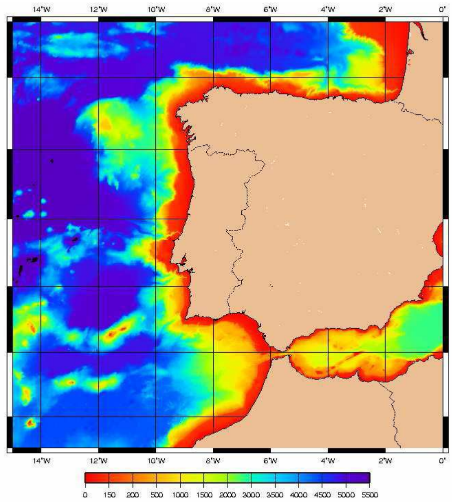
« *Modélisation des fines échelles internes*
dans la région du détroit de Gibraltar et leurs impacts »

Tâche 2 : généralisation du système de coordonnées verticales

Rapport: Eric Chassignet
Référence n° SHOM-052016-CR

Le SHOM développe, met en œuvre et exploite des modèles numériques permettant de décrire précisément la circulation océanique. Le programme stratégique PROTEVS (PREVISION OCEANIQUE, TURBIDITE, ECOULEMENT, VAGUES ET SEDIMENTOLOGIE) vise à améliorer
les systèmes d'analyse et de prévision de l'environnement marin en temps réel avec essentiellement trois objectifs : améliorer la connaissance des processus océaniques et côtiers impactant les opérations militaires, étudier la faisabilité de systèmes permettant la reconstitution en temps réel et l'évolution de l'environnement hydrodynamique et étudier la possibilité d'étendre cette reconstitution à l'environnement biogéochimique.



Une maquette du détroit de Gibraltar couvrant la zone de l'outflow méditerranéen le long des côtes portugaises (maquette *OUTMEDI*, figure 1) a en particulier été développée dans le cadre de ce programme. Cette maquette a une résolution de
1.8 km (soit un mile marin) et possède, dans un système de coordonnées verticales hybrides, 32 niveaux. Le modèle est forcé aux limites par les sorties du modèle global Mercator et par les composantes harmoniques déduites de l'altimétrie TOPEX.

Figure 1 : Maquette HYCOM sur le détroit de Gibraltar (*OUTMEDI*)

L'objet de la consultation n° SHOM-052016-CR du SHOM est la « modélisation et l'évaluation de solutions numériques dans la région du Détroit de Gibraltar ». Cette consultation comporte deux tâches distinctes :

- *la première tâche consiste à implémenter un modèle numérique qui puisse totalement relaxer l'hypothèse d'hydrostaticité dans la région du détroit de Gibraltar et à procéder à une évaluation (coût calcul/performance) de la maquette numérique ainsi proposée.*

- *la seconde tâche concerne la généralisation du système de coordonnées verticales, à partir d'une approche ALE (Arbitrary Lagrangian-Eulerian coordinate).*

Rapport Tâche 2: Generalized vertical coordinates

Le groupe de modélisation numérique de l'équipe AOC du Laboratoire d'Aérologie a accueilli pendant l'automne 2016 et le printemps 2017 le professeur Eric Chassignet sur un poste d'« Enseignant-chercheur Invité » de l'Université Fédérale de Toulouse Paul Sabatier (Faculté des Sciences et de l'Ingénierie). Eric Chassignet est professeur d'océanographie à l'Université de l'Etat de Floride (Etats-Unis), directeur du « *Centre pour la Prévision et les Etudes liées à l'Océan et à l'Atmosphère*» (COAPS, Floride) mais aussi responsable et coordinateur du code numérique océanique HYCOM.

Tâche 2.1 : S*ynthèse des difficultés*

Les modèles sont des outils de premiers choix pour aborder des questions d'océanographie en nombre et d'extension disciplinaire croissants. L'expertise nécessaire à la mise au point de tels modèles dépasse de loin ce qu'une personne ou même un petit groupe de chercheurs peut détenir. Si bien que les démarches communautaires sont celles sur lesquelles il faut s'appuyer. On trouve ainsi plusieurs classes de ces modèles numériques adossés à une large communauté de développeurs et d'utilisateurs qui interagissent en partageant leurs outils (pré et post-processing), leur savoir-faire dans des structures ad hoc (comité de développement, réunions d'utilisateurs), qui ont fait l'effort de documenter leur code à tous les niveaux et en assure la diffusion par des services web (e.g. HYCOM, NEMO, ROMS-AGRIF, …).

En modélisation de la dynamique océanique, on distingue aussi différents types d'approches numériques se différenciant notamment par le type de discrétisation spatiale et temporelle, la nature de la coordonnée verticale utilisée, la paramétrisation des échelles sous-maille. Le choix de la coordonnée verticale demeure un des aspects les plus sensibles de la conception d'un modèle océanique (Chassignet et al., 2006). En pratique, la paramétrisation des processus non résolus et la discretisation spatio-temporelle des équations sont souvent directement liées au choix de la coordonnée verticale. Les modèles de circulation océanique représentent habituellement la dimension verticale en un empilement de couches définies selon la profondeur, la densité ou en pro rata de la hauteur d'eau.

Les exercices récents d'intercomparaison de modèles ont montré que l'utilisation d'une unique coordonnée verticale ne pouvait être optimale partout. Ainsi la coordonnée isopycnale est la plus adaptée à la description de la circulation intérieure de l'océan, la coordonnée géopotentielle est la meilleure pour reproduire la dynamique de la couche mélangée en surface et enfin la coordonnée sigma est le meilleur choix pour la région côtière où la topographie est complexe et surtout les variations de la surface libre sont significatives par rapport à la hauteur de la colonne d'eau.

Parmi les modélisateurs en océanographie physique, il y a désormais un consensus général sur le fait qu'une coordonnée hybride dans un système de coordonnée complètement généralisée permettant de mimer les différents types de coordonnées en fonction de la région et du régime hydrodynamique est probablement le meilleur compromis (Griffies et al., 2000). Certains modèles utilisent déjà de façon courante la coordonnée verticale généralisée (HYCOM: NOAA/NCEP, U.S. et French Navies) ou bien commence à l'utiliser (MOM6: NOAA/GFDL; MPAS : Los Alamos National Laboratory).

Pour un système de coordonnée complètement généralisée, les équations primitives doivent être réécrites dans une système de coordonnées (x,y,s) ou s est un coordonnées verticales généralisée non spécifiée (Bleck, 2002). Ce qui donne le système d'équations où :

$$\frac{\partial \mathbf{v}}{\partial \mathrm{t}_s} + \nabla_s \frac{\mathbf{v}^2}{2} + (\varsigma + \mathrm{f})\mathbf{k} \times \mathbf{v} + \left(\dot{s} \frac{\partial p}{\partial s} \right) \frac{\partial \mathbf{v}}{\partial p} = p \nabla_s \alpha - \nabla_\alpha M - g \frac{\partial \tau}{\partial p} + \left(\frac{\partial p}{\partial s} \right)^{-1} \nabla_s \cdot \left(\nu \frac{\partial p}{\partial s} \nabla_s \mathbf{v} \right) \quad (1)$$

$$\frac{\partial}{\partial \mathrm{t}_s} \left(\frac{\partial p}{\partial s} \right) + \nabla_s \cdot \left(\mathbf{v} \frac{\partial p}{\partial s} \right) + \frac{\partial}{\partial s} \left(\dot{s} \frac{\partial p}{\partial s} \right) = 0 \quad (2)$$

$$\frac{\partial}{\partial \mathrm{t}_s} \left(\frac{\partial p}{\partial s} \theta \right) + \nabla_s \cdot \left(\mathbf{v} \frac{\partial p}{\partial s} \theta \right) + \frac{\partial}{\partial s} \left(\dot{s} \frac{\partial p}{\partial s} \theta \right) = \nabla_s \cdot \left(\mu \frac{\partial p}{\partial s} \nabla_s \theta \right) + \mathrm{H}_\theta \quad (3)$$

où :

- $\mathbf{v}$ = (u,v) sont les composantes horizontales de la vitesse,
- p est la pression,
- θ représente n'importe quel traceur actif,
- $\alpha = \rho^{-1}$ est le volume potentiel spécifique,
- $\varsigma = \partial v / \partial x - \partial u / \partial y$ est la vorticité relative,
- $M = gz + p\alpha$ est le potentiel Montgomery,
- f est le paramètre de Coriolis,
- $\mathbf{k}$ le vecteur unitaire vertical,
- ν et μ sont les coefficients de viscosité et de diffusivité,
- τ est un tenseur surfacique de contrainte qui représente la tension de vent en surface ou le frottement au fond,
- H_θ est la somme de tous les termes sources de θ diabatiques qui comprennent notamment le mélange diapycnal.

Les indices indiquent quelle variable est constante au cours de la dérivation. Les distances dans les directions x et y ainsi que les dérivées temporelles de u et v sont mesurées en projection sur un plan horizontal. Cette transformation conduit à un système de coordonnées non-orthogonales dans l'espace 3D mais élimine les termes de métriques relatifs aux pentes des isosurfaces s (Bleck, 1978). Les autres termes de métriques, créés quand les opérations sur les vecteurs impliquent les opérateurs $(\nabla\cdot)$ ou $(\nabla\times)$ sont évalués sur une grille non cartésienne (i.e. en coordonnées sphériques) et sont cachés dans les termes de base en évaluant la vorticité et la divergence horizontale du flux dans les équations (1) à (3) comme une intégrale le long de chaque maille (Griffies et al., 2000 pour plus de détail). Il est notable que l'opérateur ∇ appliqué à un scalaire comme $\mathbf{v}^2/2$ dans l'équation (1), ne donne naissance à aucun terme de métrique. En second lieu, en intégrant sur la verticale entre surfaces s_{top} et s_{bot}, l'équation de continuité (2) devient une équation prognostique pour le poids de la couche par unité de surface, $\Delta p = p_{bot} - p_{top}$ ·

$$\frac{\partial \Delta p}{\partial \mathrm{t}_s} + \nabla_s \cdot (\mathbf{v} \Delta p) + \left(\dot{s} \frac{\partial p}{\partial s} \right)_{\mathrm{bot}} - \left(\dot{s} \frac{\partial p}{\partial s} \right)_{\mathrm{top}} = 0 \quad (4)$$

Le terme $(\dot{s}\partial p / \partial s)$ représente le flux de masse vertical à travers les isosurfaces de s, comptant positivement dans la direction $+p$ orientée vers le bas. En multipliant (1) par $\partial p / \partial s$, en intégrant sur l'intervalle (s_{top}, s_{bot}), en divisant par $\Delta p / \Delta s$, le terme de cisaillement devient $g / \Delta p(\boldsymbol{\tau}_{top} - \boldsymbol{\tau}_{bot})$ tandis que le terme de mélange latéral s'intègre en $(\Delta p)^{-1}\nabla_s \cdot (\nu \Delta p \nabla_s \mathbf{v})$. Tous les termes en (1) conserve leur forme. La forme intégrée par couche de l'équation (3) devient, elle :

$$\frac{\partial}{\partial \mathrm{t_s}}(\Delta p \theta) + \nabla_s \cdot (\mathbf{v} \Delta p \theta) + \left(\dot{s} \frac{\partial p}{\partial s} \theta \right)_{\mathrm{bot}} - \left(\dot{s} \frac{\partial p}{\partial s} \theta \right)_{\mathrm{top}} = \nabla_s \cdot (\mu \Delta p \nabla_s \theta) + \mathrm{H}_\theta \qquad (5)$$

Les équations pronostiques ci-dessus sont complétées par différentes équations diagnostiques, notamment l'équation traduisant l'équilibre hydrostatique , $\partial M / \partial \alpha = p$; une équation d'état qui lie la température potentielle, la salinité et la pression à la densité potentielle et une équation qui prescrit le flux de masse vertical $(\dot{s}\partial p / \partial s)$à travers les iso-surfaces de s. La relaxation de l'hypothèse d'hydrostaticité doit être examinée. Finalement, il est nécessaire de combiner les avantages des différents types de coordonnées verticales de façon optimale à l'aide d'un générateur de coordonnées hybrides. Le vocable « coordonnées hybrides verticales » est un peu ambigu et peut avoir différente signification. :

- Ce peut être une combinaison linéaire de deux coordonnées conventionnelles ou plus (Barron et al., 2006)
- Ce peut être une vraie coordonnée généralisée qui vise à mimer différents types de coordonnées en différentes localisations de la grille de calcul (Bleck, 2002; Adcroft and Hallberg, 2006; Chassignet et al., 2006). Adcroft et Hallberg (2006) ont classé les modèles océaniques à coordonnées verticales généralisées en modèles océaniques à coordonnées lagrangiennes (Lagrangian Vertical Direction, LVD) ou à coordonnées eulériennes (Eulerian Vertical Direction, EVD). Les modèles à coordonnées verticales lagrangiennes résolvent l'équation de continuité qui fournit le terme de tendance des épaisseurs de couches par intégration temporelle (forward) et une technique arbitrairement Lagrangienne-Eulérienne (ALE) pour remapper la coordonnée verticale et prescrire différents types de coordonnées sur la grille. Les modèles à coordonnées eulériennes qui suivent la topographie (typiquement les coordonnées sigma) se servent de l'équation de continuité pour calculer la vitesse verticale. Deux générateurs de coordonnées hybrides existent : HYCOM et MOM6. Ces derniers sont des modèles communautaires, mais diffèrent dans leur approche. Le générateur d'HYCOM date de 2002 et a continuellement évolué depuis tandis que celui de MOM6 est beaucoup plus récent (été 2015).

Le groupe de travail consistant de Francis Auclair, Remy Baraille, Laurent Debreu, et Florian Lemarié s'est rencontré plusieurs fois, ensemble ou individuellement pour faire une évaluation du code CROCO et de la difficulté qu'il y aurait d'implémenter le système de coordonnées généralisées. Il s'avère que le code CROCO est écrit de telle façon qu'il est relativement simple de le faire tourner en coordonnées isopycniques (approche LVD), la première étape nécessaire avant d'implémenter une technique arbitrairement Lagrangienne-Eulérienne (ALE) pour remapper la coordonnée verticale. Laurent Debreu a donc rajouté une routine pour l'équation de continuité et a pu faire tourner quelques cas tests rapidement (2 couches, fond plat) pour démontrer cette capacité.

Recommandations : Afin d'implémenter complètement l'option isopycnique et ensuite ALE, il faut que (1) les épaisseurs des couches isopycniques puissent aller à zéro (implémentation d'un schéma de type FCT pour l'équation de continuité et pour les traceurs) et (2) l'expression du gradient de pression soit exacte pour tout choix de cordonnées verticales (i.e. Adcroft et al., 2008). Une offre de post-doc par Florian Lemarié devrait permettre d'avancer assez vite sur ces options avec un schéma de discrétisation pour la conservation de la masse (pour le moment, seulement le volume est conservé) préservant la positivité des épaisseurs de couche et compatible avec le schéma de discrétisation temporel utilisé dans les autres équations de conservation. Les travaux prévus d'implémentation et de tests qui font l'objet d'une partie du contrat se poursuivent désormais dans l'équipe de Florian Lemarie. Un post-doctorant est en cours de recrutement. Le professeur Chassignet participera à l'encadrement du postdoc et l'accueillera dans son laboratoire. Les résultats obtenus seront alors adossés à ce rapport.

Tâche 2.2 : *ALE et remapping*

L'étape suivante est d'implémenter ALE. Pour un modèle traditionnel exprimé en coordonnées Eulérienne fixe, les équations sont (Adcroft, 2016, ALE workshop)

Integrate down from top b.c.

$$\partial_z p = -g\rho(z, S^n, \theta^n) \qquad \rightarrow p$$

$$v_h^{n+1} = v_h^n + \Delta t\left(-\frac{1}{\rho_o}\nabla_z p + \cdots\right) \qquad \rightarrow v_h^{n+1}$$

$$\partial_z w = -\nabla \cdot v_h^{n+1} \qquad \rightarrow w$$

Integrate up from solid bottom

$$\theta^{n+1} = \theta^n - \Delta t\left[\nabla \cdot \left(v_h^{n+1}\theta^n\right) + \partial_z(w\theta^n) + \cdots\right] \rightarrow \theta^{n+1}$$

Explicit vertical transport
Conditionally stable

$$\boxed{\frac{\Delta t w}{\Delta z} < 1}$$

Implications for topographic representation

Lorsque les coordonnées peuvent se déplacer de leur positions fixes pour permettre à des ondes de se propager (Leclair and Madec, 2011), les équations sont souvent exprimées comme (Adcroft, 2016, ALE workshop) :

$$\partial_z p = -g\rho(z, S^n, \theta^n)$$

$$v_h^{n+1} = v_h^n + \Delta t\left(-\frac{1}{\rho_o}\nabla_z p + \cdots\right)$$

(Leclair & Madec, 2011, use this form)

$$\delta_k(w^* + w_g) = -\nabla \cdot h^n v_h^{n+1}$$

Specify motion of grid, w_g, here

$$h^{n+1} = h^n + \Delta t \delta_k\,(w_g)$$

Still have explicit transport

$$h^{n+1}\theta^{n+1} = h^n\theta^n - \Delta t\left[\nabla \cdot \left(h^n v_h^{n+1}\theta^n\right) + \delta_k(w^*\theta^n) + \cdots\right]$$

- If $w_g = 0$, then grid is fixed and we recover Eulerian algorithm
- $w^* = w - w_g$ is motion relative to grid
- If we want $w^* = 0$ then we must specify $\partial_z w_g = -\nabla_h . v_h^{n+1}$
- Note that if $w_g \neq 0$ then the grid is moving

Ce qui permet de spécifier les mouvements de la grille verticale. L'analyse du code CROCO montre donc que l'implémentation ALE du type I comme ci-dessus est déjà existante et que cela devrait permettre de tester les coordonnées généralisées assez rapidement dès que la positivé des épaisseurs de couches et le gradient de pression généralisé est en place. Cette approche est cependant limitée par un critère CFL (voir plus bas).

L'ALE type II est celle qui est en place dans HYCOM et MOM6 (Adcroft, 2016, ALE workshop),

$$\partial_z p = -g\rho(z, S^n, \theta^n)$$

$$v_h^\dagger = v_h^n + \Delta t\left(-\frac{1}{\rho_o}\nabla_z p + \cdots\right)$$

$$h^\dagger = h^n - \Delta t \nabla \cdot (h^n v_h^\dagger)$$

Grid moves as if $w^* = 0$

$$h^\dagger \theta^\dagger = h^n \theta^n - \Delta t\left[\nabla \cdot \left(h^n v_h^\dagger \theta^n\right)\right]$$

No vertical transport

- At this point (†), the grid has moved (Lagrangian-ly)
- If the grid is not where we want it, then we remap:

$$h^{n+1} \leftarrow \delta_k Z\left(z^\dagger\right) ; \theta^{n+1} = \theta^\dagger\left(Z(z^\dagger)\right) ; \ldots$$

It's the same thing!

- Specifying Z is potentially simpler than specifying w_g

mais sans critère CFL. Pour récapitulation :

Eulerian	**A.L.E. (flavor 1)**	**A.L.E. (flavor 2)**
$\partial_z p = -g\rho(z, S^n, \theta^n)$	$\partial_z p = -g\rho(z, S^n, \theta^n)$	$\partial_z p = -g\rho(z, S^n, \theta^n)$
$v_h^{n+1} = v_h^n + \Delta t\left(-\frac{1}{\rho_o}\nabla_z p + \cdots\right)$	$v_h^{n+1} = v_h^n + \Delta t\left(-\frac{1}{\rho_o}\nabla_z p + \cdots\right)$	$v_h^\dagger = v_h^n + \Delta t\left(-\frac{1}{\rho_o}\nabla_z p + \cdots\right)$
$\partial_z w = -\nabla \cdot v_h^{n+1}$	$\delta_k(w^* + w_g) = -\nabla \cdot h^n v_h^{n+1}$	$h^\dagger = h^n - \Delta t \nabla \cdot (h^n v_h^\dagger)$
$\theta^{n+1} = \theta^n - \Delta t \begin{bmatrix} \nabla \cdot \left(v_h^{n+1}\theta^n\right) + \\ \partial_z(w\theta^n) + \cdots \end{bmatrix}$	$h^{n+1} = h^n + \Delta t \delta_k(w_g)$	$h^\dagger \theta^\dagger = h^n \theta^n - \Delta t\left[\nabla \cdot \left(\begin{matrix} h^n v_h^\dagger \theta^n \\ + \cdots \end{matrix}\right)\right]$
	$h^{n+1}\theta^{n+1} = h^n\theta^n - \Delta t \begin{bmatrix} \nabla \cdot \left(h^n v_h^{n+1}\theta^n\right) \\ +\delta_k(w^*\theta^n) + \cdots \end{bmatrix}$	$h^{n+1} \leftarrow \delta_k Z\left(z^\dagger\right)$
$\boxed{\frac{\Delta t w}{\Delta z} < 1}$	$\boxed{\frac{\Delta t w^*}{\Delta z} < 1}$ $\quad w^* = w - w_g$	$\theta^{n+1} = \theta^\dagger\left(Z(z^\dagger)\right)$

Une fois tout cela en place, il faudra préciser le rezoning, c'est-à-dire le choix de la position des coordonnées généralisées. Cela dépend beaucoup des applications et ce choix devra être fait pour des applications CROCO, i.e. principalement côtières. Cela veut donc dire un match avec les coordonnées HYCOM au large pour les conditions aux limites et des coordonnées sigma le long des côtes. Dans le cas global couplé avec l'atmosphère, Adcroft montre que la prise de chaleur par l'océan est diminuée de 30% lorsque le choix de distribution des coordonnées est fait comme dans HYCOM.

Ce qui est aussi important pour la communauté CROCO, c'est de suivre l'effort qui a lieu aux USA pour unifier l'approche ALE et partager les expériences.

Le premier meeting a eu lieu en Octobre 2016. Les recommandations sont :

- Partage de code
- Création d'une communauté ALE
- Unification des codes HYCOM/MOM6
- Exploitation de la diversité des approches ALE

Le rapport complet est disponible en Annexe A.

Le second meeting a eu lieu en May 2017 et s'est surtout concentre sur la faisabilité d'un merger

HYCOM/MOM6 et sur le développement de code ALE en commun. Rapport complet en Annexe B.

Tâche 2.3 : *Meeting utilisateurs CROCO*

Afin d'encourager l'utilisation du modèle CROCO et d'informer les utilisateurs des derniers avancements, Eric Chassignet a organisé avec Rachid Benshila le premier metting des utilisateurs CROCO. L'agenda de ce meeting est en Annexe C.

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Annexe A :

Executive Summary
Workshop on Improving ALE Ocean Modeling NOAA Center for Weather and Climate Prediction College Park, MD
October 3-4, 2016

A one-and-a-half-day workshop on ocean models that employ the ALE (Arbitrary Lagrangian-Eulerian) method to permit general vertical coordinates was held at NCWCP on October 3-4, 2016. Four different ALE models (GO2, HYCOM, MOM6, and MPAS-Ocean) were discussed. Workshop participants included users and developers of these models, from academia and from seven different national modeling centers (ESRL, GFDL, GISS, LANL, NCAR, NCEP, NRL). A more detailed report on the workshop follows this executive summary, and a workshop agenda with a list of workshop speakers is attached as an appendix.

A number of recommendations for future action were developed during the meeting. The recommendations fall into four broad categories: Code Sharing, Community Building, Code Merger and Performance and Future Development. The recommendations are listed below.

1. Code Sharing

Sharing of common codes for the equation of state, grid generation and remapping, and column physics such as mixing parameterizations, is recommended. The group suggested making vertical remapping/grid generator routines an open source package that can be shared in the manner of CVMix.

a. The development of prognostic equations for the grid generator based upon physical mixing should be considered.
b. We recommend open-source GIT repositories (hosted on code-sharing sites such as Github) for submodules such as CVMix.
c. We recommend the development of common tests for self-consistency, conservation, and known solutions.

2. Community Building

d. The ALE modeling group should consider whether semi-regular meetings similar to this workshop should be undertaken; perhaps via merger/inclusion with the Layered Ocean Model workshop.
e. Following on successful efforts in the atmospheric modeling community, our community should consider developing ocean model development workshops. The long term health of the ocean modeling activity would be significantly enhanced through the sustained sponsorship of integrative activities that develop early career talent and, subsequently, provide cross-model fertilization.

3. Code Merger

f. HYCOM and MOM6 have enough similarities to consider a code merger, bringing the strengths of each to a common code base.

4. Performance and Future Development

g. The modeling community must confront the physics of boundary layers (at both the top and bottom boundaries) in order to fully exploit the power of ALE models.
h. The group expressed unanimous agreement on the value of funding different approaches to ALE modeling. Impressive results from the DOE MPAS-Ocean and NASA GISS GO2 models demonstrate the need for diversity in ALE modeling. Only by funding a few different ALE streams can we, as a community, be assured that innovations will continue to be developed.
i. To avoid flooding storage silos with large model output datasets, model users should consider, where possible, analyzing runs as they take place rather than afterwards.

Report on “Improving ALE Ocean Modeling Workshop” NCWCP
October 3-4, 2016

A one-and-a-half-day workshop on ocean models that employ the ALE (Arbitrary Lagrangian-Eulerian) method to permit general vertical coordinates was held at NCWCP on October 3-4, 2016. Four different ALE models (GO2, HYCOM, MOM6, and MPAS-Ocean) were discussed. Workshop participants included users and developers of these models, from academia and from seven different national modeling centers (ESRL, GFDL, GISS, LANL, NCAR, NCEP, NRL). A list of acronyms appears later in this document. A workshop agenda with a list of workshop speakers is attached as an appendix.

The first day included agency overview talks, a discussion of previous attempts to create a unified home for ALE code development, overview talks from all of the modeling groups, discussions of numerical implementation issues, and an overview of applications enabled by ALE models. A few key points that emerged are that (1) ALE is an algorithm for the vertical grid choice, (2) ALE is versatile and permits general vertical coordinates, that include traditional z, isopycnal, and terrain-following coordinates as well as hybrid combinations of the former and other creative treatments yet to be formulated and explored, (3) ALE can eliminate vertical CFL restrictions and minimize velocity errors, and easily enables wetting and drying, (4) a weakness of sorts for ALE models is that grid choice is important, not a simple black box usage, and (5) the MOM6 group has found that model errors have been reduced with the use of a finite-volume pressure gradient force.

The second half-day was set aside for discussions and recommendations. The general topics discussed were numerics and performance, model issues and necessary improvements, code sharing and potential collaborations, and next generation ALE models and future directions. Some key points and recommendations from the discussions held on the second day follow below.

There was some discussion about HPC performance issues that are experienced by all ocean modeling groups including ALE model groups—e.g. limitations on scalability, bit-for-bit multi-CPU reproducibility, refactoring for vector instructions, the low computational intensity of ocean models, and ocean model performance on coming future architectures. In response to a request from David McCarren, workshop participant Alan Wallcraft produced a summary of these issues, attached to this report as an appendix.

The problem of analyzing the massive outputs that large models can generate was discussed. This problem is particularly acute in the case of large high-resolution ensembles. One proposed solution to the large output problem is to analyze model output on the fly as it is running, rather than saving enormous amounts of high-spatial and temporal resolution output for later analysis. For example, in the context of data assimilation (an application for which large ensembles are likely to be used), the capability to output model fields interpolated to specified observation locations would considerably reduce I/O costs. In data assimilation algorithms, the model state must be interpolated to the observation locations in order to compute the analysis adjustments to be made to the model forecast. Without such a feature embedded in the model, 4D-EnKF and 3D-FGAT ("first guess at the appropriate time") methods would require outputting the full model state at or near the observation frequency to achieve similar results. For example, in the context of data assimilation (an application for which large ensembles are likely to be used), the capability to output model fields interpolated to specified observation locations would considerably reduce I/O costs. In data assimilation algorithms, the model state must be interpolated to the observation locations in order to compute the analysis adjustments to be made to the model forecast. Without such a functionality embedded in the model, 4D-EnKF and 3D-FGAT ("first guess at the appropriate time") methods would require outputting the full model state at or near the observation frequency to achieve similar results. For example, an EnKF with a 50-member ensemble assimilating hourly along-track SST data and randomly located in situ profiles over a 24-hour analysis cycle would require 50*24=1200 full model states to be output. With an embedded interpolation scheme, only the model state interpolated to the satellite tracks and sparse in situ profiles would need to be output at those same times, plus the 50 full model states at the analysis time.

This online approach applies most clearly to a reanalysis scenario, in which the observation locations are known in advance. But even in a forecast scenario it may be more efficient to rerun the ensemble of models and supply them with the observation locations to do an online computation of the required interpolations than to output all the model states during the original forecast and then compute the interpolations offline. The observation-minus-forecast and observation-minus-analysis data are the fundamental pieces of information produced in the data assimilation, and these are likely the primary ensemble data to be maintained and stored after the DA processing.

ALE-specific modeling issues were also discussed during the second half-day. For example, the HYCOM group will work to implement the Adcroft et al. 2008 pressure gradient approach, as part of an NRL Nordic Seas project. The HYCOM group will also explore using interface, rather than layer-average, density to guide vertical remapping.

There was much discussion of vertical remapping. Community users of model output generally want output in z-space (or pressure levels for non-Boussinesq configurations). The remapping to z levels has to be done carefully within an ALE model in order to respect conservation laws. An interesting idea that came up is development of prognostic equations for the grid generator based upon physical mixing. It was pointed out that ALE models can be made non-hydrostatic, but this feature has not been implemented yet because ALE models have not been run athorizontal resolutions fine enough to merit this approach. Another important point that came up is that the modeling community must confront the physics of boundary layers (at both the top and bottom boundaries) in order to fully exploit the power of ALE models.

It became clear at the meeting that different groups were using different names for the same type of grid related computation. The term regridding was suggested to be confusing and should be replaced with remapping. Alistair Adcroft suggested normalizing the nomenclature for future clarity. The group also suggested making vertical remapping/grid generator routines a common package that can be shared in the manner of CVMix. The discussions on code sharing and potential collaborations occupied a longer time than the other themed discussions, and led naturally into the final session on next generation ALE models and future directions. The group recommends open-source GIT repositories (hosted on code-sharing sites such as Github) for submodules and common codes to be developed. Sharing of common codes for the equation of state, grid generation and remapping, and column physics such as mixing parameterizations (via CVMix), was recommended. There was widespread support for the development of common tests for self-consistency, conservation, and known solutions.

The idea was floated that this ALE modeling group consider meeting annually or bi-annually, and that one potential format is to absorb such meetings into the Layered Ocean Model (LOM) meetings that have been taking place biannually for
many years. The latter idea found favor with some but not with all. An advantage of incorporating ALE workshops into LOM meetings is that it would entail less travel.
A potential disadvantage is that the LOM meeting has many presentations on science issues and incorporating the ALE workshops into it may make it too large. The question of whether future ALE workshops should be held, and whether they should be held during LOM meetings, was left unresolved.

One very important point made near the end of the discussions is that the ocean numerical model development community is small and that there is a need to entrain more early-career scientists into the field. The atmospheric modeling community has been very successful in this realm. For example, the Dynamical Core Model Intercomparison Project summer schools (https://goo.gl/7WDpSX) pair international atmophere modeling groups with aspiring graduate students and postdocs. In addition, since the mid 1990s the atmosphere modeling community has nurtured a core capability in computational physics through the bi-annual PDEs on the Sphere workshop. These activities not only develop early-career scientists but also provide an incubator for new ideas. The ocean modeling community lacks similar integrative activities and, instead, has tended toward model-centric workshops (e.g. NCAR OMWG, LOM, ROMS). The long term health of the ocean modeling activity would be significantly enhanced through the sustained sponsorship of integrative activities that develop early-career talent and, subsequently, provide cross-model fertilization.

Another critical point made was that some groups that use similar model codes consider merging their codes for the benefit of both groups. One such potential merger is between the HYCOM and MOM6. A merged model code that incorporated HYCOM's real-time data assimilation packages into a MOM6 dynamical core would partially satisfy the Navy's stated needs to upgrade HYCOM's dynamical core by ~2023, and would satisfy NOAA's desire for a common dynamical core to use in climate modeling, seasonal-interannual forecasting, and near-real-time ocean forecasting. **The group generally agreed that a closer working relationship between NOAA, NRL, and academic partners such as University of Michigan and Florida State University, involving an as-yet-to-be-determined merger between HYCOM and MOM6, was desirable.** It is important to note that such a merger does not prevent any scientist from continuing to use their own versions of HYCOM and MOM6 as they see fit. NRL, GFDL, and Michigan are already working on a MOM6 test run on NRL's 1/12th degree HYCOM grid with atmospheric and tidal forcing. A comparison of results from this MOM6 test run with a twin HYCOM run is expected to be very informative. The group recognized that an inter-agency project to set up and run a model for the benefit of both agencies is a time-consuming endeavor, that will need to be supported with dedicated resources. **The group noted that code sharing is different from**

code merging. HYCOM and MOM6 have enough similarities to consider a code merger, bringing the strengths of each to a common code base. The grid structure for MPAS-Ocean and GO2 are sufficiently different to preclude a code merger. However, there remain opportunities for code sharing of vertical column physics.

Finally, the group expressed unanimous agreement on the value of funding different approaches to ALE modeling. Impressive results from the DOE MPAS-Ocean and NASA GISS GO2 models demonstrate the need for diversity in ALE modeling. Only by funding distinct ALE streams can we be assured that innovations will continue to be developed. On a related note, the group recognized that ocean modeling involves people as much as it involves codes; as noted above, the nurturance of young talented model developers is critical for the long-term health of the field.

A number of recommendations for future action were developed during the meeting. The recommendations fall into four broad categories: Code Sharing, Community Building, Code Merger and Performance and Future Development. The recommendations are listed below.

1. **Code Sharing**
   a. The group suggested making re-mapping/grid generator routines an open source package that can be shared in the manner of CVMix. .
   b. The group recommends open-source GIT repositories (hosted on code-sharing sites such as Github) for submodules such as CVMix.
   c. Sharing of common codes for the equation of state, grid generation and remapping, and column physics such as mixing parameterizations, was recommended.
   d. There was widespread support for the development of common tests for self-consistency, conservation, and known solutions.

2. **Community Building**
   a. The ALE modeling group should consider whether semi-regular meetings similar to this workshop should be undertaken; perhaps via merger/inclusion with the Layered Ocean Model workshop.
   b. Following on successful efforts in the atmospheric modeling community, our community should consider developing ocean model development workshops. The long term health of the ocean modeling activity would be significantly enhanced through the sustained sponsorship of integrative activities that develop early-career talent and, subsequently, provide cross-model fertilization.

3. **Code Merger**
   a. HYCOM and MOM6 have enough similarities to consider a code merger, bringing the strengths of each to a common code base. The grid structure for MPAS-Ocean and GISS are sufficiently different to preclude a code merger. However, there remain opportunities for code sharing of vertical column physics.

4. Performance and Future Development

a. The development of prognostic equations for the grid generator based upon physical mixing should be considered.
b. The modeling community must confront the physics of boundary layers (at both the top and bottom boundaries) in order to fully exploit the power of ALE models. The group expressed unanimous agreement on the value of funding different approaches to ALE modeling. Impressive results from the DOE MPAS-Ocean and NASA GISS GO2 models demonstrate the need for diversity in ALE modeling. Only by funding a few different ALE streams can we as a community be assured that innovations will continue to be developed.
c. Ocean models and ALE models, in particular, haven't been designed for some of the potential new computer architectures. Ocean models tend to perform little computational work relative to the memory access. Moving ocean models to these new architectures will require substantial development effort. To avoid flooding storage silos with large model output datasets, model users should consider, where possible, analyzing runs as they take place rather than afterwards.

Acronyms:
ALE: Arbitrary Lagrangian-Eulerian DOE: Department of Energy
ESPC: Earth System Prediction Capability ESRL: Earth System Research Laboratory GFDL: Geophysical Fluid Dynamics Laboratory GISS: Goddard Institute for Space Studies
GO2: Goddard Ocean Model 2
HPC: High Performance Computing HYCOM: HYbrid Coordinate Ocean Model LANL: Los Alamos National Laboratory LOM: Layered Ocean Model meeting
MIT: Massachusetts Institute of Technology MOM6: Modular Ocean Model version 6
MPAS-Ocean: Model for Prediction Across Scales - Ocean NASA: National Aeronautics and Space Administration NCAR: National Center for Atmospheric Research
NCEP: National Centers for Environmental Prediction NCWCP: NOAA Center for Weather and Climate Prediction NOAA: National Oceanic and Atmospheric Administration NRL: Naval Research Laboratory
NWS: National Weather Service OMWG: Ocean Model Working Group
OSTI: Office of Science and Technology Integration ROMS: Regional Ocean Modeling System

Workshop organizers:
Brian Arbic, University of Michigan Robert Hallberg, NOAA GFDL Avichal Mehra, NOAA NCEP
James Richman, Florida State University

Workshop participants:
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Dan Eleuterio, Office of Naval Research
David McCarren, NOAA
Jesse Carman, NOAA

Appendix 1. Agenda: Workshop on Improving ALE Ocean Modeling

Venue
NCWCP College Park, MD, Oct, 3-4, 2016

Preamble
In the past few years, a number of research groups in the US have shifted ocean general circulation models from a fixed or single vertical coordinate to an Arbitrary Lagrangian Eulerian (ALE) vertical coordinate system. This shift takes advantage of the superiority of different vertical coordinate systems in different model locations (e.g., shelf vs. deep-ocean, weakly stratified mixed layer versus well-stratified interior). These relative performance advantages have led to a diversity of ocean models. The ALE framework offers the potential for a single model to exploit these relative advantages. However, a convergence in the vertical coordinate system doesn't imply convergence to a single ocean model. The numerical, dynamical and physical implementation and choices of these models differ substantially. Yet, there are aspects of the models that are similar and could be leveraged to improve all ALE models.

Goals of the Workshop
This workshop will gather experts associated with 3 in-use ALE Ocean Models, HYbrid Coordinate Ocean Model (HYCOM), Modular Ocean Model (MOM6) and Model for Prediction Across Scales- Ocean (MPAS-Ocean), as well as ocean modeling and forecasting leaders from academia and national laboratories, to exchange information about the strengths and weaknesses of the ALE models, their numerical, dynamical and physical implementations, and new developments in ALE modeling. The aim of this exchange is fostering improvements in the models by using the strengths of one model to address the weaknesses of another. We will also discuss the applications enabled by ALE models.

Day 1 Monday, October 3

0800 Jim Richman and Brian Arbic: Welcome and goals of Workshop

National Overview

0815 Henrick Tolman: NWS/NGPPS Modeling Plans
0900 Dan Eleuterio: National Earth System Prediction Capability Perspective
0930 Eric Chassignet: Previous attempt to create a unified home for ALE code development (remote presentation)
1000-1030 Coffee Break

ALE Numerics

1030 Rainer Bleck: Historical overview of ALE development
1100 Alistair Adcroft: MOM6 ALE overview + ALE-enabled general coordinates 1130 Darren Engwirda: MIT & GISS High-order accurate reconstructions,
re-gridding and pressure gradient evaluation for an ALE ocean model. 1200-1330 Lunch

Model overviews

1330 Max Kelley: GISS The new ALE-enabled GISS ocean model
1400 Mark Petersen and Todd Ringler: Overview of MPAS-Ocean ALE efforts
1430 Alan Wallcraft: Overview of HYCOM ALE efforts
1500-1530 Coffee Break

ALE Applications

1530 Bob Hallberg: Applications enabled by ALE modeling
1600 Future directions/Collaborations

Day 2 Tuesday, October 4 (half day)

0800 Numerics and performance. Mehra lead and Shriver rapporteur: Long range simulations require faster performance ~6 min/model day versus current HYCOM ~30 min/model day Resolution versus high order operators I/O limitations
0900 Current model issues and necessary improvements. Wallcraft/Adcroft lead and Hogan rapporteur: Thermobaric instability in HYCOM Velocity remapping with ALE operator
1000-1030 Coffee Break
1030 Code sharing and potential collaborations Hallberg lead and Richman rapporteur
1130 Next generation ALE model and future directions Arbic lead and Penny rapporteur

1230 Meeting close

Appendix 2. Computational Aspects of Global Ocean Models

Introduction: Historically structured grid codes have dominated ocean models with some unstructured and semi-structured codes. The models are 3-D but with some of the characteristics of a 2-D problem. Vertical scales of the ocean models are much different from horizontal scales. HYCOM 1/25th degree fully-global: 9000 x 6595 in horizontal with 41 vertical levels. Typically, the models use a 2-D domain decomposition. The vertical dimension is “on-chip” and often treated implicitly. Ocean models have fast surface gravity waves O(100m/s) which is O(100)x faster than advection and internal gravity wave speeds, motivating a separate 2-D sub-problem with a split-explicit or (less often) semi-implicit time step.

Limits on Ocean Model Scalability

A major problem for ocean models is that little computational work is performed compared to the memory access. For the 2-D sub-problem, memory accesses are required for the 2-D Halo exchanges and/or 2-D global sums with relatively little computational work between memory accesses. Thus, performance is highly dependent on communication latency. For the 3-D sub-problem, memory accesses are required for the 3-D Halo exchanges with still relatively little computational work per halo exchange (or per memory access) and still dependent on communication latency. Typically no overlap between I/O and computations. Thus, I/O eventually limits scalability. Can get good scalability with a large enough grid or ensembles. HYCOM 1/25th dgree global tripole (9000 x 6595 x 32): in practice almost exactly 16x faster on 16,000 vs 1,000 cores of Cray XC40 or SGI ICE systems.

Bit-for-Bit Multi-CPU Reproducibility

A requirement for porting to new architectures and different numbers of processors is bit-for-bit reproducibility. Repeating a single processor run produces identical results under this condition. However, repeating a multi-processor run, produces different results, using either OpenMP or MPI. e.g. fastest global sum is non-reproducible unless programmer explicitly avoids non-reproducible operations. We require reproducibility on any number of processors. Then we can test a compiler/system setup once, rather than for every core count. However, we can’t use the highest level of compiler optimization ifort -fp-model precise -no-fmafp-model precise because vector and scalar operations have different rounding, so the start and end of loop extents can’t be scalar if the middle is vector. fused multiply-add is new with AVX2, it has different rounding and so must be used for all operations in a loop or none. The Intel compiler is not providing the fastest possible reproducible results. In some cases this can be worked around with extra coding, but should not be necessary.

Refactoring for Vector Instructions

Earlier generations of ocean models targeted Cray vector shared memory, but recently replaced by models targeting distributed memory (MPI) “scalar” systems. However, all modern processors either include vector instructions or work well with vector constructs (GPGPUs). HYCOM is 5% faster on Xeons if its 1st array dimension is a multiple of 8. The best example of this organization is vertical column physics. To vectorize the vertical column, we would “push” a horizontal index into the routines. This index is promoted back outside the routine in modern codes. Taken to an extreme, the single column routine can be very inefficient. Generally, the best approach is to have a shallow nest of subroutines which a compiler (e.g. on GPGPUs) might be able to in-line into the outer loop to expose the parallelism. One possible approach to vector refactoring of column physics. Pack the horizontal dimensions into one index with no land. Have all column arrays aligned for vectorization with exactly the native vector length (pad the length in the last call). Use compile time constants and compiler directives to force maximum vectorization of the column physics routines. The native vector length would be system dependent

Ocean Models on Attached Processors

The low computational intensity of ocean models has been an issue on attached processors. The cost of repeatedly moving arrays from system (host) memory to attached memory is prohibitive. Only viable approach: Copy all model arrays to attached memory. Run MPI across attached processors (without involving the host). Use the host only for start up and I/O.

I/O includes error reporting, which may require re-factoring the error handler. This means that "incremental" approaches to porting won't work. We can't do one subroutine at a time and the attached processor must have enough memory to hold all arrays. 1/25th degree global HYCOM requires 850GB of memory plus tiling overhead. We still must face the low computational intensity bottleneck and may not get good performance without major code re-factoring.

Ocean Models on Future Systems

The memory and programming limitations of attached processors are being reduced over time, which makes host memory more accessible and increase size of "fast" memory. Host-less "attached" processors, with "fast" memory treated as a cache, may provide an option, Host-less approach involves "more slower cores" vs "fewer faster cores." Currently Intel Knights Landing single socket node with 72 cores per socket vs Intel Xeon dual socket nodes with ~18 cores per socket. Knights Landing has enhanced vector operations but may require more use of hyper-threading for good performance, for example,72 vs 36 cores per node. The question remains which is a) faster per node, b) faster per watt, or c) faster per dollar? In the future ARM server chips with vector extensions will join the "more slower cores" class. In general, ocean models can scale well (favors more cores) but may need re-factoring to take advantage of vector hardware. Knights Landing may need hyper-threading for maximum performance. Increase the number of MPI tasks, or use MPI and OpenMP.

Future Architectures of Interest

Two new architectures are emerging to explore these issues. IBM Summit/Sierra (2018) 140PFlops at 10MW; 14GF/W 3,400 to 4,200 nodes Multiple IBM POWER9s and multiple NVIDIA Volta GPGPUs per node 512GB RAM per node (high BW memory + DRAM) 800GB NVRAM per node (either extension to memory or burst buffer) NVLink on-node interconnect (CPUs and GPUs in a common memory space) Dual-rail IB-4X EDR (200Gbps) between node interconnect GPFS Parallel Filesystem (120 PB; 1TB/s) Intel/Cray Aurora (2019) 180PFlops at

13MW; 14GF/W 50,000+ nodes 1 Intel Knights Hill (3rd generation Phi) per node 128GB+ RAM per node (high BW memory + DRAM) Intel Omni-Path Gen 2 between node interconnect Intel SSD burst buffer in each node Lustre Parallel Filesystem (150 PB; 1TB/s)

Annexe B :

Arbitrary Lagrangian-Eulerian (ALE)
Working Group Meeting

Silver Spring
9-10 May 2017
Executive Summary

A one-and-a-half day working group meeting was held on 9-10 May 2017 in Silver Spring, MD, as a follow-on to the larger October 2017 workshop on ocean models that employ the ALE (Arbitrary Lagrangian-Eulerian) method for general vertical coordinates. The working group meeting included broad representation by NOAA, Navy, NCAR, NASA and university ocean modelers with the goal of discussing the feasibility of a common ocean model framework for operations and research, suitable for both high-resolution, short time scale work as well as coarser resolution, longer time scale modeling.

Speakers presented their organizational and modeling needs, and the group created a notional list of requirements for a common community ALE-based ocean modeling effort, which should:

- support as many agencies and modeling centers as possible, testable by each center's own metrics
- be an efficient, scalable code to permit high resolution modeling
- be a global multi-scale effort, capable of supporting nests for regional modeling
- consist of modular code so that ALE modeling groups in NASA GISS and DOE LANL could exchange modules, and thus enhance development
- allow many eyes throughout the community to look at the model, leading to model improvements

The group agreed on the need to converge to a single, modular ocean modeling framework for all time scales. To address this need, the group agreed to perform preliminary feasibility tests of MOM6 and HYCOM with the goal of merging HYCOM features into MOM6, and to develop a formal proposal. Pending successful feasibility results, the working group recommended the proposal be presented for funding to enable progress toward this goal.

Introduction

A one-and-a-half day working group meeting on ocean models that employ the ALE (Arbitrary Lagrangian-Eulerian) method to permit general vertical coordinates was held in Silver Spring on May 9-10, 2017. The working group meeting was a follow-up to an ALE workshop held at NOAA/NCWCP in October 3-4, 2016. A key point that emerged from the October 2016 workshop is that ALE is versatile and permits general vertical coordinates including traditional z, isopycnal, and terrain-following coordinates, as well as hybrid combinations of the former and other creative treatments yet to be formulated and explored. A general feeling that the time for ALE modeling has arrived permeated the October 2016 workshop. The October 2016 workshop recommended that the ALE community consider a code merger between HYCOM and MOM6, bringing the strengths of each to a common code base. The May 2017 working group meeting built upon this recommendation with a focus on talks that discussed the specific agency/institutional needs that need to be considered and met in such a merger, the need for metrics to determine whether models met agency needs, and plans for going forward. The need for code modularity was stressed, to allow for code-sharing with other ALE models such as the NASA GO2 model and the DOE MPAS-Ocean model, as it was in the October 2016 meeting.

Summaries of Talks

Agency perspectives on collaboration potential and drivers

An agenda for the May meeting listing all of the presentations is included later in this document.

The May 2017 working group meeting began with a summary of the October 2016 workshop, given by Brian Arbic and Avichal Mehra. The October 2016 workshop brought together developers and users of several ALE models, from several modeling centers as well as academia. The October 2016 workshop was a follow-up to Town Hall meetings, held at large AGU and AMS meetings, on the future of ocean modeling. The October 2016 meeting discussed the future of ALE modeling, and the opportunities for collaboration between different modeling groups. The convergence of interests between long-term and short-term forecast communities was noted, as was the launching of ambitious programs for global forecasting by NOAA and the US Navy, for instance the Department of Defense National Earth System Prediction Capability (ESPC), and the NOAA Unified Modeling Framework. Both NOAA and the US Navy envision operation of a next-generation ocean model by FY23. The October 2016 workshop recommended code sharing, community building, consideration of a code merger between HYCOM and MOM6, and several issues related to model performance and future development, for instance the physics of boundary layers, and the value of funding different approaches to ALE modeling.

The second May 2017 working group meeting talk, given by Jessie Carman, was on the national ESPC effort and inter-agency collaboration. The ESPC represents an effort to bridge the gap for decision support between synoptic, or daily/weekly, timescales, with longer time scales such as seasonal, interannual, and decadal time scales. There is an increasing realization that using the same model for short- and long-scale predictions yields numerous benefits and efficiencies.

The perspective from the office of the Oceanographer of the Navy, given by Dave McCarren, is that there is a need to make the ocean model more scalable, so that it does not take up such a large percentage of the available cores as it does now. The Navy needs scalable models, to support high spatial resolution, coupling with ice models (especially in the Arctic, a region of intense current interest), and data assimilation.

As discussed by Hendrik Tolman, NOAA has recently published white papers on the benefits of unified modeling. NOAA NCEP views the partnerships with GFDL and with NRL as hugely beneficial for both its near-real-time and seasonal prediction efforts. NCEP needs a closer assessment on the best approach for a single framework and how to fund the work as it cannot be a major sponsor of the ocean part of the unified model. NCEP supports the multi-model ensemble concept by allowing diverse code bases under a unified framework, and would leverage other centers for model development. Forecasters need multi-model ensembles to communicate uncertainty.

Modeling state: HYCOM/MOM6

As noted in a discussion led by Alan Wallcraft, efforts to perform direct comparisons of HYCOM and MOM6 simulations in nearly-identical configurations are already underway. NOAA/GFDL has succeeded in running MOM6 on a $1/12^{th}$ degree HYCOM grid, with simultaneous atmospheric and tidal forcing. NRL has attempted to run MOM6 on a $1/12^{th}$ degree HYCOM grid, but so far has not succeeded due to issues that should be fixable. Alan Wallcraft plans to travel to GFDL in June to collaborate on getting MOM6 running on the HYCOM grids and on Navy machines. This trip will be discussed in more detail later in this document.

Carlos Lozano has led an effort at HYCOM-MOM6 comparison at NOAA NCEP. He has been running the models in a global $1/12^{th}$ degree, 32-layer configuration, and comparing the HYCOM RTOFS simulations to Argo observations.

Agency/office requirements on ocean models; interest in participation

Steve Penny talked about data assimilation, which is a critical topic for operational centers such as NOAA NCEP and NRL/NAVO. There are two major camps in data assimilation-one espousing Ensemble Kalman Filter methods, and the other espousing variational methods including the adjoint, and the trend has been towards merging these into hybrid methods. Penny sees multiple spatial and temporal scales as one of the approximately 6 big challenges facing the ocean and coupled data assimilation community today, and recommends active collaboration between modeling and data assimilation communities throughout development.

Alan Wallcraft discussed needs of NRL and NAVO. NAVO needs better “feature placement” of mesoscale eddies. The Navy is most concerned with acoustics and near-surface currents. The Navy’s interest in the National ESPC program is focused on 90-day forecasts for strategic guidance. Wallcraft noted that MOM6 and HYCOM already share many features. However, in order for MOM6 to meet Navy operational needs some of its existing capabilities, including its non-Boussinesq capability, would need to be extensively tested on global high horizontal resolution grids and several capabilities currently available in HYCOM would need to be added to MOM6, including the use of terrain-following coordinates in shallow seas, spatially varying target layer densities, robust support for tides, 3DVAR data assimilation, the use of steric sea surface height as a diagnostic field, atmospheric pressure loading, the ability to nest for regional modeling, and higher-order advection operators. Wallcraft noted that all of this would represent a substantial effort, appropriate for a multi-center NOPP project.

Carlos Lozano and Avichal Mehra gave presentations on NOAA NWS operational requirements for a global ocean model. NWS desires efficient and accurate (numerical) representation of mesoscale ocean variability from shelves to the deep ocean driven by atmospheric forcings; river and runoff; tidal forcings; ice melting, freezing, and drift; and surface gravity waves. NWS desires a non-Boussinesq formulation, and like NRL/NAVO, will provide data assimilation expertise for ocean forecasting. For NWS seasonal forecasts a lower resolution version of MOM6 will be used. NWS real-time forecasting will use high-resolution ocean models, as in the present RTOFS system. Because NOAA NWS will run this model on an operational basis, the model must be "bulletproof;" i.e. robust enough to run in near-real-time on a regular basis. This also applies to use of the model for Navy operational ocean modeling. Lozano and Mehra again emphasized the need for reduced complexity of the NCEP Production Suite, as well as a unified, collaborative strategy for model development across NOAA. The JEDI system for data assimilation is part of this effort.

Bob Hallberg and Alistair Adcroft presented an overview of their MOM6 development efforts. MOM6 represents a vision for a community ocean model. GitHub allows for immediate dissemination of improvements. Robust testing, documentation, and community engagement are all key features of the MOM6 vision. GFDL sees NRL and NOAA NCEP as providing operational/data-assimilation expertise to the proposed HYCOM/MOM6 merger effort. NCAR will use a complementary (not identical) configuration to that used by GFDL, and, like GFDL, will focus on longer time scales. GFDL notes that managing the collaboration will be one of the biggest challenges for this effort. Different centers have different needs, and everyone is stretched for time.

Frank Bryan discussed NCAR ocean model needs as well as the contributions they make to the modeling community. NCAR provides coarse-resolution (about 1 degree) ocean models for long-time-scale studies of the Earth system, as part of the Community Earth System Model (CESM) framework. CESM modeling efforts include even coarser resolution configurations for paleoclimate studies, as well a small number of higher-resolution configurations (of order 1/10th degree) for studying the role of ocean eddies in coupled atmosphere-ocean simulations. NCAR does use data assimilation, for decadal prediction. The adoption of MOM6 will represent a new direction for NCAR, which has not previously used ALE models, and NCAR scientists will have to "learn the ALE psychology" as they proceed. Additionally, there will be a considerable effort to educate CESM users in both the ALE based model formulation and analysis simulations using ALE based models. NCAR expects to expend considerable research effort in the area of scale-adaptive lateral closures to ocean modeling.

Rainer Bleck and Darren Engwirda discussed NOAA ESRL and NASA GISS needs for, and contributions towards, ALE ocean modeling. Both centers run simulations for long-time-scale forecasts, and both centers are involved in ALE model development. NOAA ESRL is running a version of HYCOM on an icosahedral grid, while NASA GISS is running a new ALE model (GO2). Both Bleck and Engwirda emphasized their plans to continue to run their own ALE models (not the proposed HYCOM/MOM6 merger code), thus contributing to the important goal of maintaining model diversity. At the same time, if the proposed HYCOM/MOM6 merger code is written in a modular manner, then it will be easy for Bleck and Engwirda to swap parts of code in and out, thus contributing greatly to the quality of the HYCOM/MOM6 code.

Brian Arbic briefly discussed the contributions that academia makes towards large-scale ocean modeling efforts. Academia serves as a training ground for young scientists, some of whom participate in process studies that can lead to important improvements in ocean models, and some of whom undertake significant model-observation comparison studies. Another contribution that academia can make towards ocean model development is the entrainment of young scientists with strong computational science backgrounds into the field. The number of ocean model developers is small and needs to be increased. Steve Penny concurred with these points.

Distillation of content:

To summarize the first day of the working group meeting, presentations on ALE modeling were given by practitioners from several agencies and modeling centers. The needs of different agencies and modeling centers, as well as the contributions they can make towards the ALE modeling community, were discussed. There is general interest on the part of NOAA and the US Navy in conducting further tests on the feasibility of a HYCOM/MOM6 code merger, and there is general interest on the part of other agencies and centers (e.g., NASA GISS, and, we hope, DOE) in creating modular codes to promote code sharing between HYCOM/MOM6 and other ALE models such as GO2 and MPAS-Ocean. Tests of HYCOM and MOM6 in identical configurations will be conducted shortly.

In the discussion at the end of the first day of the workshop, the following points were made about a potential HYCOM/MOM6 merger:

- it should continue to be a community ocean model, based primarily on MOM6 with added HYCOM capabilities
- it should satisfy and involve as many agencies and modeling centers as possible
- each center should test the code with its own metrics
- it should be done with modular code so other ALE modeling groups in NASA GISS and DOE LANL could exchange modules and so that it could form the framework for other ALE-based ocean model designs
- it would allow many eyes throughout the community to look at the model, leading to model improvements
- it should be a global multi-scale effort
- it should be capable of supporting nests for regional modeling
- it should be an efficient, scalable code

Agency motivations to participate

There are several motivations underlying agency participation in this project.

a. Program managers are looking for efficiencies in times of tight agency budgets. It is more efficient to maintain one common, modularized code base than two similar code bases (e.g., HYCOM and MOM6).
b. A common, modularized code base implies many “eyes on the model”; in other words, many model users and developers will examine the proposed HYCOM/MOM6 code base, especially because routines can be swapped in and out from other models such as

GO2 and MPAS-Ocean. The many "eyes on the model" also includes participants looking at the simulation outputs, and comparing them to observations, all of which will lead to model improvements.

c. A common code base makes it much simpler to upgrade the code when new machines are put into place; it precludes the need for updating multiple codes as would need to be done now at, for instance, NCEP, which currently maintains two ocean codes (HYCOM and MOM4).

d. The new code base will help some agencies to modernize their code base relative to the comparatively old codes that they are currently using. The proposed merger project could be a route for the Navy, and for NOAA NCEP, to meet their stated goals to upgrade their ocean model dynamical core by FY23.

e. A common, shared code base will allow some agencies to borrow from the strengths of other agencies. For example, the Navy expertise in data assimilation will allow for development of assimilative codes that will also be useful for NCEP. Similarly, the development of the MOM6 code at GFDL will ease the pressure at other modeling centers (e.g., the US Navy, NCAR, and NCEP) to develop ocean codes all by themselves; they will instead be able to focus on adapting the HYCOM/MOM6 merged code to local agency/center needs.

f. A common code base can be used for "unified modeling" across a wide range of spatial and temporal scales—another type of efficiency that is increasingly being recognized as important. For instance, in the atmospheric modeling community, the boundaries between weather models and seasonal-to-interannual prediction models are increasingly blurring. With this document we are making a similar argument for ocean models.

Agency contributions/expertise

NOAA/GFDL has created the existing MOM6 code base, building upon in-house ALE modeling expertise. GFDL will develop code-testing protocols, and has already provided several working configurations. Finally, GFDL will provide oversight on the dynamical core and the code repository. NOAA/ESRL provides additional ALE modeling expertise, while NOAA/EMC provides expertise in real-time forecasting, data assimilation, coupling frameworks, and code management. NOAA/NOS provides coastal modeling operations and expertise, along with connections to coastal modeling communities, within US coastal waters. NCAR provides a network to a large user community in academia and elsewhere, connections to biogeochemistry support, investment in community support (e.g., tutorials for young scientists), and development of model physics. The Navy hosts the existing HYCOM database, and has a history of expertise in ALE modeling, data assimilation, real-time forecasting, and coastal modeling at locations around the world. GISS brings expertise in ALE modeling, numerical model development, access to a different coupled earth system model framework, and development of a different ALE modeling code base (GO2). Academic partners contribute expertise in ALE modeling, process studies, model evaluations, and training of young scientists.

Next Steps

Proof-of-Concept Test

Alan Wallcraft will visit GFDL and, in collaboration with GFDL scientists Bob Hallberg, Matt Harrison, and Alistair Adcroft, develop initial tests of MOM6 on ¼ and $1/12^{th}$ degree grids. The ¼ degree test will be run for 10 years, while the $1/12^{th}$ degree test will be run for 5 years. NCEP may send someone to GFDL during Wallcraft's visit there. It is important to test whether MOM6 functions well when run in "semi-operational" mode (short time scales and high spatial resolution). The computational speed/scalability of MOM6, and its ability to perform an initial simple forecast, will also be tested. For the latter, we will test whether we can get incremental insertion from NCODA working. We will test a 5-day forecast from a Nowcast that looks reasonable.

Separately, Brian Arbic and his postdoc Joseph Ansong will work with Wallcraft to develop one- and two-layer simulations of tides in MOM6. Ansong has already developed MOM6 into a one-layer tide model, with great success, on University of Michigan machines. Wallcraft will work to adapt these results to the HYCOM grids. The two-layer tide runs will represent a clean test of the non-Boussinesq capabiliities of MOM6.

Develop a Proposal

After the proof-of-concept test, we plan to develop a proposal that includes the following elements:

- Phase one testing - Make vertical coordinates as similar as possible, compare parameterizations, examine basin configurations, and use the "correct" equation of state for higher resolution runs.
- Run standard metrics for comparison. Brian Arbic and collaborators plan to compare eddy kinetic energy to altimetry and drifter observations, and to compare the internal tide sea surface height signal to altimetry data. The latter comparison will be an excellent indirect test of the "inviscidness" of model numerics; in models that are too viscous, the internal tides do not propagate as far as they do in altimetry data. Modeling centers will run their own suite of standard ocean model metrics.
- The proposal will provide a detailed description of partner contributions. For instance, NRL and NOAA NCEP will provide data assimilation expertise, etc.
- The proposal will include a description of the deliverable and the desired end state. Both of these can be fine-tuned later. For now, we envision a deliverable that is a version of MOM6 (with HYCOM and other code merged in) that provides a suitable backbone for ocean modeling at NOAA, Navy, and NCAR. We envision that the code base will be modular so that NASA GISS GO2 users as well as DOE MPAS-Ocean users can swap code components in and out.

The project proposal will also be modular in that a minimal path forward can be ascertained, as well as a maximal plan. This will permit progress with minimal budgets as well as flexibility to take advantage of larger budgets.

The project proposal will take into account the specific physics and features (e.g., tides, sea ice, data assimilation) that are needed by particular agencies/centers. The proposal will take into account how the potential code merger fits into the ESPC. The project will also account for both human and computational resources. For example, a "maximal" plan will likely lead to hires of new computational scientists in at least some of the centers.

Finally, the project will take into account the fact that computer architectures continue to change. In a "maximal" project, academic centers would look to entrain more young computational scientists into the field of ocean model development.

Future model discussion issues

The proposal will discuss creating a forum for configuration management and code repositories, drawing connections between various center versions and configurations. This forum should also discuss issues such as ocean model metrics. While it is likely that each agency and center will have its own metrics, sharing and comparing metrics will be beneficial. As noted previously, the proposal will outline a modular code, such that it will be simple for subroutines and modules to be added or switched by model users.

Acronyms:

3DVAR: 3-Dimensional Variational data assimilation
AGU: American Geophysical Union
ALE: Arbitrary Lagrangian-Eulerian
AMS: American Meteorological Society
CESM: Community Earth System Model
DOE: Department of Energy
EMC: Environmental Modeling Center
ESPC: Earth System Prediction Capability
ESRL: Earth System Research Laboratory
GFDL: Geophysical Fluid Dynamics Laboratory
GISS: Goddard Institute for Space Studies
GO2: Goddard Ocean Model 2
JEDI: Joint Effort for Data Assimilation Integration
HYCOM: HYbrid Coordinate Ocean Model
LANL: Los Alamos National Laboratory
MIT: Massachusetts Institute of Technology
MOM6: Modular Ocean Model version 6
MPAS-Ocean: Model for Prediction Across Scales - Ocean
NASA: National Aeronautics and Space Administration
NAVO: Naval Oceanographic Office
NCAR: National Center for Atmospheric Research
NCEP: National Centers for Environmental Prediction
NCODA: Navy Coupled Ocean Data Assimilation system
NCWCP: NOAA Center for Weather and Climate Prediction
NOAA: National Oceanic and Atmospheric Administration
NOPP: National Oceanographic Partnership Program
NOS: National Ocean Service
NRL: Naval Research Laboratory
NWS: National Weather Service
OSTI: Office of Science and Technology Integration
ROMS: Regional Ocean Modeling System
RTOFS: Real-Time Ocean Forecast System

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Darren Engwirda, MIT and NASA GISS
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Patrick Hogan, NRL
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Appendix 1. Working Group Meeting Agenda
Arbitrary Lagrangian-Eulerian (ALE) Working Group Meeting
NOAA SSMC2, Silver Spring, Maryland, Room 2358
9-10 May 2017
9 May
Overviews

8:00-8:30		Check-in, refreshments
8:30-9:00	Arbic/Mehra	Recap of October workshop, summary of recommendations to develop closer ties between NOAA and Navy modeling efforts
9:00-9:20	Carman	National ESPC and Inter-agency collaboration
9:20-9:40	McCarren	Navy perspectives
9:40-10:00	Tolman/Toepfer	NOAA perspectives
10:00-10:30		Break

Nuts and bolts

10:30-11:00	Wallcraft/Hallberg/ Mehra/Arbic	What has been done to look at the differences between HYCOM and MOM6 and what are near-term activities
11:00-11:20	Penny	Ocean modeling and data assimilation needs
11:20-11:40	Wallcraft	Navy/NRL perspective on requirements for the global ocean, what needs to be done and what resources are needed
11:40-12:00	Mehra/Chawla/ Lozano	NWS perspective on requirements for the global ocean, what needs to be done and what resources are needed
12:00-1:30		Lunch onsite
1:30-1:50	Adcroft/Hallberg	GFDL perspective on requirements for the global ocean model, what needs to be done and what resources are needed
1:50-2:10	Bryan	NCAR perspective on requirements for the global ocean, what needs to be done and what resources are needed
2:10-2:30	Bleck	Using ALE models for climate research
2:30-2:50	Arbic	Brief discussion on role of academia in entrainment of computer scientists into the field of ocean model development
2:50-3:20		Break
3:20-5:00	Arbic/Mehra	Summary of key directions: what do we need to do, to go forward? (technical level)

10 May

8:00		Refreshments

8:30-10:00	Arbic/Mehra/ Carman	Highlight key points to proceed, clarify details:
		What do we need to do to go forward? Obvious first efforts Impediments to progress Who are the users for the merged model? What requirements beyond the ocean model will impact the merger? Coupling to sea ice (CICE vs SIS2, ESMF vs FMS, etc.) Tides—Who needs tides and who doesn't? Input/Output—Formats, native grids or interpolated netcdf? Data Assimilation—Forecast model needs to include DA and the ability to generate restart files Resources—people/computer
10:00-10:30		Break
10:30-12:00	All	Formulation of a technical plan/proposal
12:00		Lunch and end of meeting

Appendice C :

CROCO's Users Meeting 2017
May 22-24, 2017
Toulouse, France

Draft Agenda

Monday, May 22: CROCO 1.0 - Overview

9:00-9:30 Registration & Coffee

9:30 Welcome & Logistics
9:40 Philosophy behind CROCO *(X. Capet, R. Benshila, L. Debreu)*
10:00 Detailed introduction of the code *(R. Benshila)*
10:45 Coffee
11:15 Advection-diffusion schemed *(F. Lemarie)*
12:00 Lunch
13:30 Non-hydrostatic option 1 *(F. Auclair)*
14:15 Non-hydrostatic option 2 (*G. Roullet*)
14:45 Coffee
15:15 Multi-grid option *(L. Debreu*)
16:00 Coupling *(S. Jullien)*
16:45 Near-shore capabilities *(R. Benshila)*
17:30 Adjourn

Dinner on your own

Tuesday, May 23: Applications

9:00 An example of ROMS/CROCO regional and realistic simulation around southern Africa : Set-up, run and downscaling capabilities *(G. Cambon)*
9:30 Modulation of Western Boundary Currents by Oceanic Current Interactions with the Atmosphere *(L. Renault)*
10:00 China Sea *(Nguyen Dac Da)*
10:30 Coffee
11:00 Introduction of the effects of a barrier reef in the CROCO model for the modeling of lagoon hydrodynamic circulation: Example of the Tulear Lagoon (Madagascar) *(M. Sow, C. Chevalier, B. Ali Sow , J.L.Devenon)*
11:30 Parametrization of the wave effect on the cross-reef flux for lagoon modeling: case of the Ouano lagoon in New Caledonia. (*F. Locatelli, M. Sow, C. Chevalier, J.-L. Devenon, D. Sous)*
12:00 Lunch
13:30 Overview of operational modelling and modelling downstream services at the Marine Institute, Ireland. (*T. Dabrowski, K. Lyons, E. O'Rourke)*
14:00 How do subsurface sea temperatures vary inter-annually in the tropical western Indian Ocean off the East African Region? (*M. Manyilizu, F. Dufois, P. Penven, C. Reason)*
14:30 Some applications of the MUSTAND sediment model (*B. Thouvenin, F. Grasso, P. Le Hir, R. Verney, B. Mengual)*
15:00 Coffee
15:30 Needs And Expectations From The CROCO Project From A Benthic Ecologist Perspective (Based On A Synthesis of Past And Ongoing Applications Of MARS3D For Ecological Modelling At LEBCO, IFREMER). *(M. Marzloff, P. Cugier, A. Menesguen, Y. Thomas)*
16:00 Anthropogenic very Short Lived Halocarbons (VSLH) from seaweed farming in South East Asian region (*A. Kumar)*
16:30 Linking the traits diversity of autotrophic plankton to the environment forcing in coastal waters with coupled biological/physical models. *(M. Sourisseau, M. Cadier, L. Memery, T. Gorgues, G. Le Gland, V. Le Guennec, A. Chapelle, M. Plus)*
17:00 On teaching ocean numerical modelling - lessons from the classroom *(A. Sepulveda, O. Artal)*
17:30 Adjourn

Dinner on your own

Wednesday, May 24: Breakout sessions on CROCO's next steps

9:00 Presentation of the breakout sessions and goals
9:15 Breakout sessions
10:15 Coffee
10:45 Plenary reports
11:30 Plenary discussion
12:00 Adjourn

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