Stochastic Forcing for Ocean Uncertainty Prediction

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LONG-TERM GOALS

Our research vision is to develop and transform ocean modeling and data assimilation to quantify regional ocean dynamics on multiple scales. Our group creates and utilizes new models and methods for multiscale modeling, uncertainty quantification, data assimilation and the guidance of autonomous vehicles. We then apply these advances to better understand physical, acoustical and biological interactions. We seek both fundamental and applied contributions to build knowledge and benefit naval operations.

A main focus of this research is the role of stochastic forcing on ocean uncertainty and variability predictions. The work includes collaborations with NRL-Stennis to prepare the transfer of a subset of the capabilities and software developed by our Multidisciplinary Simulation, Estimation, and Assimilation Systems (MSEAS) group. The research thrusts of interest to both NRL and MIT, as well as the specific goals of the work, are below.

Research Thrusts:
- *Stochastic forcing and uncertainty/variability predictions*
- *Sensitivity analysis for forecast quality control, data-model comparisons and data error models*
- *Multiscale covariance modeling and mapping*
- *Ensemble initialization and generation, towards non-Gaussian ensemble initialization*

OBJECTIVES

Our specific objectives are to:
i) Develop, demonstrate and transfer techniques for stochastic error modeling and stochastic boundary forcing for improved ensemble uncertainty predictions with NCOM and COAMPS
ii) Develop and transfer software for ocean data management, quality control and automated robust distribution, including data error-models and data-model comparison codes
iii) Demonstrate and transfer techniques for multiscale covariance modeling and level-set-based objective analysis codes for mapping data in complex coastal/archipelago domains
iv) Develop and demonstrate ensemble initialization and generation schemes, towards non-Gaussian ensemble initialization
v) Apply the above advances in collaborative sea exercises of opportunity
vi) Strengthen existing and initiate new collaborations with NRL, using and leveraging the MIT Naval Officer education program

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APPROACH

The proposed applied research in stochastic modeling and ocean uncertainty prediction is linked to two growing fundamental fields: prediction and reduction of uncertainties; and, estimation of properties by combining models with data. From a fundamental viewpoint, uncertainty is characterized by a probability density function (pdf). One of the aims of the applied research and collaborations with NRL will be to improve the prediction of such pdf's.

WORK COMPLETED

Stochastic Forcing and Uncertainty/Variability Predictions

Evaluation of Uncertainty Forecasts**:** A manuscript is being completed describing the evaluation of the real-time forecasts of ocean probability density functions (pdfs) issued during the two-month QPE IOP09 experiment off the coast of Taiwan during Aug-Sep 2009. The oceanographic features and their evolution are outlined. Uncertainties were forecast in real-time using the MSEAS nonlinear free-surface primitive equation model and Error Subspace Statistical Estimation (ESSE). The variability in the pdfs are illustrated and discussed, including effects of Typhoon Morakot and internal tides. The ESSE ensemble forecasts are compared to the measured errors between the central forecasts and seasoar data.

Uncertainty Prediction for Nonlinear Dynamical Systems for Ocean Modeling**:** Equations and software have been completed to integrate a generic class of stochastic non-autonomous linear and nonlinear systems. The class of systems includes classic nonlinear chaotic systems (e.g. Lorenz, Kraichnan-Orszag, etc.) and other systems we engineered, but in our studies, they have uncertainty in initial and boundary conditions and are forced by additive and multiplicative random processes. The software is used to inter-compare multiple uncertainty prediction schemes in terms of accuracy and computational effort. To allow accurate integration of uncertainty due to external stochastic forcing, two new polynomial chaos schemes were derived: the reduced space KLgPC scheme and the modified TDgPC scheme. We also used the software to simulate the probability density function of shallow water waves governed by Korteweg-de Vries (KdV) dynamics with stochastic forcing.

Uncertain Boundary Conditions and DO Equations**:** A manuscript is in preparation.

Hybrid Discontinuous Galerkin (HDG) Finite Element Schemes**:** A high order HDG non-hydrostatic ocean code with unstructured grids continues to be developed using Python and C/C++. The method of manufactured solutions is employed to complete a detailed code verification on the existing Python model implementation. Classes of manufactured solutions are developed and utilized for testing the HDG boundary conditions, the hydrostatic and non-hydrostatic portions of the code, as well as the conservative properties. Results of numerical convergence studies are also completed. Several routines have been ported from Python to C/C++ for high performance, parallelism, and insertion of arbitrary numbers of components and Dynamically Orthogonal (DO) stochastic PDEs. These C/C++ routines have been tested for proper numerical convergence rates and parallel scalability, and they run several times faster than their Python counterparts. In the C/C++ implementation, the PETSc library is used to parallelize the existing data structures and linear solvers, while the community-standard netCDF library (with CF conventions) is used for model and data I/O.

Sensitivity analysis for forecast quality control, data-model comparisons and data error models

Time-dependent Sponge Boundary Conditions: A sponging scheme with a novel, efficient, time dependent sponging external solution was designed to inhibit spurious reflections from open boundaries while preserving the incoming tidal forcing and permitting realistic sub-tidal dynamics (e.g. permitting the advection of eddies and upwelled water in and out of the computational domain). The temporal updating of the external solution was also incorporated into the open boundary conditions.

Data/software management**:** New and improved MSEAS software packages have been released for distribution. In addition to the improved open boundary treatments (mentioned above) and the improvements to the level-set based objective analysis codes (mentioned below), a package for preparing tidal fields for use in PE simulations was released. In addition to interpolating the tidal fields to the PE grid, this package optimizes the tides to satisfy the discrete coastlines and the exact discretized conservation of mass for the PE grid.

Multiscale covariance modeling and mapping

Dynamics- and Data-Constrained Estimation and Optimization of Initial Velocity and Transports*:* A manuscript has been completed on our methodology for dynamically balanced initialization and mapping. The over-all algorithm is outlined, including data use and quality control, the creation of the first guess velocity using the desired dynamics and the fitting of that velocity field to the bathymetry, coasts and discretization for the desired simulation. New algorithms to optimally fit the velocities and transports and to optimize the velocities and transports between islands in complex coastal regions are then derived. These algorithms are direct methods with exact solutions that optimize cost functions. Options are provided to also enforce strong constraints on the transports through specific straits and/or weak constraints on the average velocities in the straits. The methodology is illustrated and evaluated in the Taiwan/Kuroshio region, around the Hawaiian Islands of Kauai/Niihau and in the Philippines Archipelago. The optimization methodology is compared to an averaging method for obtaining the transports through straits.

Level-set-based Multiscale Covariance Modeling and Objective Analysis Codes**:** A number of extensions were made to the MSEAS Fast-Marching Method Objective Analysis (FMM-OA) method and released in software package. A new option for higher-order interpolation was implemented to obtain the distances between each pair of observation points based on the distances previously computed (using the FMM) between each observation point and each grid point. A profile of the execution of the package was used to find computational bottlenecks. These were addressed by writing C/C++ versions of a few routines and interfacing them with the remainder of the Matlab code using the Mexing utility. New algorithms were derived and coded for spatially variable correlation functions and for direct FMM-OAs along any 2D surface. The specific application was to enable direct FMM-OAs of data along the ocean floor in the Middle Atlantic Bight region. This domain spans the coastal, shelf, slope and abyssal oceans, including a shelfbreak. The new FMM speed employed for this purpose is a function of the local bathymetric gradients and depths and of the bathymetric depth at the observation point. This FMM speed allows maintaining correlations between locations in similar regions (e.g. data and grid points both on the shelf) while decreasing correlations between locations in different regions (e.g. points on either side of the shelfbreak front). An additional option was introduced that provides an initial background field (into which observations are OA'ed) that is not a constant field. This new background field is a slowly varying field on the shelf and slope/abyss with a fairly sharp transition at the front. Additional options include the averaging of nearby observations (i.e. within a single numerical grid cell) into a single observation and the ability to save the FMM distance calculations and reuse them in subsequent OA's, so as to substantially increase efficiency.

RESULTS

Stochastic Forcing and Uncertainty/Variability Predictions

***Evaluation of Uncertainty Forecasts*:** The manuscript studying the skill of real-time ocean pdf forecasts first outlines the regional dynamics. During Aug-Sep 2009, the "cold dome", a semi-persistent temperature feature off of northern Taiwan, was present on Aug 14, decayed through Aug 28, strengthened through Sep 5 and decayed afterwards. Eddies of "cold dome" waters were estimated to spin-off to the north-northeast about every 2 days. In addition, the "cold dome" was strongly modulated by tidal effects mostly of shelfbreak and Taiwan-tip origin and long filaments entrained by the Kuroshio. RMS statistics show a good agreement between forecast and measured errors after the real-time numerical bias is removed. Pdfs of the forecast errors are shown to capture and evolve non-Gaussian statistics. Comparing the Kullback-Leibler divergences for the forecast errors with a climatological error distribution shows a 50-100% improvement in the pdf forecasts over the climatology. Pdfs of the forecast error for each observation are shown to capture time scales of internal tides and evolve non-Gaussian statistics over the course of an individual survey. The logarithm score shows 25-50% improvement in the forecasts over the climatology. The choice of deterministic or stochastic tidal forcing is shown to strongly impact the forecasts of velocity error on the shelf. Reanalysis with improved numerics and parameters removed biases and improved error comparisons.

***Uncertainty Prediction for Nonlinear Dynamical Systems for Ocean Modeling*:** We showed that the two new KLgPC and modified TDgPC schemes we derived and the DO equations can integrate both additive and multiplicative noise over large time intervals. To do so, classic nonlinear dynamical systems with stochastic forcing as well as engineering test cases were employed. We also compared the Monte-Carlo and DO schemes to time-integrate shallow water surface waves governed by KdV equations with external stochastic forcing. We find that the DO scheme is computationally efficient. We expect that it can simulate shallow water waves with stochastic wave forcing and the coupling of these surface waves with internal waves and background flows, resolving the interactions between deterministic dynamics and stochastic forcing (Fig. 1).

***Hybrid Discontinuous Galerkin (HDG) Finite Element Schemes*:** A PhD thesis was completed and several manuscripts are in final preparation.

Sensitivity analysis for forecast quality control, data-model comparisons and data error models

Time-dependent Sponge Boundary Conditions: The new sponge was first tested in an idealized shelfbreak setup periodic in the along-shelf direction. The along shelf boundary on the shelf was closed (coast). The remaining (offshore) boundary was open and forced with an idealized M2 tide. The resulting simulation fields were then decomposed into internal tide modes. Figure 2 shows the time evolution of the energy flux of modes 1 & 2 along a cross-slope line through the middle of the domain for two simulations. Figure 2a shows energy fluxes of the first 4 days from the base-line simulation without sponging. A relatively strong reflection is seen coming off of the open boundary (left side of figures, positive energy fluxes), in spite of the radiation conditions applied there. Figure 2b shows the twin fields from a simulation employing the new sponge. The reflection at the open boundary is suppressed, while maintaining the correct solution structure elsewhere. Fig. 2c is as 1b but for the last 4 days of the simulation, showing that the spurious reflections are suppressed for the entire 42 days. To see the effects of our new sponging scheme that allows the time dependence of the external solution, a realistic data driven simulation in the Middle Atlantic Bight region is shown in Figure 3. The surface temperature overlaid with velocity vectors is shown for 3 simulations containing different combinations of sponging and boundary conditions. Fig 3a shows the results where the sponging relaxes towards the initial conditions. Due to wind forcing, waters have upwelled along the coast since the initialization. Near the shelf outflow boundary (38N,75W) this sponging erroneously maintains the warmer ICs and prevents the upwelled water from being advected out of the domain. Fig 3b shows the results when the sponging external solution is allowed to evolve in time using our new algorithm that slowly "forgets" the ICs. The band of persisted ICs is considerably narrowed to the boundary. Fig 3c adds the time evolution algorithm to the boundary conditions. The upwelled waters are now advected out of the domain.

Multiscale covariance modeling and mapping

Dynamics- and Data-Constrained Estimation and Optimization of Initial Velocity and Transports: The Taiwan/Kuroshio test of the initialization methodology is a relatively "benign" initialization: (i) there is only one large island (Taiwan) with a number of small islands that introduce small perturbations and (ii) the main currents are not strongly affected by Taiwan, e.g. the Kuroshio remains on the Pacific side of Taiwan. The differences between the transports and velocities produced by our optimization methodology and those produced by the averaging method are largest by the coasts and in the Strait of Taiwan. While the absolute magnitudes are small (less than 0.1 Sv in transport and 1 cm/s in velocity) the relative differences can be large (50% across the Peng-Hu channel on the northwest side of Taiwan). Compared to the geostrophic first guess velocity used, the differences are larger (5-10 cm/s) near the coasts but remain small (<0.1cm/s) away from land, confirming that the optimization is maintaining the original currents. The Hawaiian test is more challenging, with the currents directly impinging on the island of Kauai. Figure 4 shows the barotropic velocity fields from this test. Fig. 4a shows the initialization using the averaging method. Fig. 4b shows the barotropic velocities using the optimization method which produces a current that more naturally follows the contours of the ridge between Kauai and Niihau. This is in agreement with historical observations which also show that the currents are primarily around Kauai/Niiha rather than between them. Several tests were performed in the Philippines Archipelago. The averaging method overestimates the transports through many of the straits, with peak barotropic velocities reaching 110 cm/s. The solution obtained using our optimization method reduces the peak barotropic velocity to 48 cm/s. Optimization weights which lead to a minimization of velocity were shown to control spurious velocities better than weights which lead to a minimization of transport. The options to directly impose transports through select straits were used to reverse the flow in two straits. This was accomplished while maintaining sensible velocities elsewhere. Nested initializations show that it is better to utilize the optimization method for all straits in the nested subdomains and thus refine transports in accord with the refined resolution than directly impose the corresponding optimized transports from the coarse domains.

Level-set-based Multiscale Covariance Modeling and Objective Analysis Codes: The option for higher order interpolation of the distances between observation points based on the distances previously computed (using the FMM) between each observation point and each grid point was tested in open ocean domains. The resulting FMM-OA fields were compared to those obtained from a standard OA (using Euclidean distances). When the higher order interpolation is combined with second order FMM schemes and our improved FMM initialization, the differences in the temperature fields are O(1.0e-4), well within observation error. The computational profile of the FMM-OA code revealed that 91% of the time was spend in the routine that updates the FMM distances. Coding in C/C++ increased the speed of this routine by a factor of 7 and reduced the run-time of the entire code by a factor of 5. The new ability to make the correlation a function of position was used to map bottom temperature data off the eastern coastline directly, i.e. without having to compute a 3D OA. The region covered the Middle Atlantic Bight through the Gulf of Maine and the Scotian Shelf, see Fig. 5. The bathymetry is highly variable including the shelf, shelfbreak, slope, Georges Bank (41N, 67.5W) and Gulf of Maine basin. Fig 5a shows the mapped bottom temperature, while fig. 5b shows the error field, indicating the data locations. The variable correlation is able to separate the shelf and slope regions, and correctly preserves the signature of Georges Bank. The ability to map the fields directly along this variable-depth 2D surface eliminated the previous need to perform a full 3D volume of analysis just to obtain the bottom temperature. The 3D analysis was expected to require at least 60 vertical levels. The new analysis, directly along the bottom, coupled with the 5x speed up of the code led to an over-all 300x speed up of the whole FMM-OA process.

IMPACT/APPLICATIONS

Better understanding and modeling of physical and interdisciplinary regional ocean dynamics are essential to multiple applications, including efficient real-time at-sea research experiments, naval operations and coastal seas management. Mathematical and computational methods and systems are necessary to predict and study ocean dynamics. Scientific progress occurs from the comparison and optimal combination of measurements and models via data assimilation. Interdisciplinary linkages include the traditional ocean sciences and atmospheric sciences, but also new relationships with other research disciplines within the framework of complex system sciences and engineering.

TRANSITIONS

Methods, software and data sets were transitioned to other research groups. They include: UMass-Dartmouth, WHOI, MIT-OE, NRL-Stennis, U. Bologna, NATO Center for Maritime Research and Experimentation (CMRE), NCSU, TNO, UCSD.

RELATED PROJECTS

Without the present effort, several of our other projects would not be feasible. Interactions also occurred with other research groups, including: UMass-Dartmouth, WHOI, MIT-OE/EAPS, NRL-Stennis, U. Bologna, NURC and TNO (F-P. Lam).

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Ueckermann M.P., 2013. *High Order Hybrid Discontinuous Galerkin Regional Ocean Modeling*. Ph.D. Thesis, Massachusetts Institute of Technology, Department of Mechanical Engineering, September 2013

FIGURES

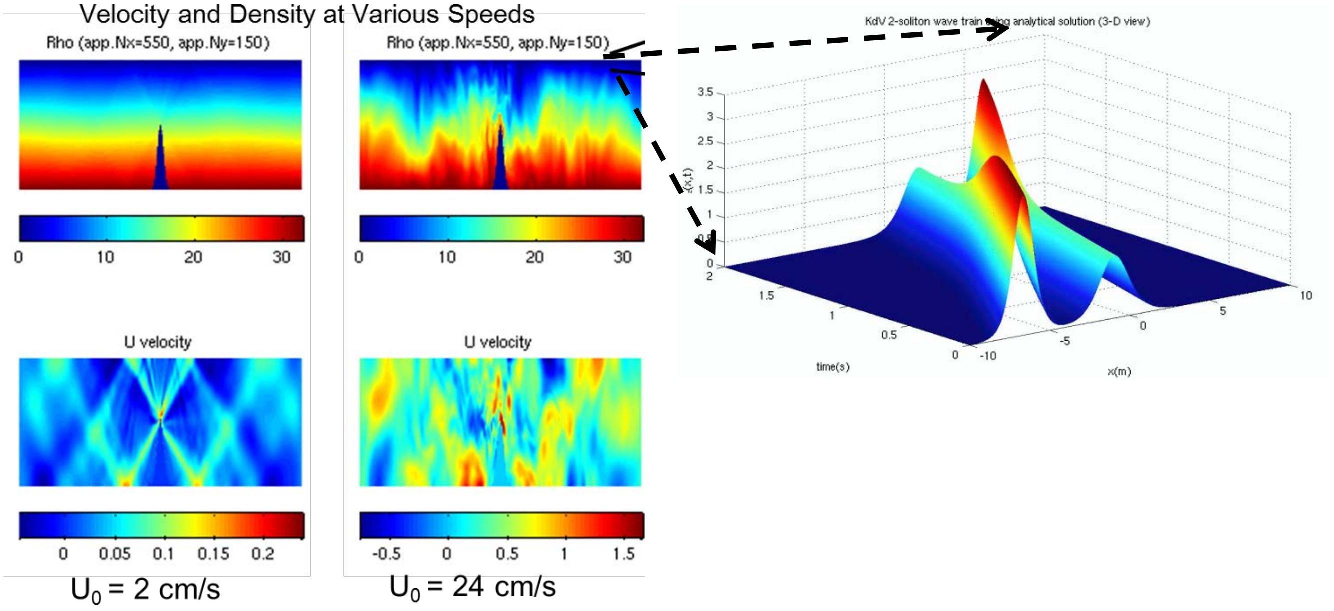

Figure 1. *Results towards coupled internal waves, background flow and surface waves*. Idealized 2d internal tides with background flow interactions are coupled to shallow water waves that are stochastically forced to represent unresolved spectrum. The coupled pdfs are integrated using DO equations.

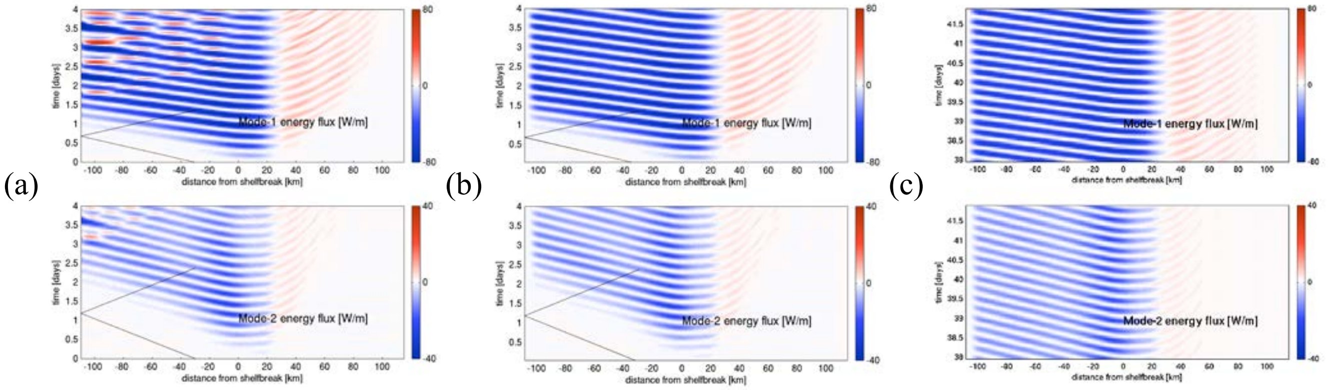

Figure 2. ***Effects of new sponging algorithm.*** An idealized shelfbreak domain was set-up with idealized M2 tidal forcing on the (open) offshore boundary (left side of each panel), closed boundary on the shelf (right side of each panel) and periodic in the along shelf direction. Each panel shows the time evolution (vertical axis) of the internal tidal energy flux for modes 1 & 2 along a line through the middle of the domain. (a) First 4 days of baseline simulation with no sponging. Notice the spurious reflections (positive flux in red) from the open boundary (left side of panels). (b) First 4 days of simulation with new sponging algorithm. Spurious reflection suppressed, fluxes away from open boundary undisturbed by sponging. (c) As (b), but last 4 days of simulation. Reflections suppressed for entire simulation.

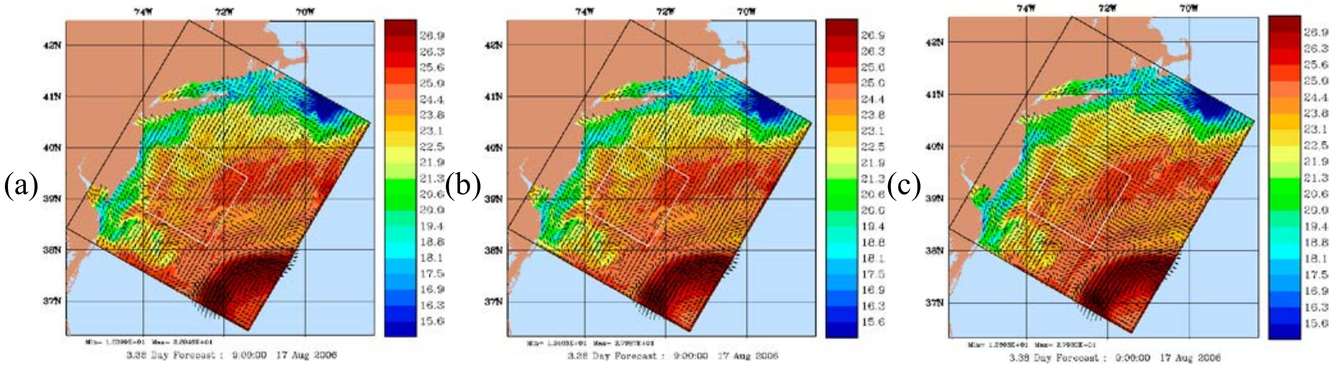

Figure 3. ***Adding time evolution to sponging and boundary conditions.*** Surface temperature overlaid with velocity vectors are shown for 3 simulations in the Middle Atlantic Bight region with different combinations of sponging and boundary conditions. (a) Sponging towards initial conditions. Cool water is upwelled by the coast during the simulation. Near the shelf outflow boundary (38N, 75W) the sponging maintains the warmer initial conditions. (b) As (a), but with a sponging external solution that evolves in time, “forgetting” the past. The band of persisted initial conditions is narrowed considerably. (c) As (b), but including the same time evolution in the boundary conditions. The upwelled waters are now advected out of the domain.

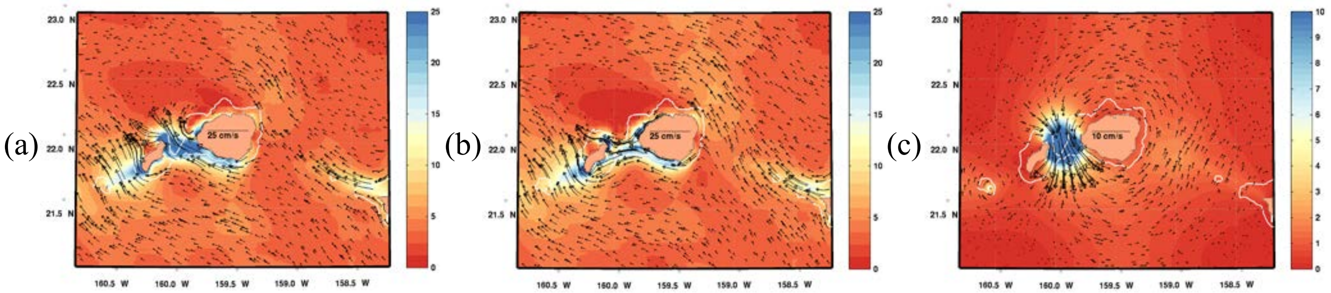

Figure 4. ***Testing the initialization methodology around the islands of Kauai and Niihau.*** Colormaps of the velocity magnitudes are show, overlain with the velocity vector. (a) The barotropic velocity field from an initialization employing an averaging method to obtain the transport between Kauai and Niihau. (b) as (a) but employing the direct minimization algorithm to obtain the transport. Note that the flow between the islands is greatly reduced, in agreement with historical observations. (c) the difference field of (b)-(a).

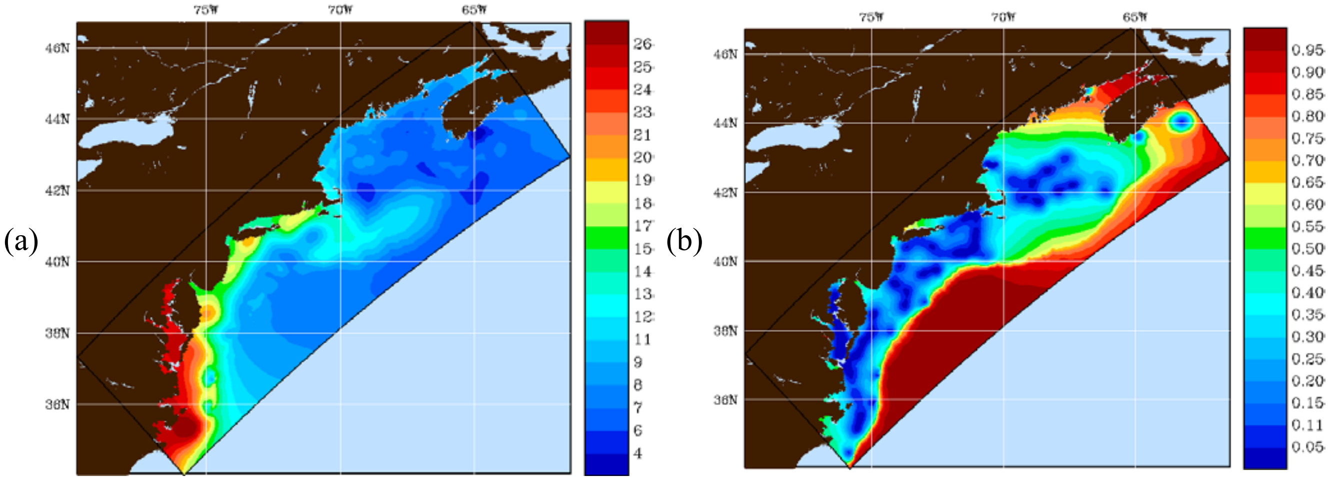

Figure 5. ***Objective analysis along the ocean bottom.*** The FMM-OA is used to objectively analyze temperature along the ocean bottom from the Middle Atlantic Bight through the Gulf of Maine. (a) Mapped bottom temperature. (b) Non-dimensional error, lowest errors around data positions. Note that the mapped bottom temperature correctly shows the separation of shelf/slope regions and the distinctive features of Georges Bank.