

A Community Terrain-Following Ocean Modeling System (ROMS/TOMS)

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LONG-TERM GOALS

The long-term technical goal is to design, develop and test the next generation, primitive equation, ocean model for high-resolution scientific (ROMS: Regional Ocean Modeling System) and operational (TOMS: Terrain-following Ocean Modeling System) applications. This project will improve the ocean modeling capabilities of the U.S. Navy for relocatable, coastal, coupled atmosphere-ocean forecasting applications. It will also benefit the ocean modeling community at large by providing the current state-of-the-art knowledge in physics, numerical schemes, and computational technology.

OBJECTIVES

The main objective is to produce a tested expert ocean modeling framework for scientific and operational applications over a wide range of spatial (coastal to basin) and temporal (days to seasons) scales. The primary focus is to implement the most robust set of options and algorithms for relocatable coastal forecasting systems nested within basin-scale operational models for the Navy. The system includes some of the analysis and prediction tools that are available in Numerical Weather Prediction (NWP), like 4-dimensional variational data assimilation (4D-Var), ensemble prediction, adaptive sampling, and circulation stability and sensitivity analysis.

APPROACH

The structure of TOMS is based on ROMS because of its accurate and efficient numerical algorithms, tangent linear and adjoint models, variational data assimilation, modular coding and explicit parallel structure conformal to modern computer architectures (both cache-coherent shared-memory and distributed cluster technologies). Currently, both ROMS and TOMS are identical and continue improving and evolving. ROMS remains as the scientific community model while TOMS becomes the operational community model.

ROMS/TOMS is a three-dimensional, free-surface, terrain-following ocean model that solves the Reynolds-averaged Navier-Stokes equations using the hydrostatic vertical momentum balance and Boussinesq approximation (Haidvogel *et al.* 2000, 2008; Shchepetkin and McWilliams, 2005, 2009). The governing dynamical equations are discretized on a vertical coordinate that depend on the local water depth. The horizontal coordinates are orthogonal and curvilinear allowing Cartesian, spherical,

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and polar spatial discretization on an Arakawa C-grid. Its dynamical kernel includes accurate and efficient algorithms for time-stepping, advection, pressure gradient (Shchepetkin and McWilliams 2003, 2005), several subgridscale parameterizations (Durski *et al.*, 2004; Warner *et al.*, 2005) to represent small-scale turbulent processes at the dissipation level, and various bottom boundary layer formulations to determine the stress exerted on the flow by the bottom.

Several adjoint-based algorithms exist to explore the factors that limit the predictability of the circulation in regional applications for a variety of dynamical regimes (Moore *et al.*, 2004, 2009). These algorithms use the ideas of Generalized Stability Theory (GST) in order to identify the most unstable directions of state-space in which errors and uncertainties are likely to grow. The resulting singular vectors can be used to construct ensembles of forecasts by perturbing initial and boundary conditions (optimal perturbations) and/or perturbing surface forcing (stochastic optimals). Perturbing the system along the most unstable directions to the state-space yields information about the first (ensemble mean) and second (ensemble spread) moments of the probability density function. Given an appropriate forecast skill measure, the circulation is predictable if low spread and unpredictable if large spread.

There are several adjoint-based variational data assimilation algorithms available in ROMS. For cases in which the dynamics are imposed as a strong constraint (*i.e.* no model error assumed), there is an incremental 4DVar (Moore *et al.*, 2010a; Powell *et al.*, 2008) driver (I4D-Var) similar to that used operationally at some numerical weather prediction centers. In the case where errors are admitted in the model, there is an indirect representer-based weak constraint 4DVar (Di Lorenzo *et al.*, 2007; Muccino *et al.*, 2008) driver (R4D-Var) and a weak constraint Physical Space Analysis System (4D-PSAS) driver.

There are several biogeochemical models available in ROMS. In order of increasing ecological complexity these include three NPZD-type models (Franks *et al.*, 1986; Powell *et al.*, 2006; Fiechter *et al.*, 2009), a nitrogen-based ecosystem model (Fennel *et al.*, 2006, 2008), a Nemuro-type lower level ecosystem model (Kishi *et al.*, 2007), and a bio-optical model (Bissett *et al.*, 1999).

ROMS includes a sediment-transport model with an unlimited number of user-defined cohesive (mud) and non-cohesive (sand) sediment classes (Warner *et al.*, 2008). Each class has attributes of grain diameter, density, settling velocity, critical stress threshold for erosion, and erodibility constant. A multi-level bed framework tracks the distribution of every size class in each layer and stores bulk properties including layer thickness, porosity, and mass, allowing the computation of bed morphology and stratigraphy. Also tracked are bed-surface properties like active-layer thickness, ripple geometry, and bed roughness. Bedload transport is calculated for mobile sediment classes in the top layer.

ROMS is a very modern and modular code written on F90/F95. It uses C-preprocessing to activate the various physical and numerical options. The parallel framework is coarse-grained with both shared-memory (OpenMP) and distributed-memory (MPI) paradigms coexisting in the same code. Because of its construction, the parallelization of the adjoint is only available for MPI. Several coding standards have been established to facilitate model readability, maintenance, and portability. All the state model variables are dynamically allocated and passed as arguments to the computational routines via dereferenced pointer structures. All private arrays are automatic; their size is determined when the procedure is entered. This code structure facilitates computations over nested grids. There are three types of nesting capabilities in ROMS: (i) *refinement* grids which provide increased resolution (3:1 or

5:1) in a specific region; (ii) *mosaics* which connect several grids along their edges, and (iii) *composite* grids which allow overlap regions of aligned and non-aligned grids.

WORK COMPLETED

One of our major accomplishments during the last year was the overhaul of the 4D-Var data assimilation capabilities. ROMS/TOMS uniquely supports three different 4D-Var methodologies: incremental strong constraint 4D-Var (I4D-Var), a physical-space statistical analysis system (4D-PSAS), and a representer-based 4D-Var (R4D-Var). To our knowledge, ROMS/TOMS is the only open-source, ocean community modeling framework supporting all these variational data assimilation methods and other sophisticated adjoint-based algorithms.

The vertical terrain-following coordinate in ROMS/TOMS was further generalized to support an additional transformation and multiple vertical stretching functions. This development is described in https://www.myroms.org/wiki/index.php/Vertical_S-coordinate in the ROMS wiki. The vertical stretching function, $C(\sigma)$, is one-dimensional, nonlinear, continuous, and monotonic. It is defined in terms of a few input parameters and the local grid bathymetry. This allows the user to increase the vertical resolution where it is most needed in a particular application. In addition, the new vertical transformation reduces the amount of numerical diapycnal diffusion in the horizontal advection of tracers.

We held two very successful workshops. The first was held at the Jean Kuntzmann laboratory, Saint Martin d'Herès Campus, Grenoble, France (Oct 6-8, 2008; <http://www.myroms.org/2008workshop>). The second was held at the Sydney Institute of Marine Science, Sydney, Australia (Mar 31 – Apr 2, 2009; <http://www.myroms.org/2009workshop>). As in the past, several tutorials were offered in each workshop about basic and advanced ROMS algorithms. The next workshop will be held at the Hawaii Imin International Conference Center, University of Hawaii at Manoa, Honolulu, Hawaii, April 5-8, 2010 (<http://www.myroms.org/2010workshop>). We will also organize a Data Assimilation Workshop at the University of California Santa Cruz, Santa Cruz, CA, summer 2010. This will be a one week workshop that will include lectures on 4D-Var data assimilation methodology and algorithms.

RESULTS

The 4D-PSAS and R4D-Var algorithms can be configured as strong constraint (dynamical model is error free) or weak constraint (errors are admitted in dynamical model). All these algorithms are fully working, parallel and affordable. If the same *a priori* hypothesis about the errors is assumed in a strong constraint application (Moore *et al.*, 2010 a, b), they produce identical solutions and the computational cost required to identify the solution is the same in each case. This is discussed in detail by Courtier (1997) and can be used to check if the ROMS/TOMS 4D-Var algorithms are coded correctly. Figure 1, shows the 4D-Var minimization cost/penalty function \mathbf{J} , a measure of the misfit between model and observations, for a 4-day assimilation cycle (1-4 July, 2000) in a regional model of the California Current System (described in Broquet *et al.*, 2009). The left panel, Fig. 1a, shows the value of \mathbf{J} for I4D-Var (red curve, model space search) and strong constraint 4D-PSAS (blue curve, observation space search). After 35 inner loop iterations, both algorithms converge to the same \mathbf{J} value. The rate of convergence is also the same. The theoretical minimum value \mathbf{J}_{\min} of \mathbf{J} , as described in Courtier (1997) dual formulation, is also plotted (black dashed-curve). The fact that \mathbf{J} does not asymptote to this theoretical minimum indicates that one or more of our *a priori* error hypothesis was not entirely

correct. Recall that our prior hypothesis about the model error is that the model is perfect which is unlikely to be true. The right panel, Fig. 1b, shows similar values for \mathbf{J} but for the representer-based R4D-Var algorithm configured as strong constraint (blue curve) and weak constraint (black solid curve). The values for I4D-Var (red curve) are repeated here for comparison. As in Fig. 1a, both algorithms converge to the same value and rate after 35 iterations. However, the weak constraint solution (black solid curve), which accounts for errors in the dynamical model, is much closer to the \mathbf{J}_{\min} predicted by the theory. Indeed, we know that dynamical models actually have errors. These errors tend to grow and affect predictability of the ocean circulation (forecast skill).

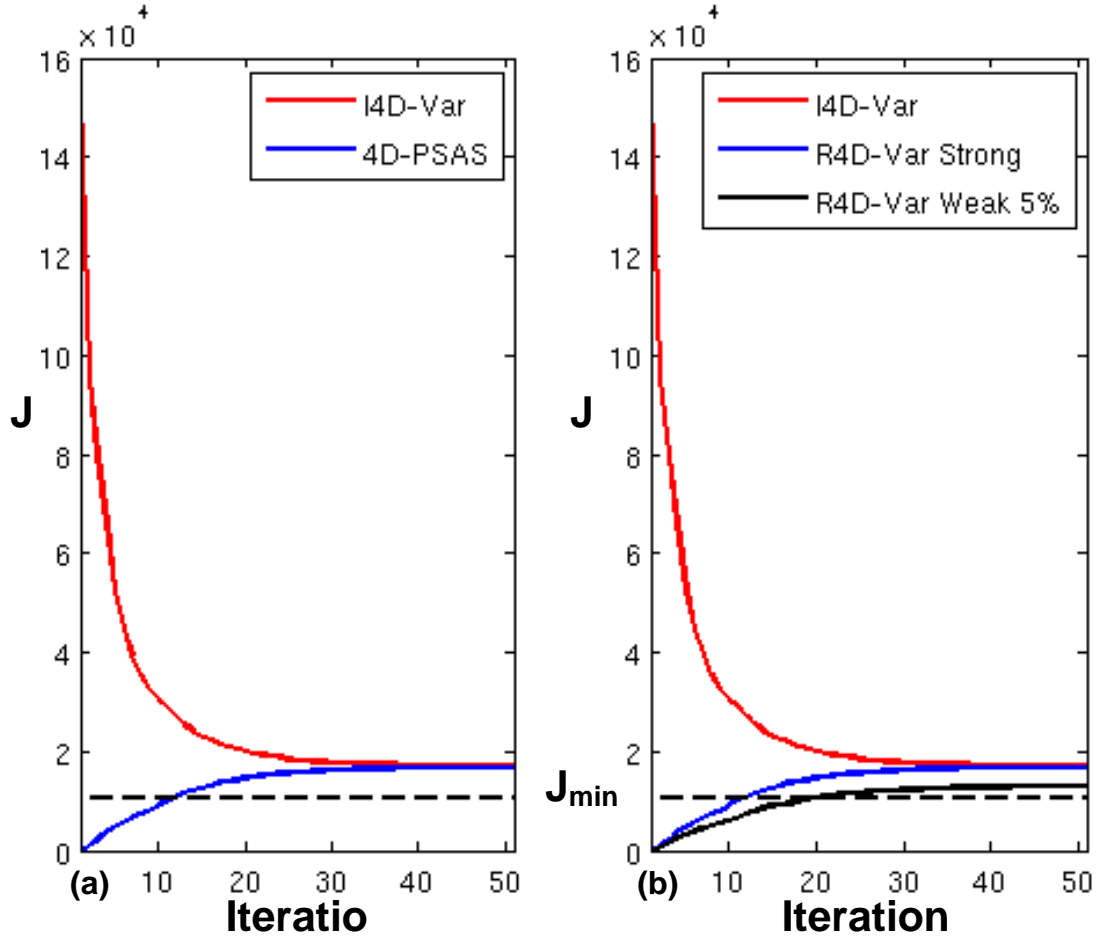


Figure 1: 4D-Var minimization cost/penalty function, J , versus number of inner loop iterations for a 4-day assimilation cycle in a regional model of the California Current System (1-4 July, 2000): (a) comparison between strong constraint I4D-Var (red curve) and 4D-PSAS (blue curve), (b) comparison between strong constraint I4D-Var (red curve), and strong (blue curve) and weak (black solid curve) constraint R4D-Var. In all cases, the initial conditions, surface forcing, and boundary conditions are adjusted. The dashed line indicates the theoretical minimum value J_{\min} of J .

This is a very important result indicating that the 4D-Var algorithms in ROMS/TOMS are correctly coded. We get identical solutions regardless of whether the minimization is done in model space search (I4D-Var) or observation space search (4D-PSAS and R4D-Var). These identical results are also shown in Figure 2. The panels show maps of sea surface temperature (SST) increments $\delta\mathbf{x}_{\text{sst}}(\mathbf{0})$, to the

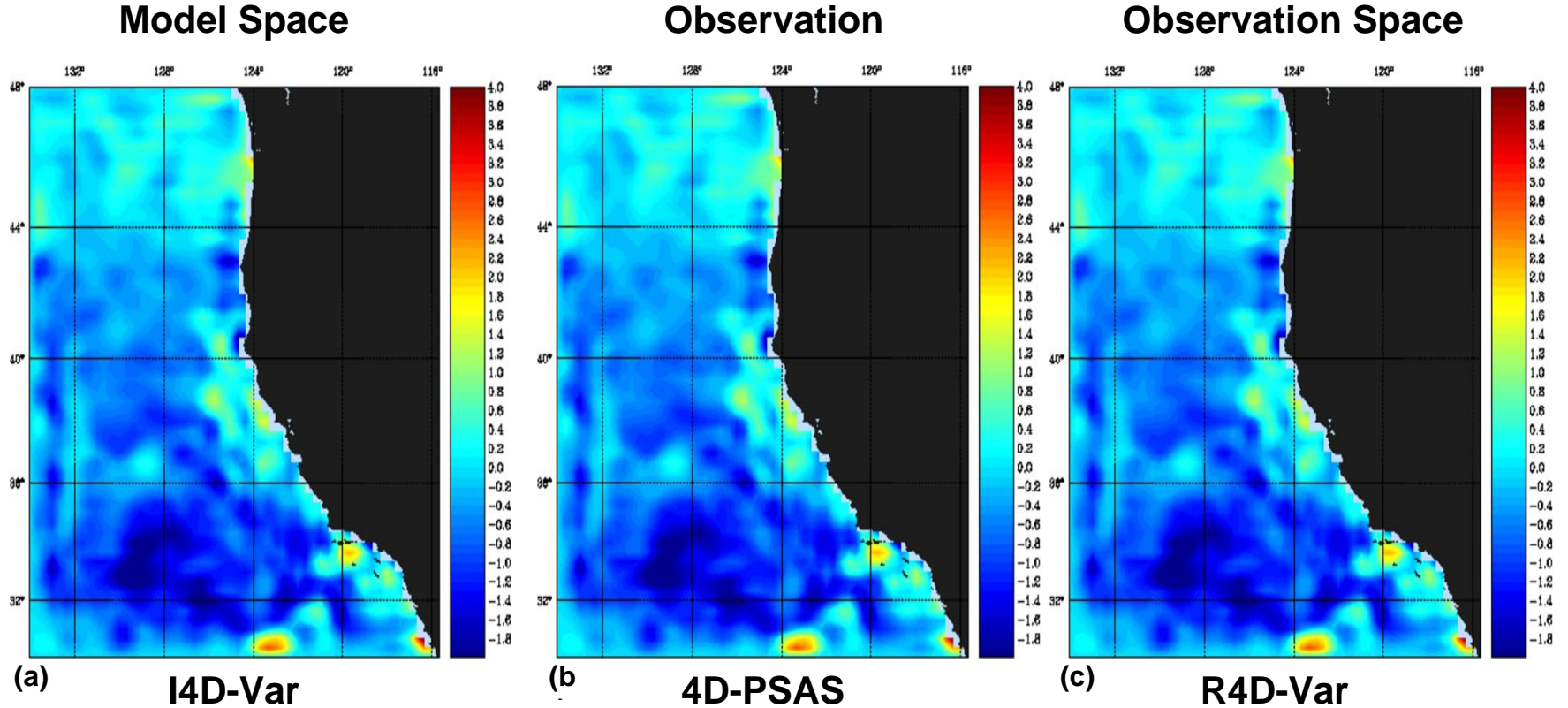


Figure 2: 4D-Var sea surface temperature ($^{\circ}\text{C}$) initial conditions increments, $\delta x_{sst}(0)$, to background or first guess value, $x_{sst}^b(0)$, from previous assimilation cycle for: (a) strong constraint I4D-Var, model space search, (b) strong constraint 4D-PSAS, observation space search, and (c) strong constraint R4D-Var. The sea surface temperature increment patterns are identical for all three 4D-Var data assimilation methodologies.

background initial conditions , $\mathbf{x}_{sst}^b(\mathbf{0})$, for (a) strong constraint I4D-Var, (b) strong constraint 4D-PSAS, and (c) strong constraint R4D-PSAS . Recall that the new analysis is $\mathbf{x}^a(\mathbf{0})=\mathbf{x}^b(\mathbf{0})+\delta\mathbf{x}(\mathbf{0})$, where $\mathbf{x}^b(\mathbf{0})$ is the background initial conditions and $\delta\mathbf{x}(\mathbf{0})$ is the 4D-Var assimilation increment.

The maps in Figure 2 are identical within round off. Notice that the data assimilation corrected the sea surface temperature associated with upwelling along the California Coast.

All critical components common to each 4DVar approach including the conjugate gradient, preconditioning, and error covariance modeling were greatly improved. Coding and testing these algorithms was technically challenging and time consuming. The conjugate gradient algorithm was completely rewritten for all three 4D-Var algorithms. It is now based on the Lanczos method, as described in Fisher (1998). Two versions of Limited Memory Preconditioners (LMP) are available. These are the *spectral* preconditioner as described in Fisher (1998), and the *Ritz* preconditioner as described in Tshimanga *et al.* (2008). The technical description of these algorithms and how to use them is documented in https://www.myroms.org/wiki/index.php/Variational_Data_Assimilation in the ROMS wiki. The error covariance modeling was enhanced by imposing a multivariate constraint via the balance operator, \mathbf{K} , as reported in Weaver *et al.* (2005). The state vector is split between balanced and unbalanced components, except for temperature, which is used to establish the balanced part of the other state variables. This allows extracting information about the unobserved variables from the observed data. It models the off-diagonal terms of the error covariance, $\mathbf{B} = \mathbf{K}\mathbf{B}_u\mathbf{K}^T$, where \mathbf{B}_u is the unbalanced error covariance matrix. Additionally, new algorithms were developed to estimate the posterior error or confidence in the resulting circulation estimates (Moore *et al.*, 2010 a,b).

IMPACT/APPLICATIONS

This project will provide the ocean modeling community with a freely accessible, well-documented, open-source, terrain-following, ocean model for regional nowcasting and forecasting that includes advanced data assimilation, ensemble prediction, and analysis tools for adaptive sampling and circulation dynamics, stability, and sensitivity.

TRANSITIONS

The full transition of ROMS/TOMS to the operational community is likely to occur in the future. However, the ROMS/TOMS algorithms are now available to the developers and scientific and operational communities through the website <https://www.myroms.org>.

RELATED PROJECTS

The work reported here is related to other already funded ONR projects using ROMS. In particular, the PI (H. Arango) closely collaborates with A. Moore (adjoint-based algorithms) at University of California, Santa Cruz, A. Miller and B. Cornuelle (ROMS adjoint and variational data assimilation) at Scripps Institute of Oceanography, E. Di Lorenzo (Southern California predictability) at Georgia Institute of Oceanography, and J. Wilkin (Mid-Atlantic Bight variational data assimilation) at Rutgers University.

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