Ocean Circulation Modeling for Operational Oceanography: Current Status and Future Challenges

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This chapter focuses on ocean circulation models used in operational oceanography, physical oceanography and climate science. Ocean circulation models are a particular branch of ocean numerical modeling that focuses on the representation of ocean physical properties over spatial scales ranging from the global scale to less than a kilometer and time scales ranging from hours to decades. As such, they are an essential building block for operational oceanography systems and their design receives a lot of attention from operational and research centers.

Introduction

cean modeling is an important branch of operational oceanography. Ocean numerical models are an essential building block of global and regional operational oceanography systems. In this context, ocean circulation models are used in conjunction with data assimilation for extrapolating both in space and in time the available satellite and in situ oceanic observations in order to build a physically consistent estimate of the ocean state and its evolution. Ocean modeling is a relatively recent discipline in the field of oceanography. The underlying principles of the algorithmic formulation of ocean circulation models were first proposed in the 1960s by Bryan (1969; see also McWilliams [1996] for an historical review). Since then, the continuous increase in computing power has allowed ocean circulation models to provide ever more meaningful and comprehensive descriptions of the ocean circulation. Ocean modeling is now recognized as an essential supplement to more traditional scientific methodologies in oceanography. The variety of oceanic physical processes accounted for in ocean circulation models has also notably broadened over past decades. The original scope of ocean circulation models was to describe oceanic properties and physical processes at scales significantly larger than the mesoscale (horizontal scales on the order of 100 km and time scales on the order of three months). But the increase in computing power and the improved physical consistency of their formulation now allow ocean circulation models to resolve routinely oceanic flows down to the submesoscale (horizontal

Le Sommer, J., E.P. Chassignet, and A.J. Wallcraft, 2018: Ocean circulation modeling for operational oceanography: Current status and future challenges. In "*New Frontiers in Operational Oceanography*", E. Chassignet, A. Pascual, J. Tintoré, and J. Verron, Eds., GODAE OceanView, 289-306, doi:10.17125/gov2018.ch12.

scales on the order of 10 km; Chassignet and Xu [2017]) and to describe internal wave and internal tides at a global scale (Shriver et al., 2012).

The range of uses and applications of ocean circulation models has diversified over the past several decades. Ocean circulation models are now used standalone for simulating ocean circulation; when integrated in a data assimilation framework, they may be used for producing short-range ocean forecasts and for ocean reanalysis; coupled to atmospheric circulation models, they may be used for seasonal to decadal forecasts; and fully integrated into Earth System Models, they are crucial to climate modeling. Scientists also use ocean circulation models as the experimental tool of choice for improving our mechanistic understanding of the ocean.

The variety of oceanic physical processes accounted for in ocean circulation models has also broadened in recent decades. Ocean circulation models were initially used to describe oceanic properties and physical processes at scales significantly larger than the mesoscale (horizontal scales on the order of 100 km and time scales on the order of three months). But the increase in computing power and improved physical consistency of their formulation now allow ocean circulation models to resolve routinely oceanic flows down to the submesoscale (horizontal scales on the order of 10 km; Chassignet and Xu [2017]) and to describe internal wave and internal tides at the global scale (Shriver et al., 2012; Savage et al., 2017).

However, despite the maturity and broad range of applications of ocean circulation models achieved to date, ocean modelers still face notable challenges. Running ocean circulation models at increased model resolution does not solve the problem of subgrid scale closures (unresolved processes), and may even question some of the underlying assumptions and algorithms of current ocean circulation models (hydrostatic vs. non hydrostatic, for example). The modularity of modern geoscientific models requires the design of robust and physically rational approaches for coupling ocean circulation models with other model components. Most importantly, there is a growing concern about the necessity to describe explicitly how model uncertainty propagates in geoscientific modeling systems. This is why ocean circulation model design is still a very active field of research and will likely remain so well into the future.

In this chapter, we aim to: (i) briefly describe the principles that underpin the formulation of ocean circulation models, (ii) review current skills of ocean circulation models, and (iii) present what we believe are the new frontiers in ocean circulation model design. Obviously, given the complexity of the issues at stake and the amount of energy that is put into ocean model development, this chapter will only briefly touch upon the above objectives. Our goal is therefore not to cover these questions thoroughly, but rather to provide an entry point to the science of ocean models. The second section of this chapter focuses on the science and applications of ocean circulation models; the third section describes ongoing research avenues geared toward improving the representation of physical processes in ocean circulation models; and the fourth section describes the ongoing paradigm shift in ocean modeling towards a more probabilistic description of oceanic flows. More general considerations regarding the future of ocean modeling are presented in the conclusion.

Ocean Circulation Models: Scope, Usage, & Fundamentals

Ocean modeling is a branch of numerical modeling that focuses on representation of the physical mechanisms governing the evolution of ocean physical properties, namely T, S, u, v, and w, where T is temperature, S is salinity, and u, v, and w are the horizontal and vertical components of the velocity V. A good understanding of a range of physical processes is required in order to build a numerical model that is capable of faithfully representing the ocean circulation. Without this physical understanding, it is easy to derive erroneous conclusions since a numerical model is constructed using discretized equations of motion. Indeed, direct numerical simulations (DNS) of the ocean (i.e., numerical representation of the smallest turbulent scale, i.e. the Kolmogorov length scale, which is on the order of 1 cm (Smyth et al., 2001)), is not possible with present-day computers. The largest simulation achievable today is on scales of 10 m (Yeung et al., 2015).

At present, we cannot represent these small scales; we can only achieve a truncated representation of the ocean and this will remain the case for the foreseeable future. The spatial and temporal scales that one can currently represent strongly depends on the model configuration and application. High resolution operational oceanography requires accurate depiction of upper ocean structure and mesoscale features such as eddies and meandering fronts. Accurate sea level representation is crucial for coastal models (response to wind, tides, and surface pressure) and seasonal-to-interannual forecasts require a good representation of the upper ocean mass field and the coupling to an active atmosphere. On global and basin scales, high horizontal resolution ($1/10^{\circ}$ to $1/25^{\circ}$ and very rarely to $1/50^{\circ}$; Chassignet and Xu [2017]) is mostly used for ocean "weather" and seasonal-to-decadal variability (Fig. 12.1). The emphasis is on short integrations (years to decades) and most models of this class are coupled to a sea-ice model but are stand-alone and use prescribed atmospheric fields. Coarser resolution ($1/4^{\circ}$ to 1°) is principally used for climate applications (Griffies et al., 2000). The emphasis for this class of models is on long integrations with fully coupled ocean-ice-atmosphere models.



Figure 12.1. Example of submesoscale permitting modeling – March 1st surface vorticity over the Gulf Stream in $a1/50^{\circ}$ North Atlantic domain (~1.5 km horizontal grid spacing). Adapted from Chassignet and Xu (2017).

In practice, ocean models consist of a numerical solution to a set of partial differential equations (PDEs) describing the ocean dynamics. These PDEs are based on an approximated version of Navier-Stokes equations adapted to our regimes of interest (see the review papers by Griffies [2004] and Griffies and Treguier [2013] for details). An ocean numerical model typically consists of 20,000 to 200,000 lines of code, usually written in FORTRAN, and can easily take up to 10 years of community development to be fully functional.

The first ocean numerical model was put forward by Bryan (1969) following in the footsteps of numerical weather prediction. The first discretized equations for an atmospheric application were solved manually by Richardson (1922) and numerically by Charney et al. (1950). The latter consisted of a 15 by 18 grid ($\Delta x = 736$ km) and demonstrated that numerical weather prediction was possible. The latest configurations use horizontal resolution Δx on the order of 1 km (Chassignet and Xu, 2017). The sheer size of the ocean problem is such that it will always require the latest generation of supercomputers, and ocean/climate models have traditionally been one of the biggest users of computer resources. This means that close collaborations with computer scientists are essential to ensure that the numerical codes run efficiently and take full advantage of the computing architecture, as this changes constantly and ocean modelers need to be flexible and ready to adopt new approaches. The main limitation is not computational speed of the processors, but access to memory and latency in reading/writing on disk drives (I/O). This limitation is not likely to change in the near future since supercomputer development is closely linked to the performance of commodity chips, which are not well-adapted to ocean applications (i.e., GPUs) and do not facilitate memory access.

There is a wide range of applications for ocean models. Without data assimilation, they are mostly used to scientifically rationalize the observed ocean by testing mechanisms underlying observations via idealized or realistic configurations. With data assimilation, they are used to perform hindcasts in order to understand past evolution and to perform forecasts that can be used for societal applications (Chassignet and Verron, 2006; Dombrowsky et al., 2009; Schiller and Brassington, 2011; Bell et al., 2015). Observational data via data assimilation sets the stage for model state estimates and forecasts (Chassignet et al., 2009). The quality of the estimates and the forecast will depend on the ability of an ocean numerical model to faithfully represent the resolved dynamics of the ocean and the parameterized subgrid scale physics. It is therefore important to realize that even using an infinite amount of data to constrain the initial conditions of an ocean model will not necessarily improve the forecast when using a poorly performing ocean numerical model.

It is also important to realize that while numerical models are necessary to understand ocean dynamics, they cannot represent reality because of limitations in computational power, incomplete understanding of subgrid scale parameterizations, poorly known forcing fields, and poorly understood interactions with other components of the earth's system such as the atmosphere and sea ice. Observations are also not an accurate representation of reality because of the many space and time gaps in the observations that give us only limited information about the ocean's state, its variability, trends, and possible instabilities and regime shifts.

In summary, while numerical models allow for hypothesis testing and experimentation, one needs to understand their limitations in order to use them to their full potential. Good modelers are aware of the strengths AND weaknesses of their models, and the main difficulty is the quantification of the truncation errors introduced by the discretization of the Navier-Stokes equations.

Truncation errors arise from the discretization of PDEs derived from the Navier-Stokes equations, which usually assume that the ocean is incompressible and make the spherical approximation (assumes the earth is a sphere), the thin-shell approximation (allows to neglect variations of the local rotation rate with respect to depth, therefore simplifying the treatment of the Coriolis acceleration), the Boussinesq approximation (neglects variation of relative density in the horizontal momentum equations), and the hydrostatic approximation (allows to neglect the vertical acceleration).

The primitive Navier-Stokes equations are

$$\frac{\partial I}{\partial t} = -\nabla \cdot (T\mathbf{U}) + D^{T} + F^{T}$$
$$\frac{\partial S}{\partial t} = -\nabla \cdot (S\mathbf{U}) + D^{S} + F^{S}$$

with U_h is the horizontal velocity vector (u,v); U, the three-dimensional velocity (u,v,w); f, the Coriolis parameter; p, the pressure; g, the gravity; ρ , the density; T, the temperature; S, the salinity; D, the dissipation; and F, the forcing. Temperature and salinity here implicitly refer to conservative temperature and absolute salinity as defined in the Thermodynamic Equation Of Seawater - 2010 (TEOS-10; McDougall and Barker, 2011). The equation of seawater relates density to temperature, salinity and pressure:

$$\rho = \rho(T, S, p)$$

Several other equations are required for setting boundary conditions at the ocean surface and at the seafloor. For instance, ocean circulation models enforce the following conditions at the ocean surface:

- Kinematic boundary condition

$$\frac{\partial \eta}{\partial t} + \mathbf{U}_h \cdot \nabla \eta = w_{|surf} + E - P$$

- Surface pressure condition

$$p_{|surf} = p_{atm}(x, y, t)$$

- Air-sea fluxes of freshwater and heat

$$K_v \frac{\partial T}{\partial z}_{|surf|} = -\rho C_p Q \qquad K_v \frac{\partial S}{\partial z}_{|surf|} = 0$$

- Air-sea fluxes of momentum

$$A_v \frac{\partial \mathbf{U}_h}{\partial z}_{|surf} = \frac{1}{\rho_0}(\tau_x, \tau_y)$$

where η is the sea surface height, *E*, the evaporation; *P*, the precipitation; τ , the wind stress; *K*, the diffusivity; A, the viscosity; and *Q*, the heat flux. Finally, one needs to use the turbulent closure hypothesis to close the system by assuming that the nonlinear terms involving correlations of variables at unresolved small scales can be fully prescribed from knowledge of the large scales.

Representation of Physical Processes in Ocean Circulation Models

In this section, we review some of the issues that arise as we strive to improve the representation of key physical processes in the ocean model component of operational systems. This includes broadening the spectrum of *explicitly represented processes* and improving the representation of *unresolved processes* in ocean circulation models.

Resolved versus unresolved physical processes in ocean circulation models.

As discussed in the previous section, ocean circulation models do not account *explicitly* for the entire range of scale interactions that control ocean circulation (Fig. 12.2). Because of the turbulent nature of oceanic flows, ocean circulation at a given scale is indeed fundamentally dependent on oceanic motions at scales ranging from global (of order 10,000 km) to dissipative (of order 1 cm; Fig. 12.3). But the finite grid resolution of a particular ocean model configuration constrains the spectrum of scales of motions that are explicitly represented in the model solution. Consider, for instance, ocean mesoscale eddies, which are known to play a fundamental role in shaping ocean circulation (McWilliams, 2008) and their representation in ocean models, which has motivated a large number of studies. Even the most high-end global ocean circulation models with grid resolutions down to just a few kilometers (Chassignet and Xu, 2017) are still not able to fully capture the dominant length scales of mesoscale eddies are therefore not explicitly represented at high latitudes in these models (Fig. 12.4).



Figure 12.2. Range of ocean physical processes (adapted from Griffies and Treguier [2013]).



Figure 12.3. Space and time scale of ocean physical processes.

Therefore, a practical challenge for most applications of ocean circulation models is to describe the broadest possible spectrum of oceanic scales of motion at a given computational cost. The overall computational budget of an application is constrained by the available computing resources and by the expected time-to-solution, the latter constraint being particularly limiting in operational applications that deliver near real-time products. The model grid of ocean model components of operational systems is also usually constrained by other practical factors. The same model grid is often used for several years because of the effort required to tune the physical model configuration, calibrate the data assimilation components, and prepare the downstream data production chains. Given these constraints, the optimal design of ocean model components in operational systems requires a robust and rational understanding of a priori what controls the spectrum of resolved process in ocean circulation models besides the model grid resolution. Developing this understanding of what controls the spectrum of resolved scales in ocean model should rely on idealized process studies, model inter-comparison exercises and confrontation of model solutions with observations.

A commonly accepted practical criteria for deciding whether a flow feature is resolved in an ocean model is that there should be no less than 2π grid points spanning the feature (see, for instance, Griffies and Treguier [2013]). This is supported by the notion of effective resolution, defined by Skamarock (2004) as the smallest resolved scale that is not significantly affected by numerical dissipation due to discretization errors. The effective resolution of an ocean circulation model is about 6 to $10\Delta x$, where Δx is the horizontal grid resolution, but the validity of the concept of effective resolution is generally restricted to model configurations with small enough grid resolutions and using high order discretization schemes (Soufflet et al., 2016).

Although effective resolution allows us to characterize the smallest scale of motion that could ideally be described without numerical error in an ocean model, it is generally impossible to distinguish unambiguously between resolved and unresolved *physical processes* in ocean circulation models. Indeed, only the physical processes with dynamics that do not depend on scales smaller than the effective resolution are unambiguously represented in a given ocean model configuration. In practice, a lot of physical processes of interest involve scales between the model grid scale and the model effective resolution. In such cases, although the model is a priori unable to fully account for the dynamics, the model solutions may still exhibit some properties of the misrepresented physical process. A good example of such a situation is discussed in a recent study by Uchida et al. (2017), who found signatures of submesoscale mixed layer instabilities in their 1/10° resolution model although their model grid resolution is a priori not able to adequately capture these dynamics.

How to broaden the spectrum of resolved processes in ocean circulation models?

Using computationally efficient numerical discretization schemes with good mimetic properties is a first approach for broadening the spectrum of resolved processes in ocean circulation models at a given computational cost. The notion of *computational efficiency* refers to the accuracy of model

solution relative to the computational cost of numerical integration. The notion of *mimetic properties* refers to the ability of a discrete model to emulate the properties of the underlying continuous mathematical model, for instance as conservation laws and geometrical symmetries. Ocean circulation models with grid resolutions approaching 1 km can be sensitive to numerical discretization schemes (Ducousso et al., 2018). This is because ocean model solutions are generally more nonlinear and less controlled by diffusion in this range of resolution. The current trend in ocean circulation modeling is, therefore, to use high order discretization schemes in order to increase model effective resolution (Soufflet et al., 2016).

Multiscale modeling approaches coming from coastal ocean modeling also provide a framework for locally increasing the effective resolution according to a particular scientific or operational objective and at a given computational cost. Multiscale modeling methods, which allow us to locally refine the grid mesh, are now commonly used in large-scale ocean circulation modeling. Applications of multiscale approaches in ocean circulation modeling can be classified according to their grid mesh topology into *structured mesh* methods (for instance as orthogonal curvilinear grids used by most ocean circulation models), *unstructured mesh* methods (e.g., see Piggott et al., 2008; Danilov et al., 2017; Ringler et al., 2013) and *block structured mesh* methods (see Blayo and Debreu, 1999; Jablonowski et al., 2006). Although many research efforts have focused on unstructured mesh ocean circulation modeling over recent years, the design of robust discretization schemes for large-scale ocean models on triangular or hexagonal meshes remains challenging (Danilov, 2013). And it should also be noted that it is still unclear how to define objective criteria for adjusting meshes and, therefore, optimally use the potential for mesh refinement and mesh adaptability of multiscale modeling approaches in large-scale ocean circulation models.

Improving the performance of ocean circulation models on modern high performance computing (HPC) platforms is also essential for broadening the spectrum of resolved scales. The current trend in HPC is toward massively parallel machines with heterogeneous multicore architectures (Giles and Reguly, 2014). However, while modern HPC platforms can deliver a peak performance in the Petaflop/s range, existing ocean circulation models are unable to exploit this potential. The *computational intensity*, i.e., floating point operations per memory access, of ocean models is very low because they are dominated by stencil operations (typical of discretized PDEs). So, they typically run at ~5% of the system's peak speed. Also, ocean models have a very small vertical dimension, typically O(10), so they scale more like 2-D domains than 3-D domains. In practice, 1/12° and 1/25° global ocean models might scale well to 8,000 and 30,000 cores, respectively. Scalability is eventually limited by the communication overhead, load imbalance, and latency inherent to spatial 2-D domain decomposition and by I/O overhead. Single processor performance depends on computational intensity, which can be improved by using higher order discretization schemes; but scalability can actually be reduced by better single processor performance because relatively more time is spent in communications.

In the future, overcoming single processor and scalability bottlenecks will require sustained collaborations between ocean modelers and computer scientists. Practical approaches will likely involve an increase in hybrid parallel programming in order to more efficiently exploit memory

hierarchy and innovative algorithms for solving the set of PDEs that govern ocean dynamics, as for instance parallelization in time in addition to spatial domain decomposition (Schreiber et al., 2017).

Looking ahead, because of the multiscale nature of oceanic flows and the needs of end-users of operational oceanography, it is necessary for ocean circulation models to account explicitly for the broadest range of physical scales possible. But this broadening of the spectrum of resolved scales will not simply be a consequence of an increase in computing power. How efficiently ocean circulation models will use computing resources will depend on the efficiency of the algorithms used for translating ocean dynamical equations into practical computation. And foreseeing what approach will be most used in the future for broadening the spectrum of resolved scales is not straightforward, but it is arguable that HPC and algorithmic aspects will be crucial in future ocean model development. New advances will most likely rely on a high level of collaboration between ocean modelers, applied mathematicians, and computer scientists.



Grid resolution (km) required for mesoscale resolving effective resolution

Figure 12.4. Grid resolution required to resolve the first baroclinic radius with 10 grid points. The figure shows the local grid resolution (in kilometers) divided by 10 as an estimate the grid resolution required for a model to effectively capture structures with wavelength close to the first baroclinic Rossby radius. The first baroclinic Rossby radius is estimated from a CMEMS 1/12° global reanalysis. The estimate of the number of points required for the effective resolution to match the first baroclinic Rossby radius is slightly more restrictive than that proposed by Hallberg (2013) following the work by Soufflet et al. (2016).

How to better account for unresolved processes in ocean circulation models

Ocean circulation models need to allow for the important physical processes that are not accounted for in their discrete approximation to the ocean dynamical equations. A common approach to the representation of unresolved processes in ocean circulation models is to use a subgrid scale (SGS) closure (aka physical parameterization). Typically, these do not focus on particular nonlinear terms in the primitive equations, but rather on particular physical processes (that may affect several terms). A rough classification of unresolved physical processes would include: (i) SGS closures for balanced turbulence (eddy closures), (ii) SGS closures for processes in the ocean surface boundary layer, (iii) SGS closures for interior mixing processes, and (iv) SGS closures for bottom boundary layer processes. The design of SGS closures associated with physical processes usually involves some combination of idealized process studies with models, realistic process studies with models, targeted field experiments at sea, and (more rarely) lab experiments. Importantly, a SGS closure should always target a particular ocean circulation model resolution because the information at the resolved scale depends on the model resolution.

Depending upon the available information from the scales assumed to be resolved in the target model, two categories of closures can be distinguished. The first is a RANS-type (cf Reynolds average) closure, implicitly based on some sort of ensemble average (in practice emulated through time average); for example, the Gent-McWilliams closure for mesoscale eddy transport (Gent, 2011). The other is a LES type closure (by analogy to Large Eddy Simulation) implicitly based on some spatial average; for example, Leith's (1968) momentum closure. LES-type subgrid closures can further be subdivided into functional and structural closures. Functional closures consider the bulk action of the subgrid terms on the resolved scales (e.g., Smagorinsly momentum closures [Griffies and Hallberg, 2000]). Structural closures aim at estimating the best local approximation of the unknown SGS term by constructing it from the known small-scale stuctures (e.g., closures defined by Taylor series expansion). A recent trend in the design of SGS closures in ocean circulation modeling deals with how to adapt them to the resolved physical scales of motions in the model solution (Bachman et al., 2017). There is also a growing concern in ocean models design regarding the complex interplay between numerical discretization errors and SGS closures, especially in the finest resolution applications (Campin et al., 2011; Lemarie et al., 2012). Another emerging approach to the representation of unresolved processes in ocean circulation models is to couple ocean circulation models with third-party code components, which are specifically designed to describe the evolution of a particular class of processes. Physical processes that are not explicitly accounted for in ocean models have been extensively studied (e.g., wave modelling) and estimates of the subgrid states associated with these unresolved processes must take into account non-local effects in space and time (e.g., propagation and dissipation of internal waves, cf. IDEMIX [Olbers and Eden, 2013]). It may also make sense to modularize, as much as possible, a complex closure so that it can be used in different ocean models and thus become an independent model library or component (e.g., https://github.com/CVMix). How to fully integrate multiple code components, each describing different aspect of the dynamics, in operational systems with data assimilation is likely to become a key research question in the future. A particularly important concern is associated with the representation of the fine-scale feedbacks between the atmospheric and oceanic boundary layers.

Towards Data-driven, Probabilistic Ocean Circulation Models

Stochastic parameterizations in ocean circulation models

Classical approaches in the design of SGS closures for ocean circulation models assumes that the bulk effect of SGS fluctuations can be deterministically predicted from the resolved scales of motions. A number of recent works have started to reconsider this assumption. These more recent studies allow the closure to be only weakly constrained by the resolved scales. Carefully designed stochastic parameterizations appear to be a promising approach to the representation of a large class of unresolved SGS processes in ocean circulation models (Berloff, 2005; Palmer and Williams, 2010; Williams, 2012; Grooms and Majda, 2013; Porta Mana and Zanna, 2014; Cooper and Zanna, 2015; Brankart et al., 2015; Andrejczuk et al., 2016). A certain amount of randomness is introduced with a stochastic procedure to account for the possible variability of fluxes at macroscales. Stochastic parameterizations seem particularly well-suited to the representation of the cross-scale exchanges of energy and momentum for SGS-balanced turbulence (in particular, energy backscatter). Notable improvement of Gulf stream dynamics has also been obtained through the stochastic representation of upscaling due to the nonlinear nature of the equation of the state of seawater (Brankart, 2013). More generally, the concept of introducing random perturbations in ocean models is also supported by another rationale coming from the theory of non-linear systems. The topology of the phase space of non-linear systems can indeed be rather complicated, showing multiple possible local energy minima. Adding perturbations could allow a system to escape from local potential wells and, therefore, explore more reliably the range of possible states.

The paradigm underpinning this idea of stochastic parameterization is actually not restricted to the design of SGS closures and could also allow us to account for more general sources of uncertainty in ocean circulation models. These include errors in their initial condition (particularly at depth), errors in the forcing function (uncertain atmospheric fields, uncertain parameter in bulk formula. etcetera), errors associated with subgrid closures (closures are imperfect models, with usually weakly constrained parameters), errors from the physical approximation use in for their continuous formulation (e.g., non-traditional Coriolis terms), and numerical discretization errors that tend to accumulate over time (even high order schemes have non-zero errors). Overall, uncertainty is a major property of ocean circulation models that physicists often tend to neglect, although some modeling frameworks are now tackling this problem more explicitly (e.g., see Brankart et al., 2015). At this point, it is arguable that further developing stochastic parameterizations for ocean circulation models will require a better understanding of their impact on the resolved scales of motion.

Toward probabilistic ocean circulation modeling through ensemble simulations

Ensemble modeling is a now common approach in operational forecast and climate modeling for accounting for the inherent uncertainty of geoscientific model solutions. Ensembles are, for instance, routinely used in operational systems to account for uncertainty in initial states, model

formulation, or forcing. Because they sample the space of possible states given such uncertainty, ensemble approaches allow for a more objective comparison of model solutions with observations, which is key to operational systems. More recently, ensemble modeling has also become an experimental tool of choice for investigating the sources of oceanic variability in eddying regimes (Sérazin et al., 2017). It should be stressed that ensemble modelling is a reasonable strategy in terms of high performance computing, because in most cases ensemble runs are entirely independent of each other and therefore 100% scalable.

The combination of ensemble and stochastic methods allows us to deal more objectively with uncertainty in ocean models (Toth et al., 2003; Palmer, 2012; Brunton et al., 2016; Bessieres et al., 2017). The purpose of ongoing efforts is to attempt to explicitly sample the probability distribution of possible states given explicitly formulated uncertainties following a Bayesian approach. This shift towards probabilistic ocean circulation modeling is arguably a paradigm transition in our field. But it is still unclear how to deal with the daemon of dimensionality. Indeed, ensemble sizes are usually constrained to several tenth of members for practical reasons while the parameter space they are sampling is orders of magnitude larger. The emergence of probabilistic ocean circulation modeling could bring several benefits to ocean model design and usage in the future. But probabilistic ocean modeling also raises several technical and scientific challenges that ought to be addressed in the future.

Final Remarks

In this chapter, we have briefly described the fundamental principles that underpin the formulation of modern ocean circulation models, shown some of their recent achievements, and discussed what we believe are the future frontiers in ocean circulation model development. This chapter has, in particular, illustrated how a modeling strategy proposed in the 1960s for solving the primitive equations has yielded ocean circulation models that are now used for a wide range of applications and that form a building block of modern operational oceanography. We have also presented the view that future frontiers in ocean circulation modeling will depend upon (i) the computational performance of ocean models, (ii) their ability to represent scale interactions either explicitly or though parameterizations, and (iii) the representation of model uncertainty with stochastic and ensemble approaches.

This chapter illustrates how the field of ocean circulation model design has reached its maturity and now involves strong collaboration between different fields of expertise. Ocean circulation model design is a very active field of research with entire scientific teams dedicated to developing or improving ocean circulation models. The maturity of the field is arguably a consequence of the high level of collaboration and merging of efforts among different groups involved in different applications and aspects of ocean circulation models. A key driver for this collaborative approach to ocean model development is this notion of *seamless* geoscientific modeling, which suggests that the same numerical code can actually be used for a range of different applications covering a range of different resolutions and dynamical regimes (Hurrell et al., 2009). Overall, this approach has improved the robustness of ocean circulation models and the sustainability of the ocean model development process over recent decades.

Although not been discussed much in this chapter, we would like to stress the importance of ocean observing networks for improving ocean circulation models. Sustained ocean observations from satellites and in situ networks are critical for routinely assessing the skills and limitations of circulation ocean models over different timescales ranging from days to decades. There is also much to be learned from targeted field observations aimed at documenting specific oceanic processes in order to improve their representation in models. For instance, recent experiments documenting fine-scale ocean processes in the ocean surface boundary layer provided a wealth of information that can be used for improving surface processes in ocean circulation models (Shcherbina et al., 2015; Buckingham et al., 2016).

An aspect that we believe has also been critical in the continuous improvement of ocean circulation models over recent decades is the shared vision in the ocean modeling community that open source is the only sustainable approach to geoscientific model development. Ocean model developers have generally been early adopters of modern practices in software development (e.g., version control, unit testing, continuous integration). All the major ocean circulation codes are also distributed under open source licenses and therefore exposed to the scrutiny of other research groups. Arguably, workflows in ocean modeling could be improved and made more reproducible, but it is fair to recognize that this community has long been concerned with these issues. Building more open and transparent data processing chains for pre- and post-processing is probably an important next step to making ocean circulation modeling more robust and reproducible in the future (Stodden et al., 2016).

In conclusion, we would like to raise what is likely to become a key issue in the future development of ocean circulation models. With a broadening of scope and an increase in the number of users, ocean circulation models have also grown in complexity. But the actual size of the community of ocean model developers is still rather small. Furthermore, most of the research questions that have been raised in this chapter would require strong and sometimes new collaborations among ocean modelers, field oceanographers, process-oriented oceanographers, applied mathematicians, and computer scientists. Sustained and proactive initiatives from major funding agencies (one good example of such an initiative being the US CLIVAR Climate Process Team scheme) will certainly be vital to the success of these interdisciplinary collaborations and to bringing more early career scientists in to contribute to the science of ocean circulation models.

Acknowledgments

EPC and AJW are supported by the Office of Naval Research and the Naval Research Laboratory. The authors also thank R. Bourdallé-Badie for providing Fig. 12.4.

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