THE REPULSIVE-PARTICLE METHOD AND THE SYMPLECTIC INTEGRATION OF THE SHALLOW-WATER EQUATIONS

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Abstract. We discuss the numerical implementation of the shallow-water equations in Lagrangian coordinates. We show that a finite-dimensional Hamiltonian approximation can be obtained based either on a moving grid or on a smooth-particle approach. We introduce a new particle method which, in some sense, combines moving mesh and smooth-particle methods. We show how this new method, which we call the repulsive-particle method, is related to the simulation of a "mesoscopic" molecular system with repulsive pairwise interactions. The resulting finite-dimensional Hamiltonian system is integrated in time by a modification of the symplectic Störmer-Verlet method.

Key words. Shallow-water equations, Lagrangian formulation, Hamiltonian systems, moving mesh methods, smooth-particle methods, molecular dynamics, symplectic time discretization

1. Introduction.

The Lagrangian formulation of fluid dynamics uses a coordinate system moving with the velocity field of the fluid. This approach can be used to perform computational fluid dynamics in a moving coordinate system. The basic idea is to represent the coordinate space by a collection of "particles" which move according to a set of appropriate equations of motion. Two choices are possible. (i) One considers the "particles" as vertices of a grid/mesh in coordinate space and defines the equations of motion as a spatial truncation of the full equations over that mesh. These methods are also called *moving mesh methods*. (ii) The particles are not restricted by a mesh but are given a spatial "extension" which defines the forces acting between the particles. We call those methods *smooth-particle methods*.

Computational fluid dynamics in Lagrangian coordinates has a long history tracing back to Courant & Friedrichs [8], von Neumann [17] and S. Ulam [18]. For recent contributions on moving mesh methods see, for example, [10, 9, 13, 7, 23]. In particular, Favorskii [9] and Holms et al. [14] suggested to truncate the Lagrangian equations of motion directly on the level of the action, the Hamiltonian function, respectively. This results in a finite dimensional model that preserves a corresponding expression of the total energy. Based on this general idea, Caramana et al. [7] developed an energy conserving discretization in space and time for Lagrangian fluid dynamics. On the other hand, following the pioneering work of Gingold and Monaghan [11] and Lucy [16], smooth-particle methods have also received much attention recently. In particular, Yserentant [24] suggested a new class of particle methods based on an appropriate ansatz for the mass density and a Lagrangian variational principle to derive the finite dimensional equations of motion. Hoover and Posch [15] show that smooth-particle simulations of barotropic ideal fluids are isomorphic to a special class of *molecular dynamics* simulations [2] and consider the smooth-particle potential as an effective molecular dynamics pair potential.

In this paper, we are interested in the numerical simulation of a family of generalized shallow-water equations as suggested by Bühler in [5]. We formulate a general ansatz that allows us to derive a finite-dimensional Hamiltonian approximation that can be based either on a moving mesh approach or on a smooth-particle approach. We also demonstrate how to combine moving mesh and smooth-particle methods in a new particle method. This method leads to equations of motion which could be character-

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ized as a "mesoscopic" molecular dynamics model with pairwise repulsive interactions. We call the new method the *repulsive-particle method.* The corresponding classical Hamiltonian equations of motion are discretized in time by a generalization of the *symplectic* and *time-reversible* Störmer-Verlet method. The fact that the method is symplectic implies that the (finite-dimensional) Hamiltonian (total energy) is very well preserved over long time intervals provided the step-size is small enough [4, 20].

2. The shallow-water equations. The standard *shallow-water equations* for a shallow homogeneous fluid in a coordinate system rotating at constant angular velocity $f/2$ are given by

$$\frac{d}{dt}h = -h\boldsymbol{\nabla}_{\boldsymbol{x}} \cdot \boldsymbol{u},$$
$$\frac{d}{dt}\boldsymbol{u} = -f\mathbf{e}_z \times \boldsymbol{u} - c_o^2\boldsymbol{\nabla}_{\boldsymbol{x}}h,$$
$$\frac{d}{dt}\boldsymbol{x} = \boldsymbol{u}.$$

Here h is the non-dimensional depth of the layer such that $h = 1$ corresponds to the undisturbed layer depth $\bar{H}$, $\boldsymbol{u} \in \mathbb{R}^2$ is the velocity field, $\boldsymbol{x} \in \mathbb{R}^2$ are the (continuous) "particle" coordinates, and c_o is a constant given by $c_o^2 = g\bar{H}$, where g is the gravitational constant. See [6] for a detailed description of this model.

These equations can lead to a steepening of gravity waves and to the formation of shocks. To prevent this, Bühler [5] suggested the generalized model

$$\frac{d}{dt}h = -h\boldsymbol{\nabla}_{\boldsymbol{x}} \cdot \boldsymbol{u}, \tag{2.1}$$
$$\frac{d}{dt}\boldsymbol{u} = -f\mathbf{e}_z \times \boldsymbol{u} - c_o^2\boldsymbol{\nabla}_{\boldsymbol{x}}F(h), \tag{2.2}$$
$$\frac{d}{dt}\boldsymbol{x} = \boldsymbol{u}, \tag{2.3}$$

where $F(h)$ is now an arbitrary function. The special choice

$$F(h) = \frac{3}{2} - \frac{1}{2h^2}$$

was shown [5] to avoid steepening of gravity waves for a one dimensional shallow-water system with $f = 0$.

One can think of the function $c_o^2F(h)$ as the local pressure field p [1]; i.e., $p = c_o^2F(h)$. The density ρ of the fluid is assumed to be constant and is formally set equal to $\rho = 1$.

The equation (2.3) defines a moving coordinate system $\boldsymbol{x}(t)$ with given initial condition $\boldsymbol{x}(0) = \boldsymbol{a}$. We now introduce the Jacobian of the associated coordinate transformation from $\boldsymbol{a}$ to $\boldsymbol{x}$, i.e.

$$\mathrm{j} = |\boldsymbol{x}_{\boldsymbol{a}}|\,.$$

Note that the Jacobian j satisfies the continuity equation

$$\frac{d}{dt}\mathrm{j} = \mathrm{j}\boldsymbol{\nabla}_{\boldsymbol{x}} \cdot \boldsymbol{u}.$$

This equation and (2.1) imply that $\mathrm{j}(t)\, h(t) = \text{const.}$ and, since $\mathrm{j}(0) = 1$, we obtain the relation

$$h(t) = \frac{h_o}{\mathrm{j}(t)}, \tag{2.4}$$

where h_o is the fluid depth at $t = 0$. Thus equation (2.1) can be viewed as a "variational equation" associated with the nonlinear system (2.2)-(2.3) and is, in a sense, redundant within the Lagrangian framework. We also note that (2.4) reflects the fact that the fluid is incompressible; i.e., changes in the depth of the layer are compensated for by changes in the density of the two dimensional cross section of the fluid.

3. Hamiltonian truncation of the equations of motion. For simplicity of exposition, we restrict the discussion to free boundaries, i.e., we assume that the fluid covers, at any time $t \geq 0$, a region $\mathcal{U}_t \subset \mathbb{R}^2$ of coordinate space with no external forces acting at the boundary $\partial \mathcal{U}_t$. Let us assume that a fixed number of "particles" $i = 1, \ldots, N$ with coordinates $\boldsymbol{q}_i(t) \in \mathbb{R}^2$ and initial values $\boldsymbol{q}_i(0) = \boldsymbol{a}_i \in \mathcal{U}_0$ is given.

The next step is to define a relation between the water depth h_i and the set of particle coordinates $\{\boldsymbol{q}_k\}$. Let us assume for a moment that such a relation has indeed been found and let us denote this relation by $h_i(\{\boldsymbol{q}_k\})$, $i = 1, \ldots, N$. We now apply the idea of *control volume discretization* [9, 7] and take the derivative of h_i with respect to time. This yields

$$\begin{aligned} \frac{d}{dt} h_i &= \sum_{j=1}^{N} (\boldsymbol{\nabla}_{\boldsymbol{q}_j} h_i) \cdot \boldsymbol{u}_j \\ &= h_i \sum_{j=1}^{N} (\boldsymbol{\nabla}_{\boldsymbol{q}_j} \ln h_i) \cdot \boldsymbol{u}_j . \end{aligned} \tag{3.1}$$

Here $\boldsymbol{\nabla}_{\boldsymbol{q}_j}$ denotes the gradient in the sense of classical mechanics [3]. Comparing (3.1) with the continuity equation (2.1), we conclude that

$$\boldsymbol{\nabla}_{\boldsymbol{x}} \cdot \boldsymbol{u}\,(\boldsymbol{q}_i) \approx -\sum_{j=1}^{N} (\boldsymbol{\nabla}_{\boldsymbol{q}_j} \ln h_i) \cdot \boldsymbol{u}_j ; \tag{3.2}$$

i.e., the divergence of the vector field $\boldsymbol{u}$ at $\boldsymbol{x} = \boldsymbol{q}_i$ can be approximated by the left-hand side of (3.2). More generally, if $\boldsymbol{v}$ is a vector field, then the divergence of this field is defined, at each point $\boldsymbol{q}_i$, by

$$\boldsymbol{\nabla}_{\boldsymbol{x}} \cdot \boldsymbol{v}\,(\boldsymbol{q}_i) \approx -\sum_{j=1}^{N} (\boldsymbol{\nabla}_{\boldsymbol{q}_j} \ln h_i) \cdot \boldsymbol{v}_j .$$

Using this approximation of the divergence operator, we now apply the concept of *support operator* [9, 7] to derive an approximation for the gradient operator. In our case, this reduces to taking the negative transpose of the discrete divergence operator. Thus, if f is a scalar field, then the discrete gradient of this field at $\boldsymbol{q}_i$ is defined by

$$\boldsymbol{\nabla}_{\boldsymbol{x}} f(\boldsymbol{q}_i) \approx \sum_{j=1}^{N} f_j \boldsymbol{\nabla}_{\boldsymbol{q}_i} \ln h_j ,$$

where $f_j = f(\boldsymbol{q}_j)$. This implies, for example,

$$\boldsymbol{\nabla}_{\boldsymbol{x}} F(h(\boldsymbol{q}_i)) \approx \sum_{j=1}^{N} \frac{F(h_j)}{h_j} \boldsymbol{\nabla}_{\boldsymbol{q}_i} h_j$$

and, still on a formal level, a finite-dimensional approximation of the generalized shallow-water equations (2.2)-(2.3) is given by

$$\frac{d}{dt}\boldsymbol{u}_i = -f\mathbf{e}_z \times \boldsymbol{u}_i - c_o^2 \boldsymbol{\nabla}_{\boldsymbol{q}_i} \sum_{j=1}^{N} \bar{F}(h_j(\{\boldsymbol{q}_k\})), \tag{3.3}$$

$$\frac{d}{dt}\boldsymbol{q}_i = \boldsymbol{u}_i, \tag{3.4}$$

$i = 1, \ldots, N$. These equations are Hamiltonian with a structure matrix

$$\boldsymbol{J}_i = \begin{pmatrix} \mathbf{0} & \boldsymbol{I} \\ -\boldsymbol{I} & \boldsymbol{\Omega} \end{pmatrix}, \qquad \boldsymbol{\Omega}\boldsymbol{u} = -f\mathbf{e}_z \times \boldsymbol{u}, \tag{3.5}$$

for each $(\boldsymbol{q}_i, \boldsymbol{u}_i)$ pair of canonical variables and with the Hamiltonian function

$$\mathcal{H} = \frac{1}{2}\sum_{i=1}^{N} ||\boldsymbol{u}_i||^2 + c_o^2 \sum_{i=1}^{N} \bar{F}(h_i(\{\boldsymbol{q}_k\})). \tag{3.6}$$

Since we must have

$$\boldsymbol{\nabla}_{\boldsymbol{q}_i} \sum_{j=1}^{N} \bar{F}(h_j) = \sum_{j=1}^{N} \bar{F}'(h_j) \boldsymbol{\nabla}_{\boldsymbol{q}_i} h_j = \sum_{j=1}^{N} h_j \bar{F}'(h_j) \boldsymbol{\nabla}_{\boldsymbol{q}_i} \ln h_j = \sum_{j=1}^{N} F_j \boldsymbol{\nabla}_{\boldsymbol{q}_i} \ln h_j,$$

the "potential energy" density $\bar{F}(h)$ is given by

$$\bar{F}(h) = \int \frac{F(h)}{h}\, dh.$$

Note that $\mathcal{H}$ is a first integral of motion, i.e. $d\mathcal{H}/dt = 0$.

To make it all work, we still have to define the relations $h_i(\{\boldsymbol{q}_k\})$, $i = 1, \ldots, N$. Two approaches seem feasible. Either we consider the particles as vertices of a moving triangular grid[1], which provides us with a definition on how much "area" each particles occupies, or we give each particle an extension, which provides us with a definition for the density of the particle system. Both approaches are explained in more detail in the following two subsections.

3.1. Moving mesh methods. We first introduce a triangular mesh over the region $\mathcal{U}_t$ at time $t = 0$, i.e., we approximate the initially given set $\mathcal{U}_0$ by M triangles with vertices $\boldsymbol{q}_i(0) = \boldsymbol{a}_i$, $i = 1, \ldots, N$. Let as denote these triangles and their images for $t > 0$ by $\{\Delta_l(t)\}$. If the corresponding vertices are numbered clock-wise and are denoted by $(\boldsymbol{q}_1^l, \boldsymbol{q}_2^l, \boldsymbol{q}_3^l) \in \mathbb{R}^6$, then the (oriented) area $\bar{A}_l$ of a triangle Δ_l is defined by

$$\bar{A}_l \mathbf{e}_z = \frac{1}{2}(\boldsymbol{x}_2^l - \boldsymbol{x}_1^l) \times (\boldsymbol{x}_3^l - \boldsymbol{x}_1^l).$$

[1] One could also consider other grid structures as well as staggered grids. In this section, we explain the basic idea of a moving mesh discretization using the triangular mesh logic as suggested by Fritts and Boris [10].

Let us denote the set of all triangles which have $\boldsymbol{q}_i$ as a common vertex by $l(i)$. Then the area A_i of the vertex $\boldsymbol{q}_i$ is defined by

$$A_i = \frac{1}{3} \sum_{m \in l(i)} \bar{A}_m.$$

This "triangular mesh logic" has been introduced by Boris and Fritts [10].

The next step is to use the area elements $\{A_i\}$ to locally approximate the exact Jacobian j via

$$\mathrm{j} \approx \mathrm{j}_i := \frac{A_i(t)}{A_i(0)} = \frac{A_i(\{\boldsymbol{q}_k\})}{A_i(\{\boldsymbol{a}_k\})}.$$

This and (2.4) yield the desired relation

$$h_i(\{\boldsymbol{q}_k\}) := h_i(0) \frac{A_i(\{\boldsymbol{a}_k\})}{A_i(\{\boldsymbol{q}_k\})}.$$

3.2. Smooth-particle methods. Instead of a defining a mesh, let us now introduce a family of "shape" functions $\psi_\tau(r)$, $r \geq 0$, with $\int \psi_\tau(r) r dr$ bounded and independent of $\tau > 0$ as well as $\psi_0(0) = 1$. Next we approximate the depth of the layer by a linear superposition of shifted shape functions; i.e.,

$$h(\boldsymbol{x}, t) = \sum_{i=1}^{N} \psi_{\tau_i}(||\boldsymbol{x} - \boldsymbol{q}_i(t)||),$$

where $\{\tau_i\}$ are appropriate constants and $\boldsymbol{x} \in \mathbb{R}^2$. This provides us with an approximation for the layer depth at each particle location $\boldsymbol{q}_i$. We denote this approximation by

$$h_i(\{\boldsymbol{q}_k\}) = h(\boldsymbol{q}_i, t).$$

The resulting equations of motion can be considered as an application of *smoothed particle hydrodynamics* (SPH) [11, 16] to the shallow-water equations (2.1)-(2.3) with special emphasize on the Hamiltonian nature of the equations of motion. Following Hoover and Posch [15], the equations of motion also fit into the framework of *molecular dynamics* with a pairwise potential energy

$$V(\{\boldsymbol{q}_k\}) = c_o^2 \sum_{i=1}^{N} \sum_{j=1}^{N} \psi_{\tau_i}(||\boldsymbol{q}_i - \boldsymbol{q}_j||)$$

provided $f = 0$ and $F(h) = h$ in (2.2).

A popular choice for the family of shape functions $\psi_\tau(r)$ is given by the Gaussian like spline function

$$\psi_\tau(r) = \frac{1}{\tau^2} \left\{ \begin{array}{ll} \frac{3}{2}\left(\frac{1}{2}u - 1\right) u^2 + 1 & 0 \leq u < 1 \\ \frac{1}{4}(2-u)^3 & 1 \leq u < 2 \\ 0 & u \geq 2 \end{array} \right. ,$$

where $u = r/\tau$.

Let us now formulate the equations of motion for the standard shallow-water equations; i.e., $F(h) = h$. In this case, $\bar{F}(h) = h$ as well. We also introduce the particle distances

$$r_{ij} = ||\boldsymbol{q}_i - \boldsymbol{q}_j||.$$

Then the finite-dimensional truncation is given by the system

$$\frac{d}{dt}\boldsymbol{u}_i = -f\mathbf{e}_z \times \boldsymbol{u}_i - c_o^2 \sum_{j\neq i}^{N} \left(\psi'_{\tau_i}(r_{ij}) + \psi'_{\tau_j}(r_{ij})\right) \frac{\boldsymbol{q}_i - \boldsymbol{q}_j}{r_{ij}}, \tag{3.7}$$

$$\frac{d}{dt}\boldsymbol{q}_i = \boldsymbol{u}_i, \tag{3.8}$$

$i = 1, \ldots, N$.

4. The repulsive-particle method. In this section, we derive a new particle method starting from a moving mesh approach and using the unified framework as provided in the previous section.

4.1. Derivation of the method. A moving mesh method can be understood as assigning an area $A_i(t)$ to each particle $\boldsymbol{q}_i$. Since the fluid is incompressible, this implies the algebraic relation

$$A_i(t)h_i(t) = \text{const.},$$

which allows us to define the layer depth h_i as a function of the area element A_i. Each area element $A_i(t)$ depends on a fixed number of particles $\boldsymbol{q}_j$ with index $j \in l(i)$. Let us assume that we use the triangular mesh logic, as described in section 3.1, and that the particles $\boldsymbol{q}_j$, $j \in l(i)$, satisfy $||\boldsymbol{q}_i - \boldsymbol{q}_j|| \approx r$. Then

$$A_i \sim r^2.$$

This suggests to replace the density layer depth $h_i(t)$, as defined above, by

$$h_i(t) = \tau_i^2 \sum_{j\in l(i)} \frac{1}{||\boldsymbol{q}_i - \boldsymbol{q}_j||^2},$$

where $\tau_i > 0$ is an appropriate scaling factor and $l(i)$ denotes now a set of indices such that $j \in l(i)$ is equivalent to the statement that $\boldsymbol{q}_j$ is "close" to $\boldsymbol{q}_i$. However, this can be interpreted as performing a molecular dynamics simulation with a repulsive $1/r^2$ pair potential taking only those interactions into account that are stored in a given, fixed neighbour list [2]. In particular, the potential energy of the shallow-water equations with $F(h) = h$ is given by

$$V(\{\boldsymbol{q}_k\}) = c_o^2 \sum_{i=1}^{N} \sum_{j\in l(i)} \left(\frac{\tau_i}{r_{ij}}\right)^2.$$

Note that

$$\boldsymbol{\nabla}_{\boldsymbol{q}_j} h_i = -2\tau_i^2 \left(\frac{1}{r_{ij}}\right)^4 (\boldsymbol{q}_j - \boldsymbol{q}_i).$$

4.2. A one-dimensional test problem. Let us, for simplicity, consider the one-dimensional shallow-water equation

$$\frac{d}{dt}u = -c_o^2 \nabla_x h(x),$$
$$\frac{d}{dt}x = u$$

with periodic boundary conditions $u(x) = u(x+1)$ and $h(x) = h(x+1)$. We assume that, initially, $h = 1$ and u some given function.

Let us first discuss the moving mesh approach. We divide the interval $[0,1]$ in N intervals of equal length Δx and introduce the mesh points $x_i = (i-1)\Delta x$, $i = 1, \ldots, N$. We approximate the layer depth h at half points by

$$h_{i+1/2} = \frac{\Delta x}{x_{i+1} - x_i}$$

which implies

$$\nabla_{x_i} h \approx \Delta x \left(\frac{1}{(x_i - x_{i-1})^2} - \frac{1}{(x_{i+1} - x_i)^2} \right).$$

Let us now develop the corresponding repulsive-particle method. With each $h_{i+1/2}$, we associate the length

$$L_{i+1/2} = x_{i+1} - x_i = r_{i+1,i}.$$

Guided by the moving mesh approach, we define the layer depth by

$$h_i = \tau \sum_{|j|=1}^{k} \frac{1}{|r_{i+j,i}|},$$

where

$$\tau^{-1} = \sum_{j=1}^{k} \frac{2}{j\Delta x}$$

and $k \geq 1$ is an appropriate constant. The corresponding repulsive-particle method is equivalent to a moving mesh method if $k = 1$; i.e., if only the nearest neighbours enter into the definition of h_i. See table 4.1 for numerical results for $k \gg 1$.

4.3. Summary of the method. We now summarize the repulsive-particle method for the generalized shallow-equations (2.1)-(2.3). Each particle $\boldsymbol{q}_i$ has a "domain of influence" $l(i)$. The layer depth h_i is defined by

$$h_i = \sum_{j \in l(i)} \left(\frac{\tau_i}{r_{ij}} \right)^2, \tag{4.1}$$

where $\tau_i > 0$ is a scaling factor such that h_i is equal to the initial layer depth at $t = 0$. The equations of motion are derived from the Hamiltonian

$$\mathcal{H} = \frac{1}{2} \sum_{i=1}^{N} ||\boldsymbol{u}_i||^2 + c_o^2 \sum_{i=1}^{N} \bar{F}(h_i)$$

Δx	k	error
0.0050	20	0.00090
0.0050	10	0.00110
0.0050	5	0.00110
0.0025	40	0.00033
0.0025	20	0.00053
0.0025	10	0.00056
0.0010	60	0.00029

FIG. 4.1. *Error in the computation of the layer depth.*

and are given by

$$\frac{d}{dt}\boldsymbol{q}_i = \boldsymbol{u}_i, \tag{4.2}$$

$$\frac{d}{dt}\boldsymbol{u}_i = -f\boldsymbol{e}_z \times \boldsymbol{u}_i + 2c_o^2 \sum_{j\in l(i)} \left(\tau_i^2 \bar{F}'(h_i) + \tau_j^2 \bar{F}'(h_j)\right) \frac{1}{r_{ij}^4}(\boldsymbol{q}_i - \boldsymbol{q}_j), \tag{4.3}$$

$i = 1, \ldots, N$.

To implement this method in a way that allows one to dynamically update the neighbor list $l(i)$ without loosing the Hamiltonian nature of the equations of motion, we modify (4.1) to

$$h_i = \sum_{j\in l(i)} \left[\left(\frac{\tau_i}{r_{ij}}\right)^2 - \left(\frac{\tau_i}{r_{ij}}\right)^\delta + \epsilon_{ij} \right],$$

where

$$j \in l(i) \quad \text{if and only if} \quad r_{ij} \le R_i := \left(\frac{2}{\delta}\right)^{\frac{1}{2-\delta}} \tau_i$$

and ϵ_{ij} is chosen such that

$$\left[\left(\frac{\tau_i}{R_i}\right)^2 - \left(\frac{\tau_i}{R_i}\right)^\delta + \epsilon_{ij} \right] = 0.$$

Here $\delta < 1$ is a sufficiently small positive number. This modification of (4.1) corresponds to a popular truncation of long-range repulsive interactions in molecular dynamics simulations [2, 19] and implies that also

$$\frac{\partial}{\partial r_{ij}} \left[\left(\frac{\tau_i}{r_{ij}}\right)^2 - \left(\frac{\tau_i}{r_{ij}}\right)^\delta + \epsilon_{ij} \right] = 0 \quad \text{for} \quad r_{ij} = R_i.$$

5. The virial theorem. The virial theorem provides a relation between the force field and the pressure in an "atomistic" molecular system [2, 19]. In this section, we show how to, formally, apply the virial theorem to the shallow-water equations and our repulsive-particle method.

Let us, for simplicity, assume that the function $F(h)$ is of the form $F(h) = h^k$, $k \neq 0$, and that the fluid is non-rotational; i.e., $f = 0$. As pointed out before [1], we can associate with $F(h)$ the pressure field p; i.e., $p = c_o^2 F(h) = c_o^2 h^k$. On the level of the discretized equations, we replace the pressure field pointwise by the expression

$$p_i = c_o^2 F(h_i) = c_o^2 \left(\sum_{j \in l(i)} \left(\frac{\tau_i}{r_{ij}} \right)^2 \right)^k .$$

Next we note that $\bar{F}(h)$ is given by $\bar{F}(h) = h^k/k$ and the Hamiltonian function for the repulsive-particle method becomes

$$\mathcal{H} = \frac{1}{2} \sum_{i=1}^{N} ||\boldsymbol{u}_i||^2 + \frac{c_o^2}{k} \sum_{i=1}^{N} \left(\sum_{j \in l(i)} \left(\frac{\tau_i}{r_{ij}} \right)^2 \right)^k .$$

with the corresponding equations of motion given by (4.2)-(4.3) and $f = 0$.

The *virial* [19] for a particle system in two dimensions is given by

$$\mathcal{V} = \frac{1}{2} \sum_{i=1}^{N} ||\boldsymbol{u}_i||^2 - \frac{1}{2} \sum_{i=1}^{N} \boldsymbol{q}_i^T \boldsymbol{\nabla}_{\boldsymbol{q}_i} \mathcal{H}$$

which, for the given repulsive-particle Hamiltonian, can be written as

$$\mathcal{V} = \sum_{i=1}^{N} \left(\frac{1}{2} ||\boldsymbol{u}_i||^2 + \mathcal{V}_i \right) ,$$

where

$$\mathcal{V}_i = \frac{1}{2} c_0^2 \bar{F}'(h_i) \sum_{j \in l(i)} (\boldsymbol{q}_i - \boldsymbol{q}_j)^T \boldsymbol{\nabla}_{\boldsymbol{q}_i} \left(\frac{\tau_i}{r_{ij}} \right)^2 = c_o^2 \left(\sum_{j \in l(i)} \left(\frac{\tau_i}{r_{ij}} \right)^2 \right)^k$$

is the *internal virial* $\mathcal{V}_i$ at q_i. Upon comparison with the expression for the pressure p_i, we see that $\mathcal{V}_i = p_i$ as one might have expected from the identity $\mathcal{V} = PV$, V the volume of the fluid and P the average pressure of the fluid. Note that we have neglected here the kinetic energy contributions to the internal virial, however,

$$\frac{1}{2} ||\boldsymbol{u}_i||^2 + \mathcal{V}_i \approx \mathcal{V}_i,$$

in general.

6. Vorticity. One of the main characteristics of the shallow water equations is the conservation of *potential vorticity.* Let us now give corresponding expressions for the finite-dimensional systems.

The *potential vorticity* field of the shallow-water equations (2.1)-(2.3) is defined by

$$q = \frac{\mathbf{e}_z \cdot \boldsymbol{\nabla}_{\boldsymbol{x}} \times \boldsymbol{u} + f}{h}$$

which satisfies $dq/dt = 0$, i.e., is constant along solution curves. Numerically, we assign a potential vorticity q_i to each particle via the formula

$$q_i = \frac{f + \omega_i}{h_i} \tag{6.1}$$

with ω_i defined by

$$\omega_i \mathbf{e}_z = \sum_{j=1}^{N} \boldsymbol{\nabla}_{\boldsymbol{q}_j} \ln h_i \times \boldsymbol{u}_j. \tag{6.2}$$

7. Symplectic time discretization. Since the finite-dimensional spatial truncation of the equations of motion is Hamiltonian with the associated flow map being symplectic, it seems only appropriate to apply a *symplectic time discretization* [22]. The standard Störmer-Verlet method [22] can be applied to (3.3)-(3.4) provided $f = 0$. The Störmer-Verlet methods can be modified such as to also cover the case $f \neq 0$. This modification is given by

$$\boldsymbol{q}_i^{n+1} = \boldsymbol{q}_i^n + \Delta t \boldsymbol{u}_i^{n+1/2}, \tag{7.1}$$

$$\boldsymbol{u}_i^{n+1/2} = \boldsymbol{u}_i^n - \frac{\Delta t}{2} \left(\boldsymbol{\nabla}_{\boldsymbol{q}_i} \sum_j \bar{F}(h_j(\{\boldsymbol{q}_k^n\})) + f\mathbf{e}_z \times \boldsymbol{u}_i^{n+1/2} \right), \tag{7.2}$$

$$\boldsymbol{u}_i^{n+1} = \boldsymbol{u}_i^{n+1/2} - \frac{\Delta t}{2} \left(\boldsymbol{\nabla}_{\boldsymbol{q}_i} \sum_j \bar{F}(h_j(\{\boldsymbol{q}_k^{n+1}\})) + f\mathbf{e}_z \times \boldsymbol{u}^{n+1/2} \right), \tag{7.3}$$

$i = 1, \ldots, N$. This method is time-reversible and symplectic, i.e., the associated one step map is symplectic under the structure matrix (3.5).

8. Numerical experiments. We now present results from two different numerical simulations demonstrating the usage of a moving mesh method and the repulsive-particle method.

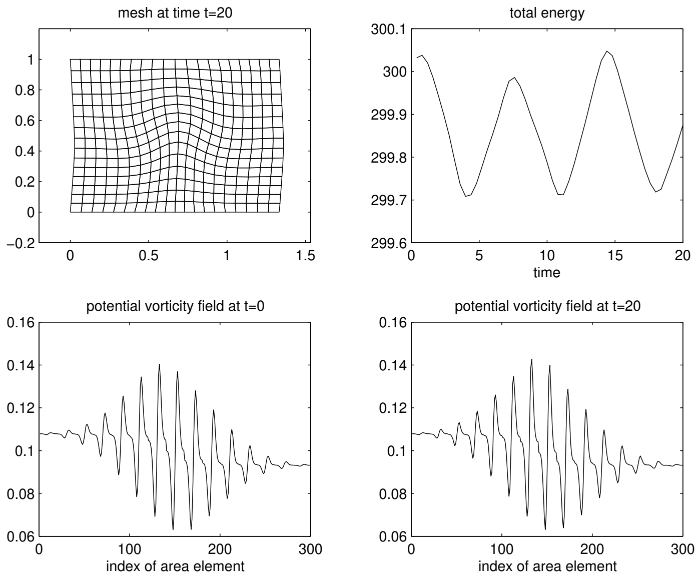

FIG. 8.1. *Numerical results for the shallow water equations using a moving mesh method.*

8.1. Moving mesh method. We implement the moving mesh Störmer-Verlet method for the following shallow water system. We take $f = 0.1$, $c_o = 0.1$, $F(h) = h$, and consider the domain which is periodic in x with length $L = 1.\bar{3}$ and has fixed extension $[0, 1]$ in the y-direction. The initial velocity field $\boldsymbol{u} = (u, v)^T$ is zero in the x direction and the v-component satisfies

$$v(x, y) = 0.01e^{-20(y-0.5)^2}e^{-20(x-L/2)^2}.$$

The initial layer depth h of the fluid is equal to

$$h(x, y) = 1 + 0.05\,\mathrm{atan}\,(20(y - 0.5)).$$

The initial domain $[0, L] \times [0, 1]$ is covered by a rectangular grid using 20×15 cells. The (oriented) area of each quadrilateral is used to define an approximate Jacobian j_i for each quadrilateral which yields a finite-dimensional Hamiltonian

$$\mathcal{H} = \frac{1}{2}\sum_j ||\boldsymbol{u}_j||^2 + c_o^2 \sum_i h_i.$$

The time discretization uses a step size of $\Delta t = 0.4$. We integrate the equations of motion over a time interval $[0, 20]$. The motion is mainly confined to the central region of the domain and the final grid can be found in Fig. 8.1.

The spatially truncated system has the Hamiltonian (total energy) as a first integral. The potential vorticity (6.1) should also be preserved. The corresponding numerical results can be found in figure 8.1. Note the excellent conservation of potential vorticity and total energy.

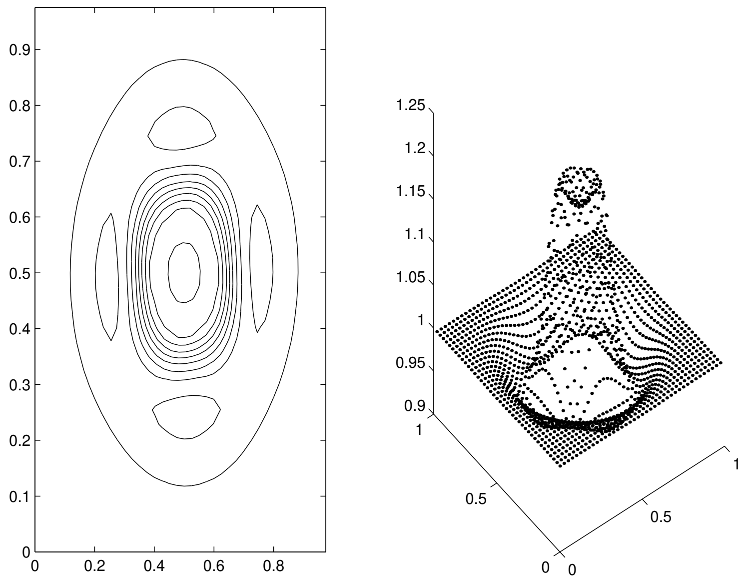

FIG. 8.2. *Numerical results for the shallow water equations using the repulsive-particle method with* 48 *nearest neighbours; layer depth at* $t = 0.05$.

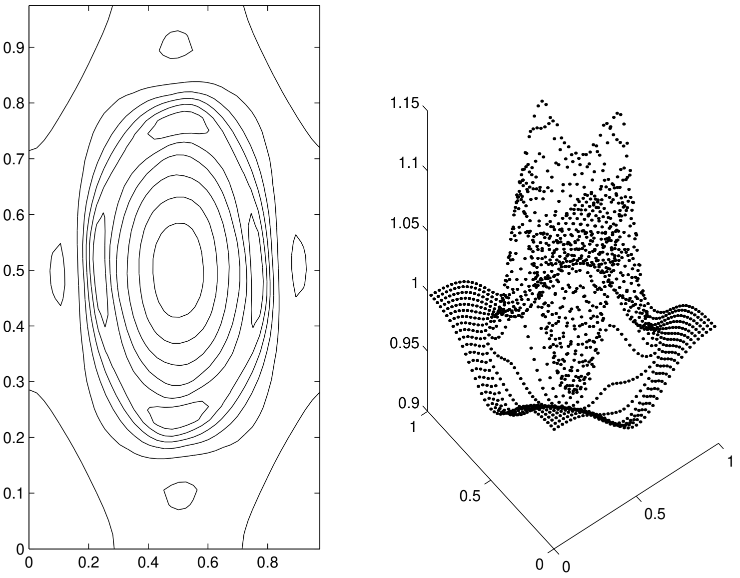

FIG. 8.3. *Numerical results for the shallow water equations using the repulsive-particle method with* 48 *nearest neighbours; layer depth at* $t = 0.1$.

8.2. Repulsive-particle method. We implement the repulsive-particle method for the following shallow-water system. We take $f = 10$, $c_o = 2$, $F(h) = h$, and consider periodic boundary conditions $\boldsymbol{u}(x,y) = \boldsymbol{u}(x+k, y+l)$, $h(x,y) = h(x+k, y+l)$, k, l integers. The initial layer depth is $h = 1$ and the initial velocity field is given by

$$u(x,y) = 2e^{-10r^2}\sin(2\pi x) \quad \text{and} \quad v(x,y) = 2e^{-10r^2}\sin(2\pi y),$$

r the distance of (x,y) from the point $(0.5, 0.5)$. The domain $[0,1]\times[0,1]$ is initially covered by a rectangular grid using 40×40 particles. Each particle $\boldsymbol{q}_i$ has a domain of influence $l(i)$ defined by its 48 nearest neighbours on the grid. The time integration uses a step-size of $\Delta t = 0.002$. See figure 8.2 for the wave form at $t = 0.05$ and figure 8.3 for the wave form at $t = 0.1$.

We also implement a moving mesh method for the same shallow-water system. The results at $t = 0.05$ are compared to those for the repulsive-particle method with 24 nearest neighbours. Both equations are integrated with a step size of $\Delta t = 0.001$. See figure 8.4.

9. Concluding Remark. We presented several discretizations for the shallow water equations. Our approach is based on a finite dimensional truncation that maintains the conservative character of the Lagrangian equations of motion. The resulting spatially truncated systems are integrated in time by a symplectic method. This results in good conservation of energy and potential vorticity. We only applied the most basic symplectic time integration methods such as Störmer-Verlet. More sophisticated choices, such as symplectic multiple-time-stepping, higher order concatenation, averaging methods etc, are clearly feasible. One could also time discretizations that exactly preserve energy [12]. However, such methods are fully implicit.

Computation of complicated flow patterns based on a moving mesh method requires restructuring of the mesh. This leads to schemes that are symplectic over each

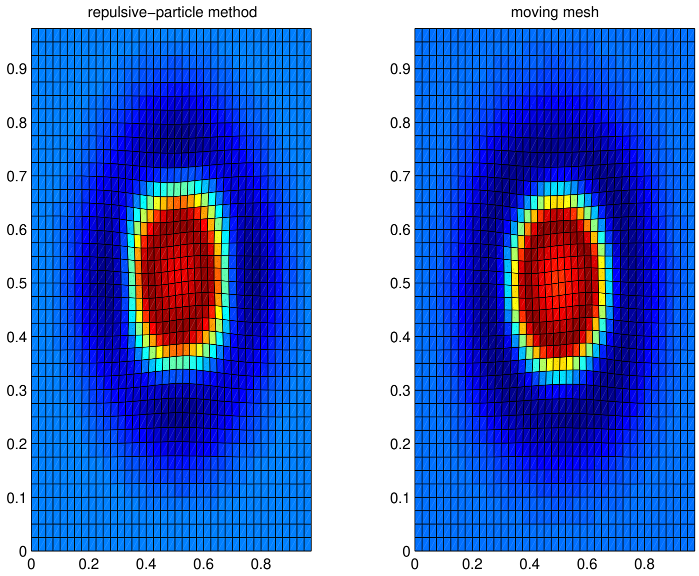

FIG. 8.4. *Numerical results for the shallow water equations using a moving mesh method with* 1600 *grid points and the repulsive-particle method with* 24 *nearest neighbours; layer depth at* $t = 0.05$.

interval of smoothly varying mesh adaption but will not be symplectic over the whole interval of integration. However, the symplectic discretizations seem to advect the (potential) vorticity field very well and this property can be maintained under mesh restructuring. This should be true in particular for the *reversible mesh restructuring scheme* as presented by Fritts and Boris [10].

We have shown how to apply smooth-particle methods to the shallow-water equations. We derived a new particle method, the repulsive-particle method, taking the properties of a moving mesh method as the starting point and combining it with the basic idea of a smooth-particle method. We anticipate that the suggested repulsive-particle method will allow us to combine the best of both particle based methods. Moving mesh methods seem better suited for laminar flows and the implementation of boundary conditions while smooth-particle methods are well suited for the computation of complicated flow patterns.

We finally mention that the repulsive particle method can also be applied to the Lagrangian description [14] of compressible ideal fluids. This generalization is discussed in [21].

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