

A Parallel Implementation of a Spectral Element Ocean Model for Simulating Low-Latitude Circulation System

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ABSTRACT

This paper is about the parallel implementation of a high-resolution, spectral element, primitive equation model of a homogeneous equatorial ocean. The present work shows that the high-order domain decomposition methods can be efficiently implemented in a massively parallel computing environment to solve large-scale CFD problems, such as the general circulation of the ocean.

1. INTRODUCTION

In the past decade or so, research on the spectral element method has made important progress in perfecting this state-of-the-art numerical method [4,10,11]. More recently, the spectral element method has shown encouraging potential in oceanic applications [5,6,7,8,9].

The equatorial ocean is well known for the richness in the structure of its currents. Equatorial currents exist not only in the upper ocean, but in the deep ocean as well [2,3]. These equatorial currents might, in some way, interact with the high-frequency, small-scale, baroclinic waves which, in turn, influence the momentum and heat budget of the tropical ocean.

The present work is about the implementation and results of a spectral element, high-resolution, three-dimensional ocean model which, in particular, is capable of resolving both the horizontal and the vertical structures of the low-latitude western boundary processes. The current version of the model is driven solely by wind stress and ignores the dynamical effects of stratification. This model is designed to study the effect of wind in the formation and variation of important meso-to-small scale equatorial ocean phenomenon, such as eddies, low-latitude western boundary currents, and vertically alternating equatorial zonal jets. The high efficiency of this model is based on an optimized coupling between the numerical algorithm and the computer architecture (algorithm-architecture). performance is further enhanced by the spectral element tensor-product factorization and spectral element parallelism.

2. GOVERNING EQUATIONS

With the hydrostatic approximation, the primitive equation model in spherical coordinates for a homogeneous ocean contains the following equations:

$$\begin{cases} \frac{du}{dt} - (2\Omega + \frac{u}{r \cdot \cos\phi})(v \cdot \sin\phi - w \cdot \cos\phi) = \\ -\frac{1}{\rho \cdot r \cdot \cos\phi} \frac{\partial p}{\partial \lambda} + A_H \Delta u + A_v \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \frac{\partial}{\partial r}) u \\ \frac{dv}{dt} + \frac{wv}{r} + (2\Omega + \frac{u}{r \cdot \cos\phi}) u \cdot \sin\phi = \\ -\frac{1}{\rho \cdot r} \frac{\partial p}{\partial \phi} + A_H \Delta v + A_v \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \frac{\partial}{\partial r}) v \\ -\frac{1}{\rho} \frac{\partial p}{\partial r} - g = 0 \\ \frac{1}{r \cdot \cos\phi} \frac{\partial u}{\partial \lambda} + \frac{1}{r \cdot \cos\phi} \frac{\partial (v \cdot \cos\phi)}{\partial \phi} + \frac{\partial w}{\partial r} = 0 \end{cases}$$

where

$$\begin{aligned} \frac{d}{dt} &= \frac{\partial}{\partial t} + \frac{u}{r \cdot \cos\phi} \frac{\partial}{\partial \lambda} + \frac{v}{r} \frac{\partial}{\partial \phi} + w \frac{\partial}{\partial r} \\ \Delta &= \frac{1}{r^2 \cos^2\phi} \frac{\partial^2}{\partial \lambda^2} + \frac{1}{r^2 \cos\phi} \frac{\partial}{\partial \phi} (\cos\phi \frac{\partial}{\partial \phi}) \end{aligned}$$

and λ is longitude, ϕ latitude, and r radial distance; u , v , and w are the velocity components in the λ , ϕ , and r directions, respectively; p is the pressure; A_H and A_v are eddy viscosities.

No-normal flow, no-slide boundary conditions are applied to all lateral boundaries. At the sea surface, we assume the rigid-lid boundary condition. The present version of the model is solely driven by the surface wind stress.

3. DISCRETIZATION SCHEMES AND SOLVERS

The computational domain, Ω , of the present model is the part of the equatorial Atlantic Ocean between 15°N and 15°S with idealized north-south meridional boundaries. Ω is decomposed into K subdomains (spectral elements), Ω_e . A strip of refined spectral elements is embedded in the western boundary region in order to resolve the narrow, strongly sheared, low-latitude western boundary currents and the retroflection eddies. The exponential convergence rate of the spectral element method lets us achieve this objective with much less computational cost than that entailed by low-order numerical methods.

The basis functions used in the present model are the the Gauss-Lobatto-Legendre polynomials. A three dimensional basis set $\{\psi_{lmn}\}$ is constructed as:

$$\psi_{lmn}(\xi, \eta, \zeta) = h_l(\xi)h_m(\eta)h_n(\zeta) \quad l, m, n \in \{0, 1, 2, \dots, N\}^3$$

Here the same elemental degree-of-freedom (N) is used in all three spatial dimensions for simplicity. This does not affect the generality of the method, and in actual implementations different elemental degrees-of-freedom can be used in each spatial direction as needed.

With well distributed interpolation points on Ω^e , it can be proved that $\{\psi_q^e\}$ is complete (when $N \rightarrow \infty$) and orthogonal. Therefore, if \mathcal{M}^e is the subspace spanned by $\{\psi_q^e\} \in \mathcal{H}^1$, then there is a projection Π_e , such that $\forall u^e(\mathbf{x} \mid \mathbf{x} \in \Omega^e) \in \mathcal{H}^1$

$$\Pi_e[u^e(\mathbf{x})] = u_h^e[\xi(\mathbf{x})] = u_q^e \psi_q^e[\xi(\mathbf{x})] \in \mathcal{M}^e \quad (0.1)$$

where u_h^e is the numerical approximation of u^e .

Then, it follows that there is a projection Π , such that $\forall u(\mathbf{x} \mid \mathbf{x} \in \Omega) \in \mathcal{H}^1$

$$\Pi[u(\mathbf{x})] = u_h = \bigcup_{e=1}^K u_h^e[\xi(\mathbf{x})] \in \bigcup_{e=1}^K \mathcal{M}^e \quad (0.2)$$

where u_h is the numerical approximation of u by the piecewise polynomials, and

$$\bigcup_{e=1}^K u_h^e \rightarrow u \quad \text{when } N^d \rightarrow \infty, \text{ or } \Delta_{max} \rightarrow 0 \quad (0.3)$$

where N^d is the dimension of \mathcal{M}^e and Δ_{max} is the maximum size of the subdomains Ω^e .

Let the solutions of the primitive equations at time t and the test functions on each subdomain Ω_e be expanded as $u^e(x, y, z, t) = u_{ijk}^e(t) \psi_{ijk}^e[\xi(x, y, z), \eta(x, y, z), \zeta(x, y, z)]$, where $u_{ijk}^e(t)$ is the value of the function u at the collocation point $(x_i, y_j, z_k) \in \Omega_e$ at time t . The relationship between the global coordinates (x, y, z) and the local coordinates (ξ, η, ζ) is given by the isoparametric mapping.

By using the same variational procedures as those in [6,7], i.e., all the integrations are evaluated by the Gauss-Lobatto quadrature scheme, which is an exact formula for $(2N - 1)^{th}$ order polynomials, the spatially discretized formulae for the primitive equations can be obtained. In particular, the isoparametric spectral element discretization formulae for the horizontal momentum equations of the present primitive equation model are virtually identical as those in [6, 7]. One advantage of using the Gauss-Lobatto-Legendre polynomials as basis functions is that we only have to deal with one set of grid points for both interpolating the solutions and evaluating the integrals.

The discretized incompressibility condition and the hydrostatic condition have the following format:

$$[D^z][w] = [g]$$

where $[D^z]$ is the matrix generated by applying variational procedures to the vertical differentiation operator; $[w]$ is the vector representing the unknown at the collocation points, and $[g]$ is a vector whose components are known.

To obtain the solution for the vertical velocity, w , we need to solve a matrix problem of the above format. It can be done by using either matrix iteration methods or direct matrix inversion. We have chosen to use the latter for the present model with regular geometries. It is especially efficient when the vertical grains of the spectral element mesh

are parallel to the z axis, since the dimension of the matrix to be inverted is the same as the number of levels in the vertical direction.

The Poisson's equation for the pressure term, however, has to be solved via a spectral element iterative solver. A preconditioned conjugate gradient iterative solver is used in the present model.

The spectral element primitive equation model has two ways to achieve better numerical precision, i.e., by increasing the dimensions of the subspaces, N^3 , and/or increasing the number of macro-elements, K . It can be very flexible and the optimum choice for these two parameters depends on each individual problem to be solved.

The time marching scheme for the hyperbolic equations of the present model is the 3rd order Adams-Bashforth scheme. This scheme has proven to be efficient in high Reynolds number, high resolution simulations, especially in a massively parallel computing environment [7]. In fact, except in the upper range of eddy viscosity (diffusion) for oceanic applications, it is likely to be more efficient to use a fully-explicit scheme because it results in diagonal stiffness matrices for the hyperbolic equations.

4. PARALLEL IMPLEMENTATION AND RESULTS

An important aspect which greatly enhances the computational efficiency of the spectral element method is the natural fit of this method to parallel computing. The main difference between the spectral element method and the spectral multi-domain method is that the C^0 and C^1 boundary conditions at the interface of the elements have to be enforced explicitly in the latter. By contrast, the spectral element method uses the variational principle to guarantee C^0 and C^1 (weakly) continuity at the interface, therefore, parallel algorithms can be implemented conveniently [4,7,8].

The spectral element primitive equation ocean model is parallelized to run efficiently on the Connection Machine Model CM5. In order to avoid unnecessary communication among processing nodes, which is of first order importance in a parallel implementation on a distributed memory, massively parallel architecture, a data mapping scheme was created so that all the information related to a given spectral element is collected in the memory of a single processor (Figure 1). Prior to assembling the global stiffness-matrices, only data related to a given spectral element are used to create the local matrices of that spectral element. At this stage, all computations are carried out at the local level, therefore, there is no communication among neighboring processors while assembling local (elemental) matrices.

The only communication which cannot be avoided is during assembling the global stiffness matrix. However, since the spectral elements are of high order, most of the costly operations are at the elemental level, which can be executed in parallel. For the same reason, the communication cost due to the information exchange among neighboring processors for the spectral element model is only a small fraction of the total cost and it is much smaller than that for the h-type finite element model partially because that many fewer redundant nodal values which are shared by more than one elements have to be stored.

The technique of partial summation provides a significant relief in cost for the stiffness-matrix/vector product, $[A][u]$, and the operation count is reduced to $O(KN^4)$. However, $[A][u]$ is still the most expensive part of the computation of the present spectral element

primitive ocean model. With massively parallel processing, we have obtained further relief for this problem.

After applying tensor-product factorization, the general expression of $[A][u] = [g]$ resulting from the spectral element discretization is of the form

$$\sum_{k=1}^K \sum_{q=1}^N C_{n,q}^k \sum_{r=1}^N B_{m,r}^k \sum_{s=1}^N A_{l,s}^k u_{q,r,s} = \sum_{k=1}^K g^k$$

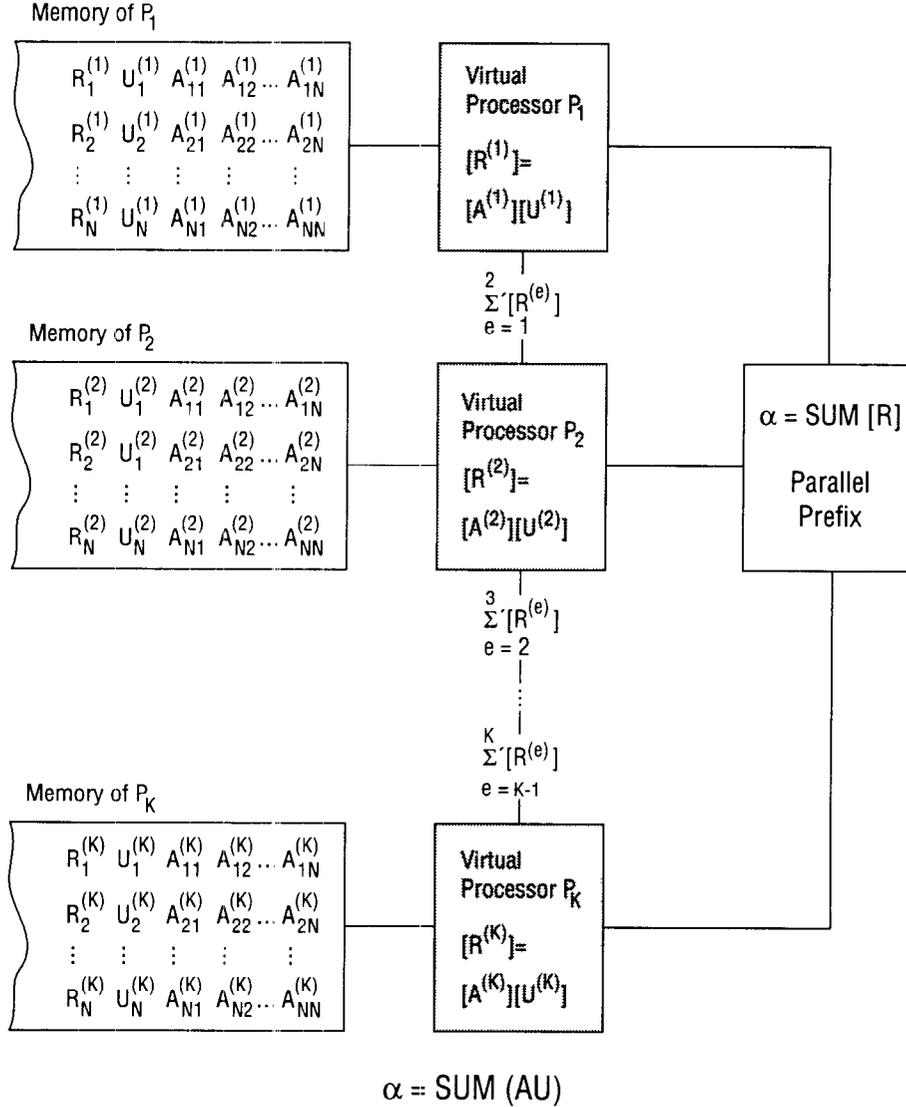


Figure 1. Flow diagram of the parallel execution of a typical spectral element matrix operation.

The direct stiffness summation in the last equation can be split into three steps, each of which admits concurrency. “Forming” is the first step, when $\sum_{q=1}^N C_{n,q}^k \sum_{r=1}^N B_{m,r}^k \sum_{s=1}^N A_{l,s}^k u_{q,r,s}$ is calculated simultaneously across K virtual processors. “Gathering” and “Redistributing” are the second and the third steps, respectively, during which contributions of

neighboring spectral elements are summed (gathering) and then given back to the corresponding nodal points (redistributing). Since the message exchange at the linkages of macro-elements, which are surfaces for the three dimensional model (Figure 2), is synchronized for all elements on the entire surface, it can provide a speedup of $K^{\frac{2}{3}}$. The cost of steps two and three is generally much smaller than that of step one, because the latter handles higher spatial dimensions. As a result, the number of clock cycles required to calculate the direct stiffness summation will then be proportional to KN^4/Q , where Q is the speedup.

Parallel Direct Stiffness Summation For [A][X]

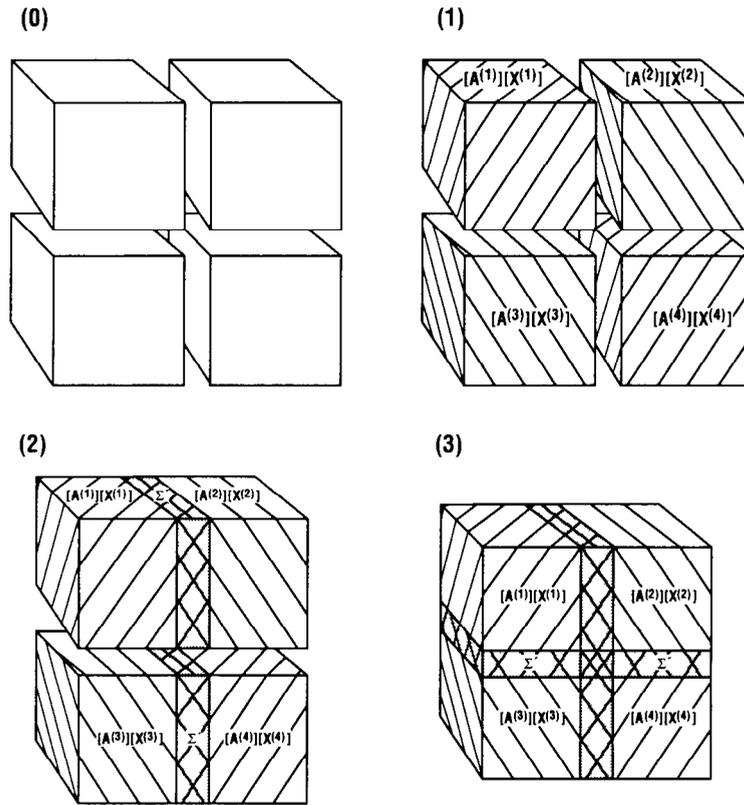


Figure 2. Symbolic diagram of direct stiffness summation with the surface-based message exchange.

In the parallel implementation of the present spectral element model on the CM5, the number of virtual processors always equals to the number of spectral elements. Therefore, we can use “equivalent speedup” = $(K * T_1)/T_K$ and “equivalent efficiency” = T_1/T_K to measure the parallel performance of the spectral element primitive equation model, where T_K is the CM5 cpu time per time step with K spectral elements. Since on a serial computer, the computational cost of the spectral element primitive ocean model is proportional to the number of spectral elements, $K * T_1$ is roughly how much time it would take to execute one time step if the CM5 had only one processor. Figure 3 shows that with a fixed number of physical processors, the performance of the spectral element

primitive equation model scales very well until the number of spectral elements becomes so large that the memory in the CM5 partition is saturated. The excellent scalability of the model recovers when the size of the CM5 partition is increased.

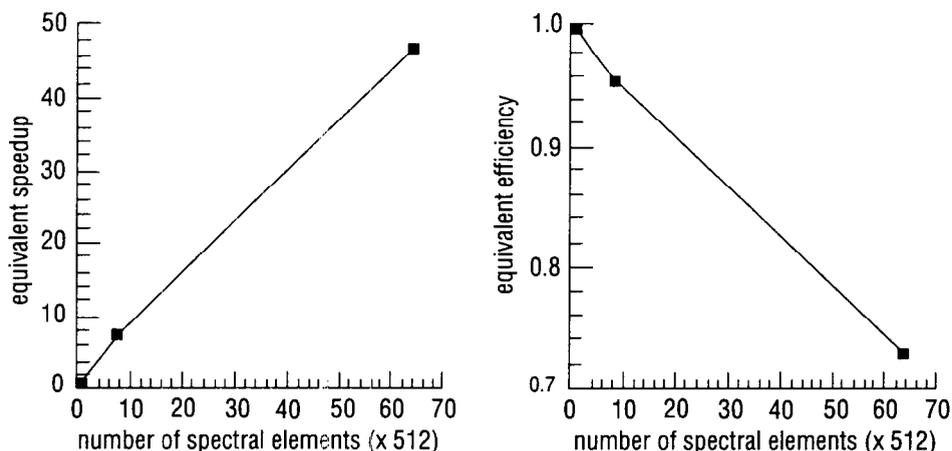


Figure 3. Parallel performance measure on a CM5 partition with 256 processors. $N = 6$.

Figure 4 is a snapshot of a meridional transection of the zonal current from a simulation run of the model driven by the climatological wind-stress over the Atlantic. The model has 67 and 2989 spectral element interpolation points in the vertical and the horizontal directions, respectively. The high computation efficiency of the spectral element primitive equation model allows the model to capture the meso-small scale oceanic processes much more efficiently than low-order numerical models. This is the first time that the north and south intermediate countercurrents and the south equatorial intermediate current are identified by a numerical ocean model. Details of the numerical simulation shall be published in a separate paper.

5. ACKNOWLEDGEMENT

This work was supported by DoD Common High Performance Computing Software Support Initiative (CHSSI). Most of the computation was carried out on the CM5 at the Army High Performance Computing Research Center.

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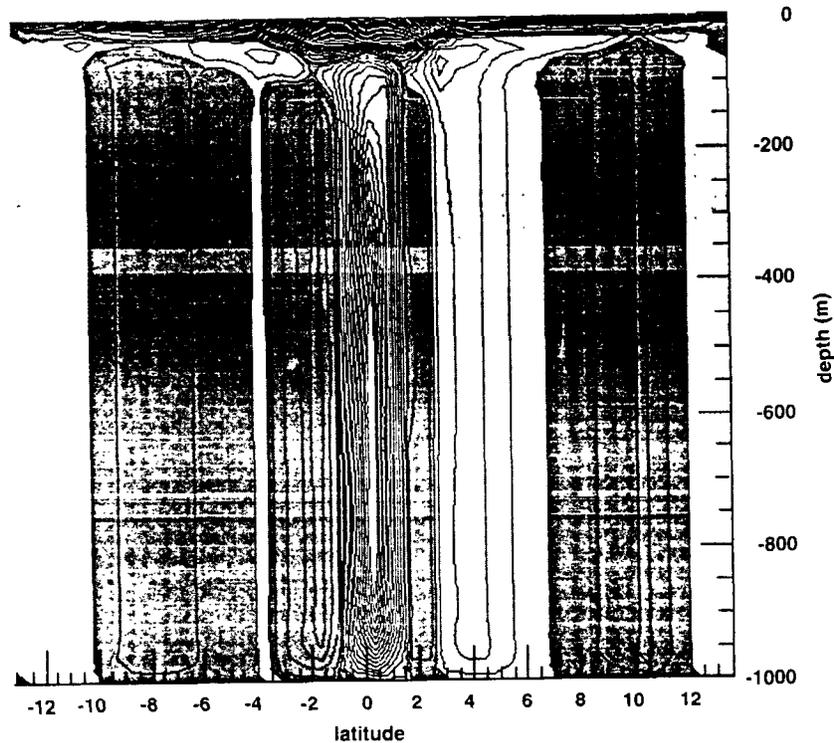


Figure 4. Section of the zonal current along 39.2°W on day 421 (contour interval=0.02 m/s). Currents in the darkly shaded areas are westward.