \mu_0(dx) f\left(\frac{i}{n} - \frac{1}{2n}\right) + \int_{[1-\frac{1}{n}, 1]} \mu_0(dx) f\left(1 - \frac{1}{2n}\right) \\ &= \int_{[0,1]} f(\Psi(x)) \mu_0(dx). \end{aligned}$$

Hence, $\mu_0^n = \Psi \# \mu_0$. Note that $|x - \Psi(x)| \leq \frac{1}{2n}$ for every $x \in [0, 1]$. Therefore,

$$\mathcal{W}(\mu_0^n, \mu_0) \leq \int_{[0,1]} |x - \Psi(x)| \mu_0(dx) \leq \frac{1}{2n} \int_{[0,1]} \mu_0(dx) = \frac{1}{2n},$$

where we obtain the first inequality by taking $\pi \in \Pi(\mu_0^n, \mu_0)$ to be $\pi := (I \otimes \Psi) \# \mu_0$. This implies that $\mathcal{W}(\mu_0^n, \mu_0) \xrightarrow{n \rightarrow \infty} 0$. This procedure generalizes to the case $d > 1$ (but with more involved notation). Let $\text{supp } \mu_0 \subset [0, 1]^d$ and let $n \in \{k^d : k \in \mathbb{N}^+\}$. Dividing the hypercube $[0, 1]^d$ into n equal subcubes, we obtain analogously that the convergence rate is $\mathcal{O}(1/\sqrt[n]{n})$.

The second way of constructing μ_0^n is probabilistic and is based on the law of large numbers as already pointed out in [9]. Suppose that the points $X_i, i = 1, \dots, n$ are independent identically distributed random variables with the same distribution $\mu_0 \in \mathcal{P}(B(r_0))$. Let μ_0^n be the empirical measure, defined by

$$\mu_0^n := \frac{1}{n} \sum_{i=1}^n \delta_{X_i}.$$

Note that in fact there is an underlying probability space Ω and $X_i : \Omega \rightarrow B(r_0)$. Hence μ_0^n is, strictly speaking, not a mere probability measure, but a mapping from Ω to $\mathcal{P}(B(r_0))$; i.e. $\mu_0^n : \Omega \rightarrow \mathcal{P}(B(r_0))$. According to [12], Theorem 11.4.1, the

sequence (μ_0^n) converges *almost surely* to μ_0 . This implies that for *almost every* realization $\bar{x}_1, \bar{x}_2, \dots$ the corresponding sequence of measures $(\bar{\mu}_0^n) \subset \mathcal{P}(B(r_0))$ given by $\bar{\mu}_0^n := 1/n \sum_i \delta_{\bar{x}_i}$, converges in the narrow topology to μ_0 :

$$\int_{B(r_0)} f(x) \bar{\mu}_0^n(dx) \rightarrow \int_{B(r_0)} f(x) \mu_0(dx), \text{ for all } f \in C_b(B(r_0)).$$

The term ‘almost every realization’ refers to the fact that the set (in Ω) on which the narrow convergence does *not* hold, has zero probability (with respect to the probability distribution on Ω). In layman’s terms, this means that if we draw a random sample $\bar{x}_1, \bar{x}_2, \dots$, it is ‘unlikely’ that the corresponding sequence $(\bar{\mu}_0^n)$ does not converge narrowly.

Assume that our random sample did yield such narrowly converging sequence $(\bar{\mu}_0^n)$. Since all $\bar{\mu}_0^n$ are probability measures on a bounded domain $B(r_0)$, their first moments are uniformly integrable (i.e. uniformly in n). Thus, Theorem 7.1.5 in [1] implies that

$$\mathcal{W}(\bar{\mu}_0^n, \mu_0) \xrightarrow{n \rightarrow \infty} 0.$$

3.6 Numerical illustration

We illustrate the theoretical convergence results presented in Sect. 3.3 by two numerical examples. The first one involves only the hydrodynamical force, as described by the first term on the right-hand side of (38). We consider both schemes derived ($\theta = 0$ and $\theta = 1$), in dimension $d = 1$ and $d = 2$. In the second example only the non-local interaction term and a drag force in (38) are present and we take $d = 2$. First, in problems of bounded domains, it is common to use the differential form of mass conservation equation, thus the time variation of the measure-valued equation for mass in (31) is evolved in time along with the momentum equation, via a leapfrog algorithm with a constant time step. The leapfrog algorithm is a second-order symplectic integrator with the property of preserving the momentum of the system. The Gaussian function, defined by

$$W_h(x) := \frac{1}{h\sqrt{\pi}} e^{-|x|^2/h^2},$$

for all $x \in \mathbb{R}$, is used for the regularization of the mass measure in the one-dimensional case. For $d = 2$, the cubic Wendland function is used, whence for all $x \in \mathbb{R}^2$:

$$W_h(x) := \begin{cases} \frac{1}{8}(1 + 3|x|/2h)(2 - |x|/h)^3, & |x| \leq 2h, \\ 0, & |x| > 2h. \end{cases}$$

These choices are made to illustrate that we can handle both bounded and unbounded support of W_h .

In order for the regularized equations of hydrodynamics to approximate the real physics well, h should be sufficiently small. Let V_0 denote a representative volume assigned to each particle based on the initial configuration. In a bounded domain, typically V_0 scales as $V_0 \sim 1/n$. It is common practice to achieve “ h sufficiently small” by taking $h = \varepsilon \sqrt[d]{V_0}$, with parameter $1.2 \leq \varepsilon \leq 1.5$, cf. [27]. However, the convergence result in Corollary 3.12 holds for h fixed, and the dependence of h on n is not investigated. Numerically, we investigate both cases. That is, we take both $h = 1$ fixed and $h = 1.5 \sqrt[d]{V_0}$, which hence varies with the number of particles. We assume that the initial measure μ_0 has a density ρ_0 such that $\rho_0(x) = 1$ for all $x \in [0, 1]^d$ and $\rho_0(x) = 0$ otherwise. We construct the measure μ_0^n , corresponding to the n -particle approximation, according to (68) or its d -dimensional counterpart. Hence, the initial particle configuration is realized for $d = 1$ by equipartitioning the initial domain $[0, 1]$ into n volumes. For the two-dimensional examples, the initial domain is the square $[0, 1]^2 \subset \mathbb{R}^2$ and particles are placed in the center of each square incremental volume partition V_0 . Masses are assigned as $m_i = \rho_0(x_i) V_0$ for each $i \in \{1, \dots, n\}$. Note that in case of more complicated initial domains, an equipartitioning may be obtained with a centroidal Voronoi tessellation.

As argued underneath (68), the sequence $(\mu_0^n)_{n \in \mathbb{N}^+}$ constructed in this way converges to μ_0 and the convergence rate is $\mathcal{O}(1/\sqrt[d]{n})$. Hence, the corresponding solutions $(\mu^n)_{n \in \mathbb{N}^+}$ converge at the same rate, due to (36).

The hydrodynamical problem considers the spontaneous expansion of a gas cloud until time $T = 1$, governed by the equation of state $P(\rho) = \mathcal{K}\rho^\gamma$, where $\mathcal{K} = 1$ is a parameter and γ the so-called *polytropic exponent*. We recall that P relates to e via $\partial e / \partial \rho = P / \rho^2$. In dimension $d = 1$, we examine the cases $\gamma \in \{1, 2, 7\}$, using a constant time step $\Delta t = 10^{-3}$, and the Gaussian function. Note that the case $\gamma = 1$ is not covered by the convergence proof (cf. Assumption 3.7 and Sect. 3.5). It is a limit case (the proof does hold for any $\gamma > 1$) and we include it for generality. We perform the calculations for $n = 2^k$ particles, where $k \in \{1, \dots, 9\}$, and compute the supremum in time of the Wasserstein distance between subsequent solutions. We compute the Wasserstein distance by solving a linear programming problem based on

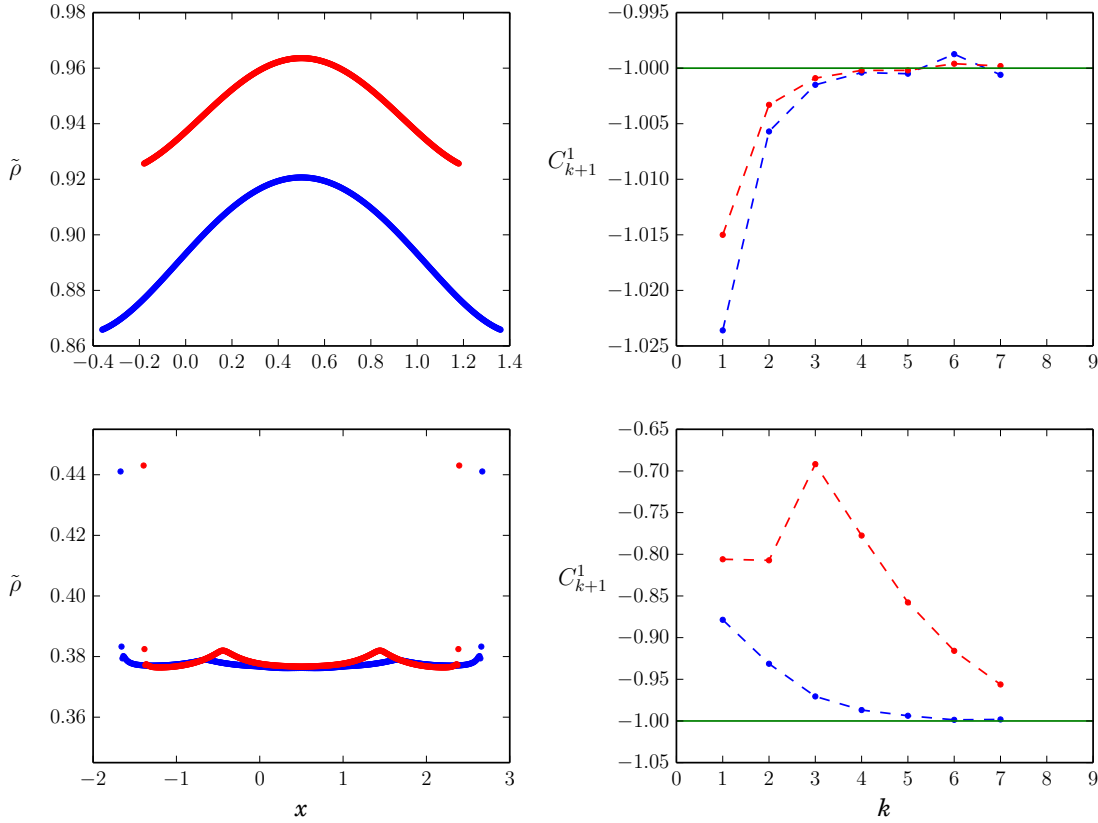


Fig. 1 For $\gamma = 1$, density $\tilde{\rho}$ at final time $T = 1$, with $n = 2^9$ particles and convergence C^1 . Red and blue plots refer to the schemes for $\theta = 0$ and $\theta = 1$, respectively. Upper plots present results for $h = 1$ fixed, while lower plots to variable $h = 1.5 V_0$.

a formulation in terms of optimal transportation. Due to the high computational cost (for large k), we use the following approximation

$$\sup_{t \in [0, T]} \mathcal{W}(\mu_t^{2^k}, \mu_t^{2^{k+1}}) \approx \max_{\tau \in I} \mathcal{W}(\mu_\tau^{2^k}, \mu_\tau^{2^{k+1}}) =: W_{k, k+1}, \quad (69)$$

to reduce the number of evaluations of \mathcal{W} . Here,

$$I := \{jT/(N_r - 1) : j = 0, \dots, (N_r - 1)\}$$

and we take $N_r = 10$. It should be noted, however that for the vast majority of the computations, the maximum distance is observed at the final time step.

The convergence rate for $d = 1$ is approximated by

$$C_{k+1}^1 := \log_2 \left| \frac{W_{k+1, k+2}}{W_{k, k+1}} \right|$$

and based on the theoretical prediction that the convergence rate is $\mathcal{O}(n^{-1})$ if $d = 1$, we expect that C_{k+1}^1 tends to the value -1 .

In Fig. 1 to 3, results are shown for the three different values $\gamma \in \{1, 2, 7\}$ respectively. Red graphs correspond to the scheme for $\theta = 0$ and blue graphs to the scheme $\theta = 1$. In these figures, the upper plots refer to computations using $h = 1$ for all resolutions and the lower plots depict computations with h varying with the number of particles used. The left plots show the result for density $\tilde{\rho}$ at $T = 1$, as obtained with the highest resolution $n = 2^9$. Additionally, the convergence of C_{k+1}^1 is plotted in the right plots.

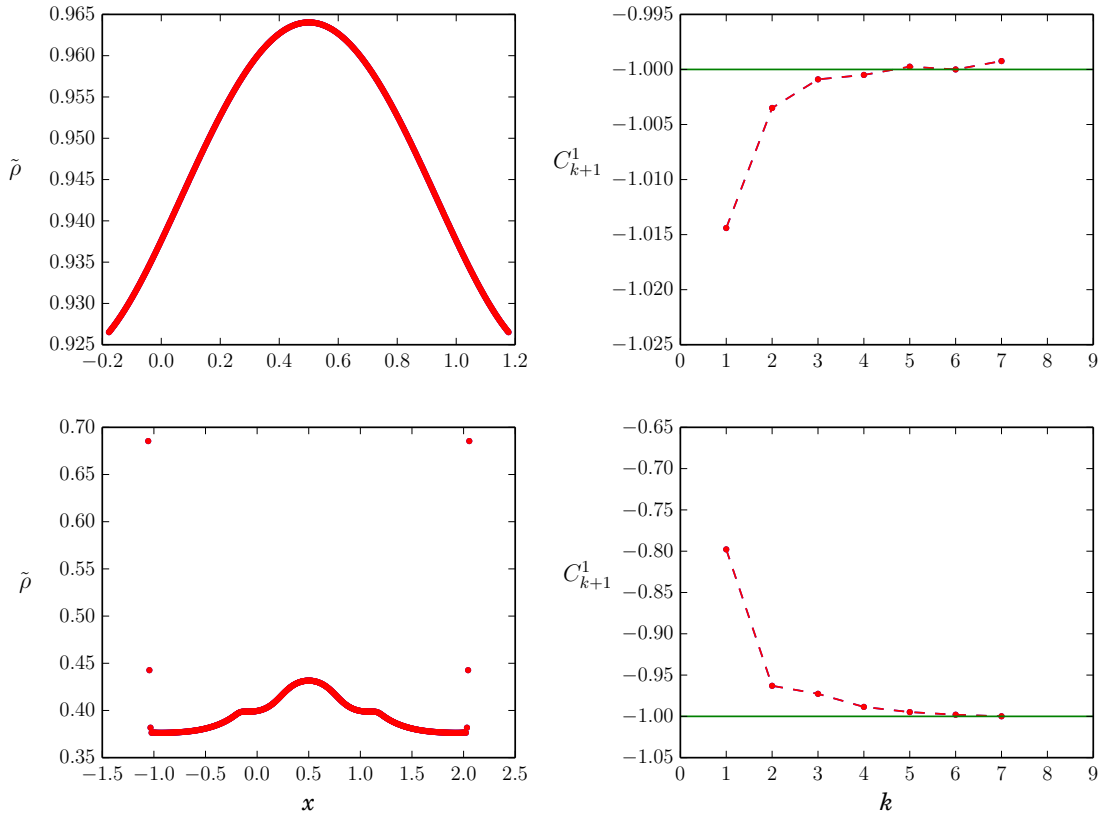


Fig. 2 For $\gamma = 2$, density $\tilde{\rho}$ at final time $T = 1$, with $n = 2^9$ particles and convergence C^1 . Red and blue plots refer to the schemes for $\theta = 0$ and $\theta = 1$, respectively. Upper plots present results for $h = 1$ fixed, while lower plots to variable $h = 1.5 V_0$.

There are several points to be mentioned about the plots. First, note that in all figures solutions, for $h = 1$ fixed and h varying, do converge to a solution by increasing the number of particles. The convergence is evident by the rate C_{k+1}^1 approaching its theoretical value -1 . Second, although convergent, solutions for $h = 1$ fixed and h varying are not the same for the same value of γ . Third, in Fig. 2 where $\gamma = 2$, the solutions obtained with the two schemes coincide. This effect is expected since for this value of γ the two schemes are identical. On the other hand, this is not true for the cases $\gamma = 1$ and $\gamma = 7$. Fourth, interestingly enough, even though the proof only covers cases for $\gamma > 1$, the case $\gamma = 1$ converges. In the same case, it is unclear why a spike is present in the convergence graph for $\theta = 0$ and varying h . Fifth, for fixed value of h all cases converge from below sharply towards the theoretical value $C_{k+1}^1 \approx -1$, while for h varying with the resolution they converge from above. Finally, for fixed $h = 1$, this large value does not permit local effects to appear on the free boundaries of the domain. These effects are exhibited in the cases of varying h as discontinuities of the density profile and therefore seem to be related to problems of applying regularization over small h -sized regions in bounded domains.

In two spatial dimensions, the hydrodynamic problem examined is the expansion of an initially square gas cloud, until time $T = 1$. In order to show that the results also hold for non-static initial conditions, a rotation described by the initial velocity field $(v_{0,x}, v_{0,y}) = (-y, x)$ is applied. The same equation of state as in the one-dimensional computation is used, with $\gamma \in \{2, 7\}$. The Wendland function and a constant time step of $\Delta t = 10^{-3}$ are employed. Note that we omit the case $\gamma = 1$, hence do not need to ‘mimic’ Assumption 3.7, and do allow for bounded support in W_h .

For $d = 2$, we approximate the rate of convergence by

$$C_{k+1}^2 := \frac{1}{2} \log_2 \left| \frac{W_{k+1,k+2}}{W_{k,k+1}} \right|.$$

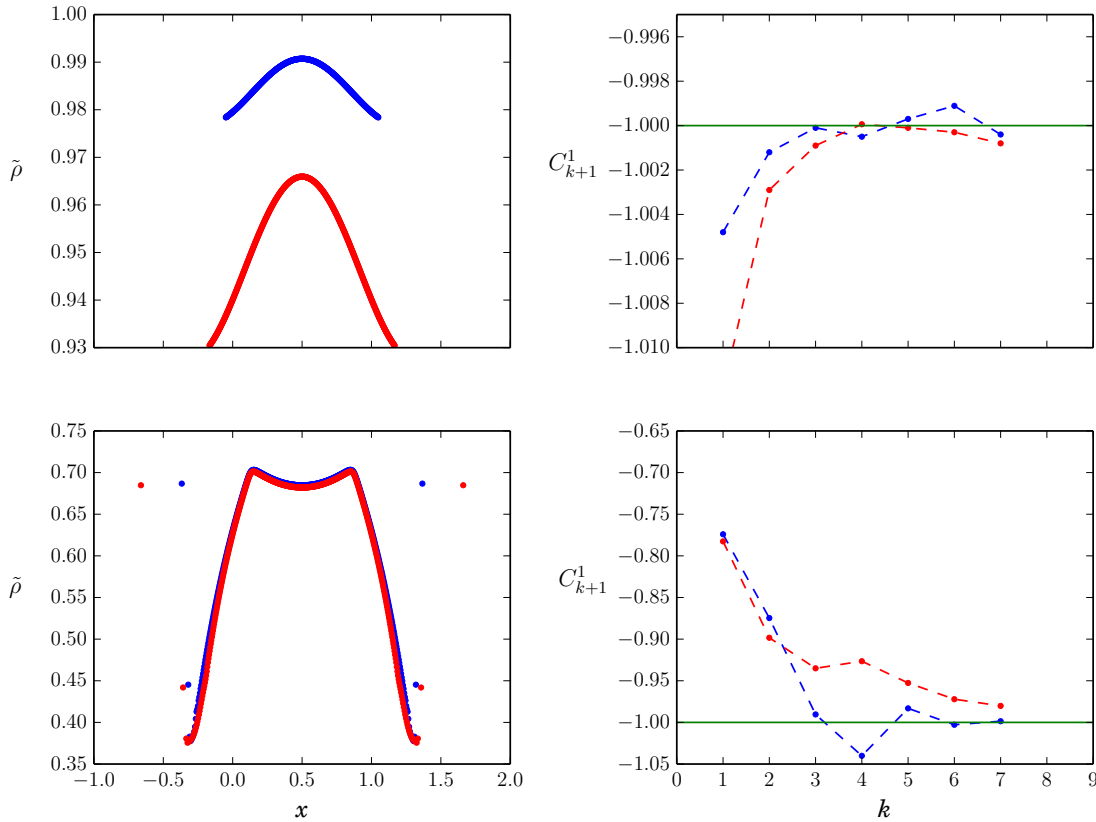


Fig. 3 For $\gamma = 7$, density $\tilde{\rho}$ at final time $T = 1$, with $n = 2^9$ particles and convergence C^1 . Red and blue plots refer to the schemes for $\theta = 0$ and $\theta = 1$, respectively. Upper plots present results for $h = 1$ fixed, while lower plots to variable $h = 1.5 V_0$.

Table 1 C_{k+1}^2 for the two-dimensional hydrodynamic computations

	k	2	3	4	5
$\gamma = 2$ h fixed	$\theta = 0$	-0.51	-0.50	-0.50	-0.50
	$\theta = 1$	-0.51	-0.50	-0.50	-0.50
$\gamma = 2$ h varying	$\theta = 0$	-0.44	-0.47	-0.49	-0.44
	$\theta = 1$	-0.44	-0.47	-0.49	-0.44
$\gamma = 7$ h fixed	$\theta = 0$	-0.51	-0.50	-0.50	-0.50
	$\theta = 1$	-0.50	-0.50	-0.50	-0.50
$\gamma = 7$ h varying	$\theta = 0$	-0.37	-0.45	-0.48	-0.48
	$\theta = 1$	-0.41	-0.43	-0.52	-0.51

Note that this definition is different from C_{k+1}^1 , since in $d = 1$ we took n of the form 2^k , while in $d = 2$ we have $n = (2^k)^2$, for $k \in \{1, 2, 3, 4, 5, 6\}$. Here, the definition of $W_{k,k+1}$ is modified accordingly to approximations by 4^k and 4^{k+1} particles, respectively. The computational effort for the calculation of the Wasserstein distance makes the investigation of higher n extremely lengthy. In the case $d = 2$, theory predicts that the convergence rate is $\mathcal{O}(n^{-1/2})$, whence we expect that C_{k+1}^2 tends to the value $-1/2$. In Table 1, the convergence rates of the two-dimensional hydrodynamic problems are shown. The theoretical value is indeed approached, but strong oscillations around this value appear in the case $\gamma = 2$ with varying h . In Fig. 4 and 5, particle configurations at final time $T = 1$ are presented for the cases $\gamma = \{2, 7\}$ respectively. The upper plots

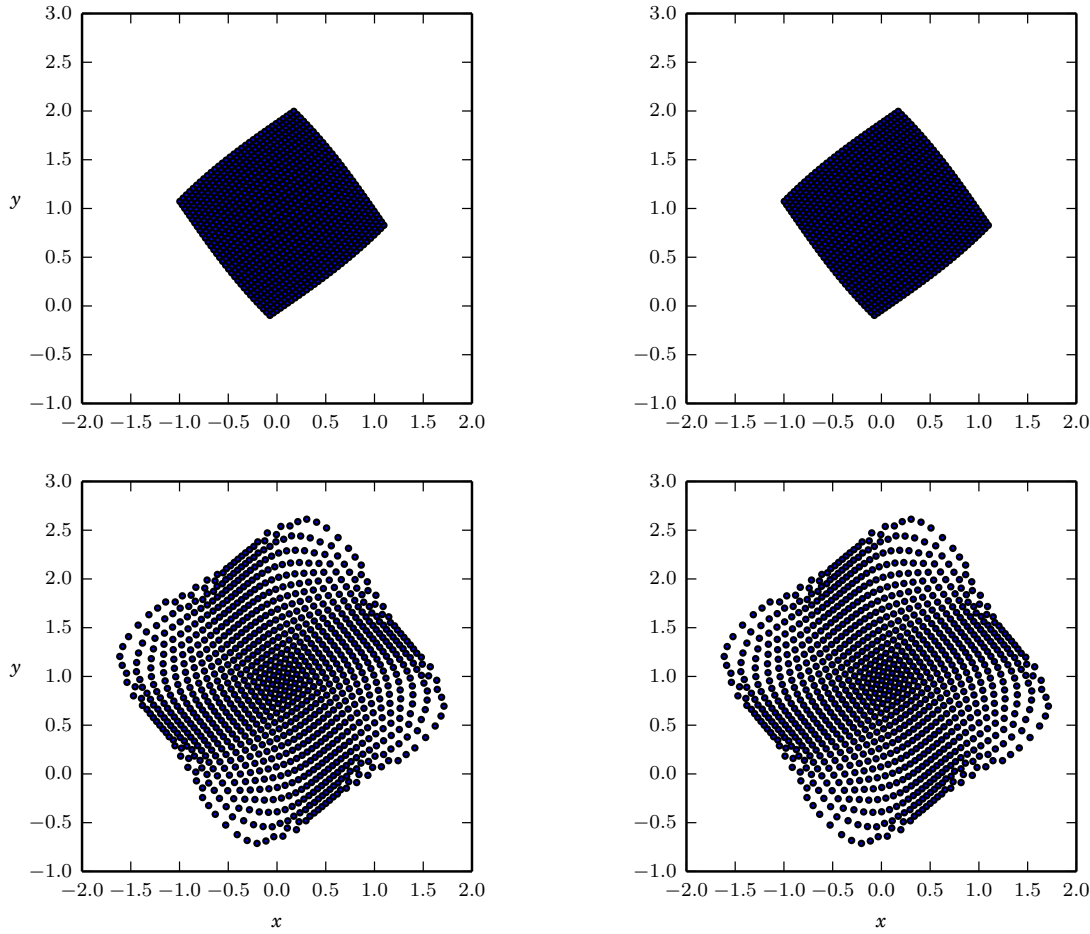


Fig. 4 For the case $\gamma = 2$, particle configurations at final time $T = 1$ for the two-dimensional hydrodynamic experiment of a rotating square; on the left-hand side with $\theta = 0$ and on the right-hand side with $\theta = 1$. The upper plots present results for $h = 1$ and $n = 512$ particles, while the lower row refers to variable $h = 1.5\sqrt{V_0}$ and $n = 512$ particles. In this case ($\gamma = 2$), the schemes for $\theta = 0$ and $\theta = 1$ are the same.

refer to fixed $h = 1$ independent of the resolution n (a choice in agreement with the convergence proof), while lower plots are obtained by h varying with the number of particles as $h = 1.5\sqrt{V_0}$. For the plots on the left-hand side the scheme with $\theta = 0$ is used, while for the plots on the right-hand side $\theta = 1$ is employed. Similarly to the one-dimensional results, the corresponding solutions for $\gamma = 2$ are identical for the schemes employing $\theta = 0$ or $\theta = 1$. On the contrary, they differ for $\gamma = 7$. Finally, it should be mentioned that the instabilities of the density profile on the boundaries of the domain, which were observed in the one-dimensional computations, have now translated into the nonhomogeneous distribution of particles.

The second numerical example considers the nonlocal force and the drag term, for which the numerical scheme corresponding to (38) does not depend on θ . Moreover, (38) does not depend on $\tilde{\rho}_t$, hence h is only relevant if we wish to plot $\tilde{\rho}_t$, and not for the computations themselves.

The Wendland function and a constant time step of $\Delta t = 10^{-1}$ are used. For the interactions, we take K such that it is the gradient of the *Morse potential*, see e.g. [11], with parameters $C_a = 2.0$, $C_r = 1.5$, $\ell_a = 1.0$, $\ell_r = 2.0$. In fact, we included a short-range regularization around the origin to the potential to enforce the required C_b^1 -regularity of K . A side-effect is that automatically self-interactions are cancelled. Two cases for the drag coefficient are examined: $\eta \equiv 10$ and $\eta \equiv 0.1$, for final time $T = 100$. In both these cases, an equilibrium has been reached. Similarly to the hydrodynamical problem, (69) is used with $n = 2^{2k}$ particles, where $k \in \{1, 2, 3, 4, 5\}$. Particle configurations and convergence rates are plotted in Fig. 6, with the upper plots referring to $\eta \equiv 0.1$ and the lower plots to $\eta \equiv 10$. The value of the convergence in this case rapidly tends to the theoretically predicted value.

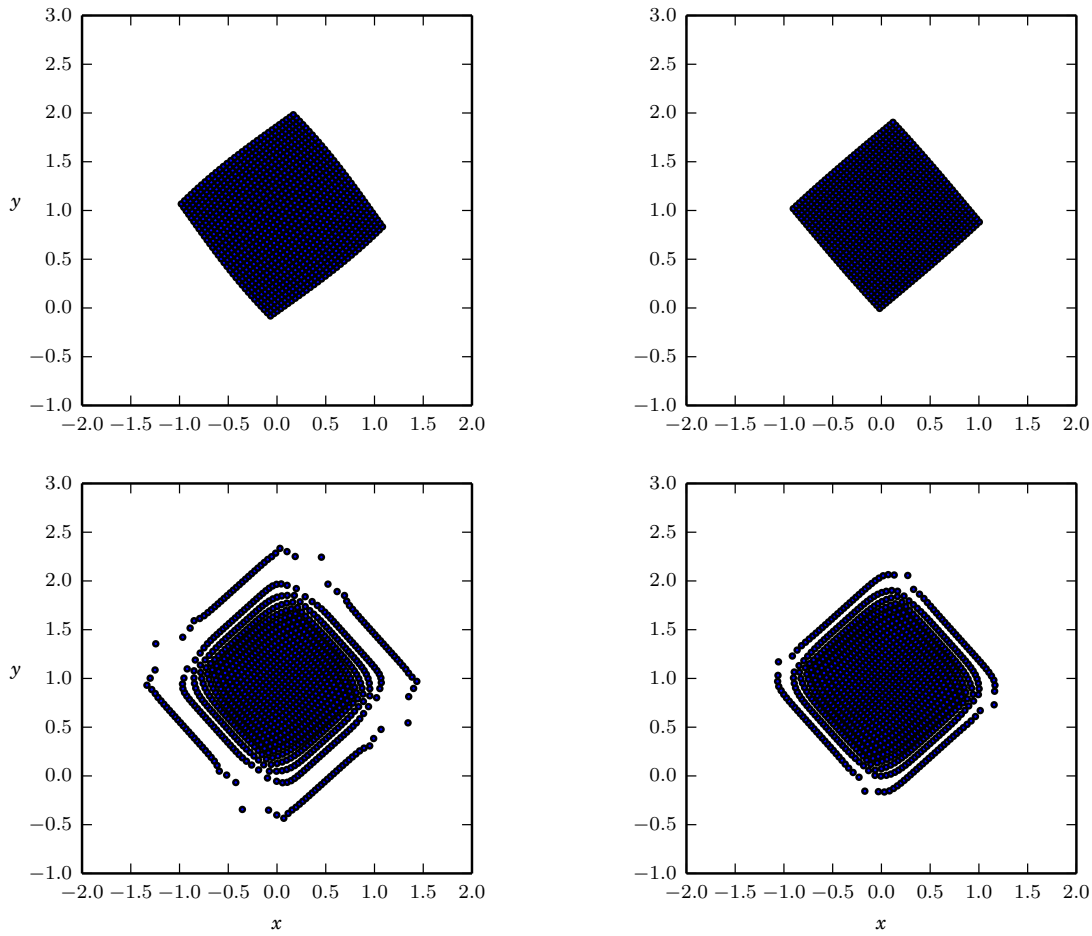


Fig. 5 For the case $\gamma = 7$, particle configurations at final time $T = 1$ for the two-dimensional hydrodynamic experiment of a rotating square; on the left-hand side with $\theta = 0$ and on the right-hand side with $\theta = 1$. The upper plots present results for $h = 1$ and $n = 512$ particles, while the lower row refers to variable $h = 1.5\sqrt{V_0}$ and $n = 512$ particles.

4 Concluding remarks and future directions

Apart from the remarks already made, there are two issues that are important to point out. One could call them shortcomings of our approach, in the sense that these are cases to which our proof of convergence does not apply. The convergence result presented in Theorem 3.11 and Corollary 3.12 does not state:

- Whether the approximations corresponding to $\theta = 0$ and $\theta = 1$, respectively, actually converge to the same limit solution. Our computations show that this is certainly not the case for $h = 1$ and (although the difference is smaller) neither for varying h , except for the trivial case $\gamma = 2$ in which the schemes coincide.
- Whether the limit $n \rightarrow \infty$ in any of the two cases $\theta = 0$ or $\theta = 1$ is actually like the ‘real physics’. To investigate this, in principle one would need to consider the limit $h \rightarrow 0$. As said before, this is beyond the scope of the current paper.

The latter point refers to a situation in which first the limit $n \rightarrow \infty$ is taken and afterwards the limit $h \rightarrow 0$. A more favourable approach (also from a numerical point of view) would be to have h depend on n in such a way that $h = \mathcal{O}(1/\sqrt[n]{n})$ as $n \rightarrow \infty$, and hence $n \rightarrow \infty$ and $h \rightarrow 0$ simultaneously. In Sect. 3.6, we anticipated this—following what is already typically done in the literature of SPH—and the numerical results there support the hope that solutions converge in the case of h varying with the number of particles.

Nevertheless, our combined theoretical-computational results establish the convergence of the classical and most-used SPH scheme and also show that the corresponding equation of motion is a true discretized version of the equation of motion of a regularized continuous medium.

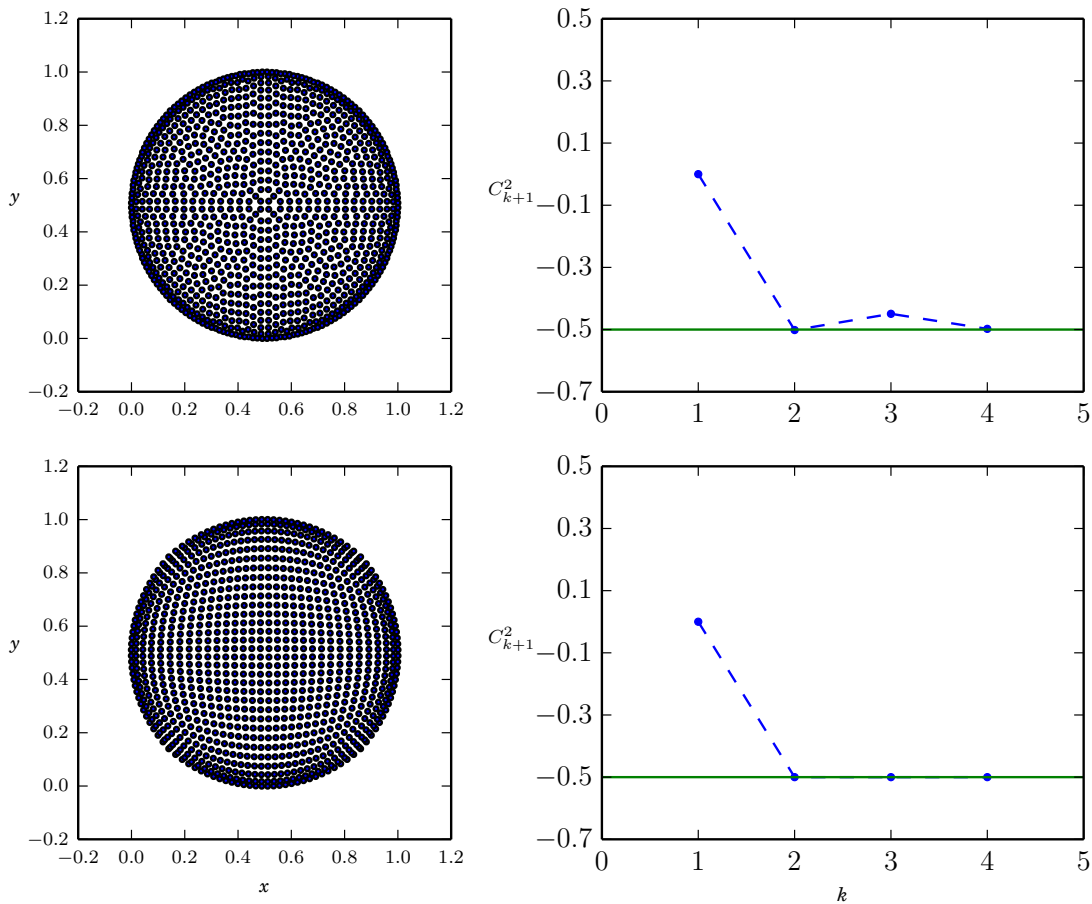


Fig. 6 For the problems involving a nonlocal force term, the particle configurations at final time $T = 100$ (left plots) and the convergence rates (right plots). Drag coefficients $\eta \equiv 0.1$ (upper plot) and $\eta \equiv 10$ (lower plot) are used.

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