

Imperial College
London

Geometric Numerical Methods for Numerical Weather Prediction

The Hamiltonian Particle-Mesh Method^a

Matthew Dixon, Colin Cotter and Sebastian Reich

Department of Mathematics, Imperial College, London

matthew.dixon@imperial.ac.uk

^a M.F.Dixon and S.Reich, Symplectic Time-Stepping for Particle Methods, GAMM, Berlin 27 (2004) N. 1, pp. 9–24
M.F.Dixon and C.Cotter, A Hamiltonian Particle-Mesh Method for Shallow Water in a Bounded Domain, in preparation.

Overview

- The Lagrangian description of shallow water
- Hamiltonian particle-mesh approximation of the shallow water equations
- Boundary conditions
- Numerical experiments of 1D and 2D shallow water flow in a channel

The Lagrangian description of fluid

- The forward map $X(\ell, t)$ is a diffeomorphism from the fluid reference space F to the fluid container C , where $X(\ell, 0) = \ell$ and ℓ is a fluid particle label.

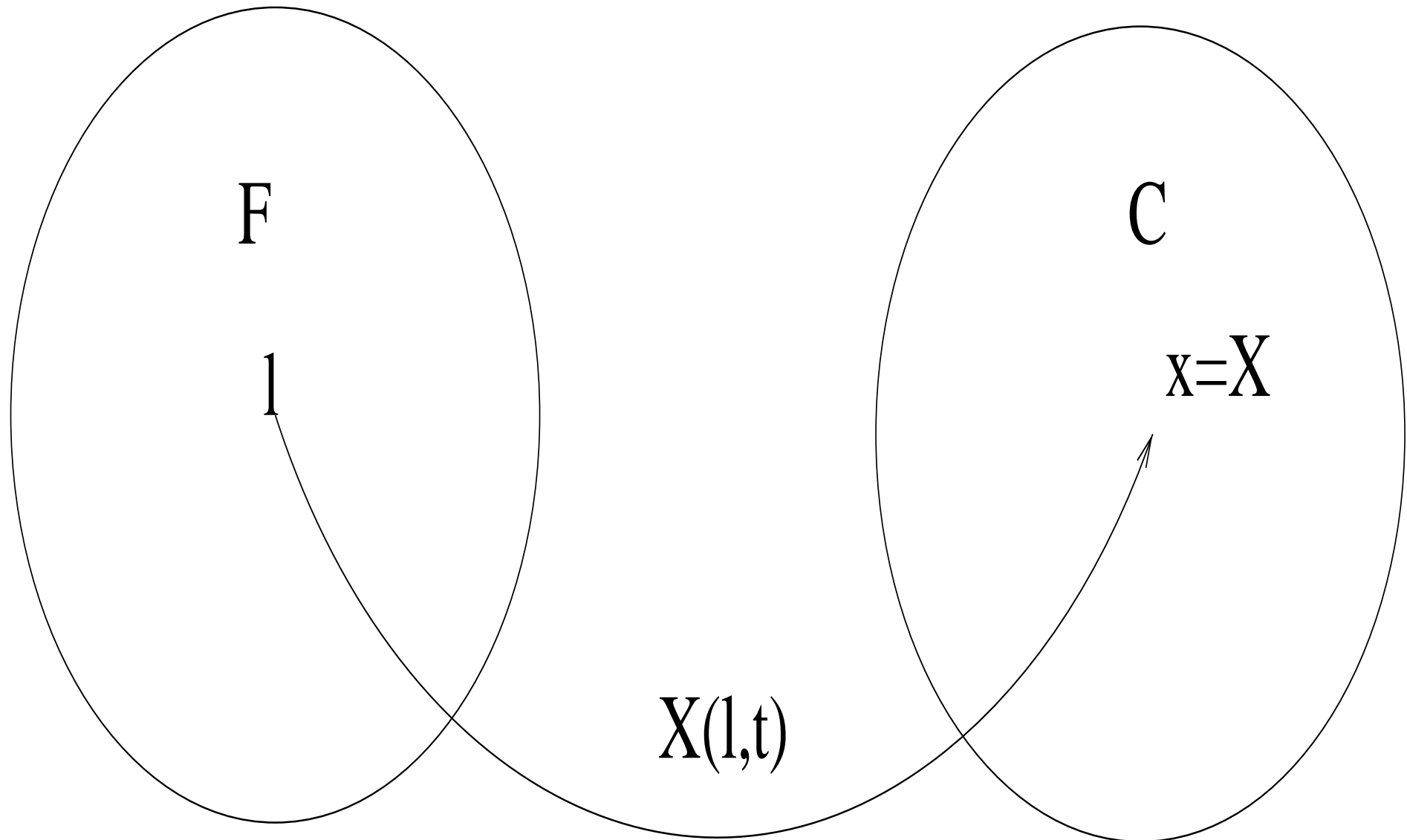
-

$$\dot{\mathbf{U}}(\ell, t) = \mathbf{F}, \text{ momentum equation}$$

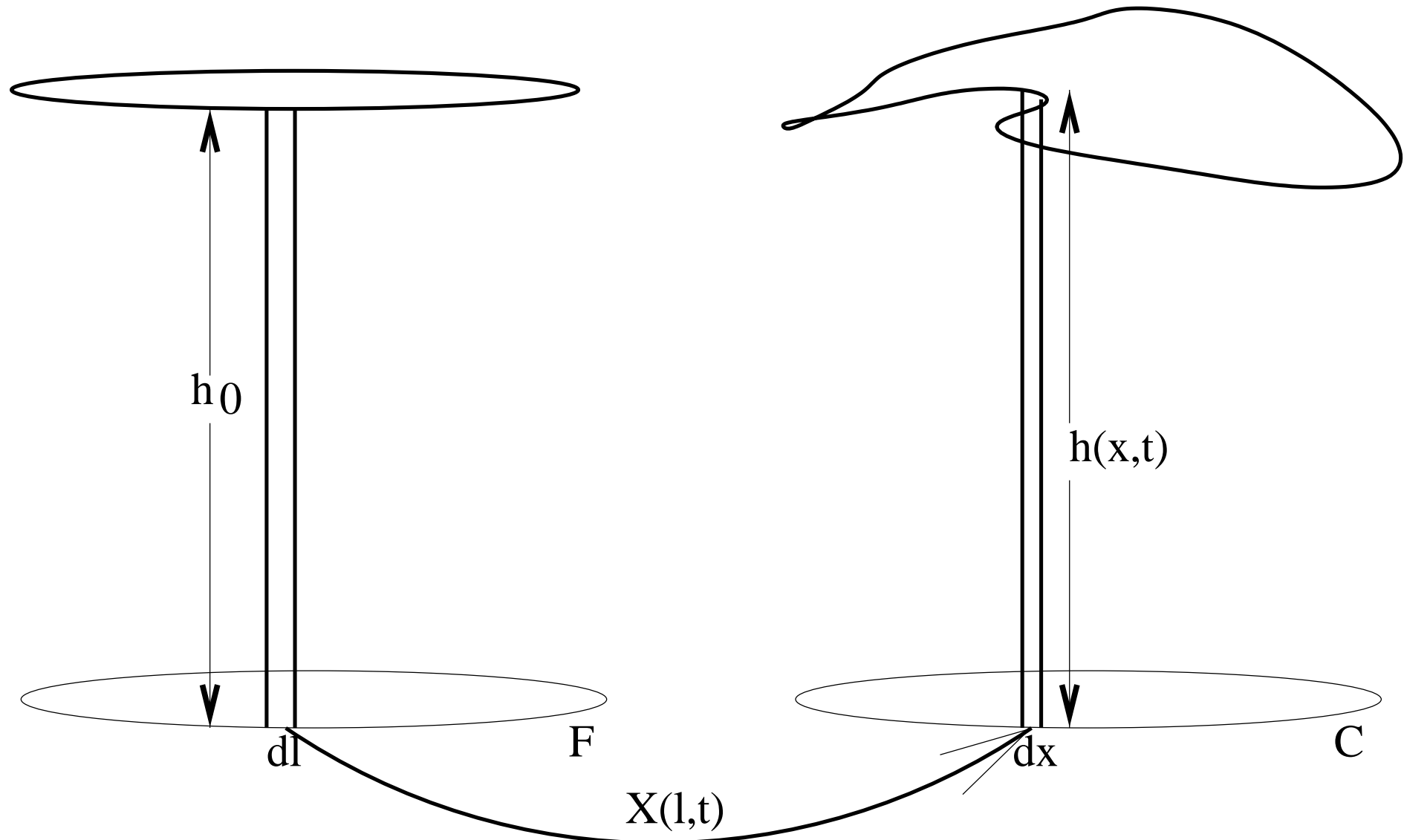
$$\dot{\mathbf{X}}(\ell, t) = \mathbf{U}, \text{ kinematic relation}$$

- $U(\ell, t)$ is the Lagrangian velocity, the tangent vector at $X(\ell, t)$ keeping the fluid label ℓ fixed.
- The Eulerian velocity $u(x, t)$ is equal to the time derivative of the forward map $u(X(\ell, t), t) := U(\ell, t) := \dot{X}(\ell, t) =: \dot{X}(t)$ at fixed $x = X(\ell, t)$.

The forward map



The Lagrangian Description of Shallow Water



The Lagrangian description of 1D shallow water on a periodic domain

- Consider the fluid container $C \equiv \Omega \equiv S^1$, the circle with circumference of length L
- The equilibrium or reference layer depth $h_0(\ell)$ is a time independent field defined on $F \equiv S^1$.
- The scaled Jacobian of the forward map
$$J = \rho_0 \frac{\partial X}{\partial \ell} = h_0(\ell) h(X(\ell, t), t)^{-1}.$$
- The Eulerian layer depth and velocity field $h(x, t)$ and $u(x, t)$ is defined on $C \times \mathbb{R}^+$.

The Euler-Lagrange shallow water equations

- The 1D Euler-Lagrange equations for shallow water motion on the velocity phase space TS^1 are

$$\dot{U} = \frac{g\rho_0^2 h_0}{J^3} \frac{\partial^2 X}{\partial \ell^2} = -g \frac{\partial h}{\partial X},$$
$$\dot{X} = U.$$

The Hamiltonian Particle-Mesh (HPM) Method

- Label space is discretised into N particles with coordinates on the momentum phase space $T^*S^1 \subseteq \mathbb{R}^2$

$$(\mathbf{X}^T, \mathbf{P}^T) = ([X_1, X_\alpha, \dots, X_N]^T, [P_1, P_\alpha, \dots, P_N]^T).$$

- Define a mesh $\Omega^h = \{x_i, x_i = (i\Delta x), i \in [0, n - 1]\}$, $\Omega^h \subseteq \Omega$ with node index i .
- Define the meshed layer depth $h_i = \sum_{\alpha=1}^N \frac{m_\alpha}{\gamma} \phi_i(X_\alpha) \Delta l$ where $\gamma = \int_{\Omega} \phi_i(x) dx$ and the basis functions $\phi_i(X_\alpha) \equiv \phi(x_i - X_\alpha)$ form a partition of unity, $\sum_i \phi_i(x) = 1$.
- $\tilde{h}_i = S_{ij} h_j$ and $S_{ij} = (1 - \hat{\alpha}^2 \delta_{xx})^{-1}$.

HPM Equations of shallow water motions

- The canonical HPM equations of 1D shallow water motion on T^*S^1 are

$$\dot{P}_\alpha = -\frac{c_0^2 m_\alpha}{\gamma} \sum_i \tilde{h}_i(t) \nabla_{X_\alpha} \phi_i(X_\alpha),$$

$$\dot{X}_\alpha = \frac{P_\alpha}{m_\alpha},$$

- with Hamiltonian

$$\mathcal{H} = \underbrace{\frac{1}{2} \sum_\alpha \frac{P_\alpha(t)^2}{m_\alpha}}_T + \underbrace{\frac{c_0^2}{2} \sum_i h_i(t) \tilde{h}_i(t)}_V. \quad (1)$$

Definition of a Symplectic Integrator

- Define the discrete flow map on momentum phase space $\mathbf{Z}^{n+1} = \Phi_{\Delta t}(\mathbf{Z}^n)$, where $\mathbf{Z}^n := [P^n \ X^n]^T$.
- The momentum phase space T^*S^1 is a symplectic manifold (\mathbf{M}, ω) , $\mathbf{M} \subseteq \mathbb{R}^2$ with symplectic two-form $\omega = dP \wedge dX$
- A symplectic integrator is a discrete flow map that is symplectic, that is $dP^{n+1} \wedge dX^{n+1} = dP^n \wedge dX^n$.

First order symplectic integrators

- the first order accurate Euler-A method,

$$X^{n+1} = X^n + \Delta t \mathcal{H}_P(P^n, X^{n+1})$$

$$P^{n+1} = P^n - \Delta t \mathcal{H}_X(P^n, X^{n+1})$$

- the first order accurate Euler-B method,

$$X^{n+1} = X^n + \Delta t \mathcal{H}_P(P^{n+1}, X^n)$$

$$P^{n+1} = P^n - \Delta t \mathcal{H}_X(P^{n+1}, X^n)$$

Second order Symplectic integrators

- the composite of half-step Euler-A and half-step Euler-B : second order accurate Störmer Verlet method,

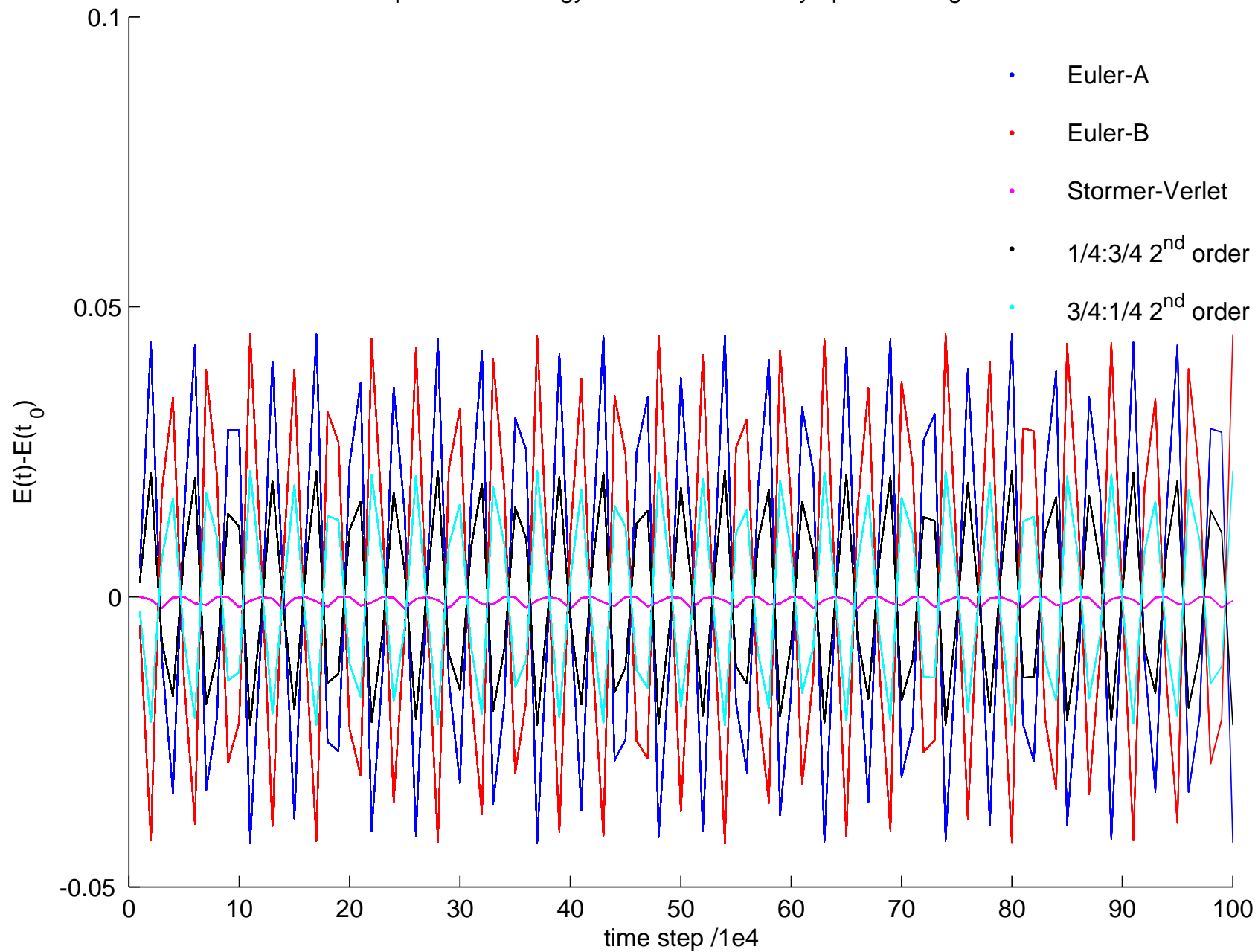
$$P^{(n+\frac{1}{2})} = P^n - \frac{\Delta t}{2} \mathcal{H}_X(P^n, X^n)$$

$$X^{n+1} = X^n + \Delta t \mathcal{H}_P(P^{(n+\frac{1}{2})}, X^n)$$

$$P^{n+1} = P^{(n+\frac{1}{2})} - \frac{\Delta t}{2} \mathcal{H}_X(P^{(n+\frac{1}{2})}, X^{n+1})$$

- the composite of quarter-step Euler-A and three-quarter-step Euler-B and
- the composite of three-quarter-step Euler-A and quarter-step Euler-B.

Comparison of energy errors for various symplectic integrators



Symplectic integration of the HPM shallow water equations

- The Störmer-Verlet method is a symplectic 2^{nd} order integrator.
- The Störmer-Verlet integration of the HPM equations of motion is

$$X_{\alpha}^{n+1} = X_{\alpha}^n + \Delta t \frac{P_{\alpha}^{n+\frac{1}{2}}}{m_{\alpha}},$$
$$P_{\alpha}^{n+\frac{1}{2}} = P_{\alpha}^n - \frac{\Delta t}{2} \nabla_{X_{\alpha}} V(X_{\alpha}^n),$$
$$P_{\alpha}^{n+1} = P_{\alpha}^{n+\frac{1}{2}} - \frac{\Delta t}{2} \nabla_{X_{\alpha}} V(X_{\alpha}^{n+1}).$$

- The Störmer-Verlet method preserves the symplectic two-form $w = \sum_{\alpha=1}^N \sum_{i=1}^d dX_{\alpha}^i \wedge dP_{\alpha}^i$.

Boundary Conditions

- Dirichlet boundary conditions on the velocity field

$$u(x, t) = 0, \quad x \in \partial\Omega \equiv \{0, L\}.$$

- Impose kinematic boundary conditions on static particles initially assigned to the boundaries

$$\dot{U}_\alpha = -c_0^2 \sum_{i \in \hat{I}} h_i \nabla_{X_\alpha} \psi_i(X_\alpha) = 0, \quad \alpha \in \{1, N\},$$

$$X_1(t_0) = 0, \quad X_N(t_0) = L, \quad U_\alpha(t_0) = 0, \quad \alpha \in \{1, N\}.$$

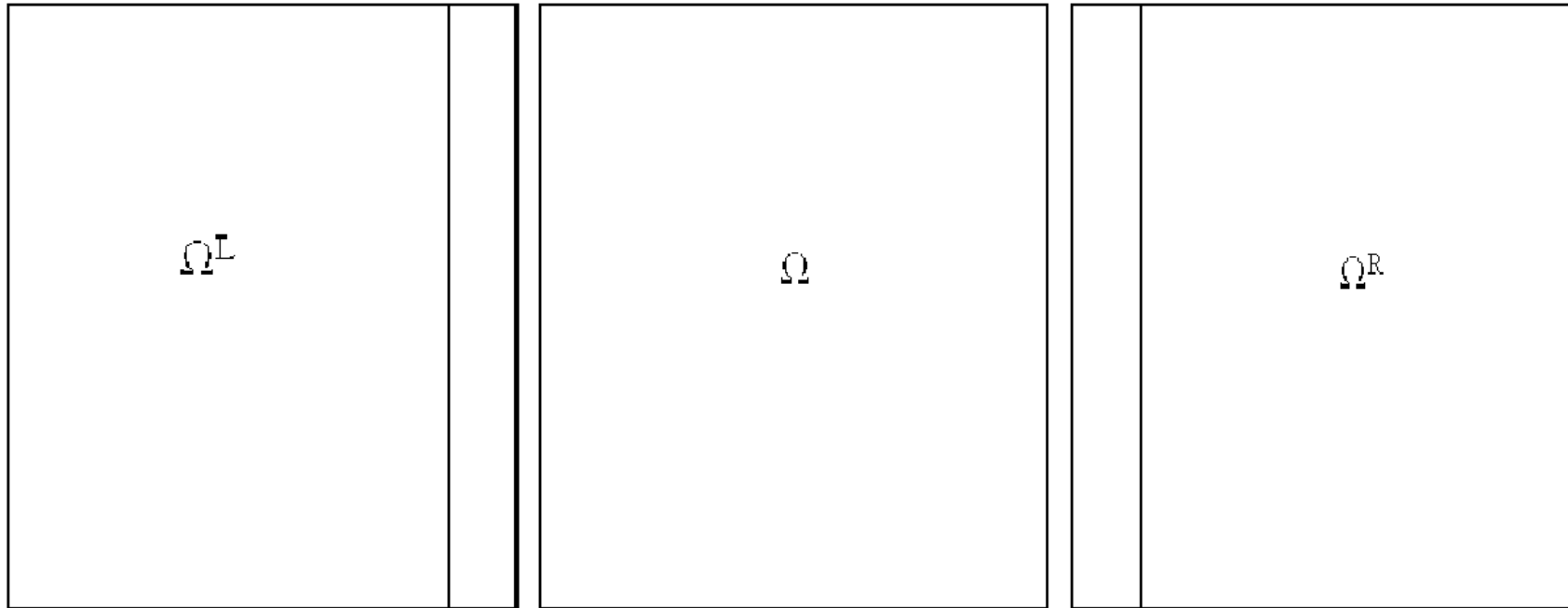
- Define the boundaries as pointwise symmetries.
- Image particles on velocity phase space $(-X_\alpha, -U_\alpha)$ and $(2L - X_\alpha, -U_\alpha)$.
- This symmetry condition implies pointwise symmetry in the layer depth.

$i=-n+1$

$i=-1$ $i=0$

$i=n-1$ $i=n$

$i=2(n-1)$



$k=-N$

$k=1$

$k=N$

$k=2N-1$

Smoothing on a Bounded 1D Domain

- The smoothed layer depth $\tilde{h} = S^x h$, where S^x is an inverse Helmholtz matrix.
- Impose a Neumann boundary condition $\mathbf{n} \cdot \nabla \tilde{h} = 0$.
- Formulate a finite element approximation

$$Mh = A\tilde{h} \Rightarrow S^x = A^{-1}M.$$

Smoothing on a 2D Periodic channel

- Smoothing can be extended to a periodic 2D channel

$$\hat{\hat{H}} = \hat{S}^y \widehat{H} \widehat{S}^x.$$

where H is a layer depth matrix and S^y is a 1D spectral approximation of the inverse Helmholtz operator.

Numerical Experiments: 1D shallow water in a tank

- Initial conditions $\{U_\alpha\} = 0$ and

$$m_\alpha = 1 + a_0 \exp(-50((X - L/2)^2)/L^2)$$

- $N=256$ particles, $n=64$ grid points, $a_0 = 5e - 3$, $\hat{\alpha} = 2\Delta x$ and $\Delta t = 0.005$.

Numerical results: 1D shallow water in a tank

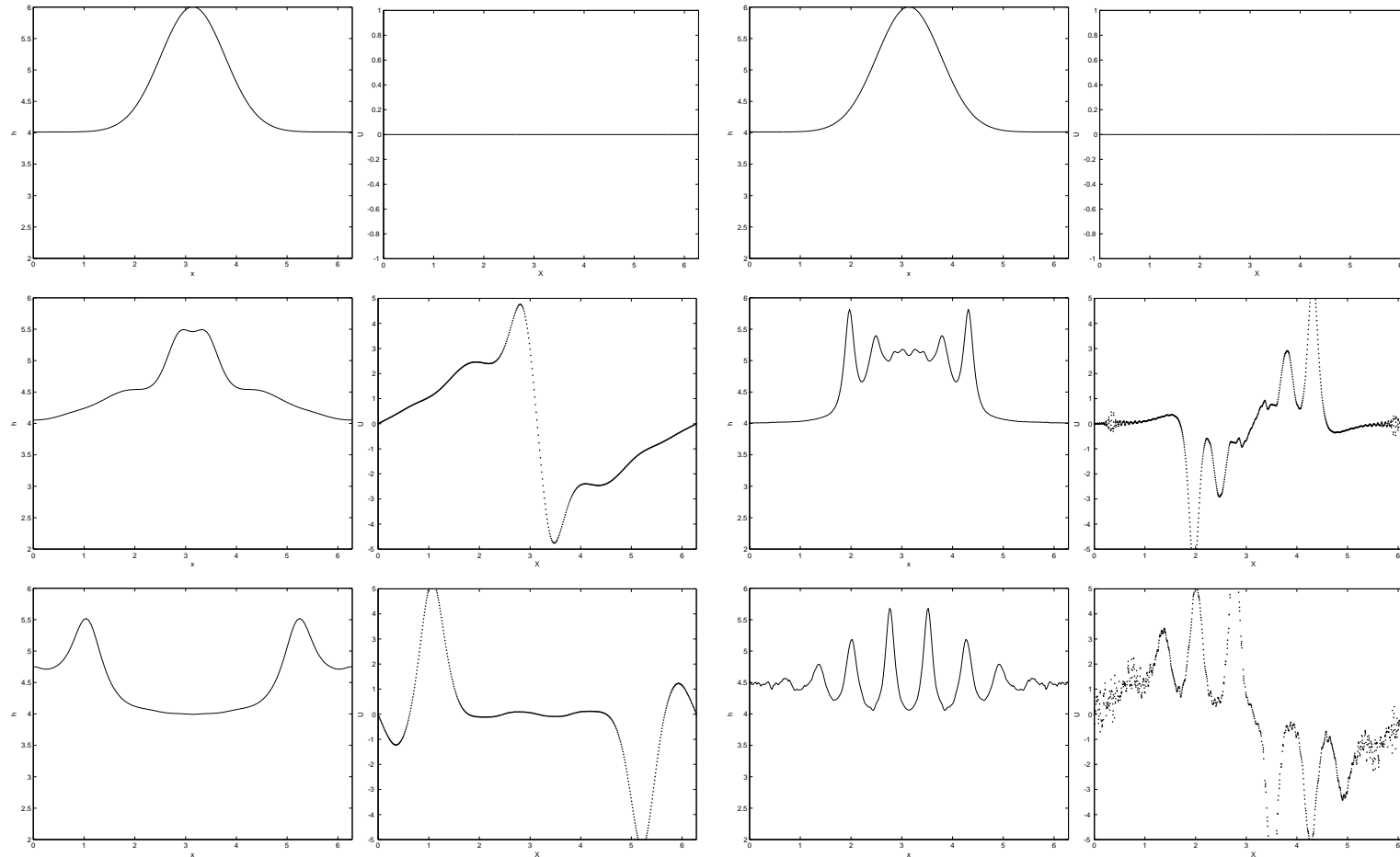


Figure 1: (far left) FEM smoothed h and (center left) u ; (center right) FD smoothed h and (far right) u . Each row is at time $t = \{0, 50, 100\}\Delta t$

Numerical results: 1D shallow water in a tank

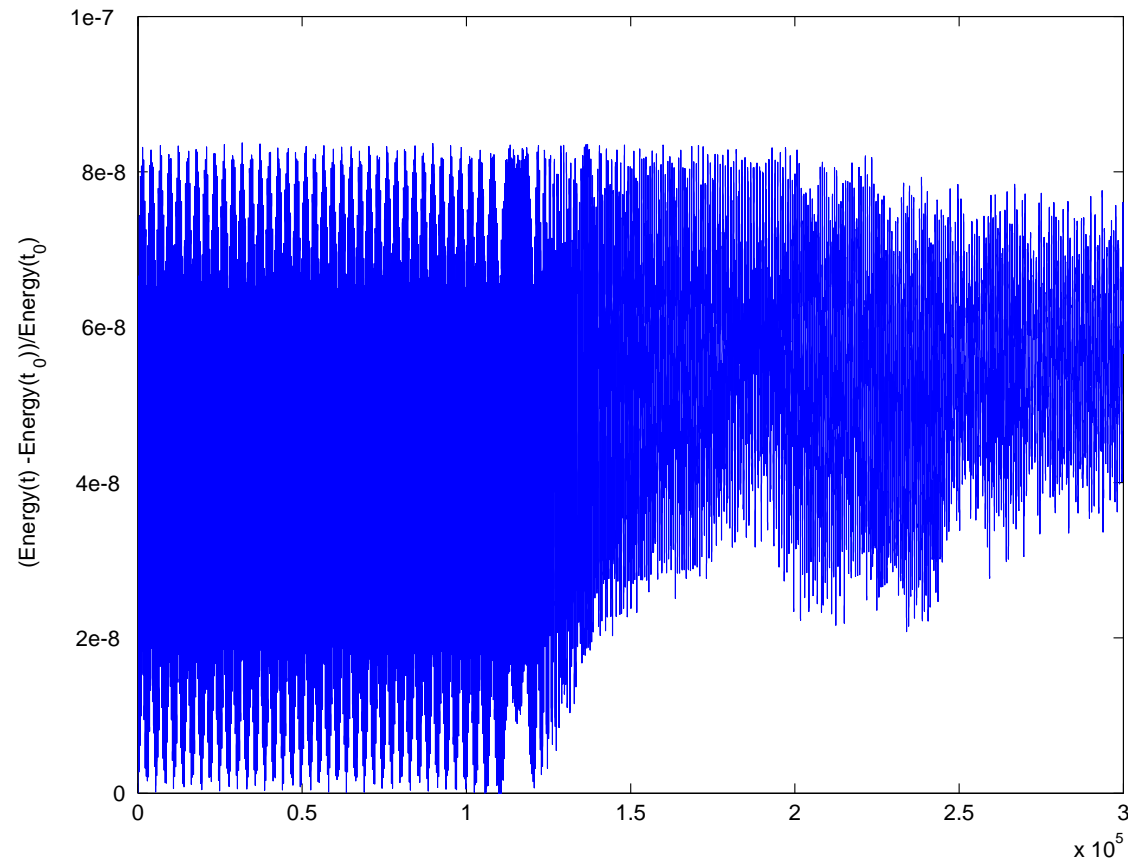


Figure 2: Relative energy error against time.

Numerical Experiments: 2D shallow water in a channel

- Initial conditions $\{U_\alpha\} = 0$, $\{V_\alpha\} = 1$ and

$$m_\alpha = 1 + a_0 \exp(-800[(X_\alpha(t_0) - L/2)^2 + (Y_\alpha(t_0) - L/2)^2]/L^2).$$

- $N= 256$ particles, $n=64$ grid points, $a_0 = 0.5$, $\hat{\alpha} = 2\Delta x$ and $dt = 5e - 4$

Numerical results: 2D Shallow water in a channel

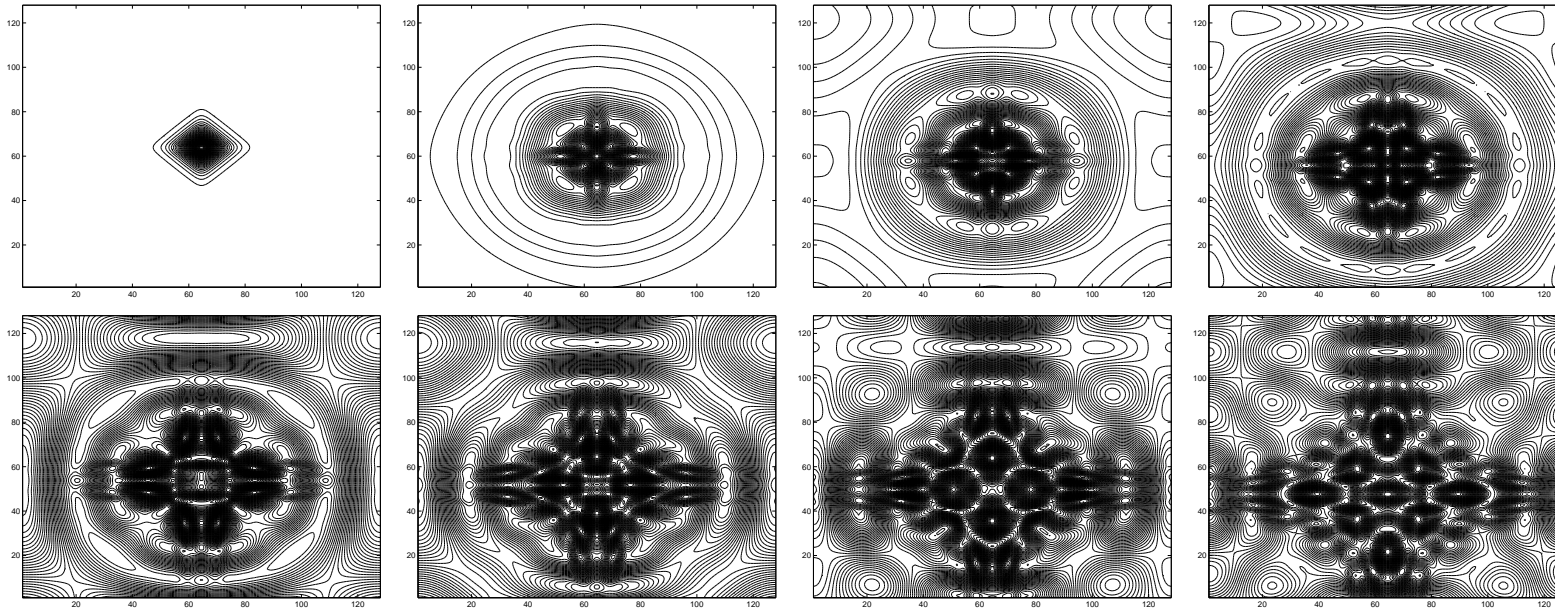


Figure 3: Layer depth of shallow water in a periodic channel.

Numerical results: boundary condition at the channel wall

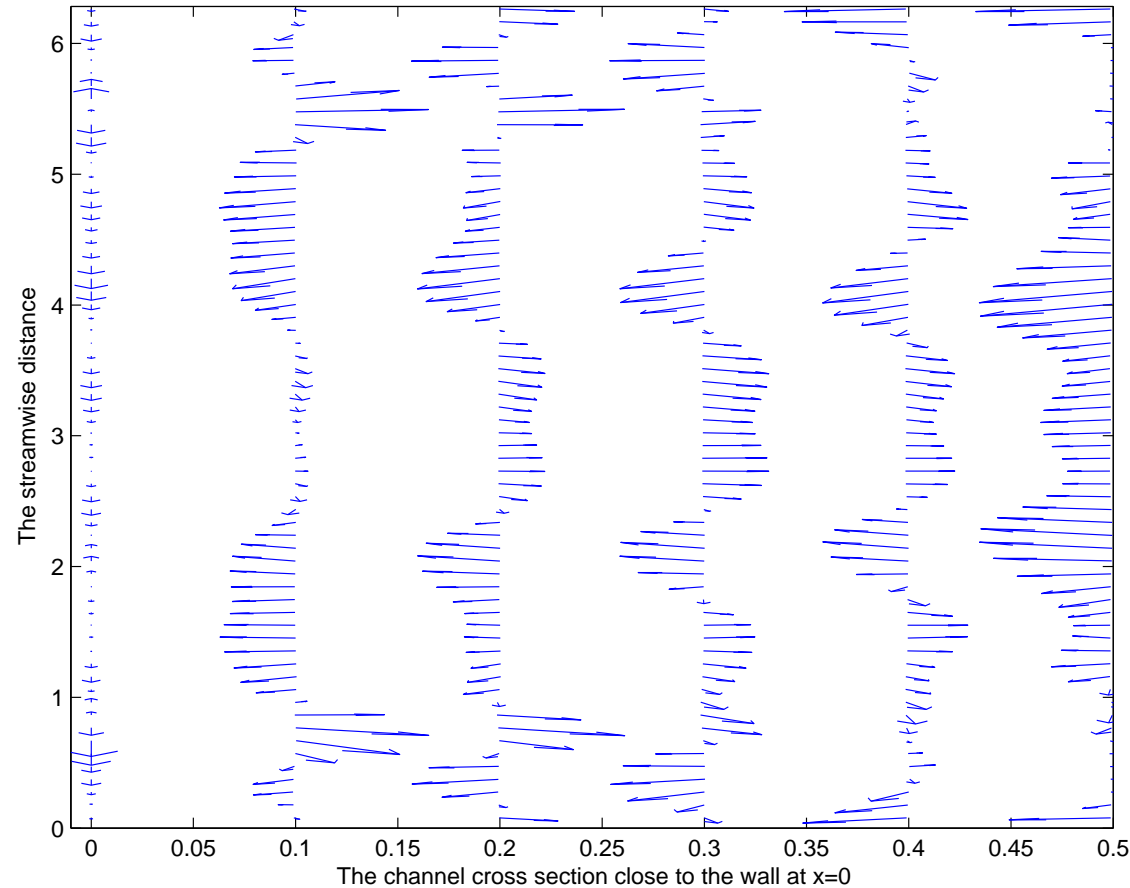


Figure 4: A vector plot of the velocity field of a region close to a planar channel wall.

Numerical results: comparison with a spectral-chebyshev method

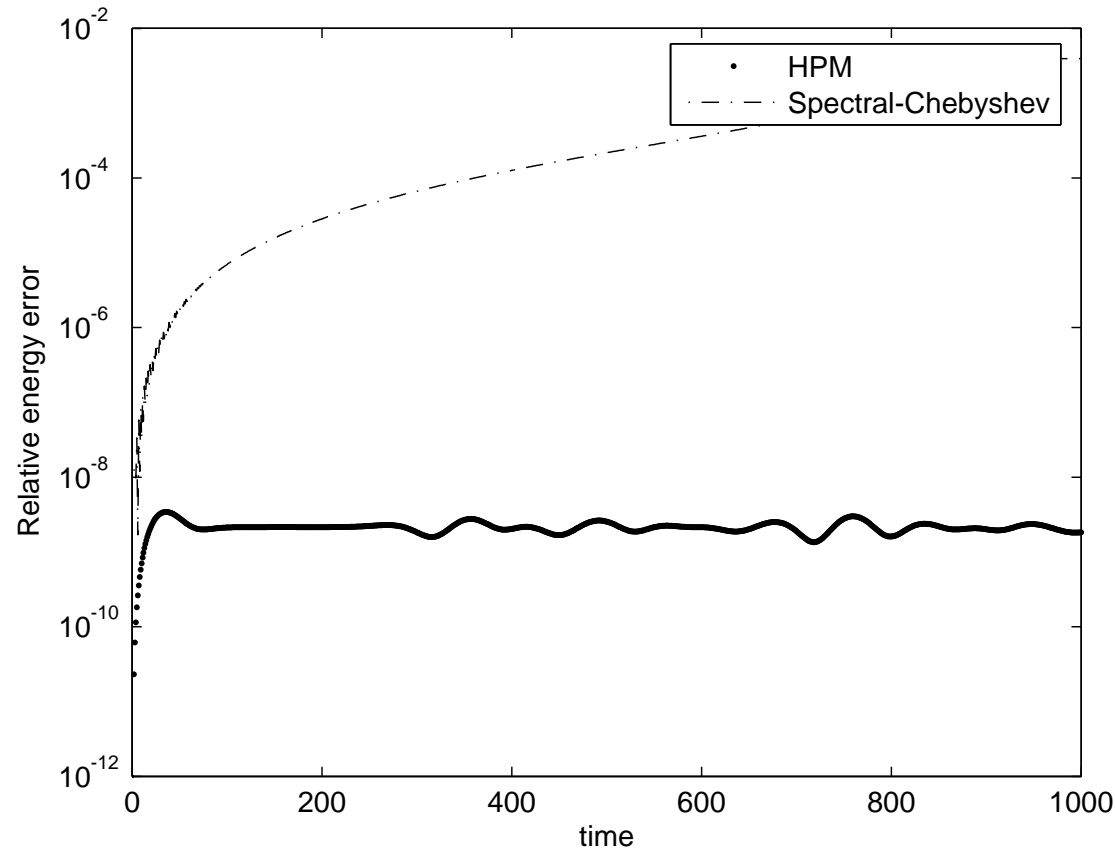


Figure 5: Relative energy error against the number of time steps.

Numerical results: comparison with a spectral-chebyshev method

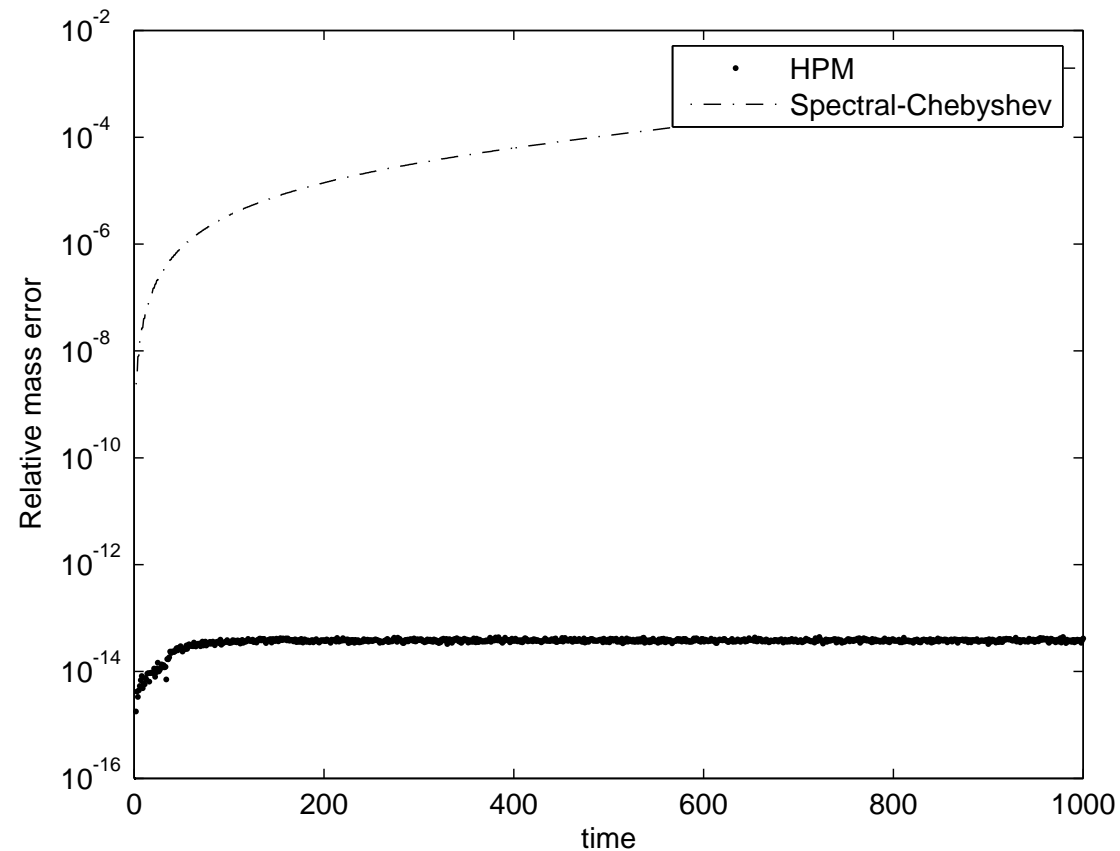


Figure 6: Relative mass error against the number of time steps.

Summary

- The HPM method approximates the regularised continuum flow with a semi-discrete finite dimensional Hamiltonian flow
- A Störmer-Verlet method is used to integrate the finite dimensional system of Hamiltonian ODEs
- Dirichlet velocity boundary conditions are implemented in the HPM method with image particles
- Neumann boundaries conditions are imposed naturally on the smoothed layer depth by a finite element approximation of a dispersive smoothing operator
- Numerical experiments show the conservative properties of the HPM approximation of 2D shallow water in a channel are vastly superior to a Spectral-Chebyshev method.

When is the shallow water model useful for weather prediction?

- When the fluid is in hydrostatic balance, that is the vertical pressure gradient $\frac{\partial p}{\partial z} = -\rho g$.
- When the aspect ratio is small, i.e. the fluid depth is small compared to the horizontal length scale of motion.
- When the fluid is incompressible and inviscid.