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MODELING A LIMITED REGION OF THE OCEAN. Amala Mahadevan and David Archer. *Department of Geophysical Sciences, University of Chicago, Chicago, Illinois 60637.* E-mail: amala@starbuck.uchicago.edu and archer@starbuck.uchicago.edu.

Many of the difficulties that arise from the specification of open boundary conditions when modeling a limited region of the ocean with the *primitive equations* can be overcome by using a nonhydrostatic set of equations that is well posed in open domains even without the viscous term. We simulate the mesoscale flow in a region of the open ocean using the flow fields from a global circulation model to provide initial and boundary data. Information flow across lateral boundaries is specified using the method of characteristics. By modeling the region at higher resolutions than the fields providing boundary conditions, we are able to resolve more structure and processes in the flow than were detectable from the initial and boundary data. This is of value for studying a region of the ocean in detail at moderate computational cost, if initial and boundary data is available. Shortcomings of the characteristics-based formulation of the boundary conditions and limitations in using such a model to selectively refine a region within a coarser model are also examined.

DISCRETE TRANSPARENT BOUNDARY CONDITIONS FOR WIDE ANGLE PARABOLIC EQUATIONS IN UNDERWATER ACOUSTICS. Anton Arnold*,† and Matthias Ehrhardt*. **Fachbereich Mathematik, TU Berlin, MA 6-2, Strasse des 17. Juni 136, D-10623 Berlin, Germany; and* †*Center for Applied Mathematics, Purdue University, West Lafayette, Indiana 47907.* E-mail: arnold@math.tu-berlin.de and ehrhardt@math.tu-berlin.de.

This paper is concerned with transparent boundary conditions (TBCs) for wide angle "parabolic" equations (WAPEs) in the application to underwater acoustics (assuming cylindrical symmetry). Existing discretizations of these TBCs introduce slight numerical reflections at this artificial boundary and also render the overall Crank–Nicolson finite difference method only conditionally stable. Here, a novel discrete TBC is derived from the fully discretized whole-space problem that is reflection-free and yields an unconditionally stable scheme. While we shall assume a uniform discretization in range, the interior depth discretization (i.e. in the water column) may be nonuniform, and we shall discuss strategies for the "best exterior discretization" (i.e. in the sea bottom). The superiority of the new discrete TBC over existing discretizations is illustrated on several benchmark problems. In the literature different WAPEs (or WAPE and the standard "parabolic" equation) have been coupled in the water and the sea bottom. We analyze under which conditions this yields a hybrid model that is conservative for the acoustic field.

CONVERGENCE OF THE EQUILIBRIUM CODE SOLGASMIX. C. F. Weber. *Oak Ridge National Laboratory, P.O. Box 2008 Oak Ridge, Tennessee 37831-6370.*

The procedure used to calculate chemical equilibrium in the code SOLGASMIX has been evaluated mathematically and applied to several examples in aqueous electrolyte chemistry. Matrix representation of the solution procedure allows convenient expression as a standard fixed-point iteration. Evaluation of sample problems illustrates the importance of certain free energy differences in theoretical convergence results. An interpolation scheme based on the oscillation of Gibbs energies yields legitimate equilibrium results in situations where the code would otherwise fail to converge properly.

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RAPID PARALLEL EVALUATION OF INTEGRALS IN POTENTIAL THEORY ON GENERAL THREE-DIMENSIONAL REGIONS. A. Greenbaum* and A. Mayo†. **Courant Institute of Mathematical Sciences, 251 Mercer Street, New York, New York 10012; and* †*IBM T. J. Watson Research Center, Yorktown Heights, New York 10598.*

We present a new, high order accurate method for the rapid, parallel evaluation of certain integrals in potential theory on general three-dimensional regions. These methods use fast methods for solving the differential equation which the kernel satisfies, and the number of operations needed to evaluate the integrals is essentially equal to the number of operations needed to solve the differential equation on a regular rectangular grid. In particular, one can evaluate integrals whose kernels are the Greens function for Poissons equation by using Fourier methods on a rectangular grid, or, a fast Poisson solver. Thus, these methods avoid the problems associated with using quadrature methods to evaluate an integral with a singular kernel. Numerical results are presented for experiments on a variety of geometries.

WEIGHTED PARTICLES IN COULOMB COLLISION SIMULATIONS BASED ON THE THEORY OF A CUMULATIVE SCATTERING ANGLE. K. Nanbu and S. Yonemura. *Institute of Fluid Science, Tohoku University, Sendai 980-8577, Japan.* E-mail: nanbu@ifs.tohoku.ac.jp and yonemura@ifs.tohoku.ac.jp.

A cumulative property of Coulomb collisions in plasmas was formulated by Nanbu. A succession of small-angle binary collisions is grouped into a unique binary collision with a large scattering angle; the law of scattering is given by the exponential cosine function. Proposed here is a Coulomb collision algorithm for weighted particles, based on that work. Three cases of the weight algorithm are considered: (1) the weights of particles are the same; (2) the weights of particles are different from species to species; and (3) the weights are different from particle to particle. Sample calculations demonstrate the accuracy of the weight algorithm.