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Physical and Interdisciplinary Regional Ocean Dynamics and Modeling Systems

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LONG-TERM GOALS

This research is concerned with the fundamental understanding and modeling of complex physical, acoustical and biogeochemical oceanic dynamics and processes. New mathematical models and computational methods are created, developed and utilized for i) ocean predictions and dynamical diagnostics, ii) data assimilation and data-model comparisons, and, iii) optimization and control of autonomous ocean observation systems.

OBJECTIVES

General objectives are to:

i) Analyze and study regional physical and acoustical-physical-biogeochemical dynamics
ii) Incubate and develop new numerical modeling systems, including next generation ocean physics, 3D acoustics and Lagrangian coherent structures predictions
iii) Update existing and create new nonlinear and adaptive assimilation schemes and systems, including parameter estimation
iv) Evolve concepts and determine methodologies for regional adaptive modeling and adaptive sampling with the intent to increase predictive capabilities
v) Quantify regional predictabilities and improve probability and uncertainty modeling
vi) Utilize several ocean models, estimate their uncertainty statistics and fuse their estimates

APPROACH

The technical approach is rooted in the comparison and optimal combination of measurements and models via nonlinear data assimilation (DA), including the development of adaptive modeling and adaptive sampling schemes based on Error Subspace Statistical Estimation. Topics specific to the present effort include: three-dimensional acoustic modeling coupled to ocean modeling; incubator for the next-generation numerical ocean modeling; interactions of mesoscales with internal tides and waves, and mixing processes; Lagrangian coherent structures and ocean features; nonlinear data assimilation and multi-model estimations.

The regional dynamics studied involves interactions of sub-mesoscale and mesoscale ocean processes in the littoral as well as effects from large-scale processes in ocean basins. Such interactions and feedbacks with scales smaller and larger than the mesoscale need be better quantified. Investigations are generic but the focus is on specific ocean regions: the Mid-Atlantic Bight (MAB) and Shelfbreak

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Front region, the Chinese-Taiwanese Seas and Philippine Seas; the Monterey Bay and California Current System (CCS) region, the Massachusetts Bay/New England shelf region, and the Mediterranean and Black Seas. Several of these regions have been or are investigated under other collaborative efforts. The present proposal is leveraging these other projects, aiming to carry out the creative and fundamental research necessary for major advances and forward leaps.

The research consists of two inter-related thematic areas: Modeling System and Ocean Dynamics. The Modeling System research involves the incubation of new ocean modeling methods and schemes, the investigation of 3D acoustic modeling, continued efforts in interdisciplinary nonlinear and adaptive DA and parameter estimation, the estimation of model uncertainties and combination of multiple models and the development of self-modifying models that learn from data. The Ocean Dynamics research includes the applications of these modeling systems to generic ocean process studies and specific ocean regions. It involves studies of frontal systems and their multiscale interactions, of coastal bays and their shelf interactions, and of semi-enclosed seas and their water-mass interactions.

WORK COMPLETED

Discontinuous Galerkin Finite Element Methods. A 2D-in-space MATLAB framework was developed in order to test novel higher order Discontinuous Galerkin Finite Element Methods (Reen and Hill, 1973). The new Hybrid Discontinuous Galerkin (HDG) method (Cockburn et al, 2009, and Nguyen et al., 2009), which offers improved numerical efficiency, was also included in this framework. Our framework (Ueckerman, 2009) offers the capability to easily and rapidly setup and solve various 2D equations, including equations governing non-hydrostatic ocean dynamics and acoustics on unstructured meshes with optional curved boundaries. The purpose of developing a framework is to significantly reduce the development time for testing and developing new high order schemes. Novel high order numerical methods on structured or unstructured meshes allow the study of new physics and improved accuracy of current simulations. Each component of the MATLAB framework was tested and validated against analytical test cases.

Effort was expended in order to improve the efficiency of the numerical solution (Ueckerman, 2009). In particular, p-multi-grid preconditioners were evaluated. Also, an algorithm was implemented on a Graphics Processing Unit to evaluate the effort required for developing on this architecture, the types of algorithms that could benefit from this architecture, and the possible speed-ups for algorithms that can be achieved. As a practical issue, important routines that were inefficient in MATAB were coded in C through the MATLAB external interface. The C routines call optimized BLAS/LAPACK libraries. The framework was used to setup three different algorithms for solving the Boussinesq equations, which governs non-hydrostatic physics. All the solution methods were based on Projection methods (Gueremond et. al., 2006). Issues with the solution of the Pressure Poisson equation were identified and resolved, although research in this area is still underway. Preliminary validation of the scheme was performed using analytical test cases to solve the Stokes problem, as well as a comparison with the Lock exchange experiment (Hartel et al., 2000).

Dynamically Orthogonal Evolution Equations for Flows with uncertainty. A closed set of evolution equations has been derived for general fields described by a Stochastic Partial Differential Equation (SPDE) (Sapsis and Lermusiaux, 2009). By hypothesizing a decomposition of the solution field into a mean and stochastic dynamical component, we derive a system of field equations consisting of a Partial Differential Equation (PDE) for the mean field, a family of PDEs for the orthonormal basis that describe the stochastic subspace where the uncertainties ‘live’, as well as a system of Stochastic Differential Equations that defines how the stochasticity evolves in the time varying error subspace. These new evolution equations are derived directly from the original SPDE, using nothing more than a dynamically orthogonal condition on the representation of the solution.

Since the basis of the error subspace is evolving according to the system SPDE, fewer modes are needed to capture most of the energy relative to the POD method that fixes the form of the basis a priori, especially for the case of transient responses. On the other hand, since the stochasticity inside the dynamically varying stochastic subspace is described by a reduced-order, exact set of SDEs, we avoid the large computational cost of Polynomial-Chaos methods to capture non-Gaussian behavior. If additional restrictions are assumed on the form of the representation, we recover both the Proper-Orthogonal-Decomposition equations and the generalized Polynomial-Chaos equations.

A numerical code was developed in Matlab to implement the new DO equations for the case of two-dimensional fluid flows described by Navier-Stokes equations with general geometry and stochastic initial conditions. We applied the code and the methodology for two cases of two-dimensional viscous flows namely, the lid-driven cavity flow and the flow behind a circular disk. Our results were validated with direct Monte-Carlo simulations that were initiated using ESSE methodology. The numerical discretization of the DO field equations was performed using a staggered grid combined with a donor-cell discretization scheme for the spatial derivatives. For the time discretization, we used Euler's method resulting in an explicit scheme for the velocities and an implicit scheme for the pressure.

Uncertainty, data assimilation and dynamics in a coastal ecosystem: the Lagoon of Venice. ESSE was used to investigate the seasonal ecosystem dynamics of the Lagoon of Venice in 2001, combining a rich data set with a physical-biogeochemical numerical estuary-coastal model (Cossarini et al, 2009). Novel stochastic modeling components were developed to represent uncertainties in the internal ecosystem dynamics model, measurement model and boundary forcing by rivers, open-sea inlets and industrial discharges. The formulation and parameters of these new additive and multiplicative stochastic error models were optimized based on data-model forecast misfits. The sensitivity to initial and boundary conditions was quantified and analyzed. Half-decay characteristic times were estimated for key ecosystem variables and their spatial and temporal variability studied. The new error models were used in the ESSE scheme for ensemble uncertainty predictions and data assimilation, and an optimal ensemble dimension was estimated. The seasonal biogeochemical-ecosystem fields and their uncertainties were estimated using ESSE and used to guide local environmental policies.

Multi-grid data assimilation into regional tidal models: A new method has been developed for nested data assimilation in barotropic tidal models resolving the topographic and coastal features (Logutov and Lermusiaux, 2008; Logutov, 2008). The method is designed to reduce representativeness errors by fitting the resolved dynamics to data consistently, across a multi-grid computational system. The set of control parameters are presently chosen to be the OBCs of the outer domain. The uncertainty from the outer domain OBCs is propagated to model tidal fields at observation locations through the set of nested domains using efficient low-rank error covariance representations. An analysis increment for these outer OBCs is computed to optimally steer the multi-grid system towards observations by minimizing the (weighted) variance of the observation-minus-forecast residuals.

Scale Estimation Schemes. The knowledge of spatio-temporal scales is fundamental to understand dynamics and is thus useful for a series of applications. In particular, scale estimates are needed in the parameterizations of correlation functions used in steady-state field estimation. Adaptive methods have been implemented to learn the largest and most energetic scales directly from ocean data (prior to mapping these data) (Agarwal, 2009). The method is based on obtaining the structure function from the available data and utilizing non-linear least square fit to a specified analytical form to estimate the scales in the data. The use of second-generation wavelet analysis is also investigated since it can provide both spatial and temporal scales directly from the data.

Objective Analysis schemes for complex geometries: Our OA scheme which utilizes the Kalman update steps of the Kalman filter has been updated for complex domains (Agarwal, 2009). The structure of the correlation function is first specified. Correlation parameters are then obtained using the separation distance estimated from two numerical techniques: a) Level Set Method (LSM) and b) Fast Marching Method (FMM). Knowledge of spatial-time scales provide a measure for the parameters of the analytical correlation function and thus improve field estimates obtained using OA. A third mapping method was also implemented. It uses a numerical diffusion equation to extrapolate the sensor data.

Ocean dynamics, modeling and assimilation: An improvement in the coupling of the barotropic mode was implemented in the free-surface, primitive equation nesting algorithm. This was accomplished by (1) averaging an intermediate estimate of the barotropic velocity (instead of the vertically averaged right-hand side of the momentum equation) in the fine domain to replace corresponding values in the coarse domain, (2) averaging the free surface elevations (lagged 1 time step behind the transfer of the other quantities) in the fine domain to replace corresponding values in the coarse domain and (3) recomputing the (lagged) barotropic velocity in the coarse domain to be consistent with the updated surface elevation. New data assimilation schemes for barotropic tidal estimates were published (Logutov and Lermusiaux, 2008). Contributions were made to our Monterey Bay research (Haley et al, 2009; Ramp et al, 2009). A special edition of Ocean Dynamics on "Multi-Scale modeling: nested grid and unstructured mesh approaches" was edited with a refereed editorial (Deleersnijder and Lermusiaux, 2008). A publication on "Many Task Computing" for multidisciplinary real-time uncertainty prediction and data assimilation was written and accepted (Evangelinos et al, 2009). Different methods for parameter estimation in straightforward diffusion problems were explored and distributed computational schemes for the automated evaluation of physical and numerical parameters of ocean models have been developed (Heubel, 2008). The dynamic coupling of models and measurements for a Dynamic Data-Driven Application System (DDDAS) is described based on examples in Massachusetts Bay, and Monterey Bay and the California Current System (Patrikalakis et al., 2009).

Acoustic predictions. Coupled ocean-acoustic fields were forecast at sea in real-time (Lam et al, 2009). A manuscript on acoustically focused adaptive sampling and onboard routing for marine rapid environmental assessment was completed (Wang et al, 2009). Lin et al. (2009) utilizes a novel EOF fitting technique for profile merging to combine time-varying data profiles from multiple sources into sound speed profiles indicative of conditions at a single site. The resulting profiles have been used in acoustics propagation modeling endeavors and have improved acoustic data-model comparisons.

Adaptive sampling. A manuscript on the quantitative planning of the paths of AUVs using Mixed Integer Linear Programming (MILP) was published (Yilmaz et al, 2008). The second part of this work, which selects the ocean sampling paths based on the ESSE-MILP forecasts of data impacts, is finalized (Yilmaz and Lermusiaux, in prep). Schemes for adaptive sampling based on genetic algorithms have been evaluated based on Observation System Simulation Experiments (manuscript in prep).

RESULTS

Discontinuous Galerkin Finite Element Methods. The analytical test cases showed optimal convergence for all components (Ueckermann, 2009). In particular, when using a p^{th} order basis, the HDG solvers showed $p+1$ convergence for both velocity and the gradient of velocity, and showed $p+2$ convergence for the post-processed velocity. These results for the analytical test case $u=sin(\pi x)sin(\pi y)$ are reported in Table 1. Problems with Gibbs oscillations appearing with higher polynomial bases in biogeochemical advection-diffusion-reaction equations with steep bathymetry were also improved and nearly resolved by using a curved boundary on the bathymetry.

We (Ueckermann, 2009) find that the p-MG preconditioners significantly reduce the iteration count for Local Discontinuous Galerkin (LDG) methods, although the application of the same preconditioners to HDG did not yield the same impressive results. It was found to be prohibitively time consuming to develop algorithms on the GPU, although significant speedups (greater than 10) are possible. Also, the architecture appears to be well suited to high order Discontinuous Galerkin methods, but realistic implementation await the development of efficient compilers for this architecture. The MATLAB routines implemented in C sped up computations by factors ranging from 10 to 500 times. Convergence results from the analytical Stokes problem can be seen in Table 2. Also, a snapshot of the solution for the lock exchange experiment at time 5 and 10 overlaid with the Hartel (2000) results are plotted in Figure 1. Excellent agreement with the (Hartel, 2000) solution is observed, and the discrepancy seen at time 10 is due to different domain sizes.

Dynamically Orthogonal Evolution Equations for Flows with uncertainty. Figure 2 presents the results for the stochastic cavity flow with Re = 1000 of the numerical code developed to implement the new evolution equations for the case of two-dimensional fluid flows described by Navier-Stokes equations with general geometry and stochastic initial conditions. The two upper left plots present the mean streamfunction and vorticity, respectively, of the response at $t = 8$. The four lower left subplots present four, two-dimensional marginal that describe the stochastic characteristics of the response, while the two columns of plots on the right present the subspace where the stochasticity “lives” (five dimensional) in terms of the streamfunction and the vorticity. In Figure 3 a direct comparison is shown with Monte-Carlo simulation involving 250 samples and 500 samples. Finally, in Figure 4 the corresponding results are presented for the flow behind a circular disk for Re=100.

Uncertainty, data assimilation (DA) and dynamics in a coastal ecosystem: the Lagoon of Venice. We find that boundary forcing and internal mixing have a significant control on the seasonal dynamics of the Lagoon and that DA is needed to reduce prior uncertainties. Higher uncertainties are predicted in the central and northern regions of the Lagoon. Based on the ESSE singular vectors, the two major northern rivers are the biggest sources of DIN uncertainty in the Lagoon. Other boundary sources such as the southern rivers and industrial discharges can dominate on certain months. For DIP and phytoplankton, dominant modes are also linked to external boundaries, but internal dynamics effects are more significant than for DIN. Our ESSE estimates of the seasonal biogeochemical fields and their uncertainties in 2001 cover the whole Lagoon (Figure 5) and provide the means to describe the ecosystem and guide local environmental policies (Figure 6). Findings include the: temporal and spatial variability of nutrient and plankton gradients; dynamical connections among ecosystem fields and their variability; strengths, gradients and mechanisms of the plankton blooms in late-spring, summer and fall; uncertainties predictions, their monthly reductions by DA and thus a quantification of data impacts and needs; and, finally, an assessment of the water quality in the Lagoon.

Multi-grid data assimilation into regional tidal models. Our new methodology based on nested domains in complicated coastal regions allowed fitting the full local tidal data only where it made sense, i.e. where the resolution of the model nests was sufficient to fully resolve the tidal dynamics. The method (Logutov and Lermusiaux, 2008; Logutov, 2008) can avoid artificial steering of the solution towards unresolved observations which is, in general, degrades accuracy. The presence of representativeness errors in data-model misfits was detected through sensitivity experiments with model resolution. In some cases, the observation-minus-forecast residuals were found to be highly sensitive to resolution. For example, in the Philippines region, a high-resolution (1-minute resolution) nested domain was setup around the Sulu, Bohol, Visayan, and Sibuyan seas, where representativeness errors were found, and the assimilation of ADCP and Topex/Poseidon data in those areas was carried out using the nested computation. Figure 7 shows the velocities at data location A1 obtained from the 5-min and 1-min resolution runs compared with the depth-averaged ADCP velocity data. The forward solution in the 5-min domain exhibits much larger errors in both amplitude and phase than the forward 1-min resolution nested computations. Figure 8 shows the comparison of the velocity field of the multi-grid inverse solution against the ADCP data. The improvement in the velocity field estimates through the use of our multi-grid inverse can be seen by comparing Figures 8(a) and 7(b).

Ocean dynamics, modeling and assimilation: Novel 2-way implicit nesting scheme for free-surface PE modeling with finite-volumes. The new nesting algorithm for the free-surface primitive equation simulations strengthened the barotropic feed-back from the fine domain to the coarse domain. Of the 3 changes specified earlier, the first moves the fine to coarse feed-back of the barotropic forcing to the latest step in the algorithm it can be before affecting the vertically integrated conservation of mass. The other modifications provide fine-to-coarse feed-backs utterly missing from the original algorithm. Tests in the middle Atlantic Bight show that a large scale O(10) cm/s drift between estimates of the barotropic velocity in coarse and fine domains in the original algorithm were reduced to, generally, under 1 cm/s. Overall, we find that embedded schemes with stronger implicit couplings among grids, especially for the velocity components, work best. We also found that time-dependent grids with volume-conserving schemes are required for strong tidal conditions over shallow seas. Results are obtained 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. A manuscript is in preparation.

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 earth sciences and engineering.

TRANSITIONS

Methods, software and data sets were transitioned to other research groups, several of which were involved in AQPE, AWACS and PHILEX. They include: UW-APL, Duke U., MIT-OE, WHOI, Princeton U., NATO Undersea Research Centre (NURC), NRL-Stennis, NPS, OASIS Inc., OGS-Trieste (Italy), CNR-Ancona (Italy), Cal. Tech, U. of Frankfurt (Germany) and Rutgers.

RELATED PROJECTS

Without the present effort, several other projects would not be feasible. In particular, this project contributed to MURI-ASAP (MIT-sub-00000917), AWACS (N00014-07-1-0501) and PHILEX (N00014-07-1-0473). Interactions also occurred with other research groups. For data assimilation, adaptive sampling and adaptive modeling, this involved: NPS (J. Joseph), MIT-OE/EAPS (N. Patrikalakis, H. Schmidt, C. Evangelinos), OASIS Inc. (K. Heaney), NURC (M. Rixen), NRL-Stennis (E. Coelho) and U. Mass (A. Gangopadhyay). For Mediterranean studies, NURC, F-P. Lam (TNO) and U. Trieste (G. Cosarini, C. Solidoro).

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Additional presentations and other publications are available from http://mseas.mit.edu/. Other specific figures are available upon request.

TABLES

Degree(p)	Mesh(n)	u_h Error	u_h Order	q_h Error	q_h Order	U_h^* Error	U_h^* Order
1	3	2.661e-01	0	8.533e-01	0	3.158e-02	0
	5	7.350e-02	1.86	2.510e-01	1.77	4.315e-03	2.87
	9	1.883e-02	1.97	6.559e-02	1.94	5.579e-04	2.95
	17	4.731e-03	1.99	1.662e-02	1.98	7.073e-05	2.98
2	3	4.442e-02	0	1.235e-01	0	4.858e-03	0
	5	5.952e-03	2.9	1.688e-02	2.87	3.225e-04	3.91
	9	7.565e-04	2.98	2.162e-03	2.97	2.029e-05	3.99
	17	9.491e-05	2.99	2.722e-04	2.99	1.266e-06	4
3	3	7.049e-03	0	1.857e-02	0	7.181e-04	0
	5	4.686e-04	3.91	1.251e-03	3.89	2.352e-05	4.93
	9	2.975e-05	3.98	7.967e-05	3.97	7.424e-07	4.99
	17	1.867e-06	3.99	5.004e-06	3.99	2.349e-08	4.98

Table 1: Errors and rates of convergence for $\tau=1$ of analytical diffusion test case $u=sin(\pi x)sin(\pi y)$

Degree(p)	Mesh(n)	u_h^*	v_h^*	P^*	$\partial_x u$	$\partial_y v$	$\partial_x P$	$\partial_y P$
1	2-3	2.8	2.8	3.2	2.4	2.4	2.9	2.9
	3-5	1.3	1.3	0.67	-0.19	-0.19	-0.29	-0.29
	5-9	2.8	2.8	2.1	1.6	1.6	0.98	0.98
	9-17	2.9	2.9	3.2	1.9	1.9	2	2
2	2-3	1.4	1.4	1.6	0.11	0.11	0.56	0.56
	3-5	3.2	3.2	2.8	1.9	1.9	1.9	1.9
	5-9	3.4	3.4	3.7	2.3	2.3	2.6	2.6
	9-17	3.9	3.9	3.3	2.9	2.9	2.4	2.4
3	2-3	1.3	1.3	2.4	-0.35	-0.35	1.1	1.1
	3-5	3.8	3.8	4.2	2.3	2.3	2.7	2.7
	5-9	5	5	4.2	3.9	3.9	3	3
	9-17	4.9	4.9	4.6	3.9	3.9	3.8	3.7

Table 2: Rates of convergence for Stokes problem with analytical solution

$$\mathbf{u}(x,y,t) = \pi \sin t(\sin 2\pi y \sin^2 \pi x, -\sin 2\pi x \sin^2 \pi y), \quad P(x,y,t) = \sin t \cos \pi x \sin \pi y$$

FIGURES

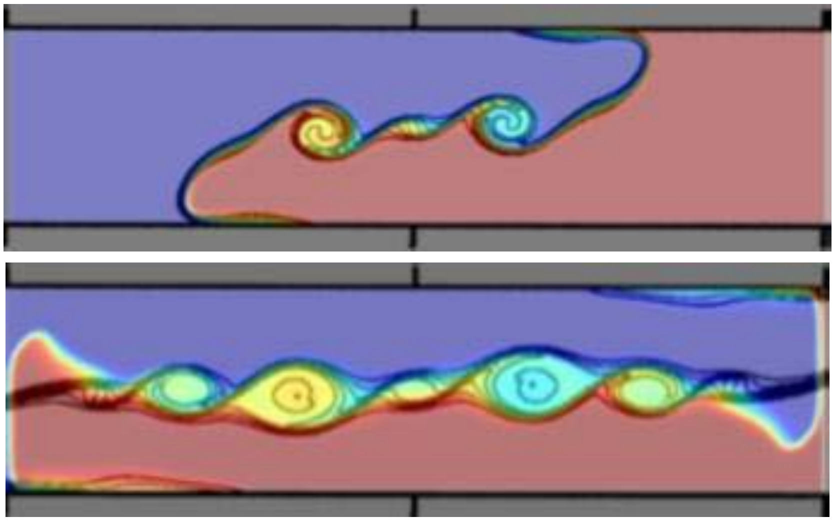

Figure 1. Comparison of our new HDG results (Ueckermann, 2009) for the Lock Exchange test case with the results of of Hartel (2000) at time=5 (top) and time=10 (bottom). Our colored solutions is overlaid on that of Hartel's.

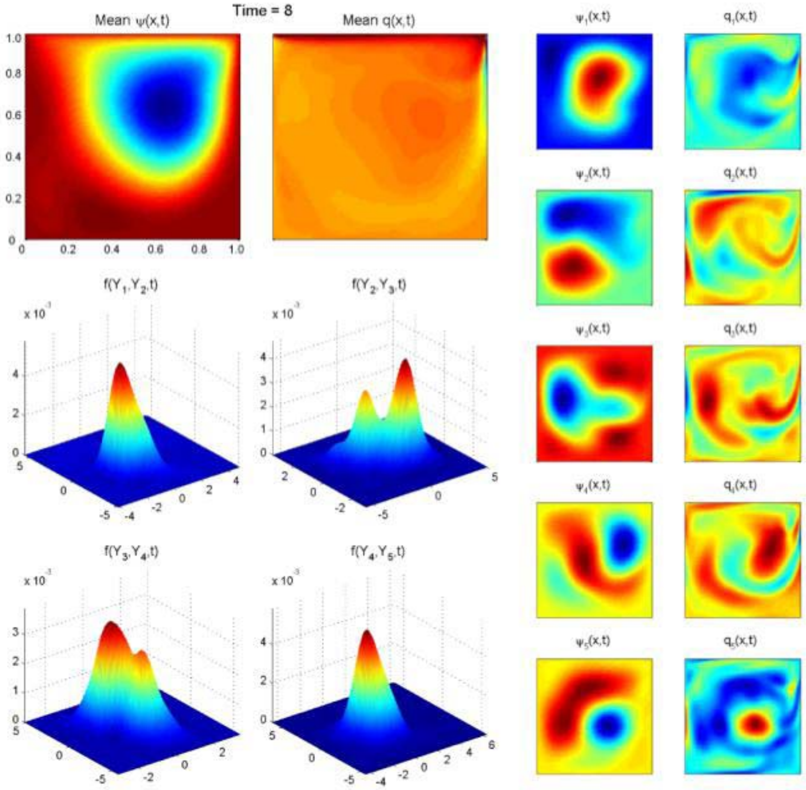

Figure 2. Response of the cavity flow with stochastic initial conditions.

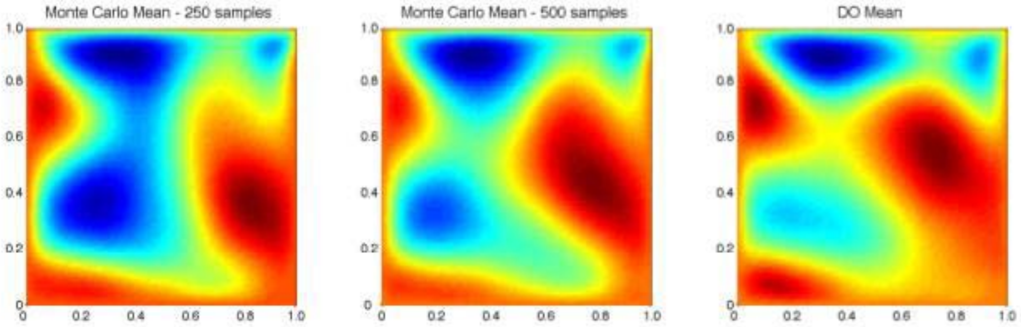

Figure 3. Monte-Carlo comparison for the stochastic cavity flow.

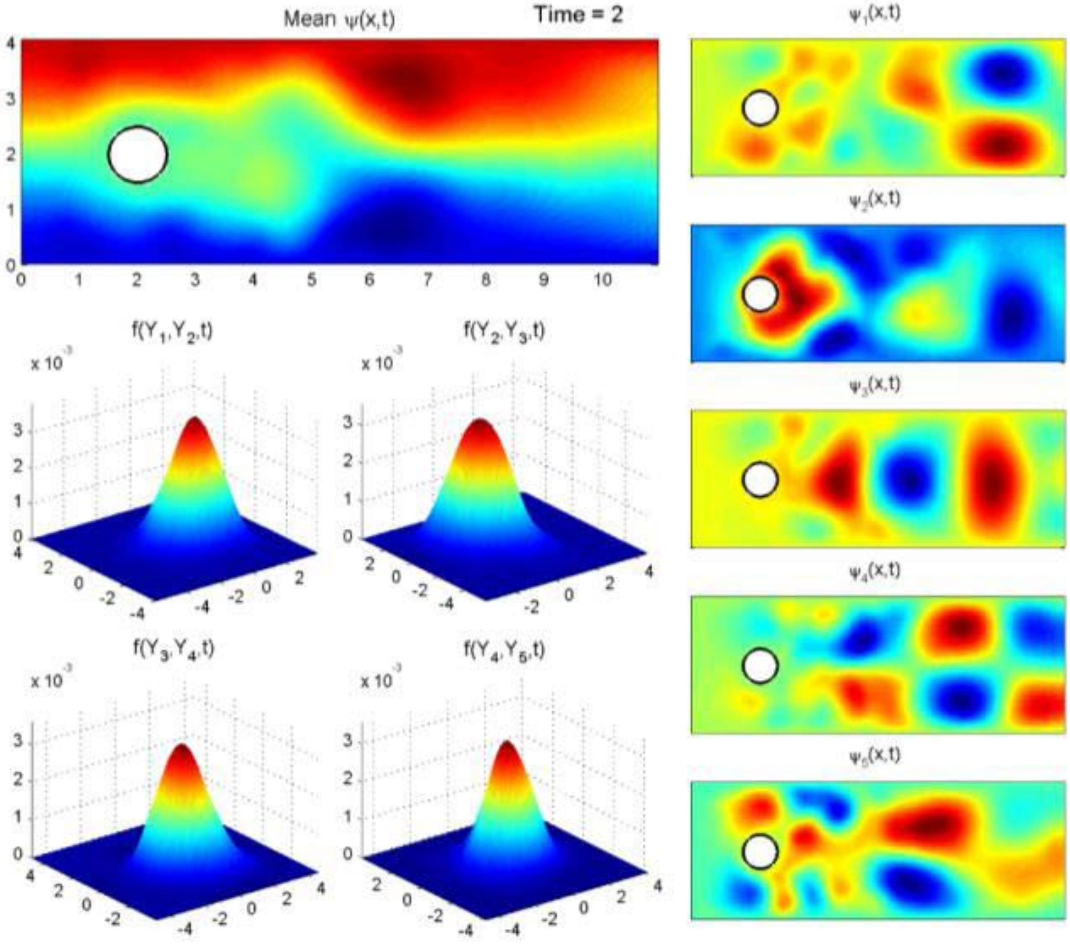

Figure 4. Response of the flow behind a circular disk with stochastic initial conditions.

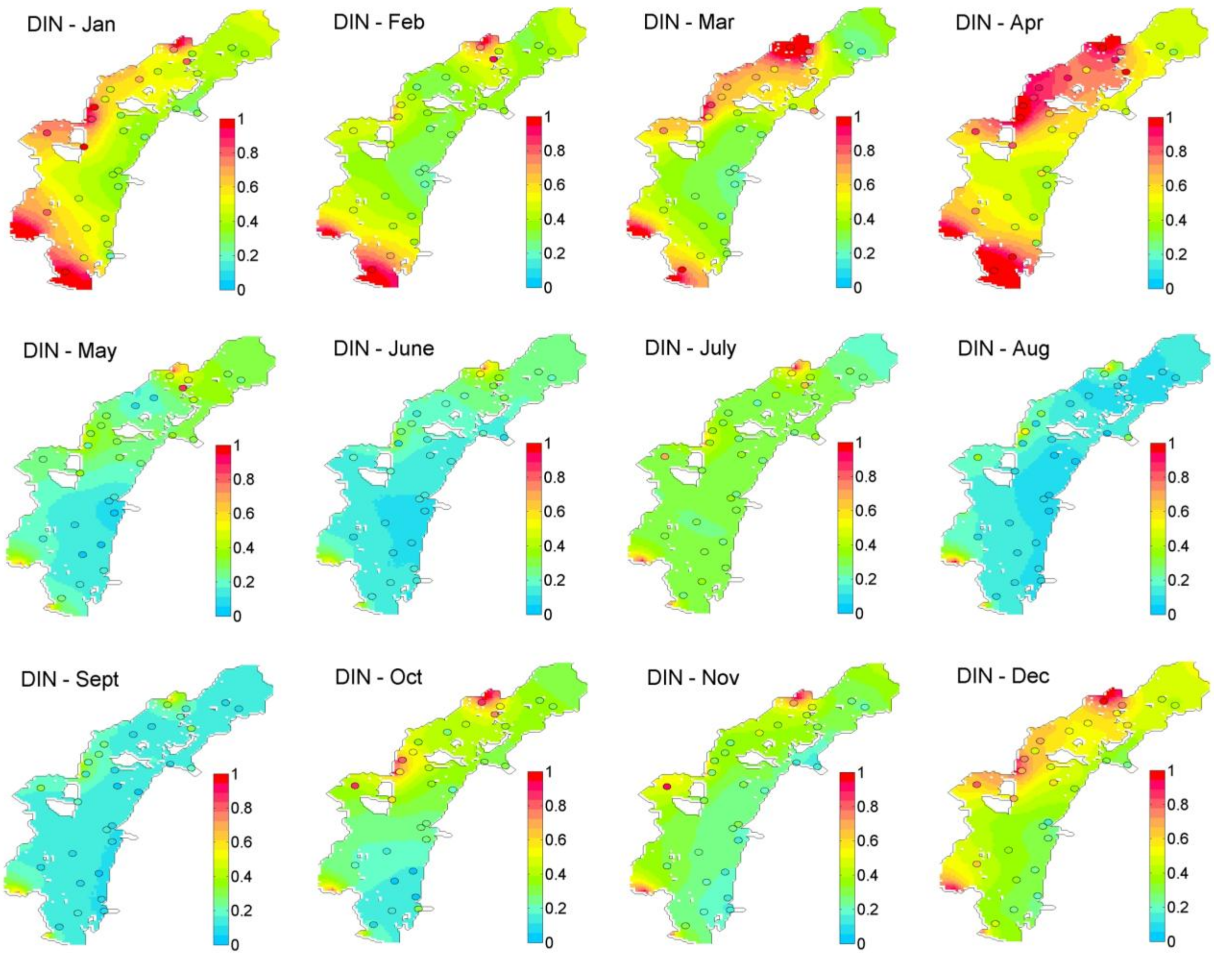

Figure 5. Evolution of the *a posteriori* fields for DIN [mg/l] (maps), and observation (overlaid colored circles) for the Lagoon of Venice in 2001. Color scale is set to 0 to 1 mg/l for all months.

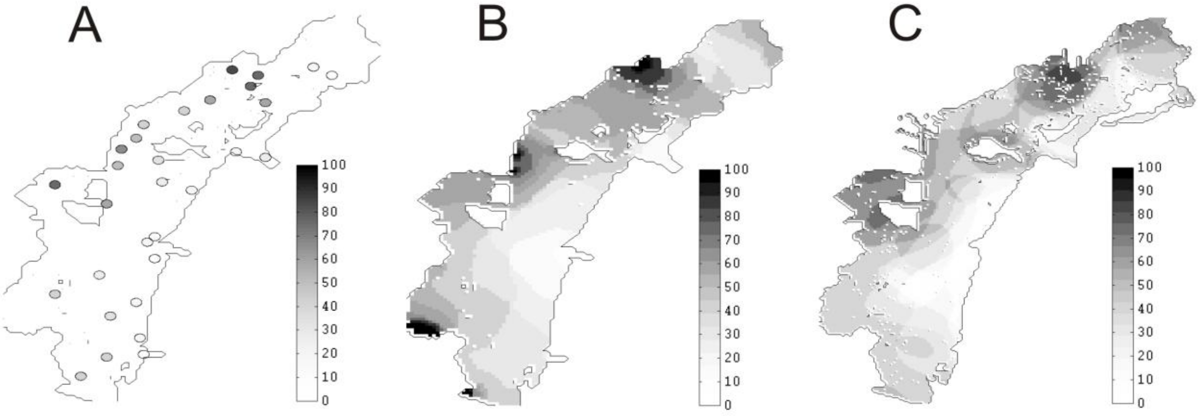

Figure 6. Percentage of time of the year during which the Lagoon of Venice is above the limit of the Water Quality Target for DIN. (a) data, (b) OA estimate, (c) ESSE estimate.

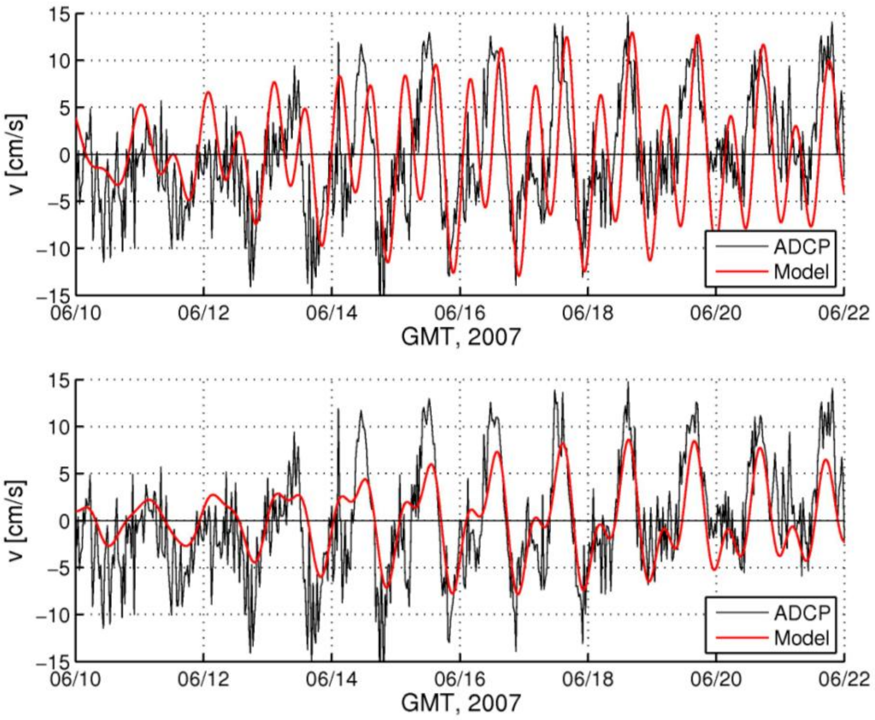

Figure 7: Observed and forward model velocity at data location A1 (see Logutov, 2008). Observed meridional depth-averaged velocity, with mean removed (black). Model velocity (red). (Top) at 5-min resolution; (Bottom) at 1-min resolution.

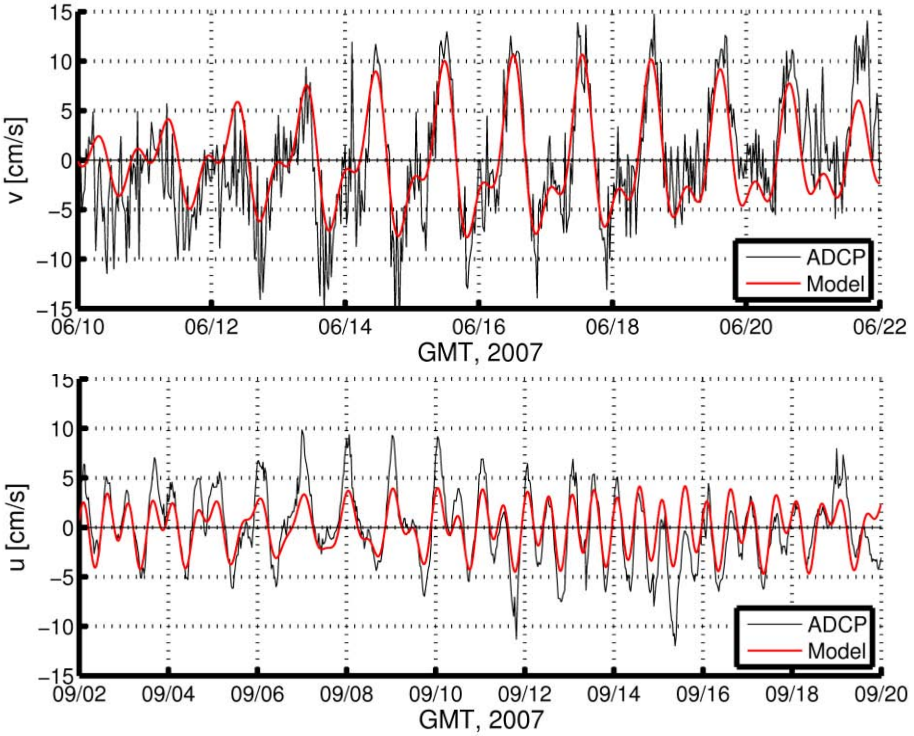

Figure 8. Observed versus inverse model velocities at A1 and A2. Plotted are the depth-averaged velocities, with mean removed. (Top) meridional velocity at A1; (Bottom) zonal velocity at A2.