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Summary Report of the CLIVAR WGOMD Workshop on Numerical Methods in Ocean Models 23-24 August 2007 in Bergen, Norway

The CLIVAR Working Group on Ocean Model Development (WGOMD), with assistance from the Layered Ocean Model (LOM) group, organized the workshop “Numerical Methods in Ocean Models” on August 23-24, 2007 in Bergen, Norway.

The evolution of ocean models is prompted by a growing range of high profile scientific and engineering applications. These applications range from refined resolution coastal and regional modelling forecast systems, to centennial-millennial global earth system models projecting future climate. Groups worldwide are working to improve the integrity of ocean models for use as tools for science research and engineering applications. This work involves a significant number of fundamental questions, such as what equations to solve, which coordinate system to solve the equations, what horizontal and vertical mesh is appropriate, what physical parameterizations are required, and what numerical algorithms allow for computational efficiency without sacrificing scientific integrity. Furthermore, given the increasing size of many applications, as well as difficulties of doing everything in just one group, there is a growing level of collaboration between diverse groups. This collaboration spans the spectrum of algorithm sharing to the merger of previously disparate code bases.

The numerical methods workshop aimed to foster the maturation of ocean models by supporting enhanced collaboration between model developers. It did so by bringing together nearly 100 of the world’s top ocean model developers and theoreticians. Presentations were given throughout each day, with plenty of opportunity for interactions, debate, and networking. The workshop emphasis was on fundamentals of design and numerical methods, with relevance of a particular approach gauged by its ability to satisfy the needs of various applications. This workshop provided a venue for participants to educate one another on the latest advances in ocean model development.

The following sessions are summarized below by the respective session Chairs:

1. Overview of equations and methods: Alistair Adcroft (GFDL, Princeton University)
2. Vertical coordinates: Robert Hallberg (GFDL)
3. Non-rectangular structured meshes and unstructured meshes: Todd Ringler (Los Alamos National Laboratory), Matthew Piggott (Imperial College), Laurent White (GFDL)
4. Parameterization of physical process: Richard Greatbatch (IFM-GEOMAR) and Martin Schmidt (Baltic Sea Research Institute)
5. Coastal/Regional modelling: Eric Blayo (Laboratoire Jean Kuntzmann, Universite Joseph Fourier), Jarle Berntsen (University of Bergen)
6. Basin and Global Models: Claus Böning (IFM-GEOMAR), Anne Marie Treguier (IFREMER) and Stephen Griffies (GFDL)
7. Ocean processes and inverse methods: Detlef Stammer (University of Hamburg)
8. Recommendations and closing comment: Stephen Griffies (GFDL)

The talks can be downloaded from the Workshop webpage at:
http://www.clivar.org/organization/wgomd/nmw/nmw_main.php.

The workshop programme is given in Appendix A at the end of the report.

1. Overview of equations and methods: Alistair Adcroft (GFDL, Princeton University)

This session was aimed at establishing a foundation of the fundamental issues involved in building an ocean model. Three presentations were made: i) on the fundamental equations and methods, ii) on algorithms for Eulerian and Lagrangian vertical coordinates, and iii) on finite difference, finite volume and finite element methods.

Building a numerical ocean climate model involves applying knowledge for physical oceanography, numerical methods, applied mathematics and computer science. Historically, large-scale ocean climate models have mostly been developed by groups, even if they were started by individuals, and have evolved into complex computer codes with of the order of hundreds of thousands of lines of code. Their size and complexity contribute to the perception that the ocean modeling community is slow moving and unwillingly to adopt ``modern'' methods now used in computational fluid dynamics and applied mathematics. To this, it is the case that many ocean models are structurally similar to the models used two decades ago. However, there are good reasons for this; large-scale, ocean climate modeling is a unique application of a very different nature to those found in other areas of fluid dynamics. The time-scales of interest in climate are centuries to millennia, the spatial scales of importance in the ocean are of order tens of kilometers and smaller and the problem as a whole is global. The shear computational cost of ocean climate calculations simply excludes many methods used in CFD, even though the community has access to some of the largest and fastest computing resources available. Ocean climate models still use structured grids and essentially grid-point methods (reminiscent of finite difference method) because they are efficient and there is yet to appear a competitive alternative. Nevertheless, progress has been made towards both incorporating new methods into existing ocean models and in the development of new ocean models based on finite element and adaptive methods. In addition to the new numerical methods, there has been much progress in the algorithms, physical assumptions and formulations. Here we will briefly discuss some of these improvements and speculate about what directions ocean models may move towards in the future.

The equations of motion that govern ocean circulation are well known and easily written down but are difficult to solve. They are the Navier-Stokes equations of motion and statements of conservation of salt mass and (heat) energy. It is impractical to solve the Navier-Stokes equations for climate calculations for two main reason:

i) the equations permit acoustic modes with characteristic speed of order 1500 ms^{-1};

ii) the dissipative scales at the end of the turbulent cascade are controlled by molecular processes and are of order millimeters. This last limitation is universally handled by "Reynolds averaging"; space-time filtering of the equations that partitions the state into a resolved components and unresolved sub-grid scale component. Correlations of the sub-grid scale components lead to Reynolds average eddy-fluxes that must be parameterized in terms of resolved or mean state. There have been significant developments in the parameterizations used in ocean climate models but is still a critical area for future research (see the session on parameterization).

Filtering of a different nature is required to deal with the acoustic modes. There are two distinct approximations that independently filter out acoustic modes; the an-elastic (or non-divergence) approximation, that removes the terms responsible for three dimensional wave propagation from the acoustic wave equation; and the hydrostatic balance approximation to the vertical momentum equation, that removes the acoustic wave propagation terms in the vertical only. If the hydrostatic approximation is used alone, there should remain an external horizontally propagating acoustic mode, known in the atmosphere as the Lamb wave; it is curious that this mode does not seem to be exhibited by hydrostatic, non-Boussinesq ocean models for reasons that are unclear.

Often associated with the an-elastic or non-divergence approximations is the Boussinesq approximation, the definition of which varies from author to author. Here, we mean the linearization of the momentum equations by replacing the in-situ density with a reference density. The Boussinesq approximation and non-divergence approximation are normally applied together and such models conserve volume rather than mass. The existence and form of geo-potential energy in the Boussinesq equations with a non-linear equation of state is a controversial issue. The use of the Boussinesq equations for ocean modeling seems to be a legacy of early ocean models that used the rigid-lid approximation and height coordinates; it is simply easier to implement rigid boundary conditions in height coordinates and the Boussinesq approximation makes the height coordinate momentum equations more tractable. Recently, however, it has been realized that the hydrostatic primitive equations written in pressure coordinates conserve mass and can properly represent non-Boussinesq effects such as steric sea level change. Ironically, in-situ observations are measured at pressure and then typically interpolated to approximate height and used in gridded data-sets; with the advent of non-Boussinesq models, the gridded data has to be

interpolated to pressure levels. There seems to be wide-spread agreement that this is the better approach and many modelling groups are moving towards non-Boussinesq formulations.
The conventional ocean climate models of old use simple coordinates, typically geopotential height ("z") or potential density (in the isopycnal class of models). A relatively new idea that has gained wide-spread acceptance in the last decade is to use hybrid coordinates (to which an entire session was devoted later in the meeting). The generalization of ocean models to work in arbitrary or hybrid coordinates involves a significant algorithmic advances over those needed to integrate the equations in "simple" coordinates. A general approach, known as the ALE (Arbitrary Langrangian Eulerian) method was presented by John Dukowicz, along with a general discussion of re-mapping. The concept of remapping and realization that advection is simply re-mapping from one grid to another allows models to become essentially "coordinate free". Although these methods are now in use (e.g. HyCOM and HyPOP), the ocean modelling community has yet to gain experience with the merits (impact, accuracy, etc.) of particular reconstruction and re-mapping approaches. It is generally accepted that these approaches will become the norm for the next cycle of ocean model development.

An overview of finite differences, finite volume, and finite element methods, presented by Mohamed Iskandarani, highlighted both the advances made in the last decade in the appearance of finite volume concepts (in place of finite difference) in ocean models and the potential for the future represented by unstructured approaches, such as is allowed by finite elements and finite volumes. While the finite element and finite volume methods are the preferred choice for the engineering/CFD communities, the merits of "structured" approaches identifiable with the finite difference method still hold sway in most of the ocean modeling community. One important reason for this is the importance of computational efficiency for climate modeling; the difference between waiting 1 week for a 100 year simulation and 1 month can make the difference between being able to conduct reasonable science or not. A session later in the meeting was dedicated to examining the issues of horizontal grids. The bottom line message from this session was that there is still much to be learned and applied from advanced numerical methods which may potentially yield major advances in ocean climate modeling.

2. Vertical coordinates: Robert Hallberg (GFDL)

The vertical coordinate used in an ocean model is often thought of as critical in discriminating between different ocean models. This choice has a large impact on the properties that a numerical ocean model will attain, and hence the applications for which a particular model is the best choice. Considerations include: how readily the pressure gradient terms can be represented and the nature and magnitude of the errors; whether the material changes in temperature, salinity, and tracer concentrations are negligible compared with changes due to physical processes; whether resolution can be easily concentrated in regions of particular interest, including boundary layers or areas of large interior gradients; how readily the top and bottom boundary conditions can be implemented exactly; and whether the vertical coordinate facilitates or hinders the analysis of simulations to answer the question of interest. Based on these considerations, there have traditionally been three distinct approaches to the vertical coordinate in ocean models – depth (or pressure), a terrain-following coordinate that is stretched between the top and bottom boundaries, or using density as the vertical coordinate. While each of these coordinate choices has its strengths and weaknesses, there is no single best vertical coordinate for all applications.

Geopotential- (Z-) or pressure coordinate ocean models have traditionally found wide-spread use in climate applications for several reasons. The equations take on a relatively simple form, and analysis of the simulations seems to be relatively intuitive for people without formal training as physical oceanographers. (Physical oceanographers often think in terms of watermasses, for which density is often the most natural coordinate.) The pressure gradient takes a particularly simple form in depth coordinates, and the errors in the pressure gradient have no baroclinicity, which is particularly useful as it avoids spinning up geostrophically balance flow. For climate studies, perhaps the biggest advantage of using a pressure- or Z-coordinate model is that with many decades of experience, unpleasant surprises are unlikely.

There have traditionally been 3 major shortcomings ascribed to Z-coordinate ocean models for climate use. Firstly, the interior ocean is exceptionally adiabatic, but Z-coordinate ocean models often exhibit much more numerical diapycnal diffusion than is observed to be present (see, for example, Griffies et al., 2000); significant progress has been made in rectifying this situation with improved tracer advection schemes, as described in a talk by S. Griffies in this session. Despite this progress, numerical diapycnal diffusion may continue to be a concern for Z-coordinate models in particularly adiabatic regions with vigorous flow along sloping isopycnals, such as in the equatorial thermocline. Secondly, Z-coordinate models have a great difficulty representing downslope flows without greatly excessive entrainment; as most of the interior ocean is filled by watermasses derived from dense overflows, this is a significant liability for climate use. Despite much effort over the past decade, the explicit representation of overflows in Z-coordinate models at horizontal resolutions that are coarser than a few kilometers and vertical resolutions that are coarser than a few tens of meters remains unsatisfactory. Thirdly, Z-coordinate models were thought to badly misrepresent the effects of topography on the large scale ocean circulation; this issue is no longer relevant, as the partial or shaved cells used by all modern Z-coordinate models largely eliminates it. At this point, the skillful representation of overflows and other terrain-following flows appears to be the greatest shortcoming of Z-coordinate models for climate applications.

Terrain-following-coordinate models (which include s- and s-coordinate models) (TFCMs) have traditionally found extensive use for coastal applications. Topography is represented very simply and accurately in TFCMs, and there is extensive experience with atmospheric modeling to draw upon. Vertical resolution can be arbitrarily enhanced near the surface. There is the impression that the vertical resolution in TFCMs can be arbitrarily enhanced near the bottom as well without drawbacks, but based on the discussion in this session, following a presentation by G. Danabasoglu, this conventional wisdom appears to be erroneous because of the need to avoid pressure gradient errors arising from overly fine vertical resolution.

There does not appear to be consensus on just how steeply sloped the bottom can be in a TFCM, but there is a clear sense that overly steep topography can be highly problematic. With modern TFCMs, the Haney (1991) “hydrostatic inconsistency condition”, requiring that

$$HIC = \left|\frac{\sigma}{D}\frac{\partial D}{\partial x}\right|\frac{\Delta x}{\Delta \sigma} < 1,$$

does not need to be satisfied. (Here x is the horizontal coordinate, *D* is the bottom depth, and $\sigma = z/D$ is the vertical coordinate.) In fact, L. Oey pointed out that the leading order pressure gradient errors exactly cancel when *HIC*=1 with the pressure gradient formulation of Mellor et al. (1994). Similarly, the constraint put forward by Beckmann and Haidvogel (1993), that the variations between the depths at adjacent grid points be smaller than 40% of the mean depth, is not general, in that it was developed for a particular simulation of flow past a seamount with 7 Chebyshev polonomials in the vertical. The question was raised of whether there is, in fact, a theoretically understood principle for how steep topography can be. To the best knowledge of all present, there is no firm limit on how steep topography can be. However, empirical experience with ROMS suggests that with modern formulations of the pressure gradient, keeping *HIC*<3 is safe, and acceptable solutions are sometimes obtained with *HIC* as high as 8 (A. Shchepetkin, pers. comm.). The exact criterion for acceptable slopes will always depend on the precise question being asked of a model, and details of the model state, such as the degree of near-bottom stratification. This consideration strongly suggests that TFCMs are likely to be useful for global-scale studies with reasonable topography only when horizontal resolution is relatively fine. For example, the topography downstream of the Denmark strait along with bottom boundary layer thicknesses of order 200 m, probably require horizontal resolutions of order 10 km or finer to study the formation of North Atlantic Deep Water in TFCMs if *HIC*<5 is required. There are very few examples in the literature of published global ocean simulations using TFCMs with horizontal resolutions coarser than ½°, and most TFCM applications use much finer resolutions than this. This limitation on bottom slope strongly suggests that TFCM use in long-term global-scale ocean applications is likely to be limited until available computational resources have increased enough to enable the use of sufficiently fine horizontal resolutions.

Isopycnal (i.e. density) coordinate models are inherently adiabatic and accept arbitrarily steeply sloped topography. The one inescapable liability of such models is that the resolution is excluded from weakly stratified (or unstratified) parts of the water column. This is inherent in the approach and cannot be cured. As the surface planetary boundary layer is of particular importance in any coupled model, this limitation is severe. To avoid this, most “isopycnal” coordinate models have attached a non-isopycnal surface region to describe the surface boundary layer, thus sharing some characteristics of the “Hybrid” coordinate models, described later. In addition, changing the role of the continuity equation from diagnostic to prognostic, along with the requirement that the continuity equation is positive definite, introduces complexities (particularly in the stability of the baroclinic-barotropic mode splitting) that are not present with fixed-grid models. Substantial progress has been made in addressing these issues, but they remain an area of active research, and the numerical algorithms employed in isopycnal coordinate models can be more costly than with other types of models.

The other long-standing challenge with isopycnal coordinate models has been that the nonlinearities of the equation of state are substantially trickier to deal with than in other models. But after several decades of work, there are now viable solutions most of these issues arising from the nonlinear equation of state, as presented to this session by R. Hallberg. Potential density with respect to surface pressure has large-scale inversions in much of the ocean – Antarctic Bottom Water has a lower potential density with respect to surface pressure than North Atlantic Deep Water – and is therefore of limited utility as a vertical coordinate. Fortunately, potential density with respect to 2000 dbar pressure (s_{2000}) is monotonically increasing with depth almost everywhere in the ocean’s large-scale climatology, except in some weakly stratified high-latitude haloclines (McDougall and Jackett, 2005); s_{2000} is now widely used as the vertical coordinate in “isopycnal” coordinate models (Sun et al., 1999). In modern isopycnal coordinate models, s_{2000} is used only to define the vertical coordinate and for nothing else. For physical consistency with the real world, all dynamical effects must be based on the in-situ density gradients. Sun et al. (1999) show the importance of using the true equation of state in the pressure gradient calculation to avoid large biases in thermal wind shears, and advocate the use of pressure gradient formulations that cancel the leading order thermobaric terms. Hallberg (2005) showed how this approximate cancellation of thermobaricity can lead to numerical instabilities in weakly stratified regions as resolution in density space is refined. Subsequent work has lead to new formulations of the pressure gradient terms in isopycnal coordinate models that perfectly avoid such instabilities (Adcroft et al, 2008).

There are several other ways in which nonlinearities of the equation of state have traditionally affected isopycnal coordinate models – all are now largely solved. If potential temperature (q) and salinity (S) are the advected state variables, cabbeling can lead to changes in potential density (s_{2000}) and a drift away from the coordinate definition. MICOM and HYCOM have avoided this with a number of options, including advecting s_{2000} along with either q or S and inverting the equation of state for the other, or advecting s_{2000} and spiciness (which is defined to be orthogonal to s_{2000} in q-S space) and inverting for both q and S (Bleck, 2006). These approaches have the profound disadvantage for global climate modeling that they do not conserve heat and salt! There was a clear consensus at this meeting (and the LOM meeting that preceeded it) that heat and salt conservation to very high precision is of extreme importance in an ocean climate model, and it was announced that steps would be taken to correct this in HYCOM. Other isopycnal coordinate models, specifically GFDL’s GOLD and a variant of MICOM being developed at the Nansen Center in Bergen, advect potential temperature and salinity, and conserve heat and salt to roundoff. The issue of what variables to advect is no longer outstanding. Cabbeling is handled naturally if temperature and salinity and advected and diffused, and double diffusion is similarly straightforward to handle. In both cases, though, there is some question as to how best to do the vertical remapping to compensate for the drifts away from the specified coordinate without introducing spurious extrema or undue diapycnal mixing. In addition, isopycnal coordinate models tend not to rotate the diffusion tensor into the neutral direction, instead relying on the relatively close approximation of their coordinate surfaces (typically s_{2000}) to neutral planes; this is clearly much less problematic than mixing along terrain-following-surfaces or geopotentials would be, but it is unclear whether this approximation of neutral surfaces by s_{2000} surfaces is generally acceptable. In summary, isopycnal coordinate models have evolved to the point where issues arising from the equation of state are not substantially more problematic than they are with other choices of vertical coordinate for an ocean model.

Hybrid vertical coordinate models appear to be the natural solution to the liabilities of the various traditional classes of ocean model (e.g., poor representation of gravity currents in pressure-coordinate models; the requirement to smooth topography to avoid pressure gradient errors in terrain-following coordinate models; the exclusion of resolution from weakly stratified regions in isopycnal coordinate models). However, care must be taken to inherent the strengths of the various classes of models while avoiding the liabilities. HYCOM in particular has been operating fairly successfully in this mode for almost a decade now, as described in a presentation by R. Bleck. Many of the numerical issues arising in HYCOM are similar to those found in its isopycnal coordinate predecessor, MICOM, but there are clear improvements in HYCOM relative to MICOM in the representation of the surface boundary layer and in shallow (and weakly stratified) marginal seas. The precise considerations behind the choice of where to put coordinates remains more an art than a science, and there are aspects of the details of how to enforce this coordinate, such as remapping without excessive diffusion, that remain elusive.

Based on this session, there are still a handful of outstanding issues related to the choice of vertical coordinate in ocean models, but it was is striking the extent to various modeling groups are tending to migrate toward choices that draw from several of the traditional types of models. These issues are all areas of active research, but it was also clear from this meeting that a number of the most intractable long-standing issues with ocean models have been largely addressed within the past decade. Based on the discussion at this meeting, it would appear that the clear identification of a particular code with a particular choice of vertical coordinate will soon be a thing of the past. This is a welcome development, as it will increase the ease with which different ocean modeling groups can exchange ideas, and the ease with which ocean models can be configured most appropriately for a particular application.

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3. Non-rectangular structured meshes and unstructured meshes: Todd Ringler (Los Alamos National Laboratory), Matthew Piggott (Imperial College), Laurent White (GFDL)

There were three main presentations during this session, each representing the state-of-the-art in non-standard mesh configurations of use for simulating the ocean. The presentations provided an overview of the following methods: 1) adaptive finite element meshes (Piggott), 2) fixed finite element meshes (White), and 3) icosahedral meshes (Ringler). The following summarizes some of the main points raised during the presentations.

Summary by Matthew Piggott

The following represent some thoughts on the session, including key questions that need to be addressed in order for these methods to be of use for ocean modeling.

Genetic diversity of models was acknowledged as a good if not crucial element in ocean modeling, especially given the inevitable convergence of "classical" methods now that the field of ocean modeling has entered into a more mature phase.

There is a need to demonstrate that models based on novel numerics (in particular the grid type used) can be competitive in terms of speed and their capabilities at modelling realistic phenomena.

The novel methods need to be tested in realistic multidecadal-multicentennial global baroclinic simulations on non-regular meshes. How well can they reproduce realistic flow patterns?

It is essential that the new methods provide for conservation in the discretisation, as well as conservative mesh-to-mesh interpolation when using adaptivity. This property is necessary for conservation of mass and tracer, which is an essential feature of ocean climate models.

What are the benefits of fully unstructured meshes (e.g., 3-dimensional unstructured) compared to an unstructured mesh in the horizontal with a structured or layered mesh in the vertical? The 3d unstructured is attractive due to its enhanced flexibility, with the model having the ability to choose to revert to something very close to a structured grid where it deems necessary. That is, 3d unstructured can include structured as a special case.

Development of mesh movement allows Lagrangian structures in the flow to be tracked if desired. Crucial importance of Lagrangian structures should mean this feature will represent another crucial development.

A hybrid capability in the vertical, in particular using mesh movement (or ALE methods) in the vertical to track isopycnal layers is important.

Can we develop the capability to use locally variable time steps with a variable resolution spatial mesh?

There is a need for robust error measures to guide the adaptive mesh and make good use out of the extra flexibility we give the model. A bad adaptive mesh will be absolutely disastrous to both the accuracy and efficiency of a simulation.

How do SGS/turbulence models work with unstructured grids – use of SGS models which assume columns is yet another reason for using meshes which are structured in the vertical.

Coupling of classical mesh adaptivity, mesh movement, and p (spectral - e.g. SEOM) type adaptivity. How does one best decide whether to increase resolution or polynomial order?

Need for new models to be included in intercomparison projects such as DYNAMO, the new CORE reference experiments, etc.

Summary by Laurent White

1. Introduction

There is a growing interest in the development of unstructured mesh numerical ocean models as one way of bridging the gap between high-resolution ocean modeling and climate ocean modeling. Due to the huge computer requirement, the former is limited to a few decades at most while the latter requires a low resolution for coupled runs over longer timescales.

A way of reconciling both approaches is to have variable mesh resolution. This could help improve a number of ocean circulation features, such as the western boundary currents, the outflows through badly-resolved straights and continental shelves dynamics for coastal ecosystems, which play a crucial role in global biogeochemical cycles.

Numerical ocean models based on unstructured meshes have been under intensive development for the past decade. The reason that none have been used in the last IPCC assessment is because they are not mature enough and unable to compete with current structured grid ocean models in a satisfactory manner.

The causes and remedies for the immaturity of the unstructured mesh approaches are explored below.

2. Model development and improvement

To convince the ocean modeling community that novel approaches are viable, we need to demonstrate that the new methods perform at least as well as the "old" ones for (almost) the same computational cost. The methods must satisfy the following properties:

1. be conservative (e.g. mass and tracer are conserved);
2. be locally consistent (e.g., constant-preserving);
3. propagate surface waves (esp. Rossby waves) without scattering and with respectable numerical dispersion properties;
4. preserve the geostrophic equilibrium without spurious scattering.

Those requirements form a minimum foundation and other considerations should build on it.

For either fixed or adaptive unstructured meshes, the new methods being conceived are much more flexible in terms of mesh resolution. It should, nonetheless, be understood that this flexibility comes at a cost. The question is How much do we want to pay for this enhanced flexibility in terms of CPU time? An ongoing -- as yet unanswered – question regards the comparison in terms of CPU time between structured and unstructured grid models (for the same horizontal and vertical resolution).

3. Important and/or controversial issues

Three different types of novel models were presented at the workshop. The first class is based on the finite volume method (on Voronoi cells), and was presented by Todd Ringler. The second class is based on the finite element method on fully unstructured adaptive meshes using tetrahedral, and was presented by Matthew Piggott. The third class is also based on the finite element method but the mesh is fixed in time and made up of prisms aligned in the vertical (thereby mimicking the topological structure of finite difference models), as was presented by Laurent White.

Each method has its advantages, and at present there is no consensus regarding which approach is the most promising. Each method builds on a priori hypotheses: finite volume methods emphasize the conservative nature of fluid flows; the fully adaptive unstructured approach is based on the multiscale (both in time and space) nature of ocean flows; the prismatic approach is based on the anisotropic nature of ocean flows (stratified and hydrostatic). All visions have great potential will require tremendous validation before being able to rule out one way of thinking or the other.

In the field of finite elements, opponents of the prismatic approach may rightfully say that by using fixed meshes, the full potential of the method is not unleashed. On the other hand, opponents of the adaptive mesh approach might have reservations as to the reproducibility of numerical results. The ratio of unresolved to resolved processes is so high in the ocean that adapting meshes might be a very challenging option insofar as the numerical solution might strongly depend on the way adaptation is performed. Other research issues with adapting meshes concern conservation and CPU time. Fixed meshes, on the other hand, may just fail to capture important processes where a clever adapting strategy would succeed.

Now, whichever one is opted for, the broader question of adaptive modelling arises, whereby the parameterizations and the equations should be modified according to the mesh resolution. In the extreme case where the horizontal (and vertical) mesh resolution is so high that non-hydrostatic phenomena could be resolved, the model should locally be switched on to a non-hydrostatic mode.

4. Parameterization of physical process: Richard Greatbatch (IFM-GEOMAR) and Martin Schmidt (Baltic Sea Research Institute)

A common theme to emerge from the session is the desirability of developing parameterizations based on the turbulent energy equations and utilizing the exchange of energy between the resolved part of the circulation and unresolved (turbulent) part. Several promising approaches were discussed in which the EKE equation is integrated prognostically as part as of the model time stepping procedure and then used to infer diffusivities. The importance of developing these parameterization based on the underlying physics (e.g. instability theory) was emphasized.

The advantages and disadvantages of treating the velocity variable in the model momentum equation as the residual mean rather than the Eulerian mean velocity needs to be explored further.

There is growing recognition that eddies also play a role in diabatic mixing processes in the ocean. Two aspects were discussed: (i) the diabatic part of the eddy buoyancy flux and (ii) the impact of a mesoscale eddy field on the dispersal and fate of near-inertial energy that is input to the ocean by synoptic wind events. The importance of the former in the surface mixed layer was noted, especially the role played by the interaction between the mesoscale eddy field and the atmosphere. Further research is required to develop parameterizations of this process. There is also a need to develop parameterizations for mixing associated with breaking internal gravity waves, although this is an area that still needs a lot of further research in the future.

Evidence was also presented that the coupling of simple parametric wave models to circulation models may provide the required information to include the influence of the wave field on surface layer mixing.

Finally, issues concerning the usefulness of eddy-resolving models for climate research were discussed. Aside from the computational expense of running such models, eddy resolving models can also be compromised by spurious mixing arising from the numerics. Progress in this area is ongoing and the emergence of new advection schemes holds the promise that this issue will be of less concern in the future. For eddy resolving models the advection of momentum also needs attention.

5. Coastal/Regional modelling: Eric Blayo (Laboratoire Jean Kuntzmann, Universite Joseph Fourier), Jarle Berntsen (University of Bergen)

1. Recommendations

1.1 On good model practise

From talk by Blayo: use open boundary conditions (OBCs) that are consistent with model equations. Typically, the use of characteristic based OBCs are recommended for the barotropic mode, and relaxation for the barotropic part of the flow.

From talk by Debreu: For two way nesting algorithms, use highly selective restriction operator to prevent aliasing on the coarse grid

From talk by Berntsen, Davies and Xing: When moving towards more non-hydrostatic modeling, the length and time scales of the non-hydrostatic pressure adjustments need to be considered. Unless the grid size is adequate to resolve these adjustments, the addition of non-hydrostatic pressure may be a waste of computer time and even give aliasing effects.

From talk by Oey: Described a simple and accurate way to extend an existing ocean model (the POM) with wetting and drying capabilities, including examples.

1.2 On targeted areas of research and development
From talk by Blayo: development of improved OBCs is presently ongoing in several groups, based on the so-called "absorbing" conditions. Since the derivation of such conditions is closely linked to the model equations, one can expect better performance of the resulting OBCs.

From talk by Berntsen, Davies and Xing: Parameterization of subgrid scale processes including interactions between stratified flow and topography, internal wave breaking and mixing, and effects of unresolved topography. There may also be feedback to the circulation from the biosphere and industrial activity (for instance trawling) that need to be considered.

1.3 On promising avenues for improving the models
From talk by Blayo: in the context of regional forecasting systems, data assimilation can be used to control and improve the interactions between large scale and local models. In addition to usual control variables like initial conditions, one can also correct for the interactions between the models.

From talk by Debreu: Use of highly flexible grid refinement (e.g. Grid Mosaics)

From talk by Roed: A systematic approach Quality Assurance, including verification, sensitivity studies, validation, and forecast skills is suggested. The users care more about the quality of the forecast than processes. Root Mean Square Errors (RMSE) may be used in quantitative skill assessment. However, RMSE may get worse with reduced grid size due to more eddies in the model field. Therefore, filtering in time and/or space may be necessary using this approach. Analysis of statistical properties like Probability Density Functions (PDFs) and also the spectral decomposition (wave lengths/frequencies) was suggested.

2. Important issues

From talk by Debreu: In the context of nested models, conservation of Mass and Tracers can be achieved by flux correction algorithms if one can write the time evolution of a variable as a flux divergence. This prevents the use of schemes that employs Asselin filtering to kill computational modes. Rendering the scheme conservative reduces the order of approximation.

Oey made it clear, based on Taylor expansion of the error term, that hydrostatic inconsistency is NOT a meaningful measure of the pressure gradient error in sigma-coordinate models. Nonetheless, this issue remains controversial and no consensus was achieved during these discussions.

6. Basin and Global Models: Claus Böning (IFM-GEOMAR), Anne Marie Treguier (IFREMER) and Stephen Griffies (GFDL)

1. Overview

Basin/global scale models have long been used for studies of ocean climate dynamics. In the last 10 years, the computer power and model numerics have improved to the point that we can explicitly permit a representation of the World Ocean's mesoscale eddy field in decade long simulations. It is anticipated that in the next few years, more groups will embark on fully coupled climate simulations with these mesoscale eddy permitting oceans. Even so, coarse resolution models will remain a key component in many applications, particularly millenial scale paleo-climate studies.

During this session of the workshop, we aimed to discuss a number of questions of primary relevance to the development and use of large-scale ocean climate models. In this summary, we revisit the questions, and provide comments based on discussions during the workshop.

2. Minimal needs for coarse models

The climate modelling community is continually in search of answers to the following question:

What are the minimal needs for coarse resolution global ocean climate models?

This question is very difficult to answer for many reasons. First, the ocean contains a huge spectrum of motions, with no clear spectral gap to provide a cutoff point for model resolution. Indeed, during the session on regional and coastal modelling, Jarle Berntsen argued that important processes related to flow over a sill remain unresolved even at 1m resolution with a non-hydrostatic model. An answer to the question of minimal needs for models also depends on details of the particular use of the simulation, with global ocean climate encompassing a huge range of applications. In addition to representing or parameterizing features of the flow, the ocean geometry plays a leading role in determining the flow characteristics. As model resolution is refined, the geometry is likewise better represented. It has proven quite difficult to parameterize certain important features of the geometry, thus making any improvements in resolution of great utility.

Given these caveats, we nonetheless propose that for ocean climate modelling, the question of minimal model needs can be restated as:

What is essential to represent explicitly and what can be reasonably parameterized?

As a partial answer to this question, we propose that (1) tropical dynamics must be explicitly represented so that the ENSO dynamics can be faithfully simulated, (2) mesoscale eddies must be parameterized with a scheme such as that proposed by Gent and McWilliams (1990) (GM90) or Greatbatch and Lamb (1990), or extensions.

2.1 Tropics

Present day high-end global models of use for climate change generally have a reasonable representation of tropical currents, thus allowing for an explicit representation of ENSO dynamics. The quality of the simulated ENSO may be improved with grid refinement of the equatorial wave guide (say moving to resolution finer than 1/3 degree), in which case transients such as tropical instability waves can be more adequately admitted. Nonetheless, the quality of the high-end ocean model simulations of the one-degree class, with refined meridional resolution in the wave guide, do capture ENSO significantly better than models in the previous generation five or ten years ago. Even though the ENSO simulations amongst various models are quite diverse (likely due to details of the atmosphere model more so than the ocean), the situation represents a major advance in the integrity of the global simulations. Namely, the ocean component at least now has an opportunity to provide sufficient realism to admit ENSO.

2.2 Mesoscale eddies

In contrast to tropical dynamics, the global models run for long term climate studies are far too coarse to resolve mesoscale eddies. Indeed, it remains unclear what it means to fully resolve the mesoscale eddy spectrum. Some have argued that a few grid points per first baroclinic Rossby radius are necessary. But is this sufficient? What about regimes where multiple baroclinic modes are critical, thus requiring resolution of the higher modes and so requiring even finer grids? What about vertical resolution? And as grid resolution continues to be enhanced, Anne Marie Treguier emphasized that sub-mesoscale processes begin to be resolved. How important are these processes? What about their interaction with non-hydrostatic processes, especially in the mixed layer? Process studies are now reaching the 1km grid scale, which is sufficient to represent these interactions, with new parameterizations proposed.

Given our inability thus far to rigorously identify when the eddy field is resolved, and given the lack of a spectral gap in the ocean, the term ‘eddy resolving’ is misleading and irrelevant. In particular, one asks ‘what eddies’? Modellers should thus use the term ‘eddying’ or ‘eddy permitting’ rather than the
presumptuous ‘eddy resolving’ when characterizing their simulations.

As a complement to the question of what it takes to represent eddying features explicitly, ocean climate modellers wish to know whether their parameterizations in coarse models are performing in a manner that maintains some fidelity to the physical effects of the subgrid scale (SGS). All models at the one-degree class possess some form of mesoscale eddy parameterization, with the parameterization derived from Gent and McWilliams (1990) (GM90) by far the most dominant. An alternative, which is gaining some attention, is the form drag parameterization of Greatbatch and Lamb (1990) (see Ferreira and Marshall (2006) for a recent implementation). The two parameterizations are equivalent when making the geostrophic assumption, but they differ significantly in details of implementation in a model. Namely, GM90 scheme affects the tracer equation in level models (geopotential, pressure, and terrain following), and the thickness equation in isopycnal models (interfacial smoothing). In contrast, Greatbatch and Lamb (1990) introduce an enhanced vertical viscosity, which is applicable regardless the vertical coordinate. Both schemes are adiabatic, in that they do not mix parcels between density classes. However, the Greatbatch and Lamb (1990) approach is manifestly adiabatic, in that it is implemented in the momentum equation, and thus is immune from potential problems with truncation errors that can spuriously introduce diabatic mixing when Gent and McWilliams (1990) is implemented in the level coordinate tracer equation.

Whether these, or other, SGS parameterizations are faithful to the unresolved eddies remains a research question. It is a very difficult question to generally answer. For example, some parameterizations enhance the integrity of a simulation due to its correct physical aspects. Others, however, improve the simulation by reducing spurious numerical effects which would otherwise be egregiously incorrect. Measurements in the real ocean are scarce, so the issue of testing parameterizations is typically addressed by running fine resolution models without a parameterization, and comparing to coarse models with the parameterization. The suite of Southern Ocean simulations presented by Hallberg is a clean example of this approach. His results raise some doubt as to whether the Gent and McWilliams (1990) scheme can accurately parameterize sensitivities of the fine resolution eddying simulations. In general, such studies are subject to caveats due to limitations of the coarse simulations (e.g., are the chosen parameterizations the ‘best’ available?), analysis methods, and prejudices of the researcher.

2.3 Recommendations

The question of minimal model needs was not firmly answered by this session. However, discussions were provocative and resulted in the following conjectures for a minimal suite of requirements for coarse resolution global ocean climate models.

- The models must explicitly represent the tropical wave guide, both horizontally and vertically, with sufficient integrity to allow for realistic tropical currents, thus providing an oceanic framework that 2 admits ENSO in coupled climate simulations. The one-degree class of models, with refined meridional resolution near the equatorial wave guide, appear to be sufficient for this purpose, so long as the upper ocean mixed layer and tropical thermocline is well resolved in the vertical. Whether the models must explicitly represent tropical instability waves, either by including a reduced level of friction or refining the grid further, remains under investigation, with particular attention given to the possible role these waves have in equatorial heat transport.

- In the sub-tropical and higher latitudes, global models must include a parameterization of mesoscale eddies. The most commonly used parameterization is that proposed by Gent and McWilliams (1990), with some renewed interest also given to the alternative approach from the Greatbatch and Lamb (1990) vertical friction method. Both schemes need to be supplemented by the neutral diffusion ala Redi (1982). This recommendation has many qualifications and details which go beyond this summary. Nonetheless, models absent one or the other scheme have proven inadequate for simulating such features as mode waters, deep water formation, and the Southern Ocean. Additionally, this recommendation transcends the vertical coordinate, with coarse resolution geopotential, isopycnal, terrain following, and hybrid models requiring some parameterization of the mesoscale eddies.

- There are many other processes which continue to be at the level of research, though with much of this research maturing. We have in mind such processes as over flow dynamics, submesoscale features, mesoscale eddy and mixed layer interactions, mixing due to breaking internal waves, etc. Each process can and should be considered as part of the suite of model SGS parameterizations in a global model, with some of the parameterizations reaching a level of maturity warranting their routine use in global models.

- The ocean fluid is contained in a very complex geometry which can have first order effects on the large-scale from very small regions, such as straits, through flows, and boundary currents. Hence, in addition to physical processes mentioned above, the question about resolution is critically associated with how well it is necessary to resolve important topographic features. It has been notoriously complicated to parameterize certain flow features closely associated with topography. It is thus difficult to make firm statements regarding what sorts of resolutions are needed for an adequate representation of the ocean geometry.

3. Eddy permitting models

As mentioned above in Section 2, eddy permitting ocean models are being used at a growing rate for simulating the global ocean. It is anticipated that within the next 5-10 years, a handful of these models will be routinely integrated for hundreds of years, if not longer. This situation then raises the following
questions:

What SGS parameterizations are required for eddy permitting simulations?
What new numerical issues arise when admitting mesoscale eddies in global climate models?

3.1 Tracer equation: SGS operators and advection

The presentation by Griffies focused on the tracer equation. He noted that the state-of-the-art eddying isopycnal models, such as the Southern Ocean MESO simulation from Hallberg (Hallberg and Gnanadesikan, 2006), employ no lateral SGS tracer operator when moving to the 1/4 degree resolution and finer. This situation strongly contrasts with the state-of-the-art in geopotential models run at global eddy permitting resolution (e.g., Roberts and Marshall, 1998; Smith and Gent, 2004). It was proposed that the nontrivial horizontal tracer operators in the geopotential models serve only to satisfy numerical closure purposes,
rather than to parameterize SGS physics. The numerical closure purposes focus on the need to 'clean' up problems with numerical tracer advection; namely, to provide a quasi-adiabatic dissipation mechanism to dispense with the dispersion errors from numerical advection. However, Griffies argued that the newer
tracer advection schemes now available are far better at reducing the tracer errors, thus enabling geopotential modellers to dispense with the lateral tracer operators.

This proposal is accompanied by one important caveat. If the simulation clearly is missing a physical process, such as a partially resolved eddy field needed for the restratification of regions of deep water formation, then it may be necessary to include an SGS parameterization. The difficulty of reintroducing SGS parameterizations at the eddying regime is that SGS operators generally act in a dissipative manner, which contrasts to the aim of allowing the flow to realize a high Reynolds number.

3.2 Friction

Lateral friction remains a necessary element of any numerical model, with levels of friction set largely by the needs of numerical closure. That is, lateral friction used by global models does not parameterize SGS physics. So modellers thus choose to engineer whatever manner of lateral friction that can retain the
numerical closure needs (e.g., suppress noise and instabilities, broaden lateral frictional boundary layers sufficiently for the grid to resolve the layer), while allowing currents to go well into a hydrodynamically unstable regime.

In contrast to lateral friction, the choices for vertical friction in models generally are generally based on physical closure requirements. In particular, vertical viscosity is often tied to the vertical tracer diffusivity with a Prandtl number on the order of unity or a bit larger. Bottom drag, wave drag, eddy drag, internal wave breaking, all contribute to determining profiles of vertical viscosity.

It was hypothesized during the workshop discussions that the need for some eddying simulations to add both a lateral Laplacian and biharmonic friction in order to facilitate a proper boundary current separation arises from missing vertical processes. Either the eddying models need to better parameterize missing vertical physics, or refine the vertical resolution to admit the processes explicitly. Adding a lateral Laplacian operator should be seen as no more than a temporary numerical closure.

3.3 Recommendations

The following recommendations arose from this session.

For geopotential coordinate eddying models, one should test the simulation integrity by dropping lateral tracer operators and replacing them with one of the more refined flux limited tracer advection schemes. By doing so, the geopotential models will be integrating the same tracer equation as the isopycnal models.

Lateral friction is used for numerical closure, meaning that all efforts should be made to reduce its impact on the simulation.

Vertical friction is generally set according to SGS physical closure. In simulations where it is found necessary to include some form of lateral friction, such as to garner a better boundary current simulation, researchers should search for missing vertical physics.

4. Running global ocean-ice climate models

After choosing the model fundamentals, such as the horizontal and vertical resolution, SGS parameterizations, vertical coordinate, etc., one then moves onto the design of the numerical experiment. There is a long history of global ocean models being run in support of coupled climate models, with the inclusion of a sea ice component generally desired in order to physically handle the liquid-solid phase transition in the high latitudes. However, the methods used to run these models are varied, with each group generally introducing defensible steps which, unfortunately, can be quite different. There are growing interests in the modelling community to compare simulations amongst groups, in hopes of improving the models and garnering a robust understanding of the results. The question arises in this context:

Can we establish useful and agreeable methods for running ocean-ice models, short of running models fully coupled to realistic atmospheric models?

4.1 Coordinated Ocean-ice Reference Experiments (COREs)

Finding a resolution to this question has been a focus of the CLIVAR Working Group for Ocean Model Development (WGOMD) for some years. The WGOMD has proposed Coordinated Ocean-ice Reference Experiments (COREs) as a tool to explore the behavior of global ocean-ice models under forcing from a common atmospheric state. Aspects of COREs formed the topic of presentations by Griffies, Böning, and Gerdes during this workshop session. Particular emphasis was given to issues that arise when designing coupled global ocean and sea ice experiments, such as difficulties formulating a consistent forcing methodology and experimental protocol. Particular focus was given to the hydrological forcing, with details key to realizing simulations with stable overturning circulations. As an outcome of this analysis is a grid resolution hypothesis, whereby models with sufficient resolution to capture certain subpolar Atlantic processes are hypothesized to be less sensitive to hydrological cycle variations.

The atmospheric state from Large and Yeager (2004) was developed for coupled ocean and sea ice models. This dataset was found to be suitable for purposes of COREs, even though evaluation of this state originally focused more on the ocean than the sea-ice. Simulations with this atmospheric state were presented from seven global ocean-ice models using the CORE-I design. These simulations test the hypothesis that global ocean-ice models run under the same atmospheric state produce qualitatively similar simulations. This hypothesis was show to hold reasonably well (with notable exceptions) for upper ocean tropical behavior, but is less valid when examining deeper properties, especially in the high latitudes.

Given the broad selection of models participating in the CORE-I study, the simulations can provide some feedback to the fidelity of the prescribed atmospheric state. That is, places where each model produces a similar behavior that is biased relative to observations may signal a problem with the atmospheric state, thus suggesting areas requiring reexamination. Conversely, an outlier model may highlight problems in the model's fundamentals and/or configuration. Identifying problem areas promotes avenues for model development aimed at reducing the bias.

One particular area of question relates to the magnitude and details of the hydrological cycle in the Arctic region. The precipitation from Large and Yeager (2004) appears to be larger than that found in other comparable datasets. All are within error bars. Nonetheless, the larger precipitation can cause problems for ocean-ice simulations, whereby the overturning circulation can become very weak. Sensitivity experiments were presented using the Kiel-ORCA model, in which the precipitation was reduced, and the resulting overturning became much stronger.

Gerdes noted that energy balance (EBM) atmospheric models may provide a useful way to reduce sensitivities to the prescribed atmospheric forcing. However, EBMs have many shortcomings and biases, which present the ocean-ice system with a sometimes poor representation of surface fluxes (see, e.g., discussion in Gerdes et al., 2006). So there remains no consensus regarding the use of an EBM, or other ‘simple’ atmospheric model for use in running ocean-ice models. Workshop participants agreed that further research would be useful to better understand how these models may play a role for ocean-ice modelling.

4.2 Reasons for COREs

Although many useful insights can be garnered from studies with ocean-ice models, it is critical to understand their limitations. Namely, it often remains difficult to ensure that results from the ocean-ice subsystem carry over to the full climate system, where climate model behavior, such as sensitivities to perturbations, can prove distinct from ocean-ice models. Quite often, problems with ocean-ice models stem from unrealistic aspects of surface forcing from a non-interactive atmosphere.

Nonetheless, even with their limitations, ocean-ice models remain a valuable climate science tool, and so can be used for fruitful scientific research and model development purposes. We summarize here a few uses which motivate a standard practice for running these models.

- Being less expensive than climate models, ocean-ice models can be formulated with refined grid resolutions thus promoting superior representations of key physical, chemical, and biological processes as well as geographic features.

- Ensembles of ocean-ice models can be run with a broader suite of algorithms and parameterizations than climate models. Such flexibility helps to develop an understanding of simulation sensitivity to model fundamentals.

- They provide a tool to study interactions between the ocean and sea ice as isolated from the complexities of atmospheric feedbacks and from biases that arise when coupling to a potentially inaccurate atmospheric model.

- Ocean-ice models forced with different atmospheric states provide a means to assess implications on the ocean and sea ice climate of various atmospheric reanalysis or observational products. As a complement, many models run using the same atmospheric state, and which show similar ocean biases, suggest that there are problems with the atmospheric states. In these ways, models can provide feedback onto the development of atmospheric states used to force ocean-ice models (e.g., Large and Yeager, 2008).

- Bulk formulae are needed to produce ocean-ice fluxes given an atmospheric state and ocean-ice state. Ocean-ice models run with the same atmospheric state yet with different bulk formulae allow one to assess the sensitivity of the simulation to the chosen bulk formulae.

- Run under realistic atmospheric forcing, models can be used to reproduce the history of ocean and sea ice variables and help to interpret observations that are scarce in space and time (e.g., Gerdes et al., 2005). This approach provides a method for ocean *reanalysis* unavailable with fully coupled climate models. Notably, there are nontrivial issues of initial conditions and ocean drifts which need to be resolved before obtaining unambiguous results from such reanalysis studies.

- One can select particular temporal or spatial scales from within the forcing data for use in running ocean-ice models for purposes of understanding variability mechanisms.

- There is great utility for model development comparing simulations from different ocean-ice models using the same atmospheric state. For example, comparisons often highlight deficiencies in the representation of physical processes, which then guide efforts to improve simulation integrity.

- Coupled ocean-ice models provide a valuable engineering step towards the development of more complete climate models. For example, many tools and methods needed to build climate models are more easily prototyped in the simpler ocean-ice models.

4.3 Recommendations

The number of research groups running global ocean-ice models is growing. Many groups are exploring these models as but a first stage in the development of a fully coupled climate model. Others are using the model as tool for studying the ocean climate. Given the difficulty running these models, yet their great utility, the workshop recommended that groups seriously consider incorporating the CORE experimental design as a baseline from which they are better able to compare with other groups, and beyond which they may expand their suite of simulations.

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7. Ocean processes and inverse methods: Detlef Stammer (University of Hamburg)

This is the summary of the session on Ocean Processes and Inverse Methods. It contains contributions from D. Stammer, M. Balmaseda and E. Chassignet. The focus of all three presentations was on time-dependent OGCM inverse problems, or data assimilation, and excluded traditional box-inversions. While the first two talks addressed climate related hind- and forecast problems, the last talk addressed specifically the question of eddy-resolving data assimilation for now-casts.

All modern assimilation approaches have in common with earlier attempts the understanding that a complete picture of the ocean for the purpose of climate research and applications will only come from a synergy between observations, modeling and data assimilation. The planning of climate research builds accordingly on the existence of global ocean reanalysis products which synthesize all available ocean observations by merging them with global circulation models to describe the state of the time-varying ocean and its interaction with the atmosphere over the past several decades.

The spectrum of assimilation applications for climate variability and prediction purposes span over seasonal-to-interannual, decadal-to-centennial, and even millennial time scales. These applications pose a range of accuracy and robustness requirements; consequently, they necessitate somewhat different data assimilation approaches and evaluation as described below. Nevertheless all those approaches have common or overlapping purposes. Examples of their use include:

1. Description of a complex local flow field and its interaction with biology;
2. Description of the interaction of the ocean with the atmosphere and associated changes in the flow fields, ocean properties, etc;
3. Use of estimated flow field for studies on CO2 sequestering, regional impacts, regional and global sea level;
4. Develop an improved base and reference data sets for climate research;
5. Deliver improved boundary conditions for regional/basin scale modeling and assimilation efforts that are being planned or performed as part of CLIVAR's regional process studies in individual basins;
6. Facilitate the initialization of coupled models for studies and prediction of seasonal-to-decadal variability.

Regardless of the purpose and with what detailed method, state estimation or “data assimilation” in general is just least-squares fitting of models to data, taking into account the model equations as constraints. There are many methods for solving constrained least-squares problems, either exactly, by iteration, or sequentially. In terms of nomenclature, they include Nudging, 4DVAR, 3DVAR, adjoint, OI, OM, Kalman filter, RTS smoother, ensemble KF, AD, Pontryagin principle, relaxation, line-searches, breeding vectors, SVD, optimals, Hessians, quelling, dual, and many more. All these apparently different methods are nonetheless just variant algorithms used to find the minimum of an objective (or cost) function measuring the deviation of the models simulation from observations, essentially varying in the extent to which an approximation to that minimum is acceptable, whether one intends to find a dynamically self-consistent solution and whether or not one seriously seeks an estimate of the error of the result.

In principle, finding a minimum of the above cost function, subject to the model’s dynamics, is a numerical issue, not a conceptual one. In practice, however, a lot of experience enters all applications, given the fact that we have to solve non-linear optimization problems with large dimensions (we typically have 10^8 – 10^{10} number of unknowns). Moreover, the nature of the minimum, in addition to the model structure, depends directly on prior information about model and data error covariances. If they are incorrect, so is the solution, no matter how wondrous the numerics and this problem is clearly an oceanographic and meteorological research problem, rather than one of simply applying numerics. Ultimately, adaptive estimation may become possible, but it remains far beyond reach. Until then a significant effort has to be put into improving our understanding of model and data errors, in improving models (ocean and atmospheric ones) and, through both, in improving ocean state estimation results. A problem that should not be underestimated is that of dynamically balanced model initialization since model adjustments can easily span a decade and more, i.e. of the same order as our data record.

Several global ocean data assimilation products are available today that in principle can be used for many climate applications. Underlying assimilation schemes range from simple and computationally efficient (e.g., optimal interpolation) to sophisticated and computationally intensive (e.g., adjoint and Kalman filter-smoother). Intrinsically those efforts can be summarized as having three different goals, namely climate-quality hintcasts, high-resolution nowcasts, and the best initialization of forecast models. One example of existing ocean state estimates, presented during the conference, was that of the GECCO 50-year ocean state estimation. It is an ocean synthesis, performed over the period 1952 through 2001 on a 1° global grid with 23 layers in the vertical, using the ECCO/MIT adjoint technology (Marotzke et al., 1999). The model started from Levitus and NCEP forcing and uses state of the art physics modules (GM, KPP). The model's adjoint (obtained using TAF) is used to bring the model into consistency with most of the available ocean observations over the full period by adjusting control parameters. At this stage control parameters are the models initial temperature and salinity fields as well as the time varying surface forcing, leading to a dynamically self-consistent solution (the next step is to include mixing). Details are provided by Köhl and Stammer (2008a, b).

Typical science questions that can be addressed by the GECCO ocean state estimation results include:

1) THE OCEANS IN THE PLANETARY HEAT BALANCE: heat storage, MOC and heat transports and ocean/atmosphere feedbacks.
2) THE GLOBAL HYDROLOGICAL CYCLE: water balance, rainfall variability, salinity and convection.
3) SEA LEVEL: sea level rise, sea level variability.

Discussed in more detail was the example of the MOC variability estimated by the GECCO effort. The meridional overturning circulation (MOC) of the ocean carries a large amount of heat poleward. The importance of this poleward heat transport for the climate of mid and high latitudes, especially of Europe, is generally accepted. Less clear is on what space and time scales the MOC varies, what the underlying processes are, what the impact of those variations is on the European climate and if the Atlantic MOC can undergo significant fluctuations that could be responsible for major climate shifts. Results showed that poleward of 30°N and 10°S the flow is mainly geostrophic. In low latitudes the Ekman component is important for the mean and the variability. A significant deviation from a geostrophic balance is caused by flow through narrow straits such as the Florida Strait where nonlinearities and mixing become important. Variability of the Ekman component is shallow, and therefore important for heat transport variations. Variability of the geostrophic component is maximum at 1000m depth and therefore not likely to significantly alter the poleward heat transport. The largest discrepancy to Bryden were diagnosed for 1957, when GECCO suggest a much lower value (could come from Florida Straight estimate). In contrast to a MOC decrease, GECCO suggests an increase in MOC strength since the 60th. An initial decline due to model adjustments underlines the need for long dynamically consistent estimation approaches with improved boundary conditions and mixing parameterizations in support of MOC analyses.

An important application of ocean state estimation is that of ocean initialization for seasonal and decadal forecasting. It is assumed that atmospheric initial conditions play a secondary role and that the ocean's initial conditions are most important for improving the skill of our forecasts on these time scales. An optimal initial condition is accordingly one that produces the best forecast. However, in complex non linear systems there is no “objective searching algorithm” for optimality. The practical approach is therefore to have subjective criteria. Theoretically, initial conditions should represent accurately the state of the real world. However, given the fact that models have errors and biases, this would not be the best initial conditions for optimizing the forecast skill. Among the practical ways of creating ocean initial conditions is to run a ocean model forward driven by atmospheric fluxes provided by NWP centres. Such an approach always leads to errors (biases) in the ocean model that cause problems when coupling the respective ocean component with the atmosphere. A practical requirement is therefore: the forecast initial conditions should be “consistent” with the model state of calibrated hindcasts. Current priorities for initial conditions of coupled models include SST and ocean subsurface temperature and salinity fields. Land/ice/snow cover become potentially also important.

There are several strategies for the initialization of coupled models, as well as those for improving the initialization procedure. Those initialization steps include uncoupled and coupled model initializations, with the former the current practice. Uncoupled initialization is the most common approach with the clear advantage that it is practical. Dependent on the detailed approach, the systematic error during the initialization is small. The obvious disadvantage is that the model used for the initialization step is different from that used during the coupled forecast. The result is an unavoidable initialization shock, besides the fact that the model error of the coupled system can be a overwhelming source of error during the forecast. Moreover, there is no synergy between ocean and atmospheric observations in that ocean information is not being propagated into the coupled system and used to improve the coupled system. To make further progress, especially in decadal forecasts and for climate scenario runs, a full coupled model initialization must be established. This step is taken now by a few that clearly demonstrated the benefits of this step for improving forecasts.

There are a variety of ocean simulation and data assimilation products available today that can be used for climate applications. Underlying assimilation schemes range from simple and computationally efficient (e.g., optimal interpolation) to sophisticated and computationally intensive (e.g., adjoint and Kalman filter-smoother). Some of the existing simulation and assimilation products span the period of the past several decades (e.g., the SODA product and the on-going multi-decadal ECCO reanalysis product); others cover only the period from 1992 to present. Some are eddy-permitting, some are coarser in resolution. In most approaches the attention has been paid to “sequential” methods (Kalman filters in various incarnations, and less commonly on completing the job with a smoother).This is probably a result of the atmospheric focus on prediction---for which the KF is optimal (up to linearization). Lagrange multiplier methods (“adjoint” or “4DVAR”) were less common in the past, because of the increased computing load. They become quite common now, partly because of the availability of semi-automatic differentiation (AD) tools (like TAF).

To assess the merits of different assimilation approaches, a careful evaluation of the quality and consistency of all existing analysis/reanalysis products is required. Such an evaluation helps to identify approaches that serve different needs (e.g., analysis of ocean/climate dynamics versus initialization of coupled models) best and will serve as the basis for recommendations for future resource planning. Evaluation efforts were performed under CLIVARS’s “Global Synthesis and Observations Panel” (GSOP) (http://www.clivar.org/organization/gsop/gsop.php). The global reanalysis evaluation effort is based primarily on model-data intercomparisons, and serves to:

- Evaluate the quality and skill of available global reanalysis products and determine their usefulness for CLIVAR.
- Identify the common strength and weakness of these systems and the differences among them, as well as to identify which application can be best served by which reanalysis products.
- Define climate-indices and products that should be produced in a regular manner by each reanalysis effort to support regional and global CLIVAR analyses and process studies alike and thereby to facilitate applications of reanalysis products by the climate research community.

An important aspect of a synthesis evaluation – and of any model evaluation for this matter – is to carefully define metrics against which model skills can be tested. Within CLIVAR, metrics for a synthesis evaluation were discussed with all basin panels, since they can also serve as important indices. Within the synthesis evaluation the following list of metrics were used. It would be useful if model development activities could adopt similar metrics, since computing those numbers and making them publicly available does help CLIVAR's research through easier use of model results. At the same time, a more intense use of synthesis and model results will also expedite the improvements of models.

Synthesis Evaluation Metrics:

- Systematic model-data comparison: RMS model data differences relative to prior data errors.
- Differences between first guess/constrained model.
- Comparison of model results to reference data sets, e.g., surface fluxes.
- Comparison of model results with time series stations.
- Computation of integral quantities, such as MOC strengths, heat transports, transports through key regions.
- Budgets, e.g., heat content and its change in all mayor ocean basins.
- Model-Model differences (incl. first guess).

8. Recommendations and closing comment: Stephen Griffies (GFDL)

It is difficult to provide just a few succinct recommendations from a workshop of this calibre and breadth, where we saw an amazing number of solid presentations and associated discussions. But here is an attempt to bring some closure to the workshop report:

- Workshops of this sort are few and far between. This situation is unfortunate, given the need for the ocean modelling community to fully step up to the task of fostering the development of sound scientifically based numerical tools. So the most important recommendation to arise from this workshop is to encourage the support by the community of a semi-periodic workshop that focuses on state-of-the-art in numerical methods used for ocean circulation models. This workshop should promote discussion and debate of the many issues that arise in ocean modelling, with plenty of time for networking.

- The common element required of all methods of use for ocean circulation modelling is that the discrete model equations should conserve scalar fields (mass, heat, salt, and other tracers). This property is dictated by the need to simulate an ocean fluid whose source and sink terms are physically based rather than numerical artefacts. The needs of understanding and simulating climate change, including effects on ocean biogeochemistry, necessitate models that conserve scalars. This conservation property, unfortunately, is not satisfied by all ocean models in use today. Such should be remedied in the future, as there is no fundamental reason that discrete model equations, and the associated methods used to time step these equations, cannot be written so that scalar fields are conserved to the accuracy of numerical round-off.

- The state-of-the-art in numerical methods presented at this workshop focused on two main elements of ocean models: 1/ treatment of the vertical coordinate, 2/ treatment of the horizontal grid. It is unclear whether the traditional level coordinate finite difference / finite volume methods, most popular in global modelling, will give way in some years to the hybrid coordinate finite element or non-rectangular grid methods which represent the cutting edge research. But results from many workshop presentations indicate that substantial progress has been made in recent years, moving what formerly were just novel ideas into very promising avenues of development. It is encouraging that the field of ocean modelling has progressed so far to allow for very creative approaches to be of potential use for the high-end models.

- As the needs of the models becomes more substantial (e.g., for prediction), and as the computer power increases to allow for more rich flow fields to be simulated, the requirements of numerical methods becomes more robust. There is no hiding sloppy methods under the veil of a heavily diffused model when the flow field becomes more refined and active. In turn, when customers, such as governments, call on scientists to answer tough environmental questions, our tools must be of utmost integrity, reliability, and transparency.

Appendix A

CLIVAR WGOMD Workshop on Numerical Methods in Ocean Models
24-25 August 2007 – Bergen, Norway

Programme

Thursday 23rd August: Basics

1. Overview of equations and methods (08:00-09:30): Alistair Adcroft

08:00-08:30	Equations, Approximations and Methods in Ocean Modeling Alistair Adcroft, Geophysical Fluid Dynamics Laboratory, Princeton, USA
08:30-09:00	Ocean Modeling, Remapping, and the ALE Method John Dukowicz, Los Alamos National Laboratory, USA
09:00-09:30	The different flavors of Finite Element and Finite Volume discretization for oceanic flows Mohamed Iskandarani, RSMAS/MPO, University of Miami, USA
09:30-10:00	Break

2. Vertical coordinates (10:00-12:00): Robert Hallberg

10:00-10:20	Overview - Inherent strengths and challenges of the various vertical coordinates used in ocean models Robert Hallberg, Geophysical Fluid Dynamics Laboratory, Princeton, USA
10:20-10:40	Spurious diapycnal mixing in ocean models Stephen Griffies, Geophysical Fluid Dynamics Laboratory, Princeton, USA
10:40-11:00	Issues arising from the nonlinear equation of state in isopycnal coordinate models Robert Hallberg, Geophysical Fluid Dynamics Laboratory, Princeton, USA
11:00-11:20	Are there remaining issues precluding the use of terrain-following coordinates in global climate models? Gokhan Danabasoglu, National Center for Atmospheric Research, Boulder, USA
11:20-11:40	Issues regarding the use of hybrid coordinates Rainer Bleck, NASA Goddard Institute for Space Studies, Columbia University, New York, USA

-i.e., what modeling considerations give the best of the various coordinate options, and not the worst.

11:40-12:00	Discussion What can be done to promote a unified treatment of physical parameterizations across various vertical coordinates? -or- Further discussion of other issues from this session at the discretion of the Organizer.
12:00-13:00	Lunch

3. Non-rectangular structured meshes and unstructured meshes (13:00-15:00): Todd Ringler, Matthew Piggott, Eric Deleersnijder

13:00-13:30	Voronoi Tessellations for Ocean Modelling: Methods, Modes and Conservations Todd Ringler, Los Alamos National Laboratory, USA
13:30-14:00	Unstructured meshes and adaptivity for 3D multi-scale ocean modelling Matthew Piggott, Imperial College, London, UK
14:00-14:30	Finite element ocean modeling on unstructured 'prismatic' meshes Laurent White, Université catholique de Louvain, Louvain-la-Neuve, Belgium
14:30-15:00 -	Discussion
15:00-15:30 -	Break

4. Parameterization of physical process (15:30-18:00): Richard Greatbatch and Martin Schmidt

15:30-15:55	Diabatic effects associated with mesoscale eddies Richard Greatbatch, Department of Oceanography, Dalhousie University, Halifax, Canada
15:55-16:20	Parameterizing eddies in ocean models: energetics, potential vorticity mixing and flow instability David Marshall(1) and Alistair Adcroft (2) (1) Department of Physics, University of Oxford, UK, (2) Geophysical Fluid Dynamics Laboratory Princeton, USA
16:20-16:45	Parameterizing Mesoscale Eddies with Residual and Eulerian Schemes Geoffrey K. Vallis, Geophysical Fluid Dynamics Laboratory, Princeton, USA
16:45-17:10	The energetics of internal solitary waves and the need for parameterizations of their effects Kevin Lamb, Department of Applied Mathematics, University of Waterloo, Canada
17:10-17:35	The vertical mixing role of surface waves in ocean circulation models Fangli Qiao, First Institute of Oceanography, State Oceanic Administration, China
17:35-18:00	Should we really resolve eddies in the ocean component of coupled climate models? Rüdiger Gerdes, Alfred-Wegener-Institute Bremerhaven, Germany

Friday 24th August: Applications

5. Coastal/Regional modelling (08:00-10:30): Eric Blayo, Jarle Berntsen

08:00-08:30	Open boundary conditions Eric Blayo, University of Grenoble, France

Coastal/regional models are partly driven by their open boundaries, and the conditions which are applied at these artificial interfaces have a strong influence on the solution:

- Mathematical point of view
- Practical aspects: which conditions? the role of external data
- Open issues

08:30-09:00	Two-way nesting

Laurent Debreu, Institut National de Recherche en Informatique et en Automatique, Saint Martin d'Heres, France

-Methods for ensuring transparent behaviour at boundaries, and conservation of mass and tracers: Technical and practical issues

Physical aspects (65mn talk + 25min discussion)

09:00-09:25 Internal physics
Jarle Berntsen (1), Alan M. Davies (2), and Jiuxing Xing (2)
(1) Universitetet i Bergen, Norway, (2) Proudman Oceanographic Laboratory, UK

The ocean physics in coastal/regional models can be somewhat different from the physics at a larger scale:

- Which particular physics has to be represented in coastal/regional models?
- Small-scale processes and their parameterization
- Interactions with topography
- Hydrostatic versus non-hydrostatic

09:25-09:45 Wetting and Drying
Leo Oey, Princeton University, USA

-The physical problem and its importance in coastal modelling; numerical methods and algorithms

09:45-10:15 Break

10:15-10:40 Model validation
Lars Petter Roed, Norwegian Meteorological Institute, Oslo, Norway

-How shall we do it? Examples from recent exercises

10:40-11:00 Discussion

6. Basin and Global Models: Claus Böning, Anne Marie Treguier and Stephen Griffies

11:00-11:15 Southern Ocean Simulations with and without Eddies
Robert Hallberg, Geophysical Fluid Dynamics Laboratory, Princeton, USA

11:15-12:00 Global Eddying Simulations: what is done and what should be done
Stephen Griffies, Geophysical Fluid Dynamics Laboratory, Princeton, USA

12:00-13:00 Surface Forcing of Ocean Models Claus Böning (1) and Rüdiger Gerdes (2)
(1) IFM-GEOMAR, Universitaet Kiel, Germany (2) Alfred-Wegener-Institute Bremerhaven, Germany

13:00-14:00 Lunch

14:00-14:15 Quantitative model-data comparisons using altimeter data: Dependancy of the model skill on resolution
Thierry Penduff, Laboratoire des Ecoulements Géophysiques et Industriels, Grenoble, France

14:15-15:00 Resolving Mesoscale Eddy Spectrum: What is Needed?
Anne Marie Treguier, Laboratoire de Physique des Océans, IFREMER, Brest, France

15:00-15:30 Break

7. Ocean processes and inverse methods (1530-1700): Detlef Stammer

15:30-16:00	Using Ocean Data Assimilation to Estimate Transports and Processes Detlef Stammer, Inst. fuer Meereskunde, Universitaet Hamburg, Germany
16:00-16:30	Impact of Ocean Initialization on Seasonal Forecast Skills Magdalena Balmaseda, ECMWF, Reading, UK
16:30-17:00	Data Assimilation with HYCOM Ashwanth Srinivasan, COAPS, Florida State Univeristy, Miami, USA

8. Recommendations to WGOMD and LOM (1700-1730): Stephen Griffies

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