Continued Development of 4D-Variational Data Assimilation and Adjoint-Based Methods of Sensitivity Analysis and Applications Using ROMS

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LONG-TERM GOALS

The scientific goals of this research project are:

1. To explore the factors (e.g. uncertainties in initial conditions versus those in surface forcing and boundary conditions) that limit the predictability of the circulation in regional ocean models in a variety of dynamical regimes;

2. To compare two state-of-the-art variational data assimilation strategies (4DVAR and IOM) and gain experience using both in regional ocean models;

3. To develop ensemble prediction techniques for regional ocean models;

4. Demonstrate the utility of the ROMS data assimilation framework in a real-time, sea-going environment for prediction studies in the Intra-Americas Sea (IAS) with particular emphasis in the Caribbean Sea. As such, we will demonstrate, as a proof of concept, the utility of adjoint modeling and 4DVAR data assimilation in a real-time operational setting, at sea.

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OBJECTIVES

The main objectives are: (**i**) to develop real-time data assimilation and prediction techniques for the coastal oceans and semi-enclosed seas, with particular emphasis on the IAS and U.S. west coast, based on continuous satellite-based and in-situ upper ocean monitoring systems; (**ii**) to demonstrate the utility of variational data assimilation in real-time, and in a sea-going environment; (**iii**) to demonstrate the value of collecting routine ocean observations from existing coastal ocean observing systems and specially equipped ocean vessels; and (**iv**) to develop much needed experience in both the assimilation of disparate ocean data and ocean prediction in regional ocean models using sophisticated variational data assimilation techniques.

APPROACH

The primary tool used is the Regional Ocean Modeling System (ROMS) and the Terrain-coordinate Ocean Modeling System (TOMS). This is a collaborative effort involving Drs. Arthur Miller and Bruce Cornuelle at the Scripps Institute of Oceanography, Dr. Hernan Arango at Rutgers University of New Jersey, Dr. Emanuele Di Lorenzo at the Georgia Institute of Technology, and Dr. Ralph Milliff at Colorado Research Associates. To address the aforementioned goals and objectives, we are using a newly developed suite of tools that utilize the tangent linear (TL), adjoint (AD), and finite-amplitude tangent linear (RP) versions of the ROMS/TOMS code. ROMS, TLROMS and ADROMS were developed under the support of previous ONR funding, while the development of RPROMS was supported by NSF.

As part of this effort we have also developed several toolkits that utilize the various versions of ROMS. These include: (1) a Generalized Stability Theory (GST) toolkit; (2) an adjoint sensitivity analysis toolkit; and (3) a suite of 4-dimensional variational data assimilation platforms that include strong constraint 4DVAR (S4DVAR), incremental S4DVAR (IS4DVAR), an indirect representer-based weak constraint 4DVAR (W4DVAR), and a weak constraint Physical Space Analysis System (W4DPSAS). W4DVAR is based on the Oregon State University Inverse Ocean Model (IOM) of which ROMS is also a component via a separate NSF funded effort (Di Lorenzo et al, 2006; Muccino et al, 2006). Our primary efforts during the last 12 months have involved using the ROMS adjoint sensitivity analysis toolkit and IS4DVAR platform for data assimilation and prediction studies in the IAS, and for adjoint sensitivity analysis in a coupled physical-biological model of the California Current system. These foci began as separate projects at the University of Colorado but have subsequently been merged into a single project at the University of California. We will discuss separately below the progress made in both components of the unified project.

WORK COMPLETED

IAS project component:

During our first IAS project PI meeting in Boulder in March 2005, the following general tasks were identified as important steps toward achieving the goals of this component of the project: (1) data assembly, (2) model configuration and testing, (3) experimental design, and (4) forecast experiment preparation and logistics. These goals were refined and reiterated during a second PI meeting in Boulder in October 2005. The following is an up-to-date status report with respect to the aforementioned tasks:

(1) Data Assembly

(i) Sub-daily (swath-by-swath) satellite scatterometer wind data has been processed, assembled and used for IAS ROMS simulations.

(ii) NCEP reanalysis surface data have been prepared and processed for the period 1990-2006 and used for IAS ROMS simulations.

(iii) Gridded SSH and SST data have been assembled and processed for the IAS for assimilation into IAS ROMS. The SSH data are from AVISO to which a steric height correction is applied, and SST is a blended product from several satellite platforms provided to us by Dr. Dave Foley at NOAA PFEL.

(2) Model Configuration and Testing

(i) ROMS has been configured for the IAS region at both 20km and 40km resolution, using climatological open boundary conditions derived from a long run of ROMS for the entire North Atlantic. The 40km resolution model is designed as a training tool for the IS4DVAR data assimilation, and to provide relatively low cost first-guess initial conditions for the 20km data assimilation model runs and predictions.

(ii) Forced simulations spanning the period 1990-2006 have been run at both 20km and 40km and are used as a baseline for data assimilation experiments.

(iii) A series of adjoint sensitivity calculations have been performed to explore the sensitivity of the IAS circulation to variations in different aspects of the model configuration. These are described in Chhak et al (2006) and Chhak (2006).

(iv) A series of identical twin IS4DVAR experiments have been performed using IAS ROMS which have greatly aided in the experimental design, detection of bugs in the algorithms, and tuning of algorithm performance and efficiency.

(3) Experimental Design

(i) Semi-variagram techniques have been employed to estimate the spatial correlations which are critical paremeters in the background error covariance function used in the definition of the IS4DVAR cost function.

(ii) Based on all of our preliminary experiments, many algorithmic improvements have been made to the ROMS 4DVAR platforms, which include full parallelization for multi-processor computers.

(4) Forecast Preparation and Logistics

(i) The proof-of-concept sea-trials of the IAS ROMS data assimilation and ensemble prediction system will take place aboard the *Explorer of the Seas,* a fully instrumented Royal Caribbean Cruise Line (RCCL) cruiseship based in Port Miami. In readiness for the sea-trials, the satellite SST and SSH data of 1(iii) for the period March 2005-June 2006 have been assimilated into IAS ROMS at 14 day intervals using IS4DVAR. This will continue through to the end of February 2007 when the sea-trials conclude.

(ii) A prototype real-time ensemble prediction system is currently under development and will be deployed aboard *Explorer.* Each ensemble member will have the same initial condition but will be forced with different surface fluxes of heat and momentum generated by a Bayesian Hierarchical Model (BHM) that has been developed by Milliff and collaborators for the Meditteranean under separate ONR support. The BHM will be reconfigured for the IAS.

(iii) The real-time sea-trials of the ensemble prediction system aboard *Explorer* are planned for the period 1/7/07 to 2/18/07. During this 6 week period a different project team member will travel aboard the cruiseship running a suite of ensemble forecasts (~100 per cruise). The initial conditions for each ensemble forecast will be generated using satellite SST, SSH, and IS4DVAR, and if logistics allow, using also ADCP and surface SST and SSS data collected aboard the cruiseship. As the ensemble unfolds, each member of the ensemble and the ensemble mean will be compared against new observations both from satellite and the cruiseship as they become available.

(iv) A project website has been constructed (http://marine.rutgers.edu/po/ias) which describes the project and acts as a repository for the data assimilation products. During the sea-trials this will also act as a live update for the ensemble prediction results.

California Current project component:

A comprehensive adjoint sensitivity analysis of the southern portion of the California Current system has been performed using a coupled physical-biological version of ROMS. This work is described in a paper by Moore et al (2006).

RESULTS

IAS:

Two different integrations of IAS ROMS will be compared here. In the first case, referred to as IAS-F, the model was run for the period Jan 1990-July 2006 using surface forcing fields derived from NCEP reanalysis data and satellite scatterometer wind data when available. In the second case, referred to as IAS-H, SST and SSH data were assimilated into the model every 2 weeks using a 14 day assimilation window starting in March 2005 using IS4DVAR. The first-guess used on 1 March 2005 was the model state from IAS-F on the same date. At the end of each 2 week period, a 14 day hindcast was run using the best estimate of the ocean state derived from the IS4DVAR. All cases were run using 40km horizontal resolution.

Figures 1 and 2 show two measures of the difference between the model SST and SSH and observations from IAS-F and IAS-H for the period March 2005 – June 2006. The measures used are mean squared differences between the model and observations (denoted MSE), and the pattern correlations between the model fields and observed fields (denoted CC), each computed separately for the Caribbean Sea (Fig. 1) and Gulf of Mexico (Fig. 2). In addition to IAS-F and IAS-H, the corresponding differences between the model and the observations during each 14 day assimilation cycle are also shown (denoted IAS-A). Comparing IAS-F and IAS-H reveals that in general data assimilation has a positive impact on the model hindcasts, although this is not always the case. The MSE in the Gulf of Mexico (Fig. 2) for IAS-H and IAS-A increases considerably during the period April to August 2005, and again May 2006 and exceeds that of IAS-F. This appears to be due to a combination of forcing error and model error. More detailed analyses reveal that the periods characterized by strong hurricanes (in this case Katrina, Wilma and Rita) are also problematic in the Gulf because the physical parameterizations in ROMS are not designed to handle such extreme surface conditions.

Comparing IAS-H and IAS-A, Figs. 1 and 2 show that the agreement between the model and the observations improves during data assimilation cycle, indicating that IS4DVAR is performing as it should. Figures 1 and 2 also reveal that in general the model and assimilation perform better in the Caribbean Sea than in the Gulf of Mexico. This is to be expected since the 40km resolution used in this case poorly resolves the Loop Current and its associated dynamics.

The pattern correlations CC of Figs. 1 and 2 reveal that despite the presence of persistent MSE during IAS-H and IAS-A, the SST and SSH patterns agree very well for much of the period with those observed. Exceptions are the Spring-to-Summer transition period in the Gulf of Mexico identified earlier (Fig. 2) when the model has problems recovering the circulation. The very low values of CC at all time for IAS-F indicates that the model forced by only the observed forcing is unable to capture the circulation patterns.

An example of differences in SST and SSH between the model and observations for one particular day, 29 June 2005 for IAS-F, IAS-H and IAS-A is shown in Fig. 3. Figure 3 reveals that considerable differences can exist between the model and observations in IAS-F when there is no data assimilation. These differences are reduced dramatically by IS4DVAR (IAS-A), however when data assimilation ceases and the model is run in hindcast mode using the observed surface forcing (i.e. IAS-F), the model minus observation differences can increase considerably due to uncertainties in the surface forcing, model error, and errors in the unobserved components of the circulation that are not completely constrained by the surface observations.

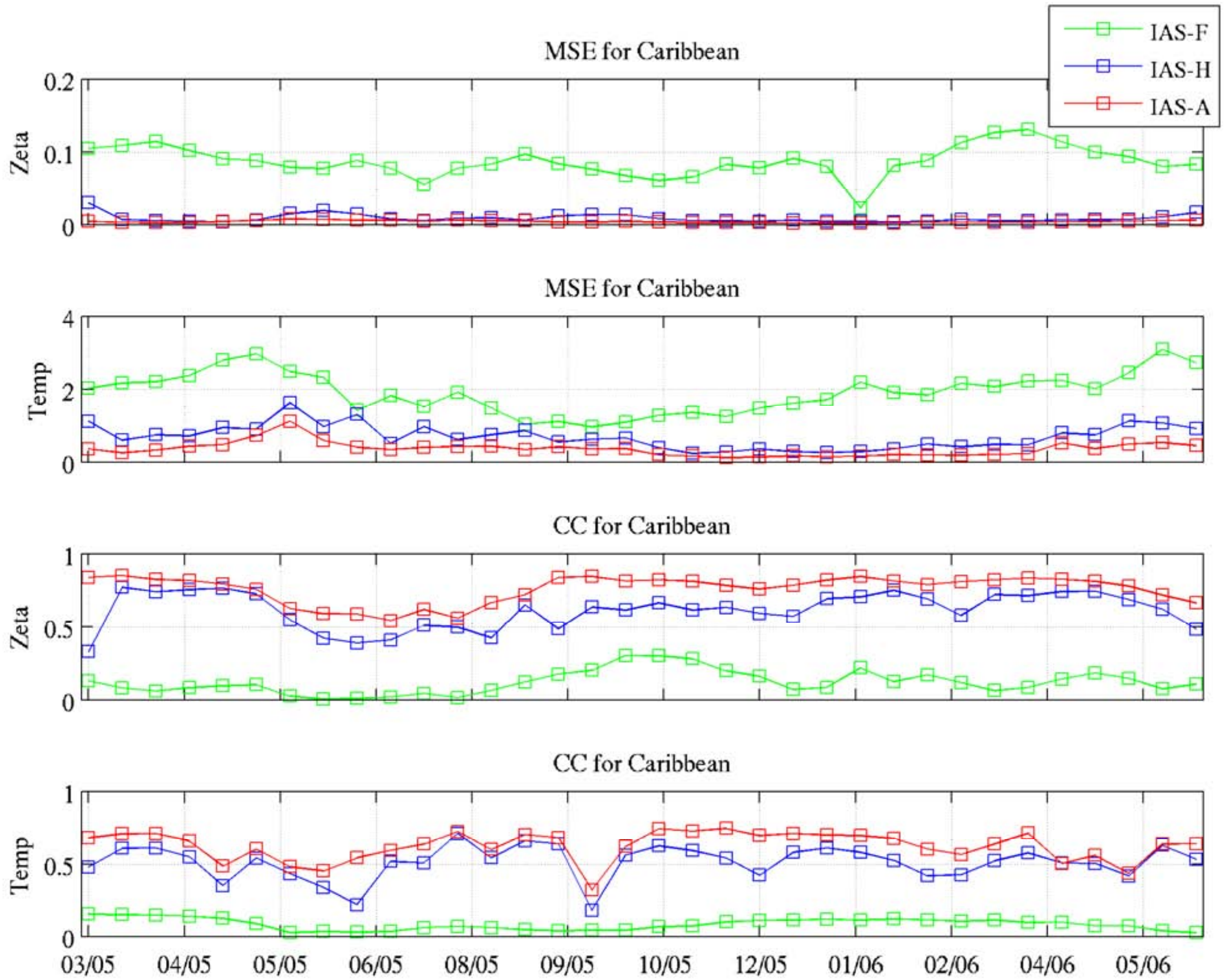

Figure 1: MSE and CC for SST and SSH computed within the Caribbean Sea for IAS-F, IAS-H and IAS-A.

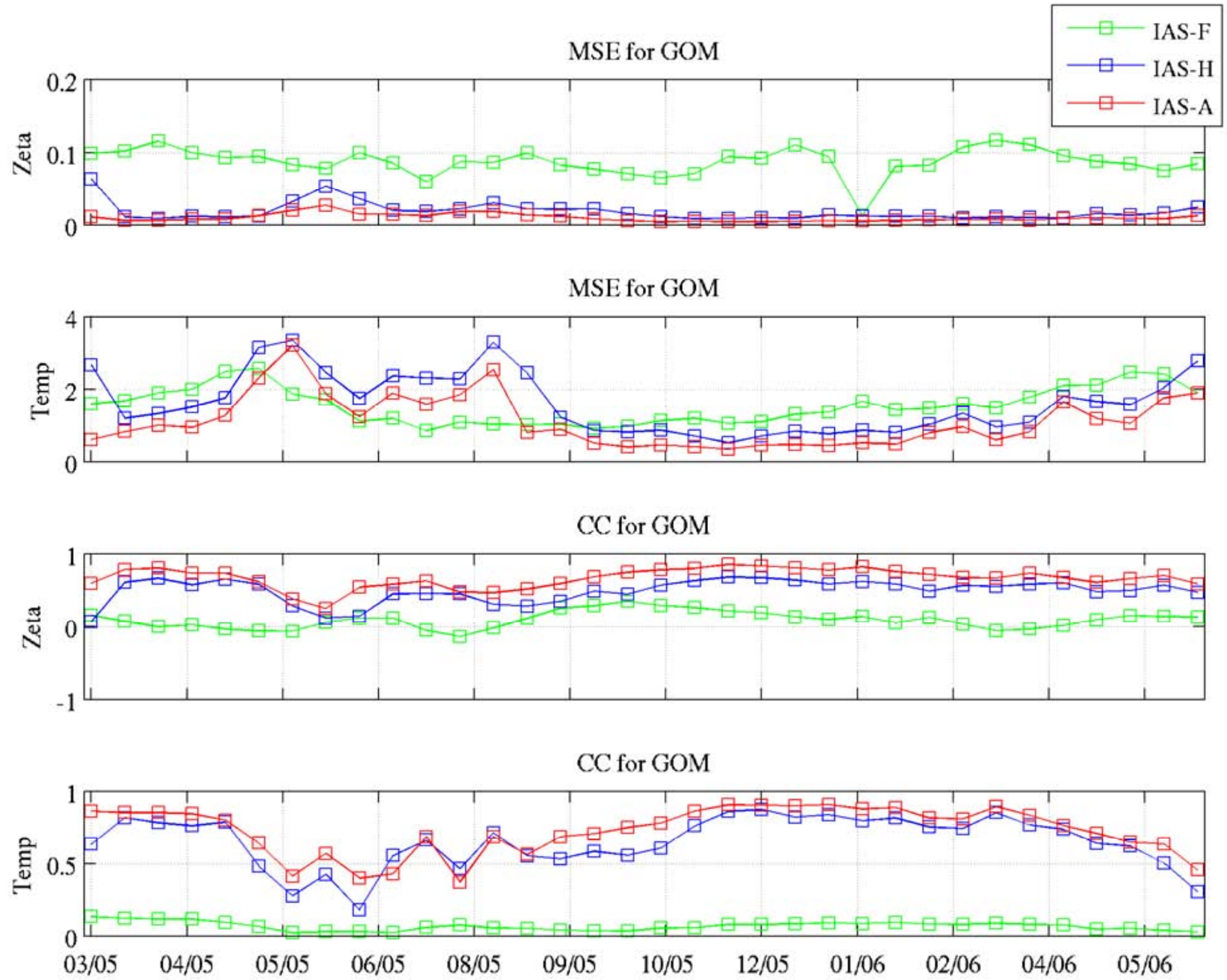

Figure 2: MSE and CC for SST and SSH computed within the Gulf of Mexico for IAS-F, IAS-H and IAS-A.

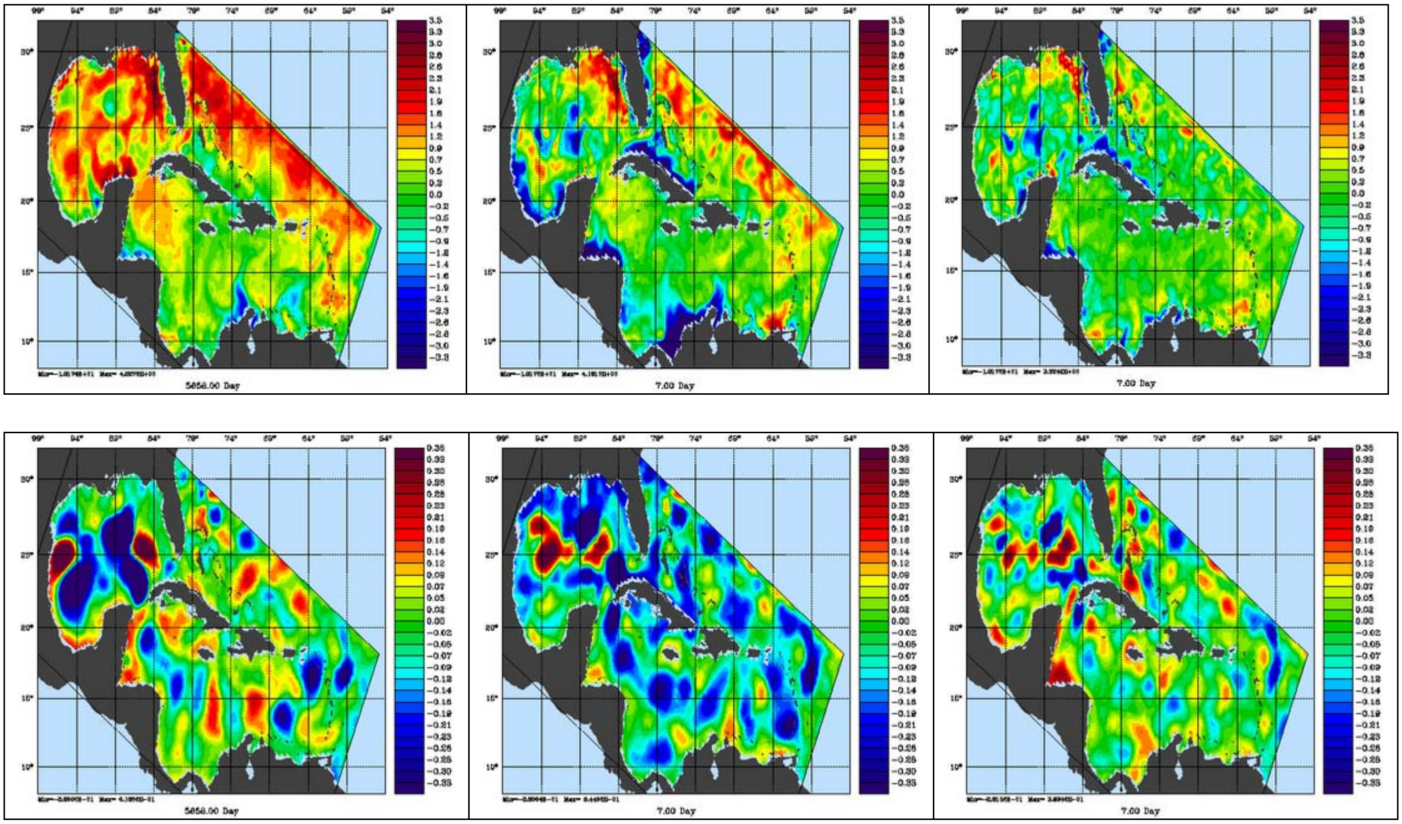

Figure 3:SST differences (top row) and SSH differences (bottom row) between the model and observations for IAS-F (left hand panels), IAS-H (center panels) and IAS-A(right hand panels).

California Current:

Indices were defined as measures of coastal SST, eddy kinetic energy, and baroclinic instability within the California Current system between Point Reyes and Point Conception on the California coast. The adjoint sensitivity toolkit was then used to quantify the monthly mean sensitivity of each index to variations in ocean surface forcing during a 5 year integration of the ROMS model configured for the central and southern California coastal region. For each index considered, there were considerable seasonal variations in sensitivity to wind stress, wind stress curl and heat flux. For the SST index, the largest sensitivities occurred during late summer and early fall associated with changes in wind stress and heat flux. The sensitivities varied by a factor of 2-4 during the course of a year, although there was considerable year-to-year variability with sensitivities between spring and fall sometimes varying by a factor of 5-10. The seasonal trends in KE sensitivity were similar to those of SST, although they exhibited a much less pronounced seasonal cycle. The sensitivities vary by a factor ~3 over the course of a year. The seasonal trends and variations in the potential for baroclinic instability were the opposite of those found for SST and KE, and peaked during the spring. Like KE, the baroclinic instability was most sensitivity to variations in wind stress, and the sensitivity varied by a factor ~2 during the course of a year. Full details of these calculations are given in Moore et al (2006).

IMPACT/APPLICATIONS

The IAS component of the project will demonstrate the utility of ROMS adjoint modeling and variational data assimilation algorithms in a real-time, sea-going environment, and will very likely strengthen the case for installing oceanographic instruments and ocean monitoring laboratories onboard other commercial or Navy cruise ships plying different routes.

The California Current component of the project demonstrates the power of the ROMS adjoint sensitivity and related toolkits for exploring and understanding the underlying dynamics of the physical and biological circulations in this region.

TRANSITIONS

The various ROMS toolkits and 4DVAR data assimilation algorithms are available from the Rutgers website and are being actively used and further developed by other research groups in the U.S., Australia and Chile. To facilitate this transition a mini-workshop on the ROMS data assimilation platforms was held at the University of California Santa Cruz in Spring 2006 and attended by students, post-docs and other researchers from Rutgers University, Scripps, and UC Santa Cruz.

RELATED PROJECTS

The work described here is intimately related to the following ONR supported projects::

"ROMS/TOMS Tangent Linear and Adjoint Models: Data Assimilation Tools and Techniques", PI Hernan Arango, grant number N00014-00-1-0227.

"ROMS/TOMS Tangent Linear and Adjoint Models: Data Assimilation Tools and Techniques ", PIs Arthur Miller and Bruce Cornuelle, grant number N00014-99-1-0045.

"ROMS Data Assimilation Tools and Techniques",PI Emanuele Di Lorenzo, grant number N00014-05-1-0365.

"Bayesian Hierarchical Models to Augment the Mediterranean Forecast System", PI Ralph Miliff, grant number N00014-05-C-0198.

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None

PUBLICATIONS

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