

Hamiltonian Particle-Mesh Method for Two-Layer Shallow-Water Equations Subject to the Rigid-Lid Approximation*

Colin J. Cotter[†], Jason Frank[‡], and Sebastian Reich[†]

Abstract. We develop a particle-mesh method for two-layer shallow-water equations subject to the rigid-lid approximation. The method is based on the recently proposed Hamiltonian particle-mesh (HPM) method and the interpretation of the rigid-lid approximation as a set of holonomic constraints. The suggested spatial discretization leads to a constrained Hamiltonian system of ODEs which is integrated in time using a variant of the symplectic SHAKE/RATTLE algorithm. It is demonstrated that the elimination of external gravity waves by the rigid-lid approximation can be achieved in a computationally stable and efficient way.

Key words. particle methods, rotating shallow-water equations, symplectic integration, rigid-lid approximation

AMS subject classifications. 76M28, 37M15, 65P10, 76U05, 76B60, 70-08, 70H05, 70F20

DOI. 10.1137/030600076

1. Introduction. Theorists frequently regard the ocean as a two-layer fluid with the interface between layers corresponding to the main thermocline. This idealization is perhaps most appropriate in the northwestern subtropical North Atlantic. Consider, then, a rotating fluid composed of two immiscible layers with different constant densities $\rho_1 < \rho_2$ over a flat bottom topography at $z = 0$. See Figure 1.1 and the excellent exposition [21]. Under the assumption that $\rho_1 \approx \rho_2$, the associated two-layer shallow-water equations are

$$(1.1) \quad \frac{D}{Dt_i} \mathbf{u}_i + f \mathbf{u}_i^\perp = \begin{cases} -g \nabla_{\mathbf{x}}(h_1 + h_2), & i = 1, \\ -g \nabla_{\mathbf{x}}(h_1 + h_2) - g' \nabla_{\mathbf{x}} h_2, & i = 2, \end{cases}$$

where $\mathbf{u}_i \equiv (u_i, v_i)^T$ is the horizontal velocity in the i th layer, $f > 0$ is the *Coriolis parameter*, $\mathbf{u}_i^\perp \equiv (-v_i, u_i)^T$,

$$\frac{D}{Dt_i} \equiv \frac{\partial}{\partial t} + \mathbf{u}_i \cdot \nabla_{\mathbf{x}}, \quad \text{and} \quad g' \equiv \frac{\rho_2 - \rho_1}{\rho_2} g$$

*Received by the editors March 3, 2003; accepted for publication (in revised form) by D. Holm November 21, 2003; published electronically March 4, 2004.

<http://www.siam.org/journals/siads/3-1/60007.html>

[†]Department of Mathematics, Imperial College London, 180 Queen's Gate, London SW7 2AZ, United Kingdom (colin.cotter@imperial.ac.uk, s.reich@imperial.ac.uk).

[‡]CWI, P. O. Box 94079, 1090 GB Amsterdam, The Netherlands (jason@cwi.nl).

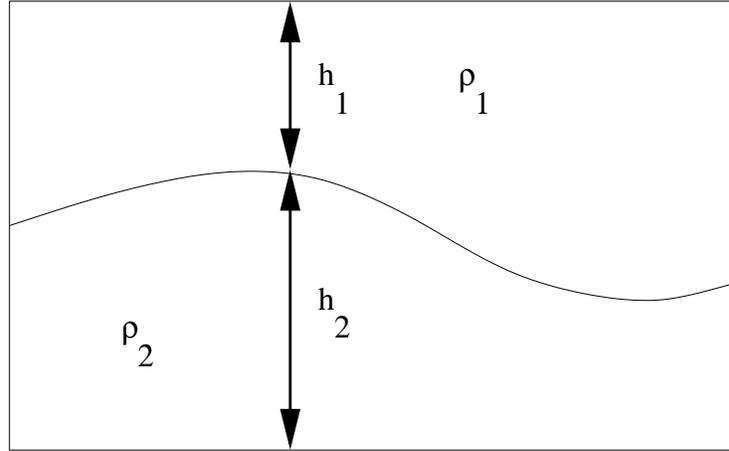


Figure 1.1. Two-layer shallow-water model with rigid lid.

is the *reduced gravity*.¹ By assumption, $g' \ll g$. Each layer-depth h_i satisfies the continuity equation

$$(1.2) \quad \frac{\partial h_i}{\partial t} + \nabla_{\mathbf{x}} \cdot (h_i \mathbf{u}_i) = 0.$$

It is also reasonable to assume that the combined flow in both layers is incompressible, which leads to the *rigid-lid* constraint

$$(1.3) \quad h \equiv h_1 + h_2 = H = \text{const.}$$

Equation (1.1) is replaced by

$$\frac{D}{Dt_i} \mathbf{u}_i + f \mathbf{u}_i^\perp = \begin{cases} -\nabla_{\mathbf{x}} p, & i = 1, \\ -\nabla_{\mathbf{x}} p - g' \nabla_{\mathbf{x}} h_2, & i = 2, \end{cases}$$

where p is the pressure field enforcing the rigid-lid constraint (1.3) which, after differentiation in time, is equivalent to

$$\nabla_{\mathbf{x}} \cdot (h_1 \mathbf{u}_1) + \nabla_{\mathbf{x}} \cdot (h_2 \mathbf{u}_2) = 0.$$

We also make the simplifying assumption that both layers have a (nondimensionalized) *mean layer-depth* of $H_i = 1$, i.e., $H = H_1 + H_2 = 2$, and replace reduced gravity g' with an appropriate constant c_0 .

In a Lagrangian description of the model, we introduce a continuum of fluid particles $\mathbf{X}_i(\mathbf{a}_i, t) \equiv (X_i(\mathbf{a}_i, t), Y_i(\mathbf{a}_i, t))^T$ in each layer $i = 1, 2$, which are *labeled/marked* by their

¹Equation (1.1) is a slight variation of the formulation given in [21, p. 85]. While (1.1) leads to a Hamiltonian formulation, no obvious Hamiltonian interpretation of (12.3) in [21] could be found. However, both formulations are identical under the rigid-lid approximation.

initial positions $\mathbf{a}_i = \mathbf{X}_i(\mathbf{a}_i, 0)$. Hence the independent variables are time t and labels \mathbf{a}_i . The material time derivative D/Dt becomes a partial derivative which, with a slight abuse of notation, we denote by d/dt .

Let $h_i^o(\mathbf{a}_i)$ denote the initial layer-depth at $t = 0$. Then the layer-depth is given at any time t by

$$(1.4) \quad h_i(\mathbf{x}, t) = \int h_i^o(\mathbf{a}) \delta(\mathbf{x} - \mathbf{X}_i(\mathbf{a}_i, t)) d^2\mathbf{a}_i, \quad i = 1, 2,$$

where δ denotes the Dirac delta function. This formula and

$$\frac{d}{dt}\mathbf{X}_i = \mathbf{u}_i$$

replace the continuity equation (1.2) in a Lagrangian description of fluid dynamics. Hence we finally obtain the constrained infinite-dimensional Newtonian equations of motion

$$\begin{aligned} \frac{d}{dt}\mathbf{u}_i &= -f\mathbf{u}_i^\perp - \begin{cases} \nabla_{\mathbf{x}_1} p, & i = 1, \\ \nabla_{\mathbf{x}_2} p + c_0 \nabla_{\mathbf{x}_2} h_2, & i = 2, \end{cases} \\ \frac{d}{dt}\mathbf{X}_i &= \mathbf{u}_i, \\ 0 &= h_1(\mathbf{x}, t) + h_2(\mathbf{x}, t) - H. \end{aligned}$$

In the following section we describe a spatial discretization for this model.

2. The Hamiltonian particle-mesh (HPM) method with rigid-lid constraint. To simplify the discussion, we assume a double periodic domain $\mathbf{x} \in \mathcal{R} \equiv [-\pi, +\pi)^2$ and introduce a regular grid \mathbf{x}^{pq} on \mathcal{R} with equal grid spacing Δx in the x - and y -direction. Let $\psi^{pq}(\mathbf{x})$ denote the tensor product cubic B-spline centered at $\mathbf{x}^{pq} \equiv (x^{pq}, y^{pq})^T$, i.e.,

$$\psi^{pq}(\mathbf{x}) \equiv \psi_{\text{cs}}\left(\frac{x^{pq} - x}{\Delta x}\right) \cdot \psi_{\text{cs}}\left(\frac{y^{pq} - y}{\Delta x}\right),$$

where $\psi_{\text{cs}}(r)$ is the cubic spline

$$\psi_{\text{cs}}(r) \equiv \begin{cases} \frac{2}{3} - |r|^2 + \frac{1}{2}|r|^3, & |r| \leq 1, \\ \frac{1}{6}(2 - |r|)^3, & 1 < |r| \leq 2, \\ 0, & |r| > 2. \end{cases}$$

These basis functions form a *partition of unity*, i.e.,

$$\sum_{p,q} \psi^{pq}(\mathbf{x}) = 1.$$

This implies

$$\sum_{p,q} \nabla_{\mathbf{x}} \psi^{pq}(\mathbf{x}) = 0,$$

which is a desirable property when computing gradients. In each layer $i = 1, 2$, we introduce N discrete particles \mathbf{X}_i^k , $k = 1, \dots, N$, with masses m_i^k such that²

$$h_i^o(\mathbf{x}^{pq}) \approx \sum_{k=1}^N m_i^k \psi^{pq}(\mathbf{X}_i^k)$$

at time $t = 0$. More specifically, we approximate the layer-depth h_2 on the grid by

$$h_2^{pq} \equiv \sum_{k=1}^N m_2^k \psi^{pq}(\mathbf{X}_2^k)$$

and the total layer-depth by

$$h^{pq}(\mathbf{X}) \equiv \sum_{k=1}^N \left(m_1^k \psi^{pq}(\mathbf{X}_1^k) + m_2^k \psi^{pq}(\mathbf{X}_2^k) \right),$$

where, for later use, we introduced the notation $h^{pq}(\mathbf{X})$ to indicate that h^{pq} depends on all particle positions \mathbf{X}_i^k collected in the vector \mathbf{X} .

So far we have essentially followed the standard methodology for deriving *particle-mesh* (PM) methods [10, 4]. The following steps are crucial to the HPM method as introduced in [7] for geophysical fluid dynamics simulations. Even though the layer-depth in rotating fluids often stays relatively smooth, the numerical approximations h_1^{pq} and h^{pq} will develop some nonsmoothness in strongly mixing flows due to the finite number of particles used to resolve the fluid motion; this tends to destabilize PM methods. We suggested in [7] to apply a (discretized) smoothing operator³

$$(2.1) \quad \mathcal{S} = (1 - \alpha^2 \nabla_{\mathbf{x}}^2)^{-p}$$

to the layer-depth over the fixed Eulerian grid \mathbf{x}^{pq} with a smoothing length $\alpha = 2\Delta x$ and an exponent $p = 2$. Let us denote the resulting smoothed approximations to h_2^{pq} and h^{pq} , respectively, by \hat{h}_2^{pq} and \hat{h}^{pq} . While this smoothing approach has been shown to work very well for compressible flows, it cannot be used to enforce a regularized incompressibility condition (1.3). To see this, note that \mathcal{S} is an invertible operator and, hence, for the (constant) layer-depth approximation,

$$h^{pq}(\mathbf{X}) = \hat{h}^{pq}(\mathbf{X}) = 0.$$

Instead, the following regularization strategy proved successful. We introduce a meta-grid with grid-spacing $\Delta\bar{x} \equiv 2\Delta x$ and grid points denoted by $\bar{\mathbf{x}}^{mn}$. Let $\phi^{mn}(\mathbf{x})$ denote the associated tensor product B-spline centered at $\bar{\mathbf{x}}^{mn} \equiv (\bar{x}^{mn}, \bar{y}^{mn})^T$, i.e.,

$$\phi^{mn}(\mathbf{x}) \equiv \psi_{\text{cs}} \left(\frac{\bar{x}^{mn} - x}{\Delta\bar{x}} \right) \cdot \psi_{\text{cs}} \left(\frac{\bar{y}^{mn} - y}{\Delta\bar{x}} \right).$$

²If the particles \mathbf{X}_i^k are initially placed on a regular grid with equal spacing Δa in the x - and y -direction, then, following (1.4), one can use $m_i^k \equiv h_i^o(\mathbf{X}_i^k) (\Delta a / \Delta x)^2$.

³In case that the direct numerical implementation of the smoothing operator \mathcal{S} is too expensive, one could replace \mathcal{S} with, e.g., a *Shapiro filter* [23]. In the present paper, we used FFT to implement \mathcal{S} .

Then an averaged (coarse-grained) total layer-depth is defined by

$$\bar{h}^{mn}(\mathbf{X}) \equiv \frac{1}{4} \sum_{pq} \phi^{mn}(\mathbf{x}^{pq}) h^{pq}(\mathbf{X}).$$

The discrete pressure approximation \bar{p}^{mn} is also defined over the coarse grid $\bar{\mathbf{x}}^{mn}$, and the resulting total force acting on particle \mathbf{X}_i^k (excluding the Coriolis contribution) is given by

$$\mathbf{F}_i^k(\mathbf{X}, \bar{\mathbf{p}}) \equiv - \sum_{p,q} \nabla_{\mathbf{X}_i^k} \psi^{pq}(\mathbf{X}_i^k) \times \begin{cases} \left(\sum_{m,n} \phi^{mn}(\mathbf{x}^{pq}) \bar{p}^{mn} \right), & i = 1, \\ \left(c_0 \hat{h}_2^{pq} + \sum_{m,n} \phi^{mn}(\mathbf{x}^{pq}) \bar{p}^{mn} \right), & i = 2, \end{cases}$$

where $\bar{\mathbf{p}}$ denotes the vector of pressure variables \bar{p}^{mn} . We observe numerically that this coarse graining keeps the pressure gradient sufficiently smooth. This regularization of the pressure field was found necessary for stable computations. Other coarse graining procedures are certainly feasible and will be the subject of further research.

We would like to point out that Holm has revealed in [11] a close relation between velocity smoothing, as fundamental to the α -Euler models [12], and a regularization of the pressure gradient. A closer investigation of our pressure regularization procedure and its relation to the results of [11] is left for future research.

Another important aspect of the HPM method is that the forces are derived from an exact gradient. This implies a number of very desirable conservation properties, such as conservation of circulation, potential vorticity (PV), total mass, and energy [8, 5]. We note that energy conserving variants of PM methods have been considered, for example, in [16] and [14] in the context of plasma physics simulations.

The discrete set of constrained Newtonian equations of motion is now

$$(2.2) \quad \frac{d}{dt} \mathbf{u}_i^k = f_i^k J \mathbf{u}_i^k + \mathbf{F}_i^k(\mathbf{X}, \bar{\mathbf{p}}), \quad J \equiv \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix},$$

$$(2.3) \quad \frac{d}{dt} \mathbf{X}_i^k = \mathbf{u}_i^k,$$

$$(2.4) \quad 0 = \bar{h}^{mn}(\mathbf{X}) - H.$$

Here f_i^k denotes the value of the Coriolis parameter at particle location \mathbf{X}_i^k . In the following, let us first assume that the Coriolis parameter f is constant, i.e., $f = f_0$. Later we will consider the more general case of variable f . Then (2.2)–(2.4) give a constrained Hamiltonian system with the \bar{p}^{mn} variables acting as Lagrange multipliers to enforce the *holonomic constraints* (2.4). The Hamiltonian is

$$\mathcal{H}(\mathbf{X}, \mathbf{v}, \bar{\mathbf{p}}) \equiv \sum_{i=1}^2 \sum_{k=1}^N \frac{1}{2m_i^k} \mathbf{v}_i^k \cdot \mathbf{v}_i^k + \frac{c_0}{2} \sum_{p,q} \hat{h}_2^{pq} (h_2^{pq} - H_2) + \sum_{m,n} (\bar{h}^{mn} - H) \bar{p}^{mn}$$

with conjugate momenta $\mathbf{v}_i^k \equiv m_i^k \mathbf{u}_i^k$. Equations (2.2)–(2.4) are equivalent to

$$\begin{aligned}\frac{d}{dt} \mathbf{v}_i^k &= f_0 J \nabla_{\mathbf{v}_i^k} \mathcal{H} - \nabla_{\mathbf{X}_i^k} \mathcal{H}, \\ \frac{d}{dt} \mathbf{X}_i^k &= \nabla_{\mathbf{v}_i^k} \mathcal{H}, \\ 0 &= \nabla_{\bar{\mathbf{p}}^{mn}} \mathcal{H},\end{aligned}$$

$i = 1, 2$, $k = 1, \dots, N$. The *symplectic two-form* [2] is given by

$$(2.5) \quad \omega \equiv \sum_{i,k} \left[d\mathbf{X}_i^k \wedge d\mathbf{v}_i^k + \frac{f_0}{2} d\mathbf{X}_i^k \wedge J^{-1} d\mathbf{X}_i^k \right],$$

which is preserved along solutions.

3. Symplectic time-stepping algorithm. Following [13] and [17], we develop a variant of the popular SHAKE/RATTLE algorithm [1, 20, 15] for Hamiltonian systems with holonomic constraints. In particular, the following two steps are performed during each time-step.

Step 1.

$$(3.1) \quad \mathbf{u}_i^k(t_{n+1/2}) = \mathbf{u}_i^k(t_n) + \frac{\Delta t}{2} \left\{ f_0 J \mathbf{u}_i^k(t_{n+1/2}) + \mathbf{F}_i^k(\mathbf{X}(t_n), \bar{\mathbf{p}}(t_{n+1/2})) \right\},$$

$$(3.2) \quad \mathbf{X}_i^k(t_{n+1}) = \mathbf{X}_i^k(t_n) + \Delta t \mathbf{u}_i^k(t_{n+1/2}),$$

$$(3.3) \quad 0 = \bar{h}^{mn}(\mathbf{X}(t_{n+1})) - H,$$

which requires the solution of a nonlinear system in the pressure variable $\bar{\mathbf{p}}(t_{n+1/2})$ to satisfy the holonomic constraint (3.3).

Step 2.

$$(3.4) \quad \mathbf{u}_i^k(t_{n+1}) = \mathbf{u}_i^k(t_{n+1/2}) + \frac{\Delta t}{2} \left\{ f_0 J \mathbf{u}_i^k(t_{n+1/2}) + \mathbf{F}_i^k(\mathbf{X}(t_{n+1}), \bar{\mathbf{p}}(t_{n+1/2})) \right\}.$$

The scheme can be rewritten in terms of the canonical momenta $\mathbf{v}_i^k(t_n)$, and the method conserves the symplectic structure (2.5) from time-step to time-step, i.e., the method is *symplectic* [22]. Backward error analysis [3, 9, 18] implies excellent conservation of energy. It is important that the method used to solve the holonomic constraints (3.3) is iterated to convergence; otherwise, the symplectic property of the algorithm is lost.

If the Coriolis parameter f is not constant, then $f_i^k \equiv f(\mathbf{X}_i^k(t_n))$ is used in (3.1) and $f_i^k \equiv f(\mathbf{X}_i^k(t_{n+1}))$ in (3.4) instead of f_0 .

The nonlinear system of equations in the pressure variable $\bar{\mathbf{p}}(t_{n+1/2})$ can be solved by the following quasi-Newton method. Let us denote the iteration index by $l \geq 0$. Then, given some approximation $\bar{\mathbf{p}}^{[l]}$, we can compute the associated approximation to the vector of particle positions $\mathbf{X}^{[l]}(t_{n+1})$ using (3.1)–(3.2) with $\bar{\mathbf{p}}(t_{n+1/2}) = \bar{\mathbf{p}}^{[l]}$. The next pressure approximation

$$\bar{\mathbf{p}}^{[l+1]} \equiv \bar{\mathbf{p}}^{[l]} + \Delta \mathbf{p}^{[l]}$$

is then found by solving

$$A \Delta \mathbf{p}^{[l]} = \bar{h}^{mn}(\mathbf{X}^{[l]}(t_{n+1})) - H.$$

The matrix A has entries

$$a_{m'n'}^{mn} \equiv \frac{\Delta t^2}{2} \sum_{k,i,p,q,p',q'} m_i^k \phi^{mn}(\mathbf{x}^{pq}) \left(\nabla \psi^{pq}(\mathbf{X}_i^k) \cdot \nabla \psi^{p'q'}(\mathbf{X}_i^k) \right) \phi^{m'n'}(\mathbf{x}^{p'q'})$$

and is computed only once at the beginning of the simulation with $\mathbf{X}_i^k = \mathbf{X}_i^k(0)$. It is found that the matrix A changes little along the numerical solutions $\mathbf{X}_i^k = \mathbf{X}_i^k(t_n)$. The initial $\bar{\mathbf{p}}^{[0]}$ is found at each time-step from the previous pressure approximation by linear extrapolation, i.e.,

$$\bar{\mathbf{p}}^{[0]} \equiv 2\bar{\mathbf{p}}(t_{n-1/2}) - \bar{\mathbf{p}}(t_{n-3/2}).$$

4. Semi-implicit methods. The step-size of the standard HPM method applied to the two-layer shallow-water equations (1.1) is restricted by the highest frequency of the external gravity waves, which is approximately

$$\omega_{\max} \equiv \sqrt{c_0 H} \sqrt{\frac{g}{g'}} k_{\max},$$

where k_{\max} is the largest computational wave number. This severe step-size restriction motivated the introduction of the constrained HPM method of the previous section. However, let us look back for a moment at the unconstrained shallow-water equations (1.1). The *semi-implicit method*, as pioneered by Robert (see [6]), avoids the step-size restriction of any standard explicit method while also being easy to implement (in particular when combined with a pseudospectral (PS) discretization in space [6]). Let us then briefly review the basic idea behind the semi-implicit method for a one-layer shallow-water model with all advection terms ignored, i.e.,

$$\begin{aligned} \mathbf{u}_t &= f_0 J \mathbf{u} - c \nabla_{\mathbf{x}} h, & c &\equiv c_0 \frac{g}{g'}, \\ h_t &= -H \nabla_{\mathbf{x}} \cdot \mathbf{u}. \end{aligned}$$

The (external) *Rossby deformation radius* [21] is equal to

$$\lambda_{\text{ext}} \equiv \frac{\sqrt{cH}}{f_0}.$$

Upon only discretizing in time, the semi-implicit method results in

$$\begin{aligned} \frac{\mathbf{u}(t_{n+1}) - \mathbf{u}(t_{n-1})}{2\Delta t} &= f_0 J \mathbf{u}(t_n) - c \nabla_{\mathbf{x}} \frac{h(t_{n+1}) + h(t_{n-1})}{2}, \\ \frac{h(t_{n+1}) - h(t_{n-1})}{2\Delta t} &= -H \nabla_{\mathbf{x}} \cdot \frac{\mathbf{u}(t_{n+1}) + \mathbf{u}(t_{n-1})}{2}. \end{aligned}$$

Let us define $\hat{h}(t_n) \equiv (h(t_{n+1}) + h(t_{n-1}))/2$. Then, at each time-step, $\hat{h}(t_n)$ is determined by the linear system

$$\left(1 - cH\Delta t^2 \nabla_{\mathbf{x}}^2\right) \hat{h}(t_n) = h(t_{n-1}) - \Delta t H \nabla_{\mathbf{x}} \cdot \mathbf{u}(t_{n-1}) - \Delta t^2 f_0 H \nabla_{\mathbf{x}} \times \mathbf{u}(t_n).$$

This gives

$$\left(1 - cH\Delta t^2 \nabla_{\mathbf{x}}^2\right) \hat{h}(t_n) = h(t_n) + \mathcal{O}(\Delta t^2),$$

which, upon ignoring terms of order $\mathcal{O}(\Delta t^2)$, we will now use as a defining equation for $\hat{h}(t_n)$, i.e.,

$$\hat{h}(t_n) \equiv \mathcal{A}h(t_n), \quad \mathcal{A} \equiv \left(1 - cH\Delta t^2 \nabla_{\mathbf{x}}^2\right)^{-1}.$$

With this new definition, the semi-implicit method becomes “explicit,” i.e.,

$$\begin{aligned} \frac{\mathbf{u}(t_{n+1}) - \mathbf{u}(t_{n-1})}{2\Delta t} &= f_0 J \mathbf{u}(t_n) - c \nabla_{\mathbf{x}} \mathcal{A}h(t_n), \\ \frac{h(t_{n+1}) - h(t_{n-1})}{2\Delta t} &= -H \nabla_{\mathbf{x}} \cdot \frac{\mathbf{u}(t_{n+1}) + \mathbf{u}(t_{n-1})}{2}. \end{aligned}$$

This reformulation has the same stability properties as the original semi-implicit method and easily generalizes to the fully nonlinear shallow-water equations.

The important point is that the operator \mathcal{A} becomes equivalent to the smoothing operator (2.1) used in the HPM method for $p = 1$ and $\alpha = \sqrt{cH}\Delta t$. Continuing along this line of thought, we conclude that the HPM method can be made unconditionally stable if used with a smoothing operator

$$(4.1) \quad \mathcal{S} = \left(1 - cH\Delta t^2 \nabla_{\mathbf{x}}^2\right)^{-1}$$

applied to the total layer-depth $h = h_1 + h_2$ in (1.1). However, for Δt severely violating the standard CFL condition [6], we will have $\sqrt{cH}\Delta t \gg \Delta x$, and the time-stepping will lead to excessive smoothing of the total layer-depth. The same argument applies, of course, to the semi-implicit method.

5. Barotropic and baroclinic motion. Let us introduce the continuous Eulerian velocity approximation

$$\mathbf{u}_1(\mathbf{x}, t) \equiv \frac{\sum_{k=1}^N \mathbf{u}_1^k(t) \psi^{pq}(\mathbf{X}_1^k(t))}{\sum_{k=1}^N \psi^{pq}(\mathbf{X}_1^k(t))}$$

for the first layer, and

$$\mathbf{u}_2(\mathbf{x}, t) \equiv \frac{\sum_{k=1}^N \mathbf{u}_2^k(t) \psi^{pq}(\mathbf{X}_2^k(t))}{\sum_{k=1}^N \psi^{pq}(\mathbf{X}_2^k(t))}$$

for the second layer, respectively. Assuming again that $H_1 = H_2 = 1$, the *barotropic* velocity contribution to the flow is defined by

$$\mathbf{u}(\mathbf{x}, t) \equiv \frac{1}{2} \{ \mathbf{u}_1(\mathbf{x}, t) + \mathbf{u}_2(\mathbf{x}, t) \},$$

which represents synchronized motion in both layers, and the *baroclinic* mode is defined by

$$\Delta \mathbf{u}(\mathbf{x}, t) \equiv \frac{1}{2} \{ \mathbf{u}_1(\mathbf{x}, t) - \mathbf{u}_2(\mathbf{x}, t) \},$$

which represents fluid motions pointing in opposite directions (the *thermal wind*).

If initially $\Delta \mathbf{u} = 0$ and $h_2 = H_2 = 1$, then the *available potential energy* (APE)

$$E_{\text{ap}} \equiv \frac{c_0}{2} \sum_{p,q} \hat{h}_2^{pq} (h_2^{pq} - H_2)$$

is zero and the motion can be reduced to a purely barotropic single layer shallow-water model with a rigid-lid approximation (corresponding to an infinite Rossby deformation radius). On the contrary, $h_2 \neq H_2$ leads to baroclinic motion which is strongly dependent upon its length scale λ relative to the *internal Rossby deformation radius*

$$\lambda_{\text{int}} \equiv \frac{\sqrt{c_0}}{f_0} \sqrt{\frac{H_1 H_2}{H_1 + H_2}} = \sqrt{\frac{c_0}{2f_0^2}}.$$

For length-scales $\lambda \gg \lambda_{\text{int}}$, most of the energy is stored in the layer-depth variation h_2 (i.e., in the APE contribution to \mathcal{H}). This energy is eventually transformed into kinetic (barotropic) energy in a process called *baroclinic instability*. In this process the baroclinic modes are reduced to those of length-scale $\lambda \sim \lambda_{\text{int}}$ unless external forcing leads to the activation of large-scale variations in h_2 (such as tropical heating and polar cooling).

Another important concept is that of *geostrophic balance*. By this we mean that the velocities \mathbf{u}_i in each layer stay close to their *geostrophic wind* approximations

$$\mathbf{u}_{\text{gw},1} \equiv f_0^{-1} \nabla_{\mathbf{x}}^{\perp} p, \quad \mathbf{u}_{\text{gw},2} \equiv f_0^{-1} \nabla_{\mathbf{x}}^{\perp} (p + c_0 h_2)$$

if initialized appropriately. These two definitions imply in particular the balanced thermal wind relation

$$(5.1) \quad \Delta \mathbf{u}_{\text{thw}} \equiv -\frac{c_0}{2f_0} \nabla_{\mathbf{x}}^{\perp} h_2.$$

The associated *baroclinic stream function* $\tau \equiv -c_0/(2f_0)h_2$ represents the vertically averaged temperature anomaly of the fluid.

The *geostrophic approximation* is valid for small *Rossby number* flows, i.e.,

$$Ro \equiv \frac{U}{\lambda f_0} \ll 1,$$

where U and λ are the typical velocity- and length-scales, respectively, for the flow under consideration. For a precise scaling analysis see [21].

To model baroclinic instabilities within the framework of double periodic boundary conditions $\mathbf{x} = (x, y)^T \in \mathcal{R} \equiv [-\pi, +\pi]^2$, we defined a variable Coriolis parameter f by

$$f(y) \equiv f_0 + \beta \sin y.$$

Hence, near $y = 0$, we approximately reproduce a β -plane approximation $f \approx f_0 + \beta y$. See [21] for a detailed explanation of the baroclinic instability.

6. Numerical experiments. We compute the solution starting from a purely baroclinic initial state defined by

$$\mathbf{u}_2 \equiv -\mathbf{u}_1 \equiv \frac{c_0}{2f} \nabla_{\mathbf{x}}^{\perp} (S h_2^o),$$

where $c_0 \equiv 1$, $f \equiv \sqrt{2}(1 + 0.2 \sin y)$,

$$h_2^o(\mathbf{x}) \equiv \frac{1}{1 + 0.08 \exp(-0.85 \|\mathbf{x}\|^2)} + \delta,$$

with the constant δ chosen such that h_2^{pq} has a mean value equal to one. The initial state moves slowly to the left along the x -axis and breaks up into smaller (barotropic and baroclinic) vortices. The internal deformation radius is $\lambda_{\text{int}} = 0.5$.

The spatial grid resolution for the rigid-lid HPM method is $\Delta x = 2\pi/128 \approx 0.0491$ with $N = 262144$ particles per layer, i.e., $\Delta a = \Delta x/4$. The smoothing length in (2.1) is $\alpha = 2\Delta x \approx 0.0982$ and the operator \mathcal{S} is implemented using an FFT. We also implemented a PS method for the standard Eulerian formulation of the compressible two-layer shallow-water equations with $\Delta x = 2\pi/256 \approx 0.0245$ and a semi-implicit discretization in time (see [6]). We stress that no hyperdiffusion was applied. The external deformation radius for the unconstrained shallow-water model is $\lambda_{\text{ext}} = 20$, i.e., $g' = g/400$ and $c = 400$.

Both methods were implemented using MATLAB, and mex-files were used for the PM computations within the HPM method. Note that $\sqrt{g'/g} = 20$ implies that a standard HPM discretization of the unfiltered equation (1.1) would require a step-size about 30 times smaller than the rigid-lid HPM method. This severe step-size restriction does not apply to the semi-implicit PS method. However, it was found that the largest possible step-size for the rigid-lid HPM method is $\Delta t = 0.5$, while the semi-implicit PS method requires $\Delta t \leq 0.07$ to be stable for the given initial data and $t \in [0, 150]$.

Figure 6.1 shows the time evolution of the baroclinic and barotropic vorticity fields over a time interval $[0, 150]$ using a step-size of $\Delta t = 0.1$. The corresponding results from the semi-implicit PS method with step-size $\Delta t = 0.01$ and initial $h_1^o \equiv 2 - h_2^o$ can be found in Figure 6.2. Note that this step-size leads to a computational smoothing length of $\alpha \approx 0.2828 \gg \Delta x \approx 0.0245$ in (4.1). We recorded the CPU-time for both simulations and obtained about 36000 time-units for the HPM method and 48000 time-units for the semi-implicit PS method. For output purposes, the smoothing operator (2.1) was applied to the gridded vorticity fields to average out fine-scale vorticity filaments. The vorticity fields are identical up to some small-scale differences over the whole time interval $[0, 150]$.

We also prepared a few videos using the GIF format. One can access these by clicking one of the following four options:

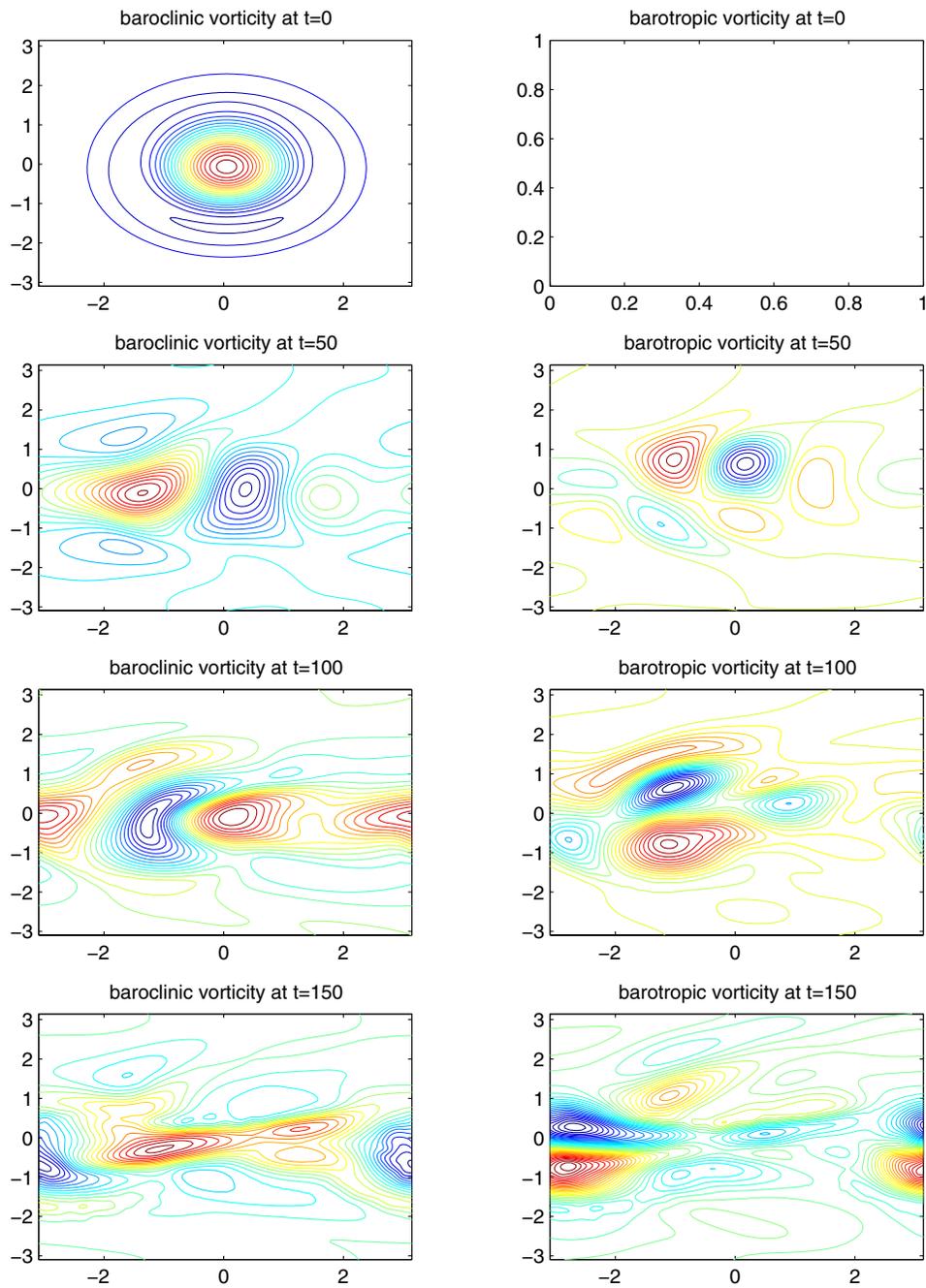


Figure 6.1. HPM simulation for shallow-water model with rigid lid. Top to bottom: time evolution of vorticity. Left: baroclinic vorticity. Right: barotropic vorticity.

- (i) particle motion in top layer,
- (ii) particle motion in bottom layer,
- (iii) baroclinic vorticity field,
- (iv) barotropic vorticity field.

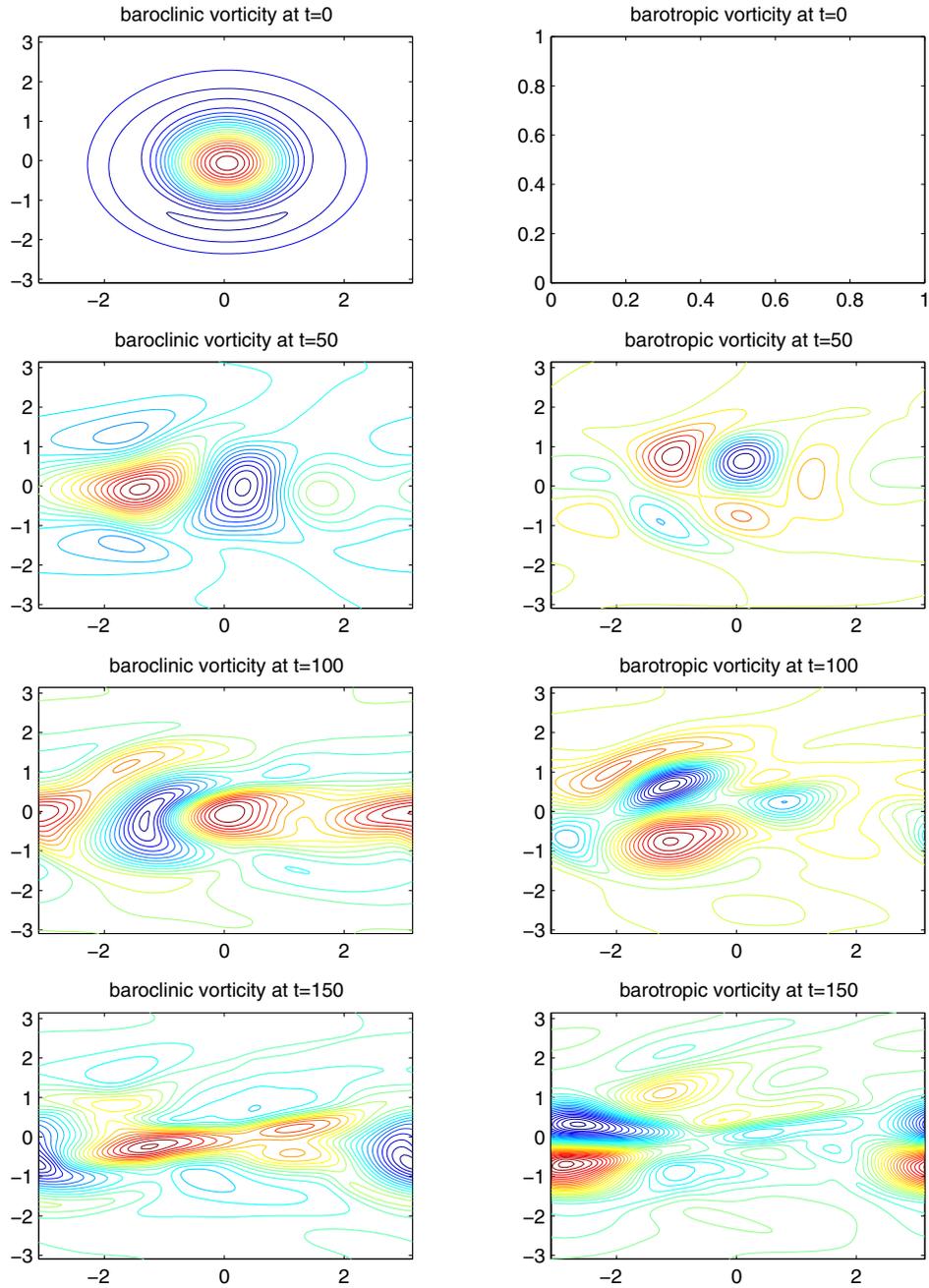


Figure 6.2. PS simulation for shallow-water model without rigid-lid. Top to bottom: time evolution of vorticity; left: baroclinic vorticity; right: barotropic vorticity.

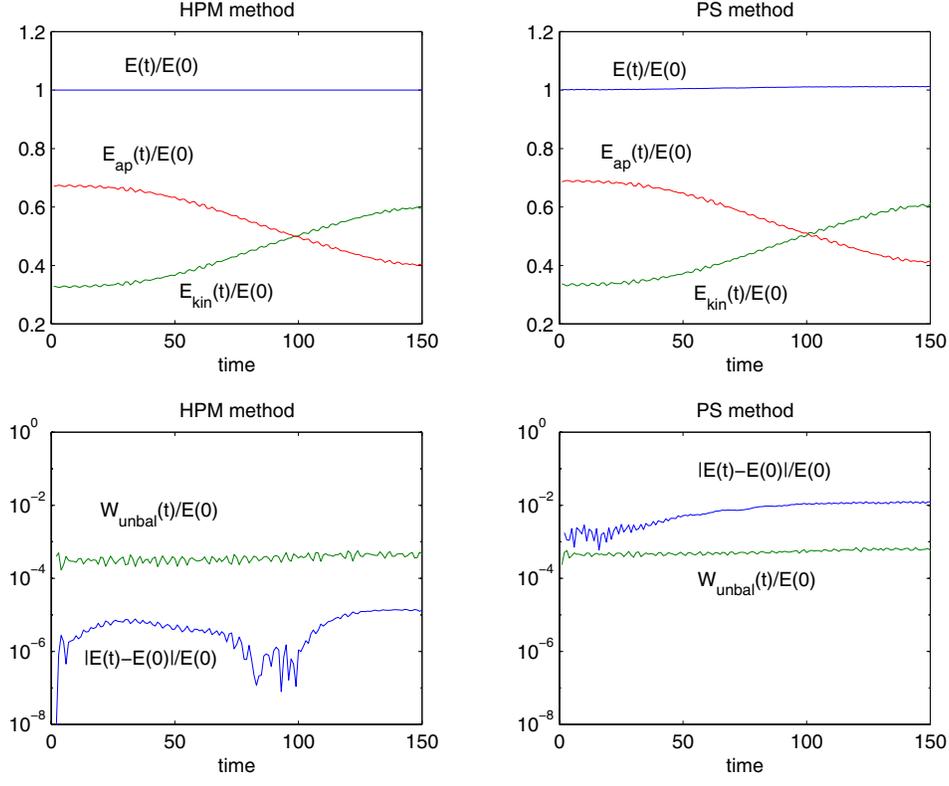


Figure 6.3. Diagnostic results.

A few diagnostic results for the rigid-lid and unconstrained simulations can be found in Figure 6.3. More specifically, let $E(t_n)$ denote the total energy of the PM model,

$$E_{\text{kin}}(t_n) \equiv \sum_{i=1}^2 \sum_{k=1}^N \frac{1}{2m_i^k} \mathbf{v}_i^k(t_n) \cdot \mathbf{v}_i^k(t_n)$$

its kinetic energy (KE), and

$$E_{\text{ap}}(t_n) \equiv \frac{c_0}{2} \sum_{p,q} \hat{h}_2^{pq}(t_n) [h_2^{pq}(t_n) - H_2]$$

its APE. For the incompressible rigid-lid model, we have $E(t_n) = E_{\text{kin}}(t_n) + E_{\text{ap}}(t_n)$. Up to a small potential energy contribution from the total layer-depth, this is essentially also true for the compressible two-layer model. We plot in Figure 6.3 the scaled quantities $E(t_n)/E(t_0)$, $E_{\text{kin}}(t_n)/E(t_0)$, and $E_{\text{ap}}(t_n)/E(t_0)$ with $t_0 = 0$. Furthermore, we also monitor the norm of the unbalanced baroclinic velocity contributions

$$W_{\text{unbal}}(t_n) \equiv \frac{1}{2} \|\Delta \mathbf{u}(t_n) - \Delta \mathbf{u}_{\text{thw}}(t_n)\|_2^2,$$

with $\Delta \mathbf{u}_{\text{thw}}$ defined by (5.1). Here all velocities are first approximated over the grid \mathbf{x}^{pq} , and then $\|\cdot\|_2$ is to be understood as the discrete l_2 -norm. The scaled variable $W_{\text{unbal}}(t_n)/E(t_0)$

and the numerically induced errors in total energy can be found in Figure 6.3. The quasi-conservation of balanced motion for both methods, as manifested by the very small ratio $W_{\text{unbal}}(t_n)/E(t_0)$, is particularly striking. The Rossby number for the simulation was $Ro \approx 0.1 - 0.2$. We also observe that the particle method conserves total energy much better than the semi-implicit PS method.

We would like to point out that the given initial purely baroclinic state is persistent in the absence of the β -plane effect. Hence the break-up of the initial state into baroclinic and barotropic motions is triggered by $\beta \neq 0$.

7. Conclusions. Three dominant themes within geophysical fluid dynamics are (i) conservation, (ii) model reduction, and (iii) multiscales. A simple model system that combines all three of these aspects is provided by the two-layer shallow-water equations. These equations are Hamiltonian, satisfy conservation laws of PV and circulation, and can be simplified by filtering out surface gravity waves via the rigid-lid approximation. Geostrophic balance is of utmost importance for the long-time solution behavior in a small Rossby number regime. In the present paper, we have demonstrated how these ideas and concepts can be filtered through to the level of numerical methods. The proposed discrete PM method is Hamiltonian and conserves circulation/PV along the lines of [8, 5]. Furthermore, symplectic time-stepping guarantees maintenance of geostrophic balance as an adiabatic invariant [19]. Finally, the rigid-lid approximation is implemented as a holonomic constraint which allows significant increases in the attainable time-steps. A coarse graining procedure has been implemented to keep the numerical pressure gradient sufficiently smooth. This technique appears to be related to regularization techniques discussed in [11].

We hope that the presented PM method can serve as a role model for further developments on more realistic model systems such as the primitive equations (see [21]).

REFERENCES

- [1] H. ANDERSEN, *Rattle: A ‘velocity’ version of the shake algorithm for molecular dynamics calculations*, J. Comput. Phys., 52 (1983), pp. 24–34.
- [2] V. ARNOLD, *Mathematical Methods of Classical Mechanics*, 2nd ed., Springer, New York, 1988.
- [3] G. BENETIN AND A. GIORGILLI, *On the Hamiltonian interpolation of near to the identity symplectic mappings with application to symplectic integration algorithms*, J. Statist. Phys., 74 (1994), pp. 1117–1143.
- [4] C. BIRDSALL AND A. LANGDON, *Plasma Physics via Computer Simulations*, McGraw-Hill, New York, 1981.
- [5] T. BRIDGES, P. HYDON, AND S. REICH, *Vorticity and Symplecticity in Lagrangian Fluid Dynamics*, Tech. report, University of Surrey, Guildford, 2002.
- [6] D. DURAN, *Numerical Methods for Wave Equations in Geophysical Fluid Dynamics*, Springer, New York, 1999.
- [7] J. FRANK, G. GOTTWALD, AND S. REICH, *The Hamiltonian particle-mesh method*, in Meshfree Methods for Partial Differential Equations, Lecture Notes in Comput. Sci. Engrg. 26, M. Griebel and M. Schweitzer, eds., Springer, Heidelberg, 2002, pp. 131–142.
- [8] J. FRANK AND S. REICH, *Conservation properties of smoothed particle hydrodynamics applied to the shallow-water equations*, BIT, 43 (2003), pp. 40–54.
- [9] E. HAIRER AND C. LUBICH, *The life-span of backward error analysis for numerical integrators*, Numer. Math., 76 (1997), pp. 441–462.

- [10] R. HOCKNEY AND J. EASTWOOD, *Computer Simulations Using Particles*, Institute of Physics, Philadelphia, 1988.
- [11] D. HOLM, *Fluctuation effects on 3D Lagrangian mean and Eulerian mean fluid motion*, Phys. D, 133 (1999), pp. 215–269.
- [12] D. HOLM, J. MARSDEN, AND T. RATIU, *Euler-Poincaré models of ideal fluids with nonlinear dispersion*, Phys. Rev. Lett., 80 (1998), pp. 4173–4177.
- [13] L. JAY, *Symplectic partitioned Runge–Kutta methods for constrained Hamiltonian systems*, SIAM J. Numer. Anal., 33 (1996), pp. 368–387.
- [14] A. LANGDON, *Energy-conserving plasma simulation algorithms*, J. Comput. Phys., 12 (1973), pp. 247–268.
- [15] B. LEIMKUEHLER AND R. SKEEL, *Symplectic numerical integrators in constrained Hamiltonian systems*, J. Comput. Phys., 112 (1994), pp. 117–125.
- [16] H. LEWIS, *Energy-conserving numerical approximations for Vlasov plasmas*, J. Comput. Phys., 6 (1970), pp. 136–141.
- [17] S. REICH, *Symplectic integration of constrained Hamiltonian systems by composition methods*, SIAM J. Numer. Anal., 33 (1996), pp. 475–491.
- [18] S. REICH, *Backward error analysis for numerical integrators*, SIAM J. Numer. Anal., 36 (1999), pp. 1549–1570.
- [19] S. REICH, *Conservation of adiabatic invariants under symplectic discretization*, Appl. Numer. Math., 29 (1999), pp. 45–55.
- [20] J. RYCKAERT, G. CICCOTTI, AND H. BERENDSEN, *Numerical integration of the Cartesian equations of motion of a system with constraints: Molecular dynamics of n-alkanes*, J. Comput. Phys., 23 (1977), pp. 327–341.
- [21] R. SALMON, *Geophysical Fluid Dynamics*, Oxford University Press, Oxford, UK, 1999.
- [22] J. SANZ-SERNA AND M. CALVO, *Numerical Hamiltonian Problems*, Chapman & Hall, London, 1994.
- [23] R. SHAPIRO, *Smoothing, filtering and boundary effects*, Rev. Geophys. Space Phys., 8 (1970), pp. 359–387.