PHYSICAL AND COMPUTATIONAL ISSUES IN THE NUMERICAL MODELING OF OCEAN CIRCULATION

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Abstract. The large-scale circulation of the world's oceans can be modeled by systems of partial differential equations of fluid dynamics, as scaled and parameterized for oceanic flows. This paper outlines some physical, mathematical, and computational aspects of such modeling. The topics include multiple length, time, and mixing scales; the choice of vertical coordinate; properties of the shallow water equations for a single-layer fluid, including effects of the rotating reference frame; a statement of the governing equations for a three-dimensional stratified fluid with an arbitrary vertical coordinate; time-stepping and multiple time scales; and various options for spatial discretizations.

Key words. numerical modeling of ocean circulation, isopycnic and hybrid coordinates, shallow water equations, layered ocean models, barotropic-baroclinic time splitting, spatial grids on a spheroid

AMS(MOS) subject classifications. 35Q35, 65M99, 76M99, 86A05

1. Introduction. The circulation of the world's oceans plays a major role in the global climate system, and numerical models of that system typically include models of atmospheric circulation, oceanic circulation, sea ice dynamics, land effects, and biogeochemistry. Local circulation in near-shore regions is also of substantial scientific and societal interest. As a result, numerous numerical models of ocean circulation have been developed in recent decades. These all involve the numerical solution of systems of partial differential equations of fluid dynamics, as scaled and parameterized for oceanic flows.

The goal of the present paper is to outline some of the physical and computational issues that are encountered when ocean circulation is simulated numerically and to suggest some areas of possible improvement that could engage mathematical scientists. The starting point is to describe some of the space, time, and mixing scales that are found in the ocean, and this is done in Section 2. In Section 3 we discuss some possible choices for a vertical coordinate in an ocean model; the elevation z is a natural choice, but other possibilities have also been developed. Section 4 describes some aspects of governing equations for oceanic flows, both the shallow water

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equations for a homogeneous (single-layer) fluid and some equations that model three-dimensional stratified flows. Some aspects of time discretization and space discretization are outlined in Sections 5 and 6, respectively.

This author has previously written a lengthy survey [6] on the subject of numerical modeling of ocean circulation. The present paper is based on the author's presentation at an IMA workshop on Societally Relevant Computing during April 2011, and it can serve as an update and relatively brief "front end" to the longer, earlier review.

In the sections that follow, some of the background information about ocean physics and ocean modeling practice is stated without explicit citations. The earlier paper [6] includes a lengthy bibliography, and the reader can refer to [6] for further details and references.

2. Multiple scales. The physical processes in the ocean exhibit a wide range of space, time, and mixing scales. This multi-scale character has a profound effect on the fluid flows that are seen and on the numerical algorithms that are used to model them.

2.1. Length scales. Ocean circulation patterns include wind-driven horizontal gyres; these are closed loops of circulation that span the widths of ocean basins, which are thousands of kilometers wide. An oceanic gyre typically includes an intense boundary current along the western edge of the basin, with a boundary current width on the order of 10^2 kilometers. Examples of western boundary currents include the Gulf Stream in the North Atlantic and the Kuroshio in the North Pacific. In general, ocean currents are not smooth, but instead they meander and shed eddies having widths in the range of tens to hundreds of kilometers. These horizontal length scales are very different from the vertical scales that are present; in the mid ocean the depth is a few kilometers (e.g., four to six), and for surface currents the kinetic energy is mostly confined to the upper few hundred meters.

For large-scale features of ocean circulation, the vertical length scale is thus far less than the horizontal length scale, and this property is known as the *shallow water condition*. It can be shown that the shallow water condition implies that the fluid is approximately hydrostatic, i.e., vertical accelerations are small. (See Section 4.1.1.) This can then lead to substantial simplifications in the system of governing equations.

However, not all of the physically relevant motions in the ocean satisfy the shallow water condition. An example arises in the thermohaline circulation, which is also known as the meridional overturning circulation, or global conveyor belt. In this circulation, a portion of the warm water of the Gulf Stream separates from the horizontal gyre and flows into the far northern Atlantic. This water then becomes colder and saltier due to atmospheric forcing, and due to its increased density the water sinks into the deep ocean in narrow convective plumes to form part of a complex three-dimensional global circulation pattern having a period of centuries.

The plumes do not satisfy the shallow water condition, and the deep convection is not hydrostatic. This convection is not resolved explicitly in present-day ocean climate models, but instead it is parameterized by some means, such as vertical diffusion. An interesting computational challenge would be to embed non-hydrostatic high-resolution models of the deep-convection zones into a lower-resolution hydrostatic global model. This process could be made difficult by the need to couple the very different dynamics of the two regimes.

2.2. Velocity and time scales. A wide range of velocities is represented in the fluid motions and wave motions that are seen in the large-scale circulation of the ocean. For the horizontal component of fluid velocity, a value of one meter per second is typical of strong currents, but elsewhere in the ocean the horizontal velocities are considerably smaller. In nearly-hydrostatic regions the vertical fluid velocity is typically far smaller than the horizontal velocity, with values such as 10^{-3} meters per second or less.

Distinct from this are the wave motions that are seen in the large-scale circulation. Here, we are not referring to the familiar surface waves that are readily visible to an observer, but instead we refer to motions having wavelengths that are long relative to the ocean depth. These motions can be classified as *external waves* and *internal waves*, and within each class are *gravity waves* and *Rossby waves.* The review paper [6] includes a derivation and discussion of this modal structure, for the case of linearized flow in a spatial domain having a level bottom.

To visualize these waves, imagine the ocean as a stack of layers separated by surfaces of constant density. If the state of the fluid consists entirely of an external wave, then at any time and horizontal location the horizontal fluid velocity is nearly independent of depth, and all layers are thickened or thinned by approximately the same proportion. The state of the free surface at the top of the fluid thus displays the mass distribution within the ocean, so the fluid motion at the upper boundary reveals nearly everything about the motion within the fluid. On the other hand, in the case of an internal wave the free surface remains nearly level; the wave motion is characterized by undulations of density surfaces within the fluid, and the mass-weighted vertical average of horizontal velocity is nearly zero. These motions are illustrated in Figure 1.

In the case of external gravity waves, the wave speed is approximately $\sqrt{gH}$, where H is the depth of the ocean and g is the acceleration due to gravity. For example, if $H = 4000$ meters then the wave speed is approximately 200 m/sec. On the other hand, for internal gravity waves the speeds are at most a few meters per second. This large difference in wave speeds can be explained by the fact that for external gravity waves the restoring force is due to the density contrast between water and air, whereas for internal waves the restoring force is due to the far weaker density contrasts within the ocean.

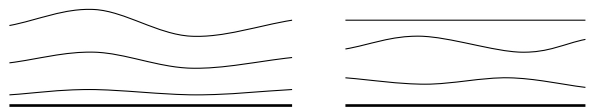

Fig. 1. *Illustrations of an external wave (a) and an internal wave (b). The figures are not to scale, as the depth of the fluid is much smaller than the horizontal length scale, and the vertical displacements are exaggerated in the figures.*

In the case of Rossby waves (Section 4.1.4) the restoring mechanism is due to vorticity instead of gravity, and these waves are generated by variations in the Coriolis parameter with latitude and/or variations in the elevation of the bottom topography. Rossby waves are typically far slower than gravity waves.

Gravity waves participate in adjustment processes, such as those that occur when a shift in prevailing winds causes a shift in quasi-balanced states in the ocean. Rossby waves are involved in the development of large-scale circulation systems.

To very good approximation, the fast external motions can be modeled by neglecting the density variations within the fluid and then applying the two-dimensional shallow water equations that are discussed in Section 4.1. On the other hand, the slow internal motions are fully three-dimensional. These properties can be exploited to develop time-stepping methods that can handle efficiently the multiple time scales that are inherent in large-scale oceanic flows, as discussed in Section 5.

2.3. Mixing scales. A major purpose of an ocean model is to simulate the transport of tracers such as temperature, salinity, and various chemical and biological species. Temperature and salinity directly affect the density of the fluid and thus its dynamics, so temperature and salinity are referred to as active tracers. Other tracers simply move with the flow and are labeled as passive tracers.

Tracers are transported in part by the bulk movement of currents, but they are also mixed by smaller-scale turbulent motions having length scales down to centimeters or less. The full extent of these motions cannot be resolved on the spatial grids of numerical ocean models, so the large-scale effects of these small-scale motions must be parameterized by some sort of diffusion operator.

The nature of this mixing depends on the location within the ocean. In the ocean's interior, the fluid is stratified, and the mixing is highly anisotropic. Empirical observations indicate that at any point in the interior, the plane of strongest mixing is nearly horizontal, and the rate of diffusion in that plane is several orders of magnitude greater than the rate of diffusion perpendicular to that plane. This phenomenon has been explained in terms of buoyancy. The plane of strongest mixing is said to be a neutral plane, and if a fluid parcel were to leave this plane then buoyancy forces would tend to restore it to the plane; on the other hand, motion within the plane experiences no such impediment and thus is far more active. The plane of strongest mixing need not be exactly horizontal, due to lateral variations of the density of the fluid. The relatively small transport across such a plane is known as *diapycnal* transport.

The preceding argument does not apply to turbulent layers along the boundary of the fluid domain. Of particular interest is the mixed layer at the top of the ocean, for which the mixing is due to wind forcing and convective overturning. At any location the structure of the mixed layer varies with time, due to weather and seasonal variations and to heating and cooling throughout the diurnal cycle. The mixed layer is generally tens of meters thick, although it can be thousands of meters thick in locations of deep convection. The mixed layer provides the means of communication between the ocean and atmosphere, so its representation is an important part of an ocean model.

3. The choice of vertical coordinate. For the vertical coordinate in a three-dimensional ocean circulation model, a traditional choice has been the elevation z. This coordinate is used, for example, in the widely-used Bryan-Cox class of ocean models (e.g., Griffies [4]). Another possibility is a terrain-fitted vertical coordinate σ, which measures the relative position between the top and bottom of the fluid domain. The top and bottom correspond to constant values of σ, so this framework is natural for representing irregular bottom topography; see Figure 2. The σ-coordinate system is widely used in modeling the ocean circulation in near-shore regions (e.g., Shchepetkin and McWilliams [10]).

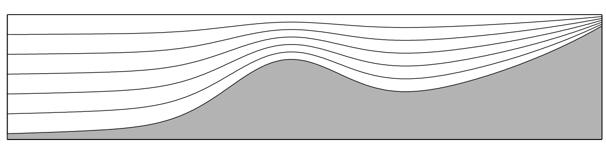

FIG. 2. *A terrain-fitted vertical coordinate. The shaded region represents variable bottom topography, and the curves are cross-sections of surfaces of constant vertical coordinate σ.*

3.1. Isopycnic coordinates. A third possibility is to use an *isopycnic coordinate*, which is a quantity related to density. A vertical discretization would then divide the fluid into layers having distinct physical properties, as opposed to using a geometrical discretization such as one found with z or σ.

A specific possibility for an isopycnic coordinate is *potential density*. To define that quantity, imagine that a fluid parcel is moved to a reference pressure, without any heat flow into or out of the parcel and without any changes in the composition of the fluid in that parcel. The resulting density is then the potential density, relative to that reference pressure. The reference pressure could be atmospheric pressure, or it could be the pressure at some specified depth. However, if atmospheric pressure is used as the reference pressure, then the resulting potential density could be non-monotonic in z in regions of weak stratification, which is not suitable for a vertical coordinate. A reference pressure at a specified depth is therefore used instead. Section 4.2.2 includes an argument for using potential density instead of true density as a vertical coordinate.

The usage of an isopycnic coordinate is motivated by the properties of oceanic mixing that are discussed in Section 2.3. For modeling the ocean's interior, an ideal coordinate would be a vertical coordinate s whose level surfaces are neutral surfaces. That is, at each point on a surface of constant s, the tangent plane is the plane of strongest mixing that was discussed previously; see Figure 3. (Such a plane is commonly described as the tangent plane to the surface of constant potential density, where the potential density is referenced to the pressure at that particular point.) Suppose that a neutral coordinate s is used, and assume that the fluid domain is discretized into layers that are separated by surfaces of constant s. The strong lateral mixing then occurs only within coordinate layers, and the only transport of tracers between layers is the much weaker diapycnal diffusion that is described in Section 2.3. The relatively warm upper layers are then distinguished automatically from the colder lower layers by the choice of coordinate system. This can be an advantage for long-term simulations, such as those that arise in climate modeling.

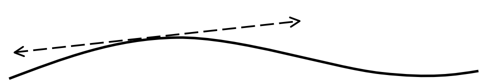

FIG. 3. *Isopycnic coordinate. The solid curve represents a cross-section of a surface of constant isopycnic coordinate. Ideally, a tangent plane to such a surface would be the plane of strongest mixing at that point. Spurious numerical diffusion in horizontal advection terms would then be confined to coordinate layers and would not mask the subtle physical diffusion between layers.*

More specifically, the transport of tracers is modeled by advection-diffusion equations, and with such equations the approximations to the horizontal advection terms typically generate spurious numerical diffusion. This diffusion is directed along surfaces of constant vertical coordinate. In the scenario described here, this diffusion is confined to the coordinate layers and does not mask the subtle diapycnal diffusion that occurs between layers. Representing the latter is then under the direct control of the modeler. On the other hand, if the vertical coordinate is z or σ then the coordinate surfaces can cross the boundaries of the physical layers, and the numerical diffusion can generate non-physical transport of tracers between those layers.

Unfortunately, the idea of isopycnic coordinate has limitations. (1) In general, exact neutral surfaces do not exist; the local picture of neutral planes does not extend globally. Instead, one must choose an approximation to this idea, and potential density (referenced to a suitable fixed pressure) is believed to be a workable proxy. (2) Isopycnic coordinate surfaces can intersect the bottom of the fluid domain, and they can also intersect the top of the fluid, due to lateral variations in temperature. This implies that the thicknesses of certain layers can tend to zero, and thus some vertical resolution is lost in such locations. (3) The physical conditions that motivate the usage of an isopycnic coordinate are valid in the oceanic interior, but not in turbulent boundary layers. Using an isopycnic coordinate over the entire ocean is thus not fully justified, on physical grounds.

3.2. Hybrid coordinates. An alternative to using purely z, σ, or an isopycnic coordinate is to use a hybrid of these three. In the case of a hybrid coordinate, an isopycnic coordinate is used in the ocean's interior, where its usage is justified by the reasoning given above. However, in vertically-mixed regions near the upper boundary, the coordinate may depart from isopycnic and become z instead. For near-shore regions, an option that is sometimes used is to transform the isopycnic surfaces into σ-coordinate surfaces. A hybrid-coordinate strategy for the ocean is described by Bleck [1], and some recent improvements are described by Bleck et al [2] in the analogous context of atmospheric modeling.

An example of a hybrid coordinate system is shown in Figure 4. The figure shows a vertical cross-section of the southern Atlantic Ocean, as computed with the Hybrid Coordinate Ocean Model [1]. This cross-section shows the top 1000 meters of the fluid domain, and it is taken at fixed longitude 54.9° W, with the latitude varying from approximately 36° S to 56.5° S. The thin, numbered curves are cross-sections of surfaces of constant potential density, as referenced to the pressure at a depth of 2000 meters (or, more precisely, to 2000 decibars). The values of potential density are obtained by adding 1000; for example, the curve labeled 36.0 represents potential density 1036.0 kg/m^3. The thicker curves are cross-sections of surfaces of constant vertical coordinate. In the ocean's interior these align with the potential density surfaces, so the coordinate is isopycnic in that region. However, near the upper boundary of the ocean, the coordinate surfaces are level.

The usage of hybrid coordinates is relatively recent, compared to the other coordinate systems described here, and it presents some physical and algorithmic challenges. In regions of the upper ocean where vertical mixing causes a loss of stratification, isopycnic layers lose their identity. In such regions the vertical coordinate cannot be isopycnic, so an alternative should be used. In addition, a given range of the isopycnic variable (e.g., potential density) may exist in some regions of the ocean but not in others;

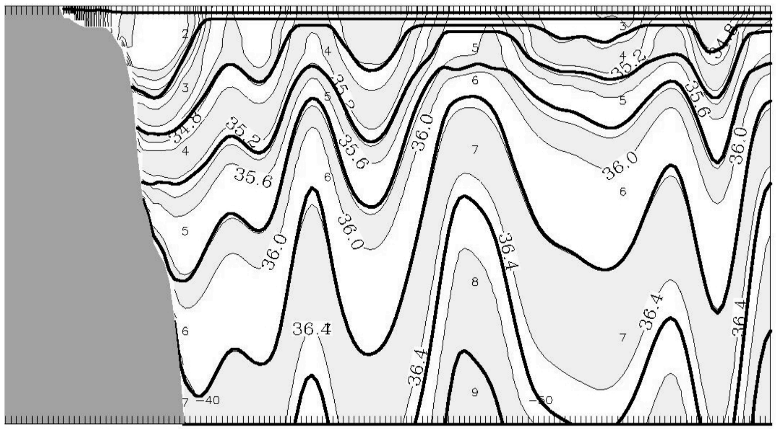

FIG. 4. *Example of a hybrid vertical coordinate. The figure shows a vertical cross-section of the southern Atlantic Ocean, for fixed longitude, as obtained from a numerical simulation. The thin curves are cross-sections of surfaces of constant potential density, and the thick curves are cross-sections of surfaces of constant vertical coordinate. In the ocean's interior, the vertical coordinate is isopycnic, and near the upper boundary the coordinate is z. In this figure the vertical extent is* 1 *kilometer, and the horizontal extent is approximately* 2300 *kilometers. (Figure provided by Rainer Bleck, NASA Goddard Institute for Space Studies.)*

in locations where an isopycnic layer does not exist physically, its mathematical representation deflates to zero thickness. It is therefore necessary to employ a grid generator that continually manages the structure of the vertical grid, which can evolve with time. For the sake of providing vertical resolution, the grid generator should maintain a minimum layer thickness for all of the coordinate layers, except perhaps those that intersect bottom topography. On the other hand, each coordinate surface should represent its "target" value of the isopycnic variable whenever physical conditions permit, i.e., the fluid is stratified at that location, and the target value is within the range that is physically present.

Depending on its design, it is possible that a grid generator could produce non-physical motions of coordinate surfaces relative to the fluid. Such motions would be represented in the vertical transport terms in the advection-diffusion equations for the transport of tracers (see Sections 4.2.1 and 4.2.2), and the spurious diffusion inherent in numerical advection schemes could then compromise the water properties in the affected regions. The vertical coordinate system should therefore be managed in a way that minimizes such coordinate movements, while maintaining adequate grid resolution in vertically-mixed regions and maximizing the volume of the ocean that is represented with isopycnic coordinates.

4. Governing equations. The survey [6] contains a detailed derivation of the equations for conservation of mass, momentum, and tracers for a hydrostatic fluid that is in motion relative to a rotating spheroid. In that derivation the vertical coordinate is arbitrary, and the horizontal coordinates are arbitrary orthogonal curvilinear coordinates.

The goal of the present section is to describe some aspects of these equations, without going into full details or derivation; the reader is referred to [6] for further information. Section 4.1 describes the two-dimensional shallow water equations for a homogeneous (single-layer) fluid, and Section 4.2 outlines the three-dimensional equations. For notational simplicity, the horizontal coordinates are taken to be Cartesian coordinates, so the equations describe motion relative to a tangent plane attached to the rotating spheroid. (At any point on the spheroid, the terms "horizontal" and "vertical" refer to directions that are tangent and normal to the spheroid, respectively.)

4.1. Shallow water equations. The shallow water equations are based on the assumption that the fluid has constant density and that the fluid satisfies the shallow water condition, i.e., the depth of the fluid is far less than the horizontal length scale for the motions of interest.

The assumption of constant density is used in certain applications, such as to model tides, tsunamis, and storm surge. However, this assumption is too restrictive for modeling the general circulation of the ocean. Nonetheless, in studies of the general circulation the shallow water equations are still of great interest, for multiple reasons. (1) These equations enable one to demonstrate, in a relatively simple setting, some of the effects of a rotating reference frame, such as geostrophic balance, conservation of potential vorticity, and Rossby waves. (2) For purposes of numerical simulations, it is highly desirable to split the full three-dimensional problem into fast and slow subsystems that are solved by different techniques. In such a splitting, the fast subsystem is very similar to the shallow water equations. (3) For a three-dimensional system with an isopycnic vertical coordinate, a vertical discretization resembles a stack of shallow-water models.

4.1.1. Implications of the shallow water condition. It was mentioned in Section 2.1 that the shallow water condition implies that the fluid is nearly hydrostatic. This conclusion can be developed via formal scaling arguments, but here we only summarize the main ideas with an informal discussion. If the horizontal velocity field displays positive divergence, then the fluid is being spread out in the horizontal, which implies that the free surface at the top of the fluid must fall. Similarly, negative horizontal divergence implies that the free surface must rise. Now assume that the shallow water condition is valid, and consider a horizontal distance L over which the horizontal velocity varies significantly. The horizontal divergence acts on the mass flux over the relatively small vertical extent of the fluid, but the effects of this divergence are spread out over the much greater distance

L. Thus the free surface elevation must change very slowly. The vertical acceleration in the fluid is then very small, i.e., the fluid is nearly in hydrostatic balance.

The case of exact balance can be formulated as follows. Let $p(x, y, z, t)$ denote the pressure in the fluid at position (x, y, z) and time t, with z increasing upward; let ρ denote the density of the fluid; and let g denote the acceleration due to gravity. (In the present paragraph, it is immaterial whether ρ is constant.) Suppose that, for each subregion V of the fluid, the vertical component of the net pressure force on the fluid in V is balanced exactly by the weight of that volume of fluid. A consideration of surface integrals and divergence theorem then implies that $\partial p/\partial z = -\rho g$ everywhere in the fluid.

For the sake of the following, let $\eta(x, y, t)$ denote the elevation of the free surface, relative to the equilibrium state $\eta = 0$. Also let p_0 denote the atmospheric pressure at the top of the fluid, and assume p_0 is constant.

Remark 4.1. *The shallow water condition and the assumption of constant density reduce the system to two horizontal dimensions (plus time), provided that the horizontal velocity is independent of z at some time.*

The reason for this is as follows. The hydrostatic condition $\partial p/\partial z = -\rho g$, together with the assumption of constant ρ, implies that the pressure in the interior of the fluid is $p(x, y, z, t) = p_0 + \rho g\big(\eta(x, y, t) - z\big)$. Thus, for a fixed elevation z within the fluid, lateral variations in pressure are due entirely to variations in the elevation of the free surface at the top of the fluid. Furthermore, the nature of that variation is independent of z. Horizontal fluid acceleration is thus independent of z; if the horizontal velocity is independent of z at some time t_0, it must therefore be independent of z for all times. The components of horizontal velocity are thus functions of (x, y, t), and the flow can described completely by this velocity and the elevation η.

4.1.2. Statement of the shallow water equations. In keeping with the preceding conclusions, let $\mathbf{u}(x, y, t) = (u(x, y, t), v(x, y, t))$ denote the horizontal velocity of the fluid; more precisely, $\mathbf{u}(x, y, t)$ is the velocity at time t of whatever fluid parcel happens to be at position (x, y) at that time. Furthermore, $\mathbf{u}(x, y, t)$ is the velocity relative to a *rotating* coordinate system, as the equations that follow describe motion relative to a tangent plane on a rotating spheroid; $\mathbf{u}(x, y, t)$ is not a velocity relative to an inertial reference frame. Also let $h(x, y, t)$ denote the thickness of the fluid layer, i.e, the vertical distance between the top and bottom of the fluid, and let $H(x, y)$ denote the thickness of the layer when the fluid is at rest. Then $\eta(x, y, t) = h(x, y, t) - H(x, y)$. These variables are illustrated in Figure 5. Due to the possibility of variable bottom topography, H need not be constant.

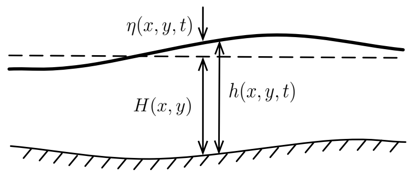

FIG. 5. *Illustration of the mass variables in the shallow water equations. The upper solid curve is a cross-section of the free surface at the top of the fluid, the lower solid curve represents bottom topography, and the horizontal dashed line represents the free surface when the fluid is at rest.*

The equation for conservation of mass is

$$\frac{\partial h}{\partial t} + \frac{\partial}{\partial x}(uh) + \frac{\partial}{\partial y}(vh) \;=\; 0, \tag{4.1}$$

or $\partial h/\partial t + \nabla \cdot (\mathbf{u}h) = 0$. Here, the layer thickness h plays the role of the mass variable; the mass of the water column on any horizontal region A is $\int_A \rho h(x,y,t)\,dxdy$, so ρh is the mass per unit horizontal area in the fluid layer.

The equations for conservation of momentum can be written in component form as

$$\frac{Du}{Dt} - fv \;=\; -g\frac{\partial \eta}{\partial x} \tag{4.2}$$

$$\frac{Dv}{Dt} + fu \;=\; -g\frac{\partial \eta}{\partial y} \tag{4.3}$$

or in vector form as $D\mathbf{u}/Dt + f\mathbf{u}^\perp = -g\nabla\eta$. Here, f is the Coriolis parameter (4.4); $\mathbf{u}^\perp = (-v, u)$; and $D\mathbf{u}/Dt = \mathbf{u}_t + u\mathbf{u}_x + v\mathbf{u}_y$, where subscripts denote partial differentiation.

The operator D/Dt is the material derivative, i.e., the time derivative as seen by an observer moving with the fluid. To see this, let $\big(x(t), y(t)\big)$ denote the position of such an observer. The velocity of the observer is then $\big(x'(t), y'(t)\big) = \big(u(x(t), y(t), t), v(x(t), y(t), t)\big)$, or $\mathbf{u}\big(x(t), y(t), t\big)$. Now let $q(x,y,t)$ be a quantity defined on the fluid region, such as a component of velocity or the density of a tracer. The value of q that is seen by the observer is $q\big(x(t), y(t), t\big)$, and the time derivative of this quantity is $q_t + uq_x + vq_y = Dq/Dt$.

The material derivative $D\mathbf{u}/Dt$ is the time derivative of velocity as seen by an observer moving with the fluid, and so it is the acceleration of that observer and thus the acceleration of a fluid parcel. However, this is the acceleration relative to the *rotating* reference frame of the spheroid. The Coriolis term $f\mathbf{u}^\perp = (-fv, fu)$ provides the necessary correction so that the sum $D\mathbf{u}/Dt + f\mathbf{u}^\perp$ gives the acceleration relative to an inertial reference frame, and it is in an inertial frame where one can apply Newton's second law to obtain a statement of conservation of momentum. The term $-g\nabla\eta$ provides the pressure forcing that produces the acceleration, and it reflects the fact that the lateral variations of pressure within the fluid are due to lateral variations in the elevation of the free surface.

4.1.3. Coriolis term and geostrophic balance. The value of the Coriolis parameter f is defined as follows. Let Ω denote the rate of rotation of the spheroid, in terms of radians per unit time. If a fluid is stationary relative to this spheroid, then the vorticity (curl of the velocity field) is the *planetary vorticity* $2\mathbf{\Omega}$. Here, the velocity is measured relative to an inertial frame attached to the axis of the spheroid, and $\mathbf{\Omega}$ is a vector with magnitude $\Omega = |\mathbf{\Omega}|$ that is aligned with the axis so that $\mathbf{\Omega}$ and the direction of rotation satisfy the right-hand rule. At any point on the rotating spheroid, the Coriolis parameter is the local vertical component of the planetary vorticity $2\mathbf{\Omega}$. That is,

$$f = 2\mathbf{\Omega} \cdot \mathbf{k} = 2\Omega \sin\theta, \tag{4.4}$$

where $\mathbf{k}$ is the unit upward vector at the point in question, and θ is the latitude. See Figure 6. At the equator, $f = 0$, so rotation does not play a role in the momentum equations (4.2)–(4.3) in that case. At the north and south poles, f equals 2Ω and -2Ω, respectively.

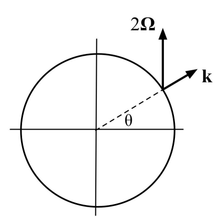

FIG. 6. *The Coriolis parameter $f = 2\mathbf{\Omega} \cdot \mathbf{k}$ is the local vertical component of the planetary vorticity $2\mathbf{\Omega}$.*

For large-scale motions of the ocean (and atmosphere), there is usually an approximate balance between the Coriolis terms and the lateral pressure forcing, except near the equator. This balance is called the *geostrophic balance*. In the case of an exact balance, the momentum equations (4.2)–(4.3) reduce to $f\mathbf{u}^\perp = -g\nabla\eta$, or

$$\begin{aligned} -fv &= -g\frac{\partial\eta}{\partial x} \\ fu &= -g\frac{\partial\eta}{\partial y} \end{aligned}$$

The left side of this system is orthogonal to the velocity vector $\mathbf{u} = (u, v)$, so $u\eta_x + v\eta_y = 0$, or $\mathbf{u} \cdot \nabla\eta = 0$. That is, the velocity is orthogonal to the pressure forcing. Equivalently, the velocity is tangent to curves of constant η, so that the level curves for the free-surface elevation are streamlines for the fluid flow. See Figure 7.

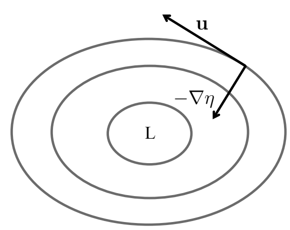

FIG. 7. *Geostrophic balance in the shallow water equations. The velocity is orthogonal to the pressure forcing, and curves of constant free-surface elevation are streamlines for the fluid flow. This behavior is due to the strong influence of the rotating reference frame. In this figure, the center is assumed to be a local minimum of the elevation, and* $f > 0$.

This result is counter-intuitive, based on our everyday experience, but it is a feature of flows that are dominated by rotation. For an analogy, suppose that you want to walk a straight path on a rotating merry-go-round. This path is curved relative to the ground, so you need to exert a side force in order to remain on that straight/curved path.

4.1.4. Potential vorticity and Rossby waves. The horizontal velocity $\mathbf{u} = (u, v)$ is the velocity relative to the rotating reference frame, and the vorticity relative to this rotating frame is then

$$\text{curl}\,\mathbf{u} \;=\; \nabla \times \mathbf{u} \;=\; \left(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}\right)\mathbf{k} \;=\; (v_x - u_y)\mathbf{k},$$

where again $\mathbf{k}$ is the unit upward vector. The quantity $\zeta = v_x - u_y$ is twice the rate of fluid rotation about the axis $\mathbf{k}$, as viewed in the rotating reference frame. As mentioned in Section 4.1.3, the planetary vorticity $2\boldsymbol{\Omega}$ is the curl of the velocity field associated with a rigid rotation of the spheroid about its axis, viewed in the inertial frame, and its local vertical (vector) component is $(2\boldsymbol{\Omega}\cdot\mathbf{k})\mathbf{k} = f\mathbf{k}$. The *absolute vorticity* of the fluid is the vorticity relative to the inertial reference frame, and it is the sum of the relative and planetary vorticities; the vertical component of the absolute vorticity is then $(\zeta + f)\mathbf{k}$.

REMARK 4.2. *Some manipulations of the mass and momentum equations (4.1)–(4.3) yield*

$$\frac{D}{Dt}\left(\frac{\zeta + f}{h}\right) \;=\; 0. \tag{4.5}$$

The quantity $q = (\zeta + f)/h$ is known as the *potential vorticity*. Since the horizontal velocity of the fluid is independent of z, the fluid moves in columns, and equation (4.5) states that the potential vorticity for each material column remains constant as the column moves with the flow.

For example, suppose that h remains constant while a water column changes latitude. Northward movement implies that f increases, so ζ must decrease; this then imparts a clockwise rotation in the fluid, relative to the rotating reference frame. Similarly, southward movement imparts a counter-clockwise rotation. These relative rotations provide restoring mechanisms for the lateral movement of water columns, and the resulting waves are known as Rossby waves. Similarly, variations in bottom topography can cause changes in the layer thickness h, and this then induces changes in $\zeta + f$ via vortex stretching.

4.2. Governing equations in three dimensions. Now consider a hydrostatic fluid for which the density is *not* constant, and assume that for each (x, y, t) the density ρ decreases monotonically as z increases. Because the fluid is hydrostatic, the pressure p must also decrease monotonically with z. Within the fluid, let s be a generalized vertical coordinate; for example, s could be z, σ, an isopycnic coordinate, or a hybrid of these three. Assume that s is strictly monotone increasing as z increases, for each (x, y, t); in order to satisfy this condition in the isopycnic case, s could be the reciprocal of potential density.

All dependent variables are then functions of (x, y, s, t). The surfaces of constant s need not be horizontal; however, the horizontal coordinates x and y shall measure distances projected onto a horizontal plane, not along surfaces of constant s. Similarly, the velocity components $u(x, y, s, t)$ and $v(x, y, s, t)$ measure velocity that is truly horizontal.

4.2.1. Conservation of mass. In the present general setting, it is not appropriate to use the density ρ as the dependent variable for mass, since in the isopycnic case ρ is essentially an independent variable. Instead, for a mass variable use

$$-\frac{\partial p}{\partial s} \;=\; -p_s \;=\; |p_s|\,.$$

(As s increases, p must decrease, so $\partial p/\partial s \le 0$.) For an interpretation of this quantity, consider two coordinate surfaces defined by $s = s_0$ and $s = s_1$, where $s_0 > s_1$. The size of $-\partial p/\partial s$ indicates the amount of mass in the layer bounded by those surfaces. In particular,

$$\int_{s_1}^{s_0} -p_s(x, y, s, t)\, ds \;=\; p(x, y, s_1, t) - p(x, y, s_0, t) \;=\; \Delta p(x, y, t) \ge 0,$$

where Δp denotes the vertical pressure difference between the two coordinate surfaces. Since the fluid is assumed to be hydrostatic, Δp is the weight per unit horizontal area in the layer, i.e., g times the mass per unit horizontal area.

The equation for conservation of mass can be written in the form

$$\frac{\partial}{\partial t}\big(p_s\big) + \frac{\partial}{\partial x}\big(up_s\big) + \frac{\partial}{\partial y}\big(vp_s\big) + \frac{\partial}{\partial s}\big(\dot{s}p_s\big) \;=\; 0. \tag{4.6}$$

Here, $\dot{s} = Ds/Dt$, the time derivative of s following fluid parcels. The last term on the left side of (4.6) is an analogue of the preceding two, as $u = \dot{x}$ and $v = \dot{y}$.

For an example of (4.6), let s be the elevation z. Then $\dot{s} = \dot{z} = Dz/Dt$, which is the vertical component w of linear velocity. Also, $p_s = p_z = -\rho g$, by the hydrostatic condition. The mass equation (4.6) then becomes

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}\big(u\rho\big) + \frac{\partial}{\partial y}\big(v\rho\big) + \frac{\partial}{\partial z}\big(w\rho\big) \;=\; 0,$$

as expected.

Equations for the transport of tracers have a form similar to (4.6), with tracer density replacing p_s, and with the addition of terms that represent the anisotropic diffusion described in Sections 2.3 and 3.1.

4.2.2. Vertical discretization. Numerical solution of the governing equations requires that the spatial domain be discretized by some means. For a vertical discretization, partition the fluid into regions separated by the coordinate surfaces $s = s_0, s_1, \ldots, s_R$, with $s_0 > s_1 > \ldots > s_R$. Now integrate the mass equation (4.6) vertically over layer r, i.e., for $s_r < s < s_{r-1}$, to obtain

$$\begin{aligned} &\frac{\partial}{\partial t}\big(\Delta p_r\big) + \frac{\partial}{\partial x}\big(u_r \Delta p_r\big) + \frac{\partial}{\partial y}\big(v_r \Delta p_r\big) \\ &\qquad\qquad + \big(\dot{s}p_s\big)_{s=s_r} - \big(\dot{s}p_s\big)_{s=s_{r-1}} \;=\; 0. \end{aligned} \tag{4.7}$$

Here, $\Delta p_r(x, y, t) = p(x, y, s_r, t) - p(x, y, s_{r-1}, t)$, and

$$u_r(x, y, t) = \frac{1}{\Delta p_r} \int_{s_r}^{s_{r-1}} u(x, y, s, t)\big(-p_s(x, y, s, t)\big)\, ds.$$

The quantity u_r is the mass-weighted vertical average of u in layer r. The mass-weighted vertical average v_r is defined similarly. In the preceding, the subscript in the quantity $\dot{s}p_s$ refers to a partial derivative, but otherwise the subscripts refer to layers and interfaces.

The terms involving $\dot{s}p_s$ represent mass transport between layers. In the case where $s = z$, this term is simply $\dot{s}p_s = \dot{z}p_z = -w\rho g$. In general, a nonzero value of $\dot{s}$ means that the value of s associated with a fluid parcel is changing with respect to time. In the case of an isopycnic coordinate, such a change could arise from a heating or cooling of the fluid. A fluid parcel could be motionless in space, but due to thermodynamic changes a surface of constant s could move across the parcel; from the point of view of the coordinate surface, the fluid parcel moves across the surface. In the case of a hybrid coordinate, a grid generator might deliberately move a coordinate surface relative to the fluid, and this action would be represented by a nonzero value of $\dot{s}$.

Related ideas explain why one would use potential density instead of true density for an isopycnic coordinate. Suppose that s were the reciprocal of true density ρ. Also suppose that, at some horizontal position (x, y), the layer between $s_r = 1/\rho_r$ and $s_{r-1} = 1/\rho_{r-1}$ is thickened due to lateral mass transport and that the effect of this thickening is move the lower boundary of the layer deeper into the fluid. Due to compressibility, the density of the fluid on this lower boundary must increase, so that its density is no longer equal to ρ_r and its vertical coordinate is no longer equal to $s_r = 1/\rho_r$. Instead, the coordinate surface $s = s_r$ must be located somewhere higher in the fluid; a portion of the water mass must therefore have crossed the surface $s = s_r$. This transport would be included in the term $\left(\dot{s}p_s\right)_{s=s_r}$. On the other hand, *potential* density is invulnerable to such effects, since by definition it is linked to a fixed reference pressure; in that case, the transport term $\dot{s}p_s$ can be reserved for subtler thermodynamic effects.

4.2.3. Conservation of momentum. In the vertically-discrete case, the conservation of horizontal momentum in layer r can be expressed by the equation

$$\frac{D\mathbf{u_r}}{Dt} + f\mathbf{u_r}^{\perp} \;=\; -\left(\nabla M - p\nabla\alpha\right) + \frac{1}{\Delta p_r}\Big[\dot{s}p_s\mathbf{u}\Big]_{s=s_r}^{s=s_{r-1}} + \mathbf{F_r}\;. \tag{4.8}$$

Here, $\mathbf{u_r} = (u_r, v_r)$, $\alpha = 1/\rho$, $M = \alpha p + gz$ is the Montgomery potential, and $\mathbf{F_r}$ denotes the effects of viscosity and shear stresses. The quantity $\dot{s}p_s\mathbf{u}$ represents momentum transport across coordinate surfaces.

The quantity $-(\nabla M - p\nabla\alpha)$ represents the horizontal pressure forcing. The differentiations in the operator $\nabla = (\partial/\partial x, \partial/\partial y)$ are taken for fixed vertical coordinate s. However, surfaces of constant s need not be horizontal, whereas the pressure forcing requires the gradient of pressure for fixed z; the difference of the two terms contains the required transformations. The hydrostatic condition $\partial p/\partial z = -\rho g$ is equivalent to $\alpha\partial p/\partial s + g\partial z/\partial s = 0$, which in turn is equivalent to

$$\frac{\partial M}{\partial s} = p\frac{\partial \alpha}{\partial s}. \tag{4.9}$$

Equation (4.9) can be discretized to communicate pressure effects between layers.

In the case of a layer of constant density, the hydrostatic condition implies that M is independent of vertical position. Suppose that a homogeneous (single-layer) fluid is bounded above by constant atmospheric pressure p_0, and let z be the vertical coordinate. In this case, $M(x,y,t)$ equals its value at the free surface, so $M(x,y,t) = \alpha p_0 + g\eta(x,y,t)$, and therefore $-(\nabla M - p\nabla\alpha) = -g\nabla\eta$. The pressure forcing used in (4.8) thus reduces, in this case, to the pressure forcing that is used in the shallow water equations.

4.2.4. Summary of the three-dimensional equations. The governing equations for the flow consist of the mass equation (4.7); the momentum equation (4.8); advection-diffusion equations for temperature, salinity, and perhaps other tracers; a discretization of (4.9); and an equation of state that relates potential density, potential temperature, and salinity. (Potential temperature has a definition analogous to that of potential density.)

In the case of an isopycnic coordinate, the quantity $\dot{s}$ is generally small, and the equations (4.7) and (4.8) for conservation of mass and momentum in layer r resemble the shallow water equations. The system of equations for the entire three-dimensional fluid can then be regarded informally as a stack of shallow-water models, with mechanisms for transporting mass and pressure effects between layers. Isopycnic and hybrid-coordinate models are therefore often referred to as *layered models*.

5. Multiple time scales and time-stepping. As noted in Section 2.2, the ocean admits motions that vary on a wide range of time scales. In particular, in the mid-ocean the external gravity waves have speeds that are two orders of magnitude greater than the other motions that are seen there. If an explicit time-stepping method is used to solve a system of partial differential equations, then the maximum allowable time step is limited by the fastest motions that are present, and in the present application the fast external gravity waves impose a severe constraint.

As described in Section 2.2, the external motions are nearly two-dimensional, in the sense that if the motion of the ocean is purely an external mode, then the motion is described approximately by the behavior of the free surface and the horizontal velocity at the top of the fluid. The irony of this situation is that the circulation of the ocean is complex and three-dimensional, yet the time step for explicit schemes is severely limited by relatively simple two-dimensional dynamics.

5.1. Barotropic-baroclinic splitting. A widely-used remedy for this difficulty is to split the problem into two subsystems. One subsystem models (approximately) the slow internal and advective motions, and it is solved explicitly with a time step that is determined by these slow motions. This system is referred to as the *baroclinic* system. The other subsystem, known as the *barotropic* system, is used to model (approximately) the fast external motions. This system is two-dimensional and resembles the shallow water equations for a fluid of constant density. The barotropic equations can either be solved explicitly with a short time step dictated by the fast external gravity waves, or they can be solved implicitly with the same long time step that is used for the baroclinic equations. Using small time steps or implicit methods raises the specter of high computational cost, but these measures are applied to a relatively simple two-dimensional subsystem instead of the full three-dimensional system. If an explicit method with short steps is used for the barotropic equations, the resulting coupled algorithm is sometimes referred to as *split-explicit* time-stepping.

An explanation of terminology is in order. In classical fluid dynamics, the term "barotropic" refers to a fluid state in which the pressure is constant along surfaces of constant density. This is approximately the case for a purely external motion, as the undulations of each density surface are synchronized with those of the free surface at the top of the fluid. (See Figure 1.) However, this is not the case with internal waves, and the term "baroclinic" is used in that situation.

In general, it is not possible to split the fast and slow motions exactly into separate subsystems; instead, approximate splittings must be sufficiently accurate. Different approaches have been used to implement the idea of barotropic-baroclinic splitting, as outlined in [6]. Generally speaking, a splitting proceeds along the following lines.

For the barotropic equations, use vertical summation and/or averaging of the mass and momentum equations. This produces two-dimensional equations in which the vertical variations in the dependent variables have been homogenized. For the three-dimensional baroclinic equations, two basic approaches can be used. For the mass equations, at each time step one could solve the mass equation in each layer and then employ some small flux adjustments to ensure that the algorithms used to solve the layer mass equations are consistent with those used to solve the vertically-integrated barotropic mass equation [5]. This has the effect of applying a time filter to the layer equations so that a long time step can be used safely. For the momentum equations, one could use an analogous approach, or an alternative is to subtract the equation for the vertically-averaged barotropic velocity from the equation for the velocity in layer r to obtain an equation for the (slowly-varying) baroclinic part of the velocity in layer r.

5.2. Remarks on constructing a time-stepping method. A time integration method that has traditionally been used in ocean modeling is the centered, three-time-level, leap-frog method. However, this method allows a computational mode consisting of sawtooth oscillations in time, and in a nonlinear model this mode can grow and swamp the solution unless it is filtered sufficiently. Accordingly, some recent work has gone into developing alternative time-stepping methods that do not suffer from this limitation. See, e.g., [4] and [10]. For example, this author [5] has developed a two-time-level method for usage with barotropic-baroclinic splitting for layered models. This method involves some predicting and correcting, is stable subject to the usual Courant-Friedrichs-Lewy condition, displays essentially no spurious numerical dissipation, and is second-order accurate.

For the sake of potential future development in this area, following are some thoughts related to the development of time-stepping methods for ocean circulation models.

(1) For reasons of computational efficiency, a time integration method should use a barotropic-baroclinic splitting, in some way or another.

(2) In such a splitting, each subsystem requires data from the other. However, somebody has to go first, and this is the reason for the predicting and correcting in the time-stepping method in [5]. The ordering and nature of operations must be chosen so as to maintain numerical stability.

(3) Suppose that the barotropic equations are solved explicitly with many short substeps of a (long) baroclinic time interval. When values of the rapidly-varying barotropic variables are communicated to provide forcing to the baroclinic equations, time averages should be used instead of instantaneous values in order to avoid problems with sampling and aliasing.

(4) Enforcing consistency between the barotropic and baroclinic equations may require some care.

(5) The Coriolis terms are energetically neutral, so their implementation should be stable and also avoid numerical dissipation. The Coriolis terms and pressure terms should be evaluated at the same time level; otherwise, the geostrophic balance will contain a first-order truncation error in time.

(6) The baroclinic equations are applied in each coordinate layer, and the forcing terms are complicated. The momentum equations include Coriolis terms, momentum flux, pressure forcing, viscosity, and shear stress. The mass equations include lateral mass fluxes and fluxes across coordinate surfaces, and it is likely that flux limiting will be necessary.

(7) Algorithms should be feasible for usage with many layers, such as dozens of layers or more. For example, the complexity of the forcing may place limitations on the number of stages that can be used in a time-stepping method. Also, the layers are coupled, and it may not be practical to use a Riemann solver over an entire water column to compute mass and momentum fluxes.

(8) For the sake of integrations over long time intervals, one could consider implicit time-stepping methods for the full three-dimensional model. Such methods require the solution of large systems of algebraic equations at each time step, and this task is substantial. One possibility for solving such systems is to use a Jacobian-Free Newton-Krylov method (e.g., Knoll and Keyes [7]), with a preconditioner based on split-explicit time-stepping.

6. Spatial discretization. In its horizontal extent, the ocean occupies a complicated domain on the surface of a spheroid. Due to the complexity of oceanic flows, one would like to use as high a spatial resolution as possible; however, for reasons given in Section 2.3, there will inevitably be unresolved processes that must be parameterized in some manner. The present section describes some horizontal spatial discretizations that have been used in ocean models and/or may be used in the future.

6.1. Rectangular grids. Logically-rectangular grids have traditionally been used in the numerical modeling of ocean circulation, and in operational ocean modeling they remain the dominant type of grid. Such grids are relatively simple and are natural for using finite difference and finite volume methods.

However, a problem with rectangular grids is the inevitable convergence of grid lines. In the case of a latitude-longitude grid, the grid lines converge at the north and south poles, and the north pole is within the fluid domain for a global ocean model. The resulting singularity in the curvilinear coordinates makes this grid unsuitable for such a model.

An alternative that has been used in operational models is a tri-polar grid. With such a grid, latitude and longitude are used to the south of a specified latitude. To the north of that latitude, each curve of constant longitude extends northward to connect smoothly with another longitude line that comes northward from another part of the earth. Orthogonal curves to these quasi-longitude curves then yield a rectangular grid. This arrangement generates two coordinate poles for the northern hemisphere, but the grid can be configured so that these two poles lie on land masses. See Figure 8.

FIG. 8. *A tri-polar rectangular grid. In the northern hemisphere, the grid has two singular points, and these are located outside the fluid domain. (Figure provided by Philip W. Jones, Los Alamos National Laboratory.)*

On a rectangular grid, there are multiple possibilities for the spatial arrangement of the dependent variables, as reviewed, for example, in [4] and [6]. In the following descriptions, regard grid rectangles as mass cells. In the 1960's, Arakawa and co-workers analyzed some possible grid arrangements and labeled these grids as A through E. For example, on the A-grid all quantities are defined at cell centers; with the B-grid, the horizontal components of fluid velocity are defined at cell corners; and in the case of the C-grid, the normal components of fluid velocity are defined at the centers of cell edges. The B- and C-grids are the ones that are generally used in existing ocean models.

Because of the staggered nature of the B- and C-grids, some spatial averaging is needed in order to implement the pressure gradient and Coriolis terms, respectively, and this averaging allows the possibility of various kinds of grid noise. Also, despite their relative superiority to other rectangular grid arrangements, the B- and C-grids can still allow substantial inaccuracy in the propagation of gravity waves and Rossby waves, depending on the grid resolution.

6.2. Unstructured grids. Compared to regular rectangular grids, unstructured grids can provide a better fit to the complicated geography of the ocean's boundary. Also, some regions of the ocean, such as the western boundary currents, are more active than other regions, so variable resolution within the fluid domain may be desirable. However, in the field of ocean circulation modeling, unstructured variable-resolution grids do not seem to be as firmly established as in other areas of computational science. A survey of some issues involved in three-dimensional ocean modeling on unstructured grids is given by Pain et al [8].

For numerical methods on such grids, one possibility is to use finite element methods, either of the continuous Galerkin or discontinuous Galerkin variety. An example of the former is the finite-element shallow-water model of White et al [11]. Discontinuous Galerkin (DG) methods have been used with the shallow water equations to model storm surges in localized regions, e.g., Dawson et al [3]. The high locality of DG methods is an appealing feature, given the massive parallelism that is needed for large-scale ocean simulations.

Another option, which represents a major break from tradition, is to employ a Voronoi grid. See, e.g., Ringler et al [9]. With such a grid, the starting point is to choose a set of points that serve as *grid generators.* (Here, the term "grid generator" has a different meaning than in Section 3.2.) For each grid generator, the corresponding grid cell is the set of points that are closer to that generator than to any other generator; see Figure 9. If the grid generators are arranged in a rectangular array on a plane, then the grid cells are rectangles. On a spheroid, the vertices in a uniform triangulation could be used as grid generators; in that case the resulting grid cells are hexagons or pentagons, mostly the former, and the triangles can be regarded as a dual grid. More generally, the grid generators can be distributed arbitrarily, so as to produce a variable-resolution grid for which the grid cells are convex polygons. When partial differential equations are discretized on a Voronoi grid, divergence and curl are computed with a discrete vector calculus that uses line integrals around the boundaries of grid cells or dual cells. The authors of [9] are presently developing models of ocean circulation and atmospheric circulation with Voronoi grids as the method of spatial discretization.

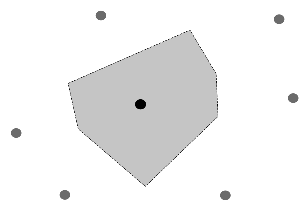

FIG. 9. *Voronoi grid. The dots represent grid generators, and the shaded region is a grid cell.*

7. Summary. This paper describes some physical and computational issues that are encountered when the circulation of the ocean is modeled numerically. These include multiple scales, the choice of vertical coordinate, properties of the governing equations, and time and space discretizations. Operational ocean models represent large-scale efforts by many people, and numerous models are already at a high state of development. However, this paper describes some areas of further work that could involve mathematical scientists, including time-stepping, hybrid vertical coordinate, variable-resolution horizontal grids, and methods for spatial discretization on such grids.

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