Multiscale Embedded Schemes for the "Multidisciplinary Simulation, Estimation and Assimilation System" (MSEAS)

Abstract

Our novel results in two-way embedded (nested) schemes for free-surface primitive-equation computations with strong tidal forcing are presented. A set of numerical two-way embedding algorithms are compared, focusing on the barotropic velocity and surface pressure components of the two-way exchanges. The different algorithms mainly differ in the level of the constraints in the fine-to-coarse scale transfers and in the interpolations and numerical filtering. We present and illustrate both the schemes that lead to divergences between grids and those that don't. We find that embedded schemes with stronger implicit couplings among grids, especially for the velocity components, work best. Volume-conserving schemes are also discussed for free-surface primitive-equation computations in large domains but including strong tidal conditions over shallow seas. Results are presented both in idealized settings such as simplified Gulf-Stream simulations over flat topography and in realistic multiscale simulations settings such as the east coast of the USA, the Philippine Archipelago and the Taiwan-Kuroshio region. For these simulations, we employ our regional modeling system, the MIT "Multidisciplinary Simulation, Estimation and Assimilation System" (MSEAS). This system includes the Harvard primitive equation model updated with new free-surface and stochastic forcing equations as well as other novel computational systems for biogeochemical and acoustic modeling, nested generalized tidal inversions, coastal objective analysis, uncertainty prediction, data assimilation and adaptive sampling.

Keywords:

1. Introduction

- Review of two-way nesting(embedding) (start with slide 8)

- MSEAS system and new components (slides 4-6)

2. Formulation of new 2-way nesting scheme for free surface primitive equation modeling

2.1. continuous free surface Primitive equations

Note:. Rewrite in integral formulation. Consider moving heat and salt equations before equation of state.

The equations of motion are the primitive equations, derived from the Navier-Stokes equations under the hydrostatic and Boussinesq approximations (e.g. Cushman-Roisin and Beckers, 2010). Under these assumptions, the conservation of mass can be expressed as

$$\int_{\mathcal{S}} (\vec{u}, w) \cdot d\mathcal{A} = 0 \tag{1}$$

where $\vec{u}$ is the two dimensional, horizontal velocity vector (u, v), $\mathcal{S}$ is the surface of the control volume $\mathcal{V}$, and $d\mathcal{A}$ is an infinitesimal area element vector pointing in the outward normal direction to $\mathcal{S}$. The conservation of momentum can be written as

$$\frac{d}{dt}\int_{\mathcal{V}} \vec{u}\, d\mathcal{V} + \vec{\mathcal{L}}(\vec{u}) + \int_{\mathcal{V}} f\hat{k} \times \vec{u}\, d\mathcal{V} = -\frac{1}{\rho_0}\int_{\mathcal{S}} p\, \hat{n}_h \cdot d\mathcal{A} + \int_{\mathcal{V}} \vec{F}\, d\mathcal{V} \tag{2}$$

$$\int_{\mathcal{S}} p\, \hat{k} \cdot d\mathcal{A} = -\int_{\mathcal{V}} \rho g\, d\mathcal{V} \tag{3}$$

where t is the time variable, f is the Coriolis parameter, $\hat{k}$ is the unit direction vector in the vertical direction, ρ_0 is the (constant) background density, p is the pressure, $\hat{n}_h$ a matrix comprised of the horizontal unit vectors, $\vec{F}$ contains the sub-gridscale terms, ρ is the variable density and g is the acceleration due to gravity. In equation (2) we have introduced the following notation for the advection terms:

$$\vec{\mathcal{L}}(\vec{u}) = \begin{pmatrix} \mathcal{L}(u) \\ \mathcal{L}(v) \end{pmatrix} \quad ; \quad \mathcal{L}(\phi) = \int_{\mathcal{S}} \phi\ (\vec{u}, w) \cdot d\mathcal{A} \tag{4}$$

To close the system a standard equation of state is introduced

$$\rho = \rho(z, T, S) \tag{5}$$

where T is the temperature and S is the salinity. The temperature and salinity are evolved using conservation equations for heat

$$\frac{d}{dt}\int_{\mathcal{V}} T\,d\mathcal{V} + \mathcal{L}(T) = \int_{\mathcal{V}} F^T\,d\mathcal{V} \tag{6}$$

and for salt

$$\frac{d}{dt}\int_{\mathcal{V}} S\,d\mathcal{V} + \mathcal{L}(S) = \int_{\mathcal{V}} F^S\,d\mathcal{V} \tag{7}$$

in which F^T and F^S contain the sub-gridscale terms.

2.2. Nonlinear "distributed-σ" discretization of the free surface Primitive equations

The equations of motion are discretized on an Arakawa B-grid (Arakawa and Lamb, 1977), the details of which can be found in Bryan (1969). In time, the discretization is mostly leap-frog, with some semi-implicit discretizations for the Coriolis and free surface terms, following Dukowicz and Smith (1994). A brief summary of this is given in Appendix B. In the vertical direction, terrain-following coordinates (σ, hybrid or double-σ, *see GRIDS manual*) which we will denote by writing depths, $z_{i,j,k}$ and vertical thicknesses $\Delta z_{i,j,k}$ as functions of all three coordinates.

Since our vertical grid is both terrain-following and time variable we define the vertical flux velocity, ω, normal to the top of finite volume elements, ζ, as

$$\omega = w - \vec{u}\cdot\nabla\zeta - \frac{\partial\zeta}{\partial t} \tag{8}$$

Using mid-point quadrature, the conservation of mass is discretized as

$$\begin{aligned} 0 &= \int_{\mathcal{S}} \vec{u}_{(3)}\cdot\hat{n}\,d\mathcal{A} \\ &= \delta^x\left(\langle u_{i+\frac{1}{2},j+\frac{1}{2},k}\rangle^x \langle\Delta z_{i+\frac{1}{2},j+\frac{1}{2},k}\rangle^y\right)\Delta y_{j+\frac{1}{2}} \end{aligned} \tag{9}$$

$$\frac{\delta\vec{u}'}{\tau} + f\hat{k}\times\vec{u}'^{\alpha} = -\frac{1}{\rho_0}\nabla p_h^n - \vec{\mathcal{L}}(\vec{u})^n + \vec{F}^{n,n-1} \tag{10}$$

$$\frac{\delta\vec{T}}{\tau} = F^T - \mathcal{L}(T)^n \tag{11}$$

$$\frac{\delta\vec{S}}{\tau} = F^S - \mathcal{L}(S)^n \tag{12}$$

$$\vec{\mathcal{F}}^{n,n-1} = \frac{1}{H}\int_{-H}^{0}\left(\vec{F} - \frac{1}{\rho_0}\nabla p_h - \vec{\mathcal{L}}(\vec{u}) - f\hat{k}\times\left[(1-2\alpha)\,\vec{u}^n + 2\alpha\vec{u}^{n-1}\right]\right)dz \tag{13}$$

$$\hat{\delta}\vec{U} + 2\alpha f\Delta t\hat{k}\times\hat{\delta}\vec{U} = 2\Delta t\left\{\vec{\mathcal{F}}^{n,n-1} - g\left[(1-2\alpha)\,\nabla\eta^n + 2\alpha\nabla\eta^{n-1}\right]\right\} \quad , \tag{14}$$

$$\alpha\theta g\tau\nabla\cdot(H\nabla\delta\eta) - \frac{2\delta\eta}{\tau} = \nabla\cdot\left[H\left(\theta\hat{\vec{U}}^{n+1} + \vec{U}^n + (1-\theta)\vec{U}^{n-1}\right)\right] \tag{15}$$

$$\vec{U}^{n+1} = \hat{\vec{U}}^{n+1} - \alpha\tau g\nabla\delta\eta \tag{16}$$

- *Note: in this context, "nonlinear" refers to applying the upper boundary conditions at $z = \eta$ instead of $z = 0$. Check MIT-GCM documentation for this terminology*

- *Note: need to also find term(s) for distributing changes in depths across all levels, instead of restricting to top level(s)*

- describe (final eqs and/or what is new) and refer to Appendix B. Look for ways to condense.

- advantages in shallow regions. *Either a subsubsection or highlighted paragraph.*

- baroclinic volume conservation (text/equations of slide 34). *This should be included in derivation, when rewritten in integral formulation.*

- open boundary conditions (take some from `surfpresssummary.tex` and/or `zuvmbcs.tex`). *Either a subsubsection or highlighted paragraph.*

- Maintaining vertically integrated continuity. *Either a subsubsection or highlighted paragraph.*

  - http://mseas.mit.edu/group/pjh/Nest/Talk/PFJL/baro_cont.ppt
  - meeting2_28Aug2001.tex

- paragraph comparing new with Dukowicz and Smith (1994).

2.3. Implicit nesting scheme

- paragraph explaining nesting scheme and relating to slide 25 and slide 26 or equivalent in table form.

- i.e. the final nesting scheme (§3.6)

- implicit vs explicit nesting

3. Ensuring consistency between estimates of barotropic fields in nested domains

- set-up paragraph on SW06/AWACS domains, topography.

3.1. Explicit Nesting

- have run, generate equivalent to slide 15

- see /projects/awacs/PE/2009/Dec07/PJH10

- since that run has blended topography around perimiter, see /projects/awacs/PE/2009/Dec07 for the equivalent final method.

3.2. Baseline Implicit nesting (mimic rigid-lid nesting)

- slide 15

3.3. Pass Uhat not RHS

- slide 18

3.4. Exchange surface pressure (at lagged time step)

- slide 21

3.5. Update ubaro (at lagged time step) as function of updated surface pressure (in region where surface pressure updated)

- slide 24

*3.6. Pass H*Uhat ("transport")*

- slide 27

4. Examples

- include some relative vorticity plot comparisons of coarse and fine domains to emphasize the additional small scales resolved in the fine domains.

4.1. Middle Atlantic Bight

- slides 28-31
- improves tidal comparison:
  - /projects/awacs/PE/2009/Dec07/PJH05
  - /projects/awacs/PE/2009/Dec07/PJH06
  - /projects/awacs/PE/2009/Dec07/PJH09

4.2. Philippines

- slides 32-33

4.3. Strait of Taiwan

- slide 34

5. Conclusions

- slide 35

Appendix A. Full details of the discretization

Anticipating some repeated averaging operations for midpoint quadrature

$$\langle u_{i,j,k}\rangle^x = \frac{1}{2}\left(u_{i+\frac{1}{2},j,k} + u_{i-\frac{1}{2},j,k}\right) \qquad \langle u_{i,j,k}\rangle^y = \frac{1}{2}\left(u_{i,j+\frac{1}{2},k} + u_{i,j-\frac{1}{2},k}\right)$$

$$\delta^x\left(u_{i,j,k}\right) = u_{i+\frac{1}{2},j,k} - u_{i-\frac{1}{2},j,k} \qquad \delta^y\left(u_{i,j,k}\right) = u_{i,j+\frac{1}{2},k} - u_{i,j-\frac{1}{2},k}$$

Since our vertical grid is both terrain-following and time variable we define the vertical flux velocity, ω, normal to the top of finite volume elements as

$$\begin{aligned}
\omega_{i+\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}} \quad = \quad & w_{i+\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}} \\
& -\langle u_{i+\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}\rangle^z \langle \delta^x z^n_{i+\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}\rangle^y \frac{1}{\Delta x_{i+\frac{1}{2}}} \\
& -\langle v_{i+\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}\rangle^z \langle \delta^y z^n_{i+\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}\rangle^x \frac{1}{\Delta y_{j+\frac{1}{2}}} \\
& -\frac{\partial z^n_{i+\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}}{\partial t}
\end{aligned} \tag{A.1}$$

Using mid-point quadrature, the conservation of mass is discretized as

$$\begin{aligned} 0 &= \int_{\mathcal{S}} \vec{u}_{(3)} \cdot \hat{n}\, d\mathcal{A} \\ &= \delta^x \left(\langle u_{i+\frac{1}{2},j+\frac{1}{2},k} \rangle^x \langle \Delta z_{i+\frac{1}{2},j+\frac{1}{2},k} \rangle^y \right) \Delta y_{j+\frac{1}{2}} \end{aligned} \tag{A.2}$$

- continue with fill discretizations

Appendix B. Review of Dukowicz and Smith Free Surface Algorithm

This appendix provides a brief summary of the free surface algorithm derived by Dukowicz and Smith (1994) (hereafter referred to as D&S) for the Bryan-Cox-Semtner model (Bryan, 1969; Semtner, 1986). Starting from equations (1-7) they decompose the velocity into a depth-averaged component, $\vec{U}$, and an internal mode, $\vec{u'}$:

$$\vec{u} = \vec{u'} + \vec{U} \quad ; \quad \vec{U} = \frac{1}{H} \int_{-H}^{0} \vec{u}\, dz \tag{B.1}$$

where H is the undisturbed depth of the ocean. They also decompose the total pressure into a surface pressure, p_s, and a hydrostatic pressure, p_h, evaluated from (3):

$$p(x,y,z) = p_s(x,y) + p_h(x,y,z) \quad ; \quad p_h(x,y,z) = \int_{z}^{0} \rho(x,y,\zeta) g\, d\zeta \tag{B.2}$$

and relate the surface pressure to the free surface elevation, η, through the hydrostatic approximation

$$p_s = \rho_0 g \eta \tag{B.3}$$

The internal components are evaluated as in the Bryan-Cox-Semtner model. To solve the external components, including the surface elevation, average equations (2) and integrate (1) all in the vertical, then substitute in equations (B.1-B.3):

$$\frac{\partial \vec{U}}{\partial t} + f\hat{k} \times \vec{U} = -g\nabla\eta + \vec{F}_{av} \tag{B.4}$$

$$\frac{\partial \eta}{\partial t} + \nabla \cdot (H\vec{U}) = 0 \tag{B.5}$$

where $\vec{F}_{av}$ now contains the advective fluxes and hydrostatic pressure gradients as well as the sub-gridscale terms:

$$\vec{F}_{av} = \frac{1}{H}\int_{-H}^{0}\left(-\frac{1}{\rho_0}\nabla p_h - \vec{\mathcal{L}}(\vec{u}) + \vec{F}\right)dz \quad . \tag{B.6}$$

Next, (D&S) introduce a particular set of time discretizations, which are simplified here following their stability conclusions

$$\frac{\delta\vec{U}}{2\Delta t} + f\hat{k}\times\vec{U}^{\alpha} = -g\nabla\eta^{\alpha} + \vec{F}_{av}^{n} \tag{B.7}$$

$$\frac{\eta^{n+1}-\eta^{n}}{\Delta t} + \nabla\cdot(H\vec{U}^{\theta}) = 0 \tag{B.8}$$

where the n superscripts indicate that a variable is evaluated at time $n\Delta t$, δ refers to the leap-frog differencing

$$\delta U = U^{n+1} - U^{n-1} \quad , \tag{B.9}$$

and the superscripts α and θ refer to the semi-implicit time discretizations

$$U^{\alpha} = \alpha U^{n+1} + (1-2\alpha)U^{n} + \alpha U^{n-1} \quad , \tag{B.10}$$

$$U^{\theta} = \theta U^{n+1} + (1-\theta)U^{n} \quad . \tag{B.11}$$

To facilitate the solution of (B.7-B.8), (D&S) split the coupling of $\vec{U}^{n+1}$ and η^{n+1} by introducing the "augmented velocity", $\hat{\vec{U}}$, as

$$\hat{\vec{U}} = \vec{U}^{n+1} + 2\alpha g\Delta t\nabla\delta\eta \quad . \tag{B.12}$$

Substituting (B.12) for $\vec{U}^{n+1}$ in (B.7) and introducing the notation

$$\hat{\delta}\vec{U} = \hat{\vec{U}} - \vec{U}^{n-1} \tag{B.13}$$

results in

$$\begin{aligned}\hat{\delta}\vec{U} + 2\alpha f\Delta t\hat{k}\times\hat{\delta}\vec{U} \quad &= \quad 2\Delta t\left\{\vec{\mathcal{F}}^{n,n-1} - g\left[(1-2\alpha)\nabla\eta^{n} + 2\alpha\nabla\eta^{n-1}\right]\right\} \\ &\quad -4\alpha^2 gf(\Delta t)^2\hat{k}\times\nabla\delta\eta \quad , \end{aligned} \tag{B.14}$$

where

$$\vec{\mathcal{F}}^{n,n-1} = \vec{F}_{av}^{n} - f\hat{k}\times\left[(1-2\alpha)\vec{U}^{n} + 2\alpha\vec{U}^{n-1}\right] \quad . \tag{B.15}$$

(D&S) then observe that the final term in the right-hand side of (B.14) is the same order, $O\left((\Delta t)^3\right)$, as the discretization error (assuming that $\delta\eta$ is $O\left(\Delta t\right)$, a necessary assumption for bounded first derivatives). Neglecting this term, they arrive at the decoupled equation for $\hat{\vec{U}}$:

$$\hat{\delta}\vec{U} + 2\alpha f \Delta t \hat{k} \times \hat{\delta}\vec{U} = 2\Delta t \left\{ \vec{\mathcal{F}}^{n,n-1} - g\left[(1-2\alpha)\nabla\eta^n + 2\alpha\nabla\eta^{n-1} \right] \right\} \quad . \tag{B.16}$$

Finally, (D&S) generate an equation for $\delta\eta$ by first averaging (B.8) with itself evaluated one time step earlier. Then they substitute for $\vec{U}^{n+1}$ using (B.12), resulting in

$$2\alpha\theta g \Delta t \nabla \cdot (H\nabla\delta\eta) - \frac{\delta\eta}{\Delta t} = \nabla \cdot \left[H \left(\theta\hat{\vec{U}} + \vec{U}^n + (1-\theta)\vec{U}^{n-1} \right) \right] \tag{B.17}$$

- *Review Dukowicz and Smith (1994) to see if need to keep θ.*

Appendix C. Review of Rigid-Lid nesting algorithm

- slide 10

Appendix D. Notes on usage of nesting code

- topography and mask matching
- initialization (rigid lid)
- initialization (free surface)
- tides? (B to C grid conversion?)

Arakawa, A., Lamb, V. R., 1977. Computational design of the basic dynamical processes of the ucla general circulation model. Methods in Computational Physics 17, 173–265.

Bryan, K., 1969. A numerical method for the study of the circulation of the world ocean. Journal of Computational Physics 4 (3), 347–376.

Cushman-Roisin, B., Beckers, J.-M., 2010. Introduction to geophysical fluid dynamics: Physical and Numerical Aspects. Academic Press.

Dukowicz, J. K., Smith, R. D., 1994. Implicit free-surface method for the bryan-cox-semtner ocean model. Journal of Gephysical Research 99 (C4), 7991–8014.

Semtner, Jr., A. J., 1986. Finite-difference formulation of a world ocean model. In: O'Brien, J. J. (Ed.), Advanced Physical Oceanographic Numerical Modelling. D. Reidel, Hingham, Mass., pp. 187–202.