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Citation: AIP Conference Proceedings **1281**, 1667 (2010); doi: 10.1063/1.3498156
View online: http://dx.doi.org/10.1063/1.3498156
View Table of Contents: http://scitation.aip.org/content/aip/proceeding/aipcp/1281?ver=pdfcov
Published by the AIP Publishing

A Parallel Communication Structure for the Multilayer Shallow Water Equations

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Abstract. We propose a horizontal discretization of the multilayer shallow water equations by the Hamiltonian particle mesh method. The equations of motion are derived by Hamiltons principle applied to the discrete energies. The structure of the particle mesh method allows a convenient parallelization. There is no communication between particles in different layers, only the data on the Eulerian mesh have to be communicated. A straightforward parallelization results in a broadcast of all layer heights. This is circumvented by a butterfly-type communication structure to keep communication at $\mathcal{O}(\log N)$, N being the number of layers.

Keywords: shallow water equations, particle methods, parallel algorithms
PACS: 65M75, 76B15, 68W10

THE MULTILAYER SHALLOW WATER EQUATIONS

In geophysical processes, hydrostatic balance plays an important role for the dynamics of air and water. The strongly stratified atmospheric flow suggests using a layer model. We assume here that flow proceeds in layers of constant density, thus relative volume $\alpha = 1/\rho$ serves as a monotonically increasing vertical coordinate - the isopycnal coordinate. For a discussion of different vertical coordinate systems, see [1], [2] [3] or [4]. In order to derive the balance law for mass, a corresponding density η is defined via $\rho dz = \eta d\alpha$. Together with hydrostatic balance we obtain in vertical columns

$$\frac{\partial z}{\partial \alpha} = \alpha\eta, \qquad \frac{\partial \Phi}{\partial \alpha} = p, \qquad \frac{\partial p}{\partial \alpha} = -g\eta. \tag{1}$$

The geophysical height z, pressure p and the Potential Φ of isopycnal motion are obtained by integration if the modified density η is known and appropriate boundary conditions on top and bottom of the model are provided. At the bottom geophysical height z_B is fixed: $\Phi - \alpha\Phi_\alpha = gz_B$. A typical boundary conditions on top is the rigid lid approach where height at the surface z_T is prescribed: $\Phi + \alpha\Phi_\alpha = gz_T$. A free surface requires pressure p_T on top to be described, where the corresponding boundary condition is $\Phi_\alpha = p_T$. The potential Φ is equivalently given by

$$\Phi = gz + p\alpha \text{ or} \qquad \frac{\partial^2 \Phi}{\partial \alpha^2} = -g\eta. \tag{2}$$

Note, that the gradient evaluates to the sum of the gradient of geopotential (potential for vertical p-coordinate) and the gradient of the potential in z-coordinates.

The dynamics of motion are described by the balance laws of momentum and mass in a rotating coordinate system

$$\frac{D}{Dt}u - fv = -\Phi_x \tag{3}$$

$$\frac{D}{Dt}v + fu = -\Phi_y, \tag{4}$$

$$\frac{D}{Dt}\eta + \eta\nabla\cdot\mathbf{u} = 0 \tag{5}$$

where $\mathbf{u} = (u,v)^T$ are the velocities, $f = 2\Omega$ is the Coriolis parameter where Ω is the angular velocity. In this presentation we use an f-plane setting, i.e. f is assumed to be constant.

In the multilayer shallow water equations fluid motion is approximated by a finite number of horizontal layers of constant density. Euklidean coordinates in the layer are $\mathbf{x} = (x,y)^T$, the quantities $\eta, \mathbf{u}$ are assumed to be independent

CP1281, *ICNAAM, Numerical Analysis and Applied Mathematics, International Conference 2010, Vol. III*
edited by T. E. Simos, G. Psihoyios, and Ch. Tsitouras

of α in each layer. The modified density η is replaced by the more meaningful layer height $h = \Delta z = \eta\alpha\Delta\alpha$ which obeys the same conservation law.

We use N layers, layer 1 being the top layer. Layer i has fixed density $\rho_i = 1/\alpha_i$. Physical upper, lower z-coordinates are $Z_{i-1/2}(t,\mathbf{x})andZ_{i+1/2}(t,\mathbf{x})$, layer height is denoted by $h_i = Z_{i-1/2} - Z_{i+1/2}$, average height is $Z_i := (Z_{i-1/2}+Z_{i+1/2})/2$. Bottom height (orography) is given by $Z_{N+1/2}(t,\mathbf{x}) = z_B(\mathbf{x})$, and whenever top height is prescribed we have $Z_{1/2}(t,\mathbf{x}) = z_T(t,\mathbf{x})$.

The multilayer shallow water equations are given by

$$\frac{D}{Dt}u_i - fv_i = -\frac{\partial}{\partial x}\Phi_i \tag{6}$$

$$\frac{D}{Dt}v_i + fu_i = -\frac{\partial}{\partial y}\Phi_i \tag{7}$$

$$\frac{D}{Dt}h_i + h_i\nabla\cdot\mathbf{u}_i = 0 \tag{8}$$

$$\Phi_i = gz_B + g\sum_{j=1}^{N}\min(1,\rho_j/\rho_i)h_j + p_T/\rho_i. \tag{9}$$

The orography value z_B is incorporated in the Potential Φ. The boundary conditions on top are applied as follows: For a free surface we have p_T prescribed. For the rigid lid setting, an additional constraint $\sum_i h_i = \text{const}$ serves to determine the unknown value p_T.

A HAMILTONIAN APPROACH TO FLUID MOTION

The equations of motion can be derived from the principle of least action (Hamiltons principle). The state variables are particle positions $\mathbf{X}$ – from these state variables we can derive density η or layer height h_i, kinetic energy E_{Kin} and potential energy E_{Pot} of the model. The Lagrangian $L = E_{\text{Kin}} - E_{\text{Pot}}$ is set up and the equations of motion are derived from the variational principle of least action

$$\delta\int_{t_0}^{t_e} L\,dt = 0. \tag{10}$$

This procedure can be applied for the vertically continuous system (3), (4), (5) as well as for the vertically discrete system (6), (7), (8). The Hamiltonian particle-mesh method [5] is obtained when this principle is applied to a particle-mesh discretization in the horizontal. Thus, a finite number of particles in a finite number of layers is utilized as a spatial discretization that describes the state of the system. Expressions for kinetic and potential energy are derived, the principle of least action is applied to derive an ODE for the particle positions.

HORIZONTAL DISCRETIZATION

The particle-mesh method (see [5]) is based on layer depth values $h_{i,mn}$ on an Eulerian grid with grid points $\mathbf{x}_{mn}$ and particles in layer i with position $\mathbf{a}_k$ at time $t = 0$ and position $\mathbf{X}_{i,k}(t)$ at time t. For sake of completeness, we repeat the crucial ingredients here.

In order to distinguish between particle departure points $\mathbf{a}$ and their actual positions $\mathbf{X}$, we denote the space of the departure points by L (the Label space) and the space of the actual positions by R (the Eulerian space), although both spaces coincide for various settings, especially on closed spatial domains like the sphere or periodic channels.

Denote the layer height in layer i at $t = 0$ by $h_{i,0}$. The particle-mesh method is based on the Lagrangian formulation of the balance of mass

$$h_{i,mn}(t) = = \int_L h_{0,i}(\mathbf{a})\delta(\mathbf{x}_{mn} - X_i(t,\mathbf{a}))d\mathbf{a}. \tag{11}$$

Thus, we need an integration formula on the label space and an approximation of the Dirac-δ function. From $h_{i,mn}(t)$ the potential $\Phi_{i,mn}$ at the Eulerian grid points is evaluated. An interpolation procedure extends Φ_{mn} to the space R, where its gradient at the particle positions can be evaluated.

In Eulerian space interpolation and integration is based on a partition of unity $N_{mn}(\mathbf{x})$ to extend grid values f_{mn} to the Eulerian space R:

$$f(\mathbf{x}) = \sum_{mn} f_{mn} N_{mn}(\mathbf{x}), \qquad \int_R f_{mn} := \int_R f(\mathbf{x}) d\mathbf{x} = \sum_{mn} \gamma_{mn} f_{mn} \text{ where } \gamma_{mn} := \int_R N_{mn}(\mathbf{x}) d\mathbf{x}. \tag{12}$$

In Lagrangian space we use a partition of unity $\hat{N}_k(\mathbf{a})$ based on the the departure points $\mathbf{a}_k$ of the particles to derive similar formulas for particle functions f_k:

$$f(\mathbf{a}) = \sum_k f_k \hat{N}_k(\mathbf{a}), \qquad \int_L f_k \approx \sum_k \hat{\gamma}_k f_k \text{ where } \hat{\gamma}_k := \int_L \hat{N}_k(\mathbf{a}) d\mathbf{a}. \tag{13}$$

Finally, we approximate the delta-function centered in $\mathbf{x}_{mn}$ by

$$\delta(\mathbf{x} - \mathbf{x}_{mn}) \approx \Psi_{mn}(\mathbf{x}) := \frac{1}{\gamma_{mn}} N_{mn}(\mathbf{x}) \tag{14}$$

We apply our discretization to equation (11) to obtain Eulerian grid point values $h_{i,mn}(t)$, where the initial layer heights $h_{0,i,k} := h_{0,i}(\mathbf{a}_k)$ have to be approximated from the initially given profile

$$h_{i,mn}(t) = \sum_k \hat{\gamma}_k h_{0,i,k} \Psi_{mn}(\mathbf{X}_{i,k}(t)). \tag{15}$$

DISCRETE HAMILTONIAN PRINCIPLE

By the principle of least action the variation of the integral over the Lagrangian $L = E_{kin} - E_{pot}$ vanishes. The kinetic energy is derived by applying the integration formula in label space (13) to the continuous energy expression. With particle masses $m_{i,k} = \rho_i \hat{\gamma}_k h_{0,i,k}$ the kinetic energy and the variation of its contribution to the action is given by

$$E_{\text{Kin}} = \frac{1}{2} \sum_{i,k} m_{i,k} \dot{\mathbf{X}}_{i,k}(t)^2, \qquad \delta \int_0^{t_e} E_{\text{Kin}} dt = - \int_0^{t_e} \sum_{i,k} m_{i,k} \ddot{\mathbf{X}}_{i,k} \cdot \delta \mathbf{X}_{i,k} dt \tag{16}$$

The potential energy is derived from the continuous energy expression in the Eulerian system where the integration formula in Eulerian space (12) and the Lagrangian form of mass conservation (15) are applied

$$E_{\text{Pot}} = \int_R \sum_i \int_{Z_{i+1/2}}^{Z_{i-1/2}} g \rho_i z dz + p_T z_T d\mathbf{x} = \sum_i \sum_{mn} \gamma_{mn} m_{i,k} \Psi_{mn}(\mathbf{X}_{i,k}) (g Z_{i,mn} + p_{T,mn}/\rho_i). \tag{17}$$

The variation of potential energy evaluates to

$$\delta E_{pot} = \sum_{i,k} m_{i,k} \sum_{mn} \Phi_{i,mn} \nabla N_{i,mn} \delta \mathbf{X}_{i,k}, \qquad \text{where } \Phi_{i,mn} = \sum_{j=1}^{N} \min(1, \rho_j/\rho_i) h_{j,mn} + p_{T,mn}/\rho_i. \tag{18}$$

Extending the Eulerian grid values $\Phi_{i,mn}$ by the interpolation formula (12) to Eulerian space via $\Phi_i(\mathbf{x}) := \sum_{mn} \Phi_{i,mn} N_{mn}(\mathbf{x})$, the Hamiltonian particle mesh method for the multilayer shallow water equations is derived

$$\frac{D}{Dt} \dot{\mathbf{X}}_{i,k} - f \mathbf{k} \times \dot{\mathbf{X}}_{i,k} = - \nabla \Phi_i(\mathbf{X}_{i,k}) \tag{19}$$

Note, that the Hamiltonian approach results in a natural approach of the continuous equations of motion and the potential. The result is a system of second order ODEs, where the different layers are coupled by the potential Φ. For temporal discretization a symplectic method is recommended because of its conservation properties [6], e.g., the Störmer-Verlet discretization. For details, see [7], [5].

A PARALLEL COMMUNICATION STRUCTURE FOR THE COMPUTATION OF THE POTENTIAL

We define the communication structure for the case where the number of layers N and the number of processors K are both powers of two. Whenever we have more layers then processors, some of the communication steps can be omitted. On the other hand, when we have more processors than layers, the particles of a layer will be distributed to several processors resulting in layers with the same density parameter ρ_i – thus we can be apply the same procedure as in the case $N = K$. In the following we assume $N = K = 2^n$.

Let $[i, i+l) := \{i, i+1, \ldots, i+l-1\}$. Our communication structure consists of n cycles of pairwise communication. It is designed such that in cycle i the processors form groups $M_{i,l}, l = 0, \ldots, 2^{n-i}$ of 2^i consecutive processors that all have computed the same intermediate values to be distributed in succeeding cycles. The first processor in group $M_{i,l}$ has number $M_{i,l}^- = 2^{i+1}l$, the last is $M_{i,l}^+ = 2^{i+1}(l+1)) - 1$. In cycle i all processors in group $M_{i,l}$ compute both $D = \sum_{j \in M_{i,l}} h_j$ and $U = \sum_{j \in M_{i,l}} \rho_j h_j$. During that cycle processor k communicates with the unique processor k' with $|k - k'| = 2^i$ being in the same group, exchanging the D- and U-values. We denote the set of processors with lower numbers in these pairs by P_i^-, the processors with higher numbers by P_i^+, and the pairs by (k, k_i^+) resp. (k_i^-, k). The communication is then accomplished by the following algorithm:

$k = getProcID()$
$U = \rho_k h_k, D = h_k$
$\Phi = g z_B + p_T / \rho_i$
for $i = 1 : n$ **do**
  if $k \in P_i^-$ **then**
    send U, D to k_i^+
    receive U^+, D^+ from k_i^+
    $U = U + U^+, D = D + D^+$
    $\Phi = \Phi + U / \rho_i$
  else
    receive U^-, D^- from k_i^-
    send U, D to k_i^-
    $U = U + U^+, D = D + D^+$
    $\Phi = \Phi + D$
  end if
end for

The communication structure is just the one that is used for the FFT, the butterfly structure. Note, when layers are distributed to 2^l processors, it suffices to communicate only D in cycles $i = 0, \ldots, l-1$. On the other hand, when several layers reside on one processor, we can use the same principle to reduce the operation count to $\mathcal{O}\left(l 2^l\right)$.

SUMMARY

We have presented a communication structure to avoid broadcast operations for the computation of the potential of the multilayer shallow water equations. The largest impact of the communication procedure is obtained when the number of processors equals the number of layers, but it is applicable as well when there is an imbalance between the number of processors and the number of layers.

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