# Statement of Research Findings and Objectives, 2007

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## Contents

# 1 Présis

My research in summary form appears first, leaving lengthier descriptions of selected topics to the Appendix.

My work in optimal estimation, aimed at finding computational methods that use models and real data, has recently become a much larger enterprise: in Fall '07 I created *The Uncertainty Quantification Group* (see our web site at [1]), a new research enterprise which aims to respond to calls by NSF's "Cyber-Enabled Discovery and Innovation Initiative" (CDI) and DOE's ASCR program, for research proposals.

Most of my work is related or inspired by geoscience problems and it is fair to say that the fact that most of my work appears in geoscience journals, rather than mathematics journals, is a testament of its relevance. Some of the work uses standard mathematics (e.g. sandbars, jets, etc), some of it may be novel applications of existing methods (e.g. wave/current interactions, optimal estimation in hydrology, etc). The remaining is new mathematics and theorems (optimal estimation, wavelets, locating eigenvalues, etc).

My applied mathematics perspective is fairly pragmatic, mostly shaped by my PhD supervisors and experiences as well as my very-long association with Los Alamos National Laboratory and Argonne National Laboratory.

# 2 Introduction

The four main themes of my work (1) the integration of multiscale ideas into flows which require both a Lagrangian and Eulerian descriptions; (2) the application of information theory, stochastic parametrization and estimation techniques to the problem of optimal estimation for highly nonlinear and non-Gaussian problem; (3) the stochastic parametrization of dissipative mechanisms in geophysical fluid flows; (4) ab-initio calculations to elucidate fundamental forces in fluid/particle interactions. Along the way I have been able to contribute to oceanography, hydrology, climate variability, scientific computing, the mathematics of nonlinear dispersive waves, sediment dynamics and morphology, and more recently, to biology.

If I had to mention specific scientific triumphs, they would be:

- The derivation of a comprehensive and general model for wave/current interactions in three-space and time at global and shelf scales, with which we clarified important oceanic interactions and showed how and why waves matter at large spatio-temporal scales.
- The stochastic parametrization for wave breaking and other dissipative mechanisms as a simpler alternative to traditional turbulence/closure ideas, with the end result of being able to better exploit the ever-growing data sets.
- I have just touched upon this, but the growing need to connect the Lagrangian and Eulerian frames in oceanic setting to capitalize on the use of drifter/buoy data and dynamical systems ideas (not mine) to infer oceanic states.
- The proposal of a variety of optimal estimation techniques to handle the nonlinear/non-Gaussian nature of data assimilation for problems not amenable by more traditional means (such as Lagrangian data assimilation).

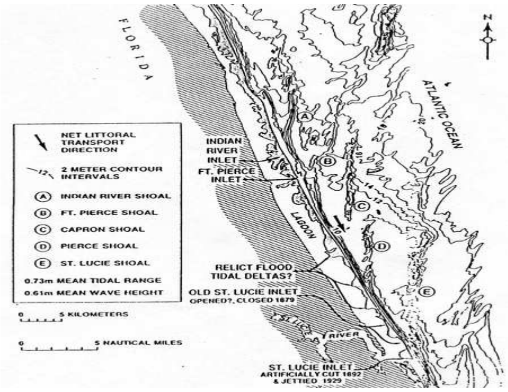


Figure 1: Shore-connected ridges off the coast of Florida

- The use of computational techniques to produce state-of-the-art experimental data on lift and drag on particles in flows. They are experimental data if you have no qualms believing that Navier-Stokes is a good model for fluid flows, of course.

## 3 Summary, Present Research

There are three main areas of interest in my research:

- **Wave/Current Interactions, Climate Variability**: Not till very recently have researchers placed a great deal of attention to formulating complete descriptions of the interactions between waves and currents. Since 1997, along with my colleague Jim McWilliams and others, we have been developing a comprehensive time-dependent and three-dimensional model for the interaction of waves and currents at global scales, shelf-scales, and more recently, in the near-shore. We have completed the conservative model and are now focusing on the inclusion of dissipative effects via stochastics and the interaction of the free surface with the atmosphere.

  In climate the research falls into the category of theoretical *climate variability.* The three major problems tackled so far have been to show that advective effects can change the simple thermohaline picture; that convective adjustments in general circulation model simulations of wind-driven circulation can lead to artificial variability. I also worked on deriving a simple model capable of reproducing the $pCO_2$ cycle during glacial and interglacial times using realistic parameters. A somewhat novel strategy in this modeling was to combine asymptotics (to generate a lowest order problem that was analytically tractable), with topological fluid mechanics to handle the higher order contributions in a simplified way. We also introduce a notion of sensitivity analysis which was suggested may replace standard metrics used to gauge climate models and their ability to capture faithfully the carbon cycle.

- **Sediment Dynamics, Erodible Beds:** Oceanic erodible beds are very complicated dynamic problems. Working at the very largest scales we have developed models that capture the phenomena of shore-connected ridges (see Figure 1) and of wave-normal ridges. We have analyzed the formation and maintenance of shore-normal sand-ridges and have also analyzed the combined effect of waves and currents in the formation and maintenance of shore-connected ridges.

Of a more fundamental nature, with my colleagues P. Fischer and G. Leaf, we have been using full 3D Navier Stokes calculations of the oscillatory fluid flow in the boundary layer to comprehensively characterize the forces of drag, lift, and torque on particles. Thus far we have fully characterized the lift, drag, and torque as a function of the particles' Reynolds number, the gap, the forcing frequency and the buoyancy. In the future we will address numerically dislogdgement and suspention of particles in the flow. We know how: we will again use a 3D Navier Stokes, however, we will modify it to conform to an accelerated frame.

With R. Goldstein I have been running experiments in an annular tank in which mono-dispersive particles are sheared, with the aim at collecting data that can be lead to insights into how sheared beds become unstable and develop bars. Here the interesting aspect is that the theory is way ahead of experiments and thus far we are able to discern from the data that many of the proposed mechanisms for the formation of bars due to shearing are woefully incomplete or wrong.

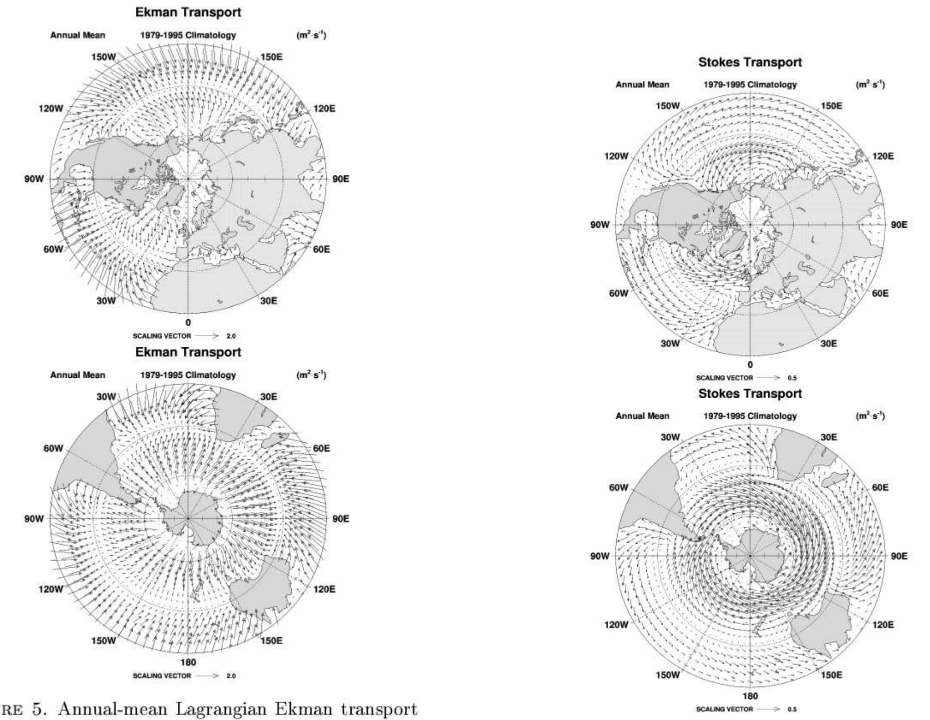
- **Scientific Computing and Optimal Estimation**

  In scientific computing I have contributed to

  - computing large-scale gradients without approximations on limited memory machines,
  - developing wavelet-Galerkin methods for the numerical approximation of PDE's,
  - locating eigenvalues of normal matrices,
  - creating efficient preconditioners using eigenvalue localization,
  - presently developing a technique to capture numerically wave runup and the morphological changes in a basin due to the effects of the floods,
  - developing a variety of software packages for wavelet computation, gradient computations, task-farming, and for complex population dynamics studies.
  - Adapting or developing new optimal estimation methods for data assimilation (smoothing and filtering).

  The frontiers in data assimilation, *i.e.* the problem of optimally combining data and models with varying degrees of uncertainty, are (1) to handle non-Gaussian and/or highly nonlinear dynamics; (2) to handle extremely large state variables, such as those that are found in meteorology problems. The errors in observations might come from the equipment used in the measurements, for example; the errors in the model come from unresolved or poorly understood physics, or because the model *is* a stochastic differential equation. We have developed a variety of new techniques for nonlinear and non-Gaussian estimation: the mean-field variational technique, particle parametrization, the path integral method for assimilation, which is sampled-based and optimal on the discretized problem. Recently we have been working on a diffusion-kernel method that relaxes optimality and promises to handle larger state estimation problems.

  The sub-optimal entropy-based technique, the Diffusion Kernel Filter, can be briefly described as follows: it picks branches of prediction for filtering and smoothing depending on the relative



(a) FIGURE 5. Annual-mean Lagrangian Ekman transport $-\hat{\mathbf{z}}\times\frac{1}{f\rho_0}\boldsymbol{\tau}^t$ from (68): (a) northern hemisphere; (b) southern hemisphere.

(b) FIGURE 4. Annual-mean Stokes transport, $\mathbf{T}_{st}$ from (67): (a) northern hemisphere; (b) southern hemisphere.

Figure 2: (a) Ekman and (b) it Stokes currents as predicted from theory using actual wind data.

entropy of the branches, it uses the tangent linear model to produce an analysis, and a bound on the covariance to sample at the filtering time step. It delivers a sub-optimal but very good approximation at a fraction of the computational cost of the more complex nonlinear/non-Gaussian methods.

A second effort is being made to exploit homogeneization, and support vector machines, along with nonlinear/nonGaussian estimation techniques to solve optimal estimation problems in hydrology: here the idea is to exploit linear methods and compartments, at the same time exploiting the most efficient elliptic nonlinear Galerkin solvers available, in order to do truly grand-scale suboptimal estimation.

## 3.1 Concrete Research Results

### 3.1.1 Wave/Current Interactions, Climate, Acoustics

1. Derivation of a theoretical framework [2] [3], the vortex force framework, which suggests how and why wave generated transport is relevant to climate dynamics, *i.e.*, to oceanic basin-scale motions (Ekman and Stokes flows appear in Figure 2 and mean sea level adjustments predicted by the theory appear in Figure 3).

2. Derivation of a model for the interactions of continental shelf waves and currents on large spatio-temporal scales [4] (see Figure 4). This is one of the most complete and consistent

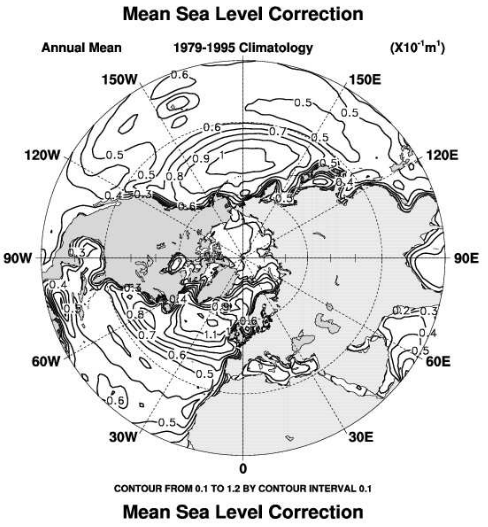


Figure 3: Mean sea level correction predicted by theory.

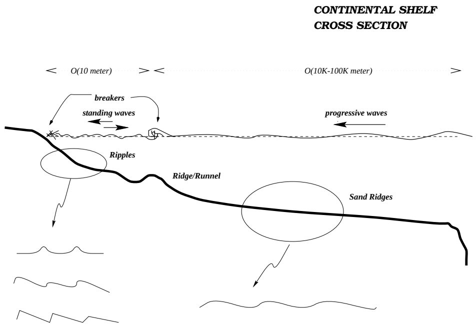


Figure 4: Cross section of the continental shelf environment.

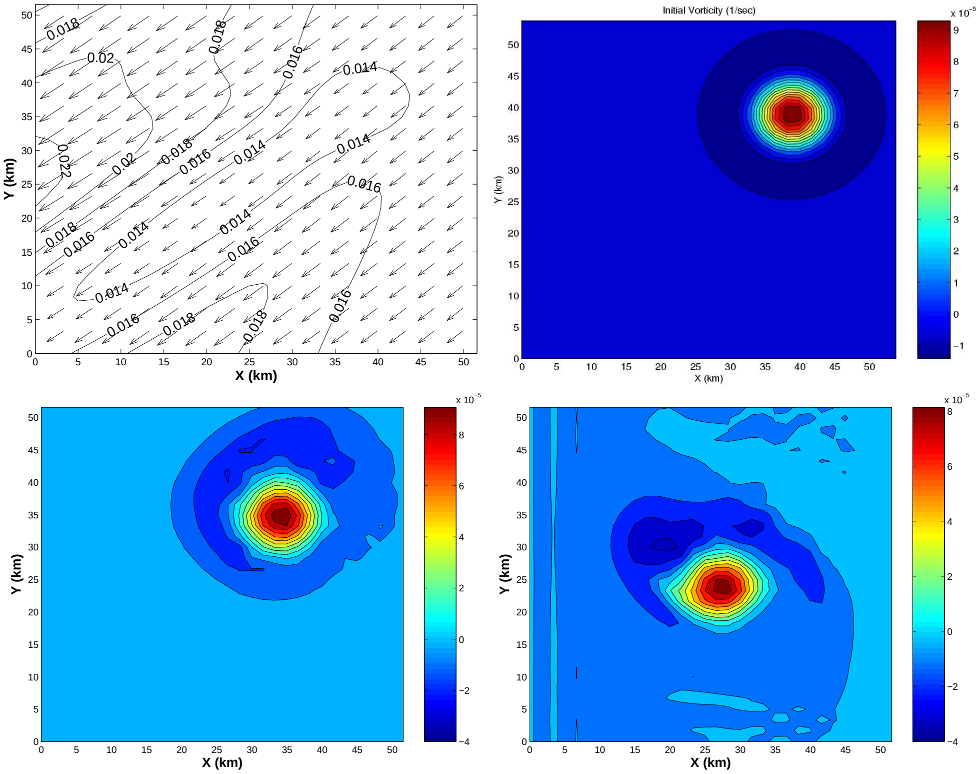


Figure 5: (a) Stokes drift due to waves, (b) initial vortex, (c) final vortex, no waves, (d) final vortex, waves.

models for the evolution of wave-current interactions, encompassing gravity waves, long waves, and currents in three space dimensions. The model is also capable of capturing the mechanics of pollutants, heat, and the transport of other tracers. Equally important is that the model is framed exclusively at the largest spatio-temporal scales, thus circumventing the computational hurdle of resolving motions which have extremely large bandwidths. See Figure 5.

3. Complete derivation of the radiation stresses in the nearshore and comparison of these to more traditional expressions for these stresses [5]. The aim of this comparison is to settle once and for all the existing misconceptions on what the stress itself yields. Furthermore, our results differ from the more generally accepted expressions, with consequences on our understanding of phenomena on which it has a bearing: rip currents, wave set-up and set-down, undertows, litoral currents.

4. Derivation of the dissipation terms in the wave-current interaction model [6]. It is not at all clear at the outset how the dissipative terms distribute among all scales. This is done by recasting the Lagrangian fluid orbit equations as stochastic differential equations and then using projection methods to infer how the stochasticity enters the Eulerian equations at the wave and current scales (see Figure 6). The resulting model explains in what manner white-capping, bottom drag and wind drag appear in the interaction evolution equations. The derivation shows that the dissipative terms appear in the currents in a manner similar to

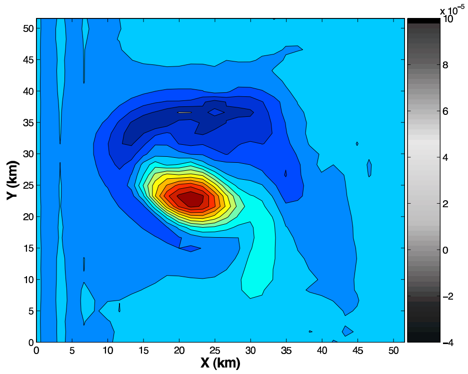
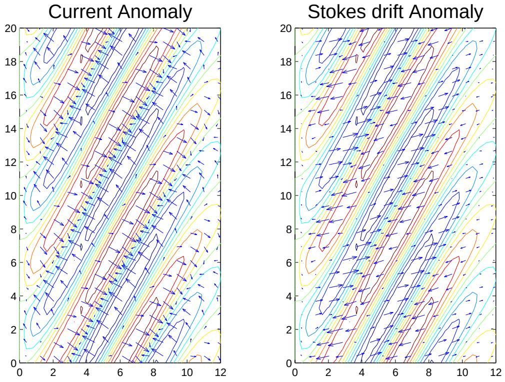


Figure 6: Final vortex, dissipation effects included. See Figure 5.


Current Anomaly

Stokes drift Anomaly

Figure 7: Current and waves anomalies showing covergences and divergences in a patter reminiscent of the shore-connected bars. The bars themselves will have a similar footprint.

Reynolds stresses, a vast modelling improvement over more ad-hoc methods currently in use. Furthermore it spells out in precise terms how the boundary conditions at the free surface has to be modified due to the presence of dissipation.

5. Stochastic effects on the dynamics of wave-generated transport in an oscillatory boundary layer were examined as well (see [7]). We found that noise enhances trapping in progressive wave fields. It has the opposite effect in the standing wave case. This result has a bearing on how wave transport in the noisy environment of natural flows manifests itself and how residual flows interact with an erodible, if present.

6. Application of the wave-current model to the study of the formation and evolution of sedimentary dynamics of shore-connected ridges [3], [8], such as those commonly found in the Middle Atlantic Bight (Figure 7). The goal was to predict how the inclusion of waves modifies the outcomes of a model with which it is conjectured that current convergences and divergences, driven by instabilities, are capable of explaining the angle, spacing, and size of the ridges. The waves are shown to modify the picture in significant ways, depending on their orientation and their frequency: they modify the celerity of the ridges, they are capable of displacing

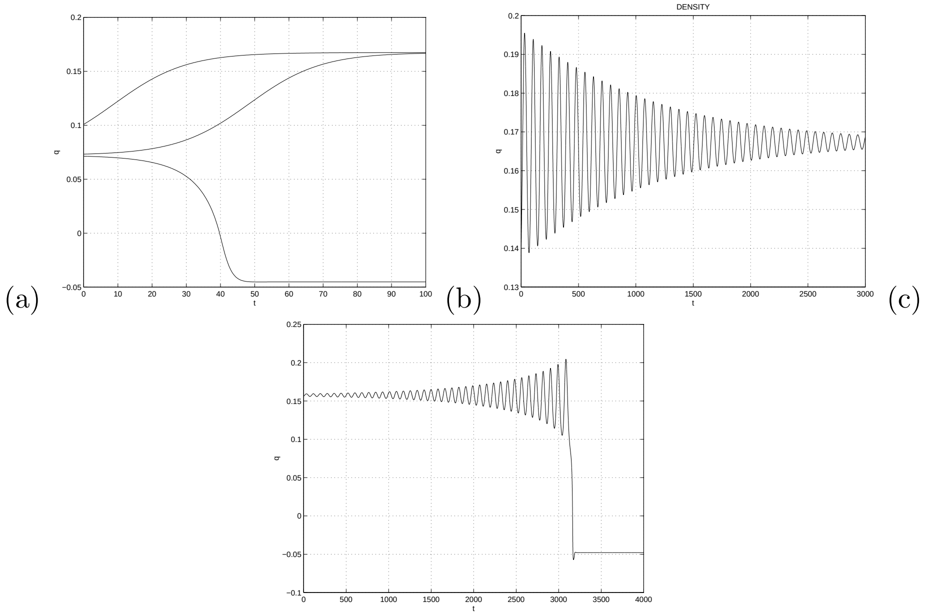


Figure 8: Stommel solution, (b) decaying oscillation due to advection; (c) sustained oscillations and climate transitions due to advection.

them, and even suppressing them.

7. Waves are mostly ignored on climate scales. The nonlinear analysis of a simple model for the thermohaline circulation with added waves or advective effects demonstrates that waves satisfying certain threshold conditions, are capable of modifying the thermohaline circulation. In particular, we show that advective effects can produce climate jumps and decaying oscillatory conditions [9] (See Figure 8). The results may have important implications on climate variability.

8. Theoretical analysis that determines the conditions under which convective adjustments will produce artificial oscillations in coarse numerical simulations of climate [10]. The model predicts the low frequency behavior of the climate system and how it is affected by real or numerically induced oscillations, an important thing to discern when climate variability is at issue. A simple algorithm is suggested that eliminates the oscillations and circumvents the use of more complex convective adjustment schemes.

9. In [11] and [12] we derived a reduced complexity model which includes an explicit dependence of the strength of the ocean's overturning flow on density gradients and a phosphate cycle. Using this model the simulated glacial-interglacial variations in atmospheric $pCO_2$ agree remarkably well with ice-core measurements. Furthermore, the predicted variations in the strength of the overturning between glacial and interglacial periods are also in close agreement with estimates based on paleo-oceanographic data. A fundamental difference between this model and other box models applied to the glacial-interglacial $pCO_2$ question is that the flow field is not prescribed *a priori*; the model also differs from previous box-models in that it uses relatively few parameters; the parameters used have values in reasonable agreement

with data-base estimates.

10. A sensitivity analysis of the reduced complexity model used in capturing glacial-interglacial variations in atmospheric $pCO_2$ referred to above shows that the model is not very sensitive to changes in the high latitude ocean (see [11]). This puts into question assertions that box models cannot be faithful to the dynamics; also it puts into question the notion that there is a robust and simple connection between sensitivity of models to high latitude effects and their ability of capturing the carbon cycle. The analysis further demonstrates that several measures for the assessment of the quality of the predictions for the many models for the problem are of questionable utility.
11. Development of regular and high frequency approximations for the covariant acoustic field scattered from randomly-rough surfaces, such as the ocean surface [13] [14].

### 3.1.2 Sediment/Particle Dynamics

1. Development of an evolutionary, parameter-free model, for the formation and evolution of sand-ridges on the continental shelf and detailed analysis of its solutions [15], [16], [17]. The model represents a possible agent of formation for ridges that are observed to occur in areas where there is no standing wave field and in which waves are normally incident on the ridges.
2. Study of the implications of wave/current interactions on the formation and evolution of sedimentary dynamics of shore-connected ridges, such as those commonly found in the Middle Atlantic Bight [3], [8]. Waves are found to modify the bars, affect their celerity and even suppress them.
3. Direct numerical calculation of the lift and drag on a sphere in an oscillatory wall-bounded boundary layer [18], [19], [20]. These are 3D Navier Stokes calculations and are considered definitive quantitative and qualitative experimental data. This is because it is impractical to measure these forces in a laboratory setting. The data is of engineering interest as well as geophysical interest. The lift, drag, and torque has been found as a function of the Reynolds number, the forcing oscillation (see Figure 9, the gap, and the moment of inertia.
4. The lift and drag forces relevant to the process of particle dislodgement and suspension in oscillatory flows is presently the focus of this effort. Again, we use a 3D Navier Stokes solver in an accelerated reference frame (see Figure 10 for the mesh configuration).
5. Established that lift forces play a role in the dynamics of sediment particles under typical oceanic settings [18]. Most every model for sediment dynamics in oceanic and fluvial settings ignores the lift force.
6. Experimental study of coherent behavior of sedimentary structures under the action of steady shearing flows (see Figure 11a for an illustration of the experimental arrangement and Figure 11b for some of the space-time data). The analysis of the data has yielded some surprising and complex bar behavior. We have been able to identify at least three types of sedimentary structures: advective, dispersive, and super-advective bars.

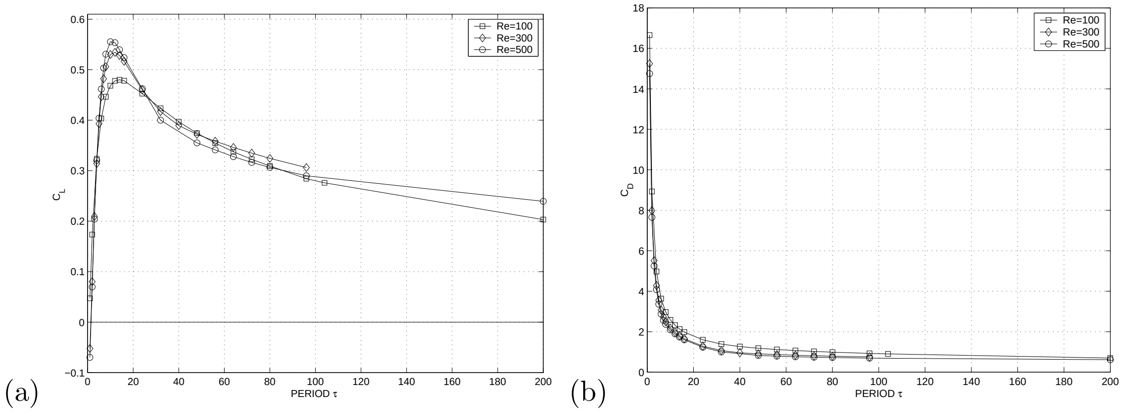


Figure 9: Lift and Drag on a particle as a function of the Reynolds number and the frequency of forcing.

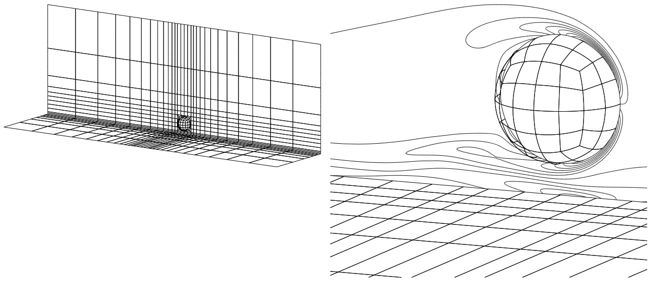


Figure 10: Configurational mesh for 3D Navier Stokes computations of lift and drag on a particle in an oscillatory flow.

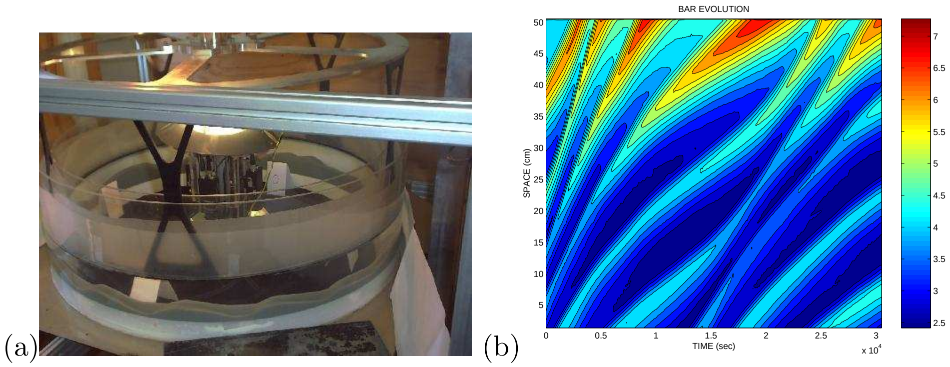


Figure 11: (a) Shearing sand experimental setup. (b) Space-time contours of the sedimentary structures. Contours represent height.

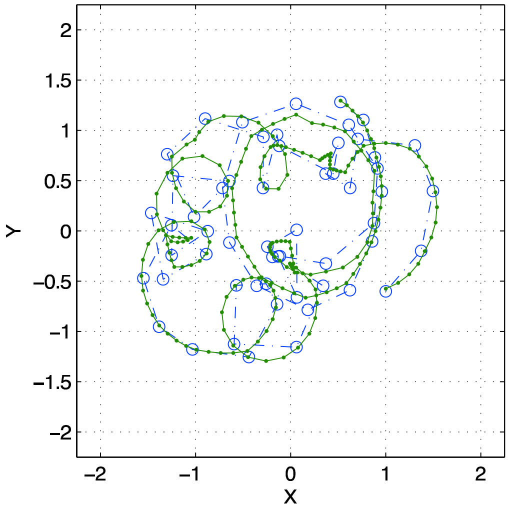


Figure 12: Noisy data (circles); assimilated data with errors in the model of order 20%.

### 3.1.3 Optimal Estimation and Scientific Computing

1. Development of a new, near optimal method for the data assimilation of possibly noisy data into highly nonlinear dynamics problems. The technique is known as the Mean Field Variational Method [21], [22], [23]. We have demonstrated the superior qualities of this method, as compared to its more common competitors, in highly nonlinear problems and far from Gaussian problems.

2. Development of the Path Integral Method for data assimilation. It is an adaptation of generalized hybrid Monte Carlo technique to the data assimilation problem [24],[25]. This nonlocal, molecular dynamics approach, the path integral approach, significantly speeds up the Monte Carlo sampling and thus enables us to use Monte Carlo sampling in the context of nonlinear and far-from Gaussian data assimilation and estimation (See Figure 12 for an assimilation of data (circles) and model for the position of a single drifter (dots) and 2 point vortices (stars)).

3. In the context of particle filters for data assimilation we investigated how parametrizations of distributions can be exploited to improve the calculation of the mean and uncertainty of histories, conditioned on observations [26].

4. Application of a recursive method to the exact calculation of gradients for large systems of equations on limited memory machines. The algorithm trades storage for added computations. However, the growth in complexity is shown to be logarithmic and hence a practical strategy [27].

5. Developed the software package for the practical implementation of the recursive algorithm described above [28].

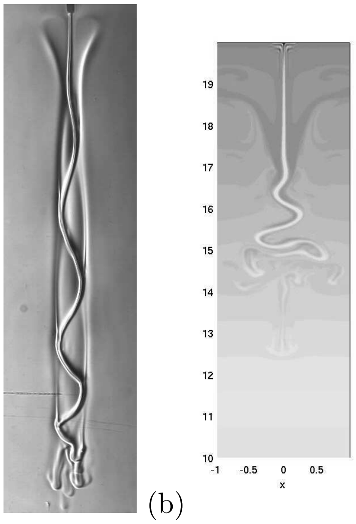
6. Use of complex polynomial approximation to develop accurately and computationally efficiently the gaps in the spectrum of a Hermitian matrix without the computation of the full

spectrum [29].

7. Developed a preconditioner for normal matrices which have gaps in their eigenvalue spectrum [30]. The technique is accurate, numerically stable. This is an alternative to more traditional methods, however, it is a very beautiful method, mathematically.
8. Computational and theoretical studies of wavelet-Galerkin methods for the solution of hyperbolic problems [31], [32]. Analytical estimates of the approximating properties of periodized wavelets.
9. Development of software for the computation of inner products using wavelets for these wavelet-Galerkin methods [33].
10. Development of a wavelet-Galerkin technique for the solution of PDE's.
11. Development of software for task farming [34]. When the code was developed it was a novel and simple way to have a heterogeneous network of computers automatically submit sequential jobs in an efficient and fully documented way. This code is now been bypassed by tools with significanly higher capabilities, such as Python, Condor, and GRID.
12. Presently developing a numerical strategy for the solution of the coupled water/sediment system which can handle a time dependent air/water/sand interfaces. Doing so will enable us to model the appearance and disappearance of islands, flooding, evaporation, ice loading. The technique combines finite volume methods with an abstraction of level set ideas. The idea here is to be capable of studying the sediment erosion problem, rip currents, wave run-up, litoral currents, tides, where it most counts: on a beach. This work is not yet published.

#### 3.1.4 Fluids, Bone Dynamics, Partial Differential Equations

1. Experimental (Figure 13a), computational (Figure 13b), and theoretical study of a the dynamics of a columnar heavy jet descending into a stratified background fluid [35] [36], [37].
2. Examination of a mechanistic model for the formation and reforming of bone tissue [38]. Found equilibrium solutions and their stability. The analysis determines very sharply the bounds of applicability of the model in capturing the dynamics of bone reforming. Also found that the model, as originally conceived, is not capable of producing sustained oscillating solutions, contrary to the published results.
3. Numerical exploration of unstable solutions to the regularized Generalized Long Wave Equation [39]. Established two regimes of parameter space in which unsable solutions become stable by shedding a train of solitary waves, thus making the transition to a more stable regime. Established that the resolution of initial data into a train of solitary waves does not require integrability of the partial differential equation.
4. Proof of the existence and stability of oscillatory solitary wave solutions (see Figure 14) to a new equation called the Benjamin equation [40]. Established with precision the physical conditions under which these may be seen in the lab or in a natural setting.



(a) (b)

Figure 13: (a) Actual jet, (b) computational jet. The images are not meant to portray the same dynamic conditions.

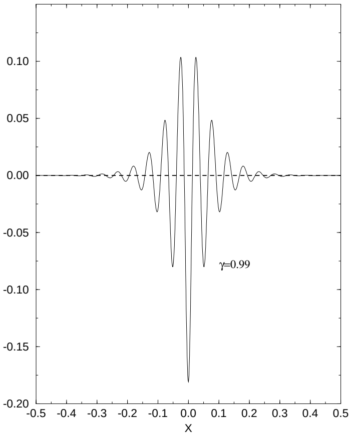


Figure 14: Traveling wave solution of the Benjamin Equation.

5. Found bound state solutions in the evolution of data under the action of the Benjamin Equation: the solutions contain particle-like behavior of waves that will interact inelastically between two other larger waves that effectively act as a potential that keep the inner waves bounded. This work is not yet published.

### 3.1.5 The Arts, Politics

1. Involvement in the production of the first-ever computer-generated music on a massively parallel distributed supercomputer [41].
2. Design and supervision of the construction of several concert halls and other complex architectural acoustics structures [42].
3. Studied the influence of exit polls on voting. In [43] we proposed a model with which to study the effect of releasing exit poll data and projections while voting is taking place, in a majority-rule, multi-party election. Will be considering the voting process during the primaries and eventual presidential election as a sequential voting scheme in which information plays a role on voting strategies.

# 4 New and Future Research

## 4.1 Biology

- **Blood**: study of the dynamics of red-blood cells in intermediate sized blood vessels. With P. Fischer and G. Leaf (ANL), Tim Secomb (Physiology, Arizona), and a graduate student, Jared Barber. Tim is very interested in developing models for the effective viscosity of blood: this is a highly nonlinear function of many things, among them the diameter of the blood vessel.

  Since the viscosity, particularly in small diameter blood vessels, depends on the dynamics and density of red blood cells, it is important to analyze and determine very precisely how blood cells move and interact with each other, with the walls, and with the background fluid. Among other things, the cells tend to tank tread and occupy the area closest to the axis of the vessel (fortunately!). They tend to react differently in the present of other cells and near walls and boundaries. The flow inside of the cell and outside of the cell is basically Stokes and thus all of the interesting complexity of the motion of the cells depends on the membrane and on the presence of walls and other cells.

  We are proposing a dynamics interacting population model for the viscosity of the blood. In addition, we are building a "blood cell dynamics" numerical solver to study the motion of the cells. Since the flow inside and outside is Stokes and a very crucial constraint of the motion of the cells is that they are membrane-surface preserving, is the following: we will use our existing Navier Stokes solver (either in a laboratory reference frame or an accelerated reference frame) to solve for the flow inside and outside. We further constrain the motion of the membrane to agree with the flow inside and outside: what is novel here we impose the surface constraint *on the grid* generator. Thus the determination of cell motions amounts to solving systems of coupled ordinary differential equations and thus easily the 3D motion of

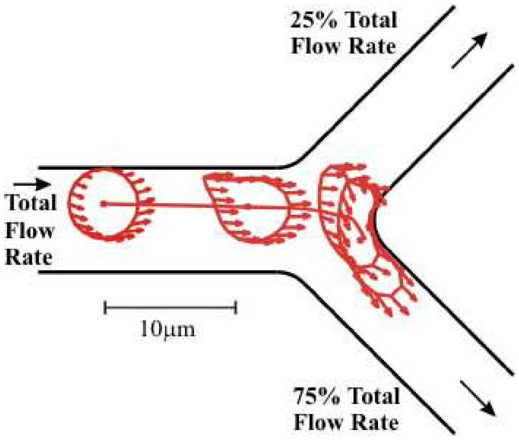


Figure 15: Bifurcating blood vessel and motion of blood cell.

the flow and the cells become computationally scalable. This is a practical method because the motion of the grid representing the cell boundary is laminar within the sea of grid points.

I doubt we will beat the computational expense of a boundary element method, however, we will be extremely competitive on the three-dimensional case and the ease in which we can simulate complex interactions does not have to rely on symmetries. The computational approach I advocate is independent of the fluid flow code and thus we can exploit tools already developed to capture the flow very precisely and in blood vessel geometries that are quite complex.

Another problem that I would like to consider is to add a magnetic field to this flow. The idea here is to model small drug and micro machine delivery systems. The small bags will be directed to a target via a magnetic field, the vesicles then disolve (delivering a small dose of iron oxide) and the drug or the machines are then put to work in a focused way. The applications range from chemotherapy to blood clot destruction, to blood vessel wall scrubbing and repair. There is, of course, one important and difficult problem to overcome: convincing the human body not to reject and filter out the delivery system. However, there is good reason to think that this problem will be solved by biochemists and biologists in the near future.

We just finished a paper on the distribution of red blood cells in bifurcating vessels ([44]): while it is approximately true that cells distribute themselves in a bifurcating vessel in a manner proportional to the blood fluxes themselves, this is not the case for very small blood vessels. See Figure 15. In our paper we propose a model to study the dynamics of blood cells in moving blood flows, apply it to bifurcating vessels after carefully calibrating the model against existing data. The end result is that we are capable of extending and correcting the range of existing estimates for blood cell distribution. The importance of knowing this distribution is because it is the concentration of red blood cells, rather than the blood itself, that determines the rate of oxygenation in tissues.

- **Bone Remodelling**: Researchers at SUNY Buffalo and NASA have been able to determine that shaking the body of an animal (a turkey, in fact) tends to preserve already healthy bone in microgravity environments. The shaking is in the order of 10-80 cps and the magnitude is just a a fraction of a $g$, moreover, the treatment to be effective requires only hours per day. This finding has obvious implications in space travel, the health of bones of bed-ridden patients, etc. Separately, there is a group at U. Washington that has been using high levels of sound radiation to induce bone growth in healthy fractured bones. Yi Jiang (LANL) and her group have been trying to use a well regarded model for bone growth developed by bone researchers to determine why the shaking works, whether there is a preferred frequency, and what dosage should be applied. The model has a natural time scale of days, and significant bone growth occurs in 60-100 days.

My analysis of a popular model used to analyze this dynamic problem lead me to conclude that is inconsistent with the physics and unable to explain how vibration has therapeutic effects.

Yi Jiang, Rustum Choksi (SFU) and I developed an alternative model ([38]) and explanation. My conjectures are (1) that the vibration and sound therapy are actually related to each other, however, their roles are not the same: the sound therapy is only capable of bringing the calcium ions close to the surfaces where they are needed, by way of acoustic streaming. The vibrations, on the other hand, are capable of creating geometric channels that allow calcium ions to penetrate deeply into the bone; (2) The latter is sensible if you take into account that the treatments cause stresses in the bones that are fractions of those present during regular exercise and daily stresses, and secondly, because the time scales at which bone reforms is in the order of months yet the effects of these oscillatory treatments are apparent on time scales that are fractions of these time scales. We are pursuing a Taylor diffusion process in the fluid-filled interstices of the hard bone. The process can be seen as a very effective way to move nutrients and other anabolic chemicals through the bone tissue. Whether or not this mechanism is related can be tested in the laboratory, as we are able to estimate time scales and extent to which material should diffuse through the bone tissue. Furthermore, we should also be able to determine in no uncertain terms how diffusion depends on the frequency, amplitude, and dosage of the vibration treatment.

## 4.2 Geosciences

- **Dissipation in Wave/Current Interations:**

  One particularly difficult problem in wave/current interactions is to figure out how dissipation enters the dynamics. The major difficulties here are that it is not at all clear what dissipation does to each of these components of the flow and how dissipation distributes itself among the waves and currents.

  We have already begun to work on this problem. We make use of stochastic differential equation theory. The main idea here is to assert that the dynamics of fluid flow in the Lagrangian frame in the presence of a periodic and spatially-dependent noise source can be modelled by a standard stochastic differential equation. We then apply projection methods and time averaging, as well as averaging over ensembles, to find how effects such as white capping and other sources of dissipation enter the full wave/current model. At present we have a fully formulated model and the answer to how white capping, for instance, enters the dynamics is this: the amplitude of the waves will have a spatially-dependent additive

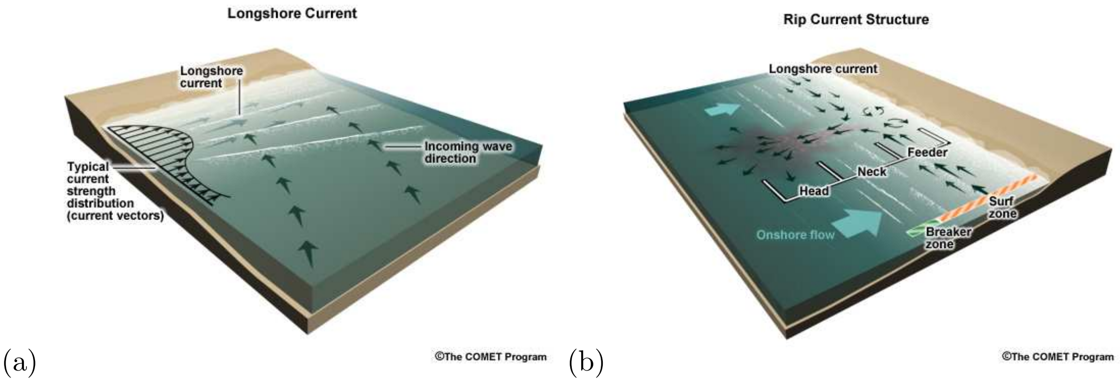


Figure 16: (a) Longshore currents, (b) Rip currents.

dissipation term. The currents, on the other hand will have a Stokes drift velocity due to the waves that has a stochastic and a deterministic component. Thus dissipation will appear in a manner similar to a Reynolds stress, however, this stress is fully determined once the stochastic distribution of the white capping is fixed.

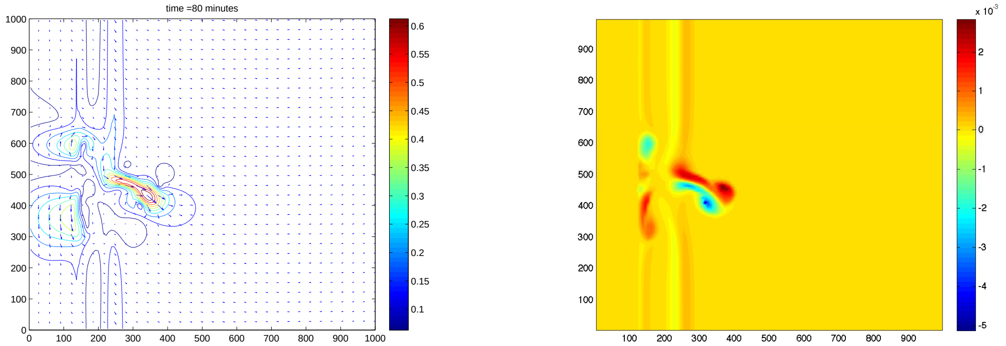
An added bonus to this approach is that it suggests a new and sensible way to include actual white capping in an operational model: what is required is ensemble averages of photographs or radio measurements of the ocean surface. This is a much preferable way to estimate dissipation than the more traditional spectral approach.

Another form of dissipation, namely that of bottom drag, can be implemented in similar fashion, however, here we can always exploit a stochastic map of the ocean bottom to transform the deterministic equations for wave propagation into stochastic partial differential equations. Whether this is a practical transformation is yet to be determined, however, formally, such formulation allows us to get a lot of mileage on what respects understanding how bottom drag modifies the flow.

- **Longshore and Rip Currents, Reevaluating the Standard Models**:

  Having derived in great detail the radiation stresses from our wave/current interaction model it is now possible to revisit these two classical problems with the aim at determining whether significant qualitative improvements over the traditional view on these problems is possible. Namely, to see if it is possible to determine the position of the runnel in the longshore wave-forced currents (see Figure 16a), and whether the spacing and extent of rip currents (see Figure 16b) is significantly modified by using our model over more traditional means. The centerpiece of our theoretical model are the *Vortex Force*, which couples the total vorticity of the flow and the residual flow due to the waves, as well as the *Bernoulli Head*, which produces an important pressure readjustment as a response to the excess mass due to the waves. The vortex force, in particular, we are finding, can explain a substantial portion of the vortex shearing that occurs in the rip current situation. This is shown in Figure 17a-b.

  Three significant findings associated with our analysis of the rip current situation are: (1) that we can offer an explanation to why biologists who measure the fluxes of biomass in shelf zones often encounter a "sticky" zone just beyond the break zone; (2) we can get rip currents



(a) (b)

Figure 17: (a) Rip current, predicted by our model, (b) the vortex force component.

of the right extent, as compared to when people have used standard models: doing so has led to a vexing problem in that the rip currents are much more pronounced and extend further out into the shelf; (3) The rip current veers downstream, there is a small contribution due to Coriolis, but the main reason for the deflection is the interaction of waves and currents, as manifested by the vortex force.

- **Rip Surges**: Randy LeVeque (Washington), Jim McWilliams and I are working on a newly-discovered form of a rip current, which I call the *Rip Surge*. This type of rip surge is new because it has only been possible to see it by the improved efforts of LeVeque's group and ours in creating a numerical solver for shallow water waves that includes a moving shoreface. In this type of rip surge, currents traveling back to the shelf are generated by the action of an excess water mass that accumulates at the shore end of a smooth-sloping beach, subjected to time-periodic waves. It is a residual flow, which when it interacts with the waves, will be guided to follow the stationary nodal lines of the waves, and develop a Kelvin-Helmholtz instability due to excess shearing.

- **Fluid Jets on Inclines**: A simple change in the configuration of the jet experiment that was described earlier allows us to consider slow gravity currents. The arrangement is that of a jet of salty water allowed to fall freely on an inclined plane into a basin of stratified flow. This is a simple representation of gravity currents that are considered extremely critical to the formation of Northern Atlantic Deep Water, among other things, and also the gravity currents that play such an important role in the pollution and mechanics of atmospheric conditions in places like Phoenix Arizona. In the experiment we can match the Richardson number and the Prantdl number of the oceanic setting. The Reynolds number, on the other hand, would be no where close to the oceanic case. Nevertheless, crucial aspects of this flow can be fully characterized both numerically and analytically: at issue are (1) how the current accomplishes mixing of fresh waters and salty waters; (2) how does this current behave as the fluid becomes denser? Both of these can be determined as a function of incline angle, input flux, and salt gradient. The rigorous determination of the mixing characteristics of this flow would be of significance, from a qualitative point of view, on the geophysical setting. This is work that I am going to pursue with Lou Howard, emeritus from MIT and Florida State.

### 4.3 Scientific Computing

The *primary* focus will be on optimal estimation. However, there are also plans for the following:

- **Ocean/Bottom Topography Interactions**: The strategy that allows us to numerically simulate flows in which the basin itself is allowed to evolve can be extended to consider a variety of problems: among them is the effect of ice loading and the evolution of river deltas. To this effect we will be generalizing the numerical solver for shallow water waves with dynamic air/water interfaces to handle these more general problems. This opens the possibility for consideration of some very difficult yet heretofore intractable problems in sedimentation and ocean dynamics.

- **Regularized Stochastic Green's Functions**: Ricardo Cortez (Tulane) has developed very robust and practical regularizations of Stokeslets which have made a host of immerse boundary method calculations possible. Here I will be adapting the strategy to generate Helmholtz Green's functions. This in itself is a straightforward task, however, the new twist is that I will incorporate the statistical aspects as well as the composite roughness strategy (see [13] and [14]) so that these Green's functions can be used in the efficient computation of scattering of scalar waves by randomly-rough surfaces.

## 5 The Uncertainty Quantification Group

This group consists of 5 faculty from computer science, mathematics, physics, statistics. It has the participation of four post-docs, roughly 8 graduate students, and 2 undergraduate students.

I created this group in order to address problems in which (1) uncertainty quantification makes a significant difference in the application of existing computational algorithms and models blended with experimental data or observations; (2) in which statistical and machine-learning techniques are exploited to affect a connection between scales in dynamics; (3) in which statistical parametrization allow one to offer an alternative to closure parametrizations, and these statistical parametrizations offer a clear advantage with regard to connecting to the ever-increasing wealth of data.

The group has been created with certain structural constraints: (a) to involve students, both undergraduate and graduate students, (b) to not hold meetings for more than one hour, (c) to encourage the creation of subgroups that have members with different strengths and skills working together, (d) to involve post-docs here at Arizona in the most rewarding and productive environment, (e) to involve mostly junior faculty, (f) to bring strengths in deterministic mathematics, in computer/computational science, statistics, machine learning and statistical mechanics.

For more information, visit our group's web site:

`http://www.physics.arizona.edu/~restrepo/myweb/UQ.html`.

### 5.1 Current UQ Projects

- Nonlinear Filtering/Smoothing in geoscience and financial forecasting.

- Optimal Estimation in Lagrangian frames with applications to oceanography.

- Homogeneizaton and optimal estimation in nonlinear/non-Gaussian hydrological data assimilation.
- Computer vision using efficient tracking.
- Stochastic regularized Green's functions.

# 6 The Computational Geosciences Program

Just as there are large efforts at many universities to modernize the education of biologists to produce a more quantitatively-skilled class of life scientists, a comparable effort should be made to produce a significant number of quantitatively-oriented geoscientists.

The demand for quantitative geoscientists is already here: I hear frequent complaints from geoscience colleagues that they cannot get students who have adequate quantitative skills if their undergraduate education was not math, physics, engineering, chemistry. I hear the same thing from government labs who wish to find skilled geoscientists to work on hydrology, meteorology, geo-statistics, climatology, glacial physics, geophysics, etc.

The Computational Geosciences Program is an educational and career strategy that addresses these problems. The details of how the program will be run, how it will recruit and place students, how it will be funded, and what it will consist in greater details, would be discussed at length in person if there is serious interest in considering its implementation.

# A Appendix: Selected Extended Descriptions

## A.1 Wave Generated Transport

The theoretical framework of wave-generated motion in the context of water, acoustic, and plasma waves rests on the fact that under certain conditions of motion the Lagrangian particle paths do not describe closed orbits and thus their time average or ensemble average leads to non-zero quantities. Perhaps the earliest theoretical studies on this phenomena are those of Stokes and Lord Rayleigh. In the early 1950's Longuet-Higgins in derived an asymptotic expression for the lowest-order drift velocity in a laminar boundary layer and showed that boundary layers, however thin, have a dramatic effect on the ensuing drift generated by monochromatic waves. For progressive waves, he showed that the drift results in a uniform current; for standing waves, on the other hand, cells form in the residual flow, commensurate with the wavelength of the waves. Hence, if tracers are present in the flow, these move on average with constant velocity in the direction of the waves when they were progressive, and form spatial structures that are on average stationary in time. Streaming also occurs when immersed objects are oscillated in a fluid. This is well documented and of considerable interest in the engineering community. It is now a classic topic in fluid mechanics monographs and textbooks.

Wave-generated transport has been shown to modify the dynamics of interacting flows. A consequence of momentum and continuity conservation is that short waves are dynamically modified by the mass and momentum fluxes due to finite amplitude long waves. The interaction of currents with the streaming induced by a wave field has been shown to generate circulation cells, which have a striking resemblance to Langmuir cells in the ocean and the atmosphere, and has been shown to modify the Ekman boundary layer in rotating flows.

My work on the subject shows that wave-generated transport is an important transport mechanism in oceanic flows relevant to climate dynamics, vertical mixing and upwelling in the near-shore, and in the transportation of suspended sediment by the interaction of waves and currents.

### A.1.1 Wave/Current Interactions

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There are a host of problems in which waves and currents are present: rivers interacting with oceans, ocean currents and gravity waves, internal waves and circulations are some of these. They also occur in other contexts, such as in plasma and particle/electromagnetic field interactions, acoustics. When the interactions are nonlinear it is not clear how each of these flows affect each other. However, in the context of oceanic fluid flows there is a fairly extensive and well trodden view of how this interaction takes place. An important premise is that the wave velocity is considered always smaller than the current velocity. In some cases this is the right assumption, and it leads to the theory that one would find in standard textbooks. It is also similar to the expressions one would find in plasma physics books. Jim McWilliams (UCLA) and I began to question the validity of this assumption on scales, and it is seldom the right scale for oceanic problems. However, when one tries to develop a theory in which the scales are such that the wave velocity is larger than the current velocity, it becomes nearly impossible to see that such approach would work. But it does, after a great deal of very hard work.

Combining asymptotics and time averaging over small scales we have built a hierarchy of models for short, intermediate and long time scale dynamics. The short scales corresponds to the gravity waves, the intermediate scale to the infra-gravity waves as well as setup and setdown, and the longest to currents. The result is a model for the interaction of these flows and a plausible explanation as to how short time scale motions modify the larger scales.

Among our results are: (1) how waves persist at ocean climate scales; (2) by developing a model prescribed specifically for the nearshore environment we also devised how one can come up with a model for the smaller scales that is formulated at the larger resolvable scales; (3) we have rederived the radiation stress under these new assumptions are able to show that the often used expressions are, to lowest order, identically zero; (4) we have developed a general framework we call the vortex force formulation which describes in a clear way how waves and currents contribute to the stresses and to the Bernoulli head in a decoupled way; (5) using a simple box model we have shown how the thermohaline circulation, a circulation that is fundamental to ocean climatology, is modified by the presence of waves; (6) The derivation of a rational model of dissipative effects in the wave/current interaction setting.

Using our formulation we can explore classical problems, such as how the spectra of water waves is affected by the presence of currents: here we expect many effects attributed to a Doppler shift to be understood as spectral interactions in the phase of the waves. We can also revisit some classical problems, such as rip and longshore currents with the aim at investigating how the application of our wave/current model differs from the more traditional approach. We have considered how sediment motion due to the coupling of waves/currents and a moving bottom topography generate bars via instabilities of the waves and the currents.

At present we are looking at how we can include several dissipative mechanisms, such as wave breaking and bottom drag. By assuming that the effect of these are stochastic processes we can show that in the long time limit the residual flow due to the waves will have two components that couple to the vorticity of the flow: one component is the standard drift velocity, the other one is a dissipative drift. We will also consider how rip currents and long trapped waves are generated in the nearshore. Our results on this will be different from the standard ones because our balances of currents and waves is diametrically opposed to the standard lore.

In a more mathematical context we are learning how to project Lagrangian paths with multiple time scales at longer time scales. We hope to produce a projective technique which (under the assumption of analyticity of the change of scales) effectively maps the small scale motions to larger scales. In reverse, this projection will wind up being a nonlinear multiresolution technique which will yield the nonlinear spectral decomposition of the dynamics.

### A.1.2 Wave Breaking Parametrization in Wave/Current Interactions

In [6] I proposed a novel way to include wave breaking effects in wave/current interactions. The basic idea is to develop a stochastic differential equation for the Lagrangian parcel path, and then use our wave/current averaging/projection. The outcome shows where the wave breaking is expected to have an effect and how. It also yields all the necessary adjustments that need to take place for the model to retain conservation of mass, momentum and energy. The two phenomena that contribute to losses are fluctuations of the particle path and these will transform part of the wave interaction terms in the currents into dissipative effects. The other effect is the enhanced mixing and the generation of stronger Reynolds stresses.

The end result, in an Eulerian time/averaged frame is a model which is far more amenable to calibration using observational data than other more turbulence-based or weak-turbulence-based models.

The ultimate goal is to produce an analogous connection between Lagrangian diffusion and wave/current motions as the one that exists between Brownian motion and molecular diffusion.

## A.2 Sediment Dynamics

Striking sedimentary structures are found on the continental shelf wherever sand is abundant (See Figure 4 for a schematic view of the continental shelf). Two common arrangements are known as sand ripples and sand ridges. These temporally evolving sand patterns have piqued the curiosity of researchers for nearly 100 years. Sediment motion has been studied for centuries now. The research is focused mainly on practical aspects of civil engineering, erosion dynamics, petroleum engineering, and industrial processes involving granular flow. Great strides have been made in the formulation of ad-hoc models, which have proven themselves useful in engineering practice. However, due to poor understanding of the dynamics of sediment motion, no evolutionary model has succeeded in accounting for the large variety of observed sedimentary structures.

In collaboration with J. Bona (UIC), a model capturing the evolution of large scale sand ridges in the deeper reaches of the shelf was developed. The results from this model imply that on the time and length scales of sand ridges, sedimentary structures are generated by nonlinear dispersive infra-gravity waves. The energetic interactions (due to nonlinear effects) and the spatial changes (due to dispersion of the spectral components in the infra-gravity range of the waves) have length scales that match those of sand ridges. These nonlinear interactions generate a coherent and structurally organized pattern in the drift velocity. This drift velocity is endowed with a structured pattern by the overlying nonlinear dispersive waves. If these nonlinear interactions are coherent and energetic enough, the drift velocity will scour the ocean bottom in ways that produce the beautiful patterns observed in sandy environments. At present we are implementing more phenomenology into the mass transport equation which forms part of the model by using an equation of state to couple a model for the suspended and the precipitated parts of the sand budget.

Two important questions which have been addressed are how the model predictions are modified if the phase of the waves changes over time, and how currents modify the solutions to the model. In order to address the first question, numerical methods were used in to study how noise and possibly under-resolved dynamics affect the structure-producing aspects of the wave-generated transport. We found that small amounts of noise can actually enhance pattern formation by significantly cutting down on the steady residual flow in the transport. Under large noise perturbations, the steady residual flow is affected even more, but the noise generates a diffusive drift which can be strong enough to suppress pattern formation.

The previously described wave-current model has been useful in consideration of an idea of Trowbridge regarding the generation and evolution of shore-connected bars and later by Falqués and others: a model which yields structures that resemble sand ridges on the inner shelf has been formulated in which exponential growth of large features results from the offshore deflection of storm-driven alongshore flows at ridge crests. This gives rise to the shore-connected oblique sand ridges commonly found in the inner shelf. Crucial to models such as that presented by Trowbridge and the others is that the waves are changing adiabatically on time scales appropriate to sediment motion. We used the wave-current model to show that this assumption cannot be valid: when the model was applied to situations examined by Trowbridge and others it was found that the bars did not resemble shore-connected structures. Furthermore, an eigenvalue calculation showed that the eigenfunctions were akin to shore-connected bars only when unstable eigen-directions of the waves are suppressed.

I have been able to contribute both in the theory and modelling of sedimentary structures and of the interaction of these structures with a fluid flow. However, it is my opinion that the most important scientific contributions one can make at present to this subject are computational and experimental. Present technology enables unprecedented computations and measurements, significantly increasing the likelihood of making important discoveries.

Laboratory sediment dynamics experiments were designed and built that give us unprecedented control over the parameters of the problem of the generation and maintenance of bars under the action of shearing flows. The focus here has been primarily with the aspect of modelling fundamental aspects of the sediment dynamics, rather than on the faithful recreation of the oceanic setting in a laboratory. An annular tank has been built in which water and sediment are sheared by a solid rotor. The shearing can be either unidirectional (both steady and accelerated motions are being investigated), or oscillatory. The apparatus includes a video system that enables viewing of the entire tank at once. The shearing rotor, the image capturing system, and the analysis routines are driven by software. At present we are studying the steady shearing case. In this case we have identified two different routes to bed instabilities. These instabilities manifest themselves in bar-like structures that precess around the tank. Transient rearrangements are also possible which lead to disturbances that travel at speeds higher than the precession velocity. We have also found that it is possible for an accumulation of sediment to slowly resolve itself in solitary-wave like structures whose speed of precession is related to their amplitude (and possibly their wavelength). This is but one of many phenomenological outcomes of this experiment. This work is a collaboration with R. Goldstein and A. Pesci (Arizona).

In addition, three-dimensional direct numerical calculation is being used to capture the drag, torque and lift forces on an isolated particle, as well as a group of particles (representative of sand). Such calculations are performed because it is impractical to measure these forces in the laboratory, where sensitivity to forces in the micro Newton range would have to be resolved. A primary goal of these experiments is to discover whether lift forces are important to the dynamics of sediment in the oceanic situation. Our work has been conclusive: we have shown that the lift force is important for small particles. A follow-up paper is in the works, in which we consider lift and drag forces on a particle in an oscillatory flow when the particle is sitting on a bed of similar particles. This sequence of experiments is aimed at documenting the process of dislodgement of particles. This initiative is a collaboration with P. Fischer and G. Leaf (ANL).

There are three components to this effort:

### A.2.1 Forces on Particles

Performing laboratory experiments aimed at determining the actual forces on a particle in an oscillatory wall bounded flow are extremely difficult to perform, even if one can scale these up. The forces, thus on sediment particles are largely unknown. However, if one is comfortable with the idea that a Newtonian incompressible flow is well modeled by the Navier Stokes equation, one can calculate these forces *ab initio*. This is in fact what we are doing (with Paul Fischer and Gary Leaf, at Argonne National Laboratory). We solve the full three-dimensional Navier Stokes equations and obtain the forces without making approximations. As such, they may be considered experimentally derived (clean) descriptions. In order to do this we are systematically adding degrees of freedom to the calculation: first we consider a fixed particle sitting on the bounding wall and compute the lift and drag as a function of the forcing frequency and the Reynolds number. We then consider the effect of having a gap. At this stage we have added a fourth parameter: we have allowed the particle to rotate and thus the moment of inertia becomes the fourth parameter. We will then consider adding translation (this can be done by recasting the Navier Stokes equations in an accelerated reference frame!). This work is reported in [20], [18], [19].

The next stage is to consider particle dislodgement and suspension. In the former we place the particle and consider only geometric constraints, we then add interparticle forces (at this point we need to use models for the forces).

### A.2.2 Experiments on Sheared Beds

Here the general idea is quite simple: we want to generate high quality descriptions of the motion of sedimentary beds under the action of a shearing fluid flow. The shear is steady at present, but later on we will consider oscillating shears. In the context of a steady shearing flow we (Ray Goldstein, Adriana Pesci, and I) have observed a multitude of different coherent structures appearing in the simple steady shearing flow. Eventually we would like to formulate models or explanations for what we observe.

### A.2.3 Modeling

There are two types of large scale sand bars that I have focused on: one is the sand ridge, fields of which are found in shallow waters, beyond the break zone. These bars are a few feet high and several tens or hundreds of meters apart. The bars are oriented flow-normal. The flow is primarily due to waves. The bars are several times larger than the wavelength of the waves and the waves are primarily unidirectional. With Jerry Bona (UIC) we developed a model which combines waves with an erodible bed equation and claim that the pattern can be produced by the spatially-varying Stokes drift, i.e. by nonlinear waves. The interbar spacing we attribute to the fact that there is a balance between nonlinear and dispersive effects and thus will necessarily lead to a spatial pattern in the drift velocity that is much longer than the wavelength of the waves. This also obviates the need to rely on a standing wave pattern in the flow which would require a significant reflected wave component. Qualitative comparisons with data are encouraging. A question was raised with regard to explaining how the phase of the waves could be maintained over the time scales of the bars: we were able to show that noise in the phase, which we propose models the erratic changes in the phase, actually contributes to the steady spatial structure of wave-induced flow under progressive waves, and destroys structure in wave-induced flow under standing waves. Another question that arose was that if the stokes drift was caused by nonlinear waves, should it not be a non-spatially dependent pattern? the answer here is simple: by a Galilean symmetry it is clear that a wave of permanent form, such as a train of solitary waves, will produce a steady drift. However, there are other solutions to the nonlinear dispersive wave equations and in fact, if the far field is a group of interacting linear waves, the outcome will not be a wave of permanent form and thus it is possible to generate a pattern in the Stokes drift.

Another sedimentary structure we have looked at are the shore-connected bars. These are bars that appear at an angle with respect to the shore. They appear as well under currents that travel in the alongshore direction. A number of researchers were able to produce a model which claims that convergences and divergences of the flow due to an instability are capable of producing the bars and under the orientation described above. We have looked at how this instability gets affected with the presence of both waves and currents. Our findings are consistent with the old ones when waves are absent but have striking morphological and dynamical differences when waves and currents are considered.

## A.3 Optimal Estimation/Data Assimilation

The aim of data assimilation is to infer the state of a system from a geophysical model and possibly incomplete or non-uniformly distributed spatio-temporal observational data. Used extensively in engineering control theory applications, data assimilation has relatively recently been introduced into meteorological forecasting and climate dynamics. Another example is the problem of recovering the release history of a groundwater contaminant, such as a chemical spill, when the porous medium and the hydrological flow-field are only statistically characterized.

There are three aspects to this effort: (1) application of Rayleigh-Ritz techniques and mean-free field approximations to the formulation of assimilation techniques; (2) overcoming important and serious computational hurdles in the calculation of the gradient of a functional, as is required in large scale minimizers that use gradient information; (3) the development of faster sampling techniques which would allow for the use of Monte Carlo-based estimation techniques.

### A.3.1 The Mean Field Approach

In such methods, conditional statistics are calculated, such as the mean and variance conditioned upon the available observations. These two statistics provide the optimal estimate and a measure of its reliability. However, to calculate such quantities, equations for the conditional probability distributions must be solved, which are hyperbolic or parabolic partial differential equation in a number of variables equal to the dimension of the dynamical phase space. Such equations are a mathematical implementation of "Bayes' formula" in probability theory. The methods simplify considerably if the stochastic system obeys linear dynamics. In that case, the optimal estimator is given by a simple variational principle, as the minimizer of a quadratic cost functional. If only future-time prediction is required, then the calculation simplifies further and the optimal estimator is given by the Kalman-Bucy filter. The calculation of the latter requires only the forward integration of a differential equation with the same number of variables as the starting dynamical system. To obtain the conditional variance a separate matrix Ricatti equation in the square of the number of variables must be solved. In such forms, optimal estimation is already being widely applied to large-scale, stochastic systems when their dynamics is, at least approximately, linear. This practice of data assimilation improves considerably the usefulness of existing models by allowing them to be coupled in the best possible way to available real data and by providing an assessment of the reliability of their predictions.

However, such methods cannot be applied to spatially-extended, many-degree-of-freedom systems with a wide range of relevant length-scales, interacting by strongly nonlinear dynamics. The important scientific prediction problems mentioned earlier all have this character. Because of the nonlinearity, the computational reduction to obtain the optimal estimator that appears for linear systems no longer holds. As has been emphasized by Kushner, the difficulties here exactly parallel the "closure problem" of turbulence theory. The equations for conditional mean and variance, which are closed for linear systems, now couple to higher-order moments. Computation of the optimal estimator thus requires the solution of a functional PDE for the entire conditional distribution, in principle, in an infinite-dimensional space and, in practice, in a space whose dimension is the size of a computational grid. The multi-scale character of the dynamics implies that such dimensions are enormous, because small-scale physics makes an essential contribution to large-scale dynamics and must be fully resolved. This makes a direct numerical computation completely impractical.

Our main thrust was to develop data assimilation techniques suited to problems with nonlinear and possibly far from Gaussian statistical distributions. Greg Eyink (Johns Hopkins) had worked on mean variational techniques for the testing of turbulence closures. Upon seeing this it was immediately clear that the same ideas could be applied to the data assimilation problem. However, the formulation was computationally intractable. Hence, a considerable effort has been put in adapting these ideas to the estimation problem and making it computationally practical. The outcome, the mean field variational approach, is suboptimal when compared to the optimal approach of Kushner and others. It is thus of great utility but only in problems with state variables no larger than perhaps order 50. We then developed closure approximations to the mean fields. These allow us to consider larger problems. We proposed a variational method to calculate such conditional statistics in a computationally efficient way. There are two main elements of our approach: (i) a new cost function, the effective action, and (ii) a variational Rayleigh-Ritz method to calculate it.

The *effective action* is a nonnegative, globally convex functional of time-histories of the variable to be estimated. Its intuitive significance is that it gives the "cost" for a particular history to occur as a fluctuation in an average over an $N$-sample ensemble of independently prepared systems. It has been shown (G. Eyink, unpublished) that the minimizer of the effective action subject to constraints approximates the ensemble means conditioned upon those constraints. The approximation involved is of "mean-field type", in that conditioning is on the $N$-sample averages rather than the individual realizations themselves. The Hessian matrix of the effective action gives furthermore an approximation of the covariance matrix of fluctuations around this optimal history, conditioned upon the same constraints. Higher-order cumulants of fluctuations can also be obtained from higher-order derivatives of the effective action.

What makes the effective action attractive as a means to approximate the required conditional statistics is the existence of a practical variational scheme to calculate it. This *Rayleigh-Ritz method* was proposed earlier by us and its detailed development initiated in a series of works. Its basis is a mathematical characterization of the effective action through a constrained variation of a dynamical action, which is a functional on the joint space of random variables (observables) and probability distributions (states). Thus, the practical computational method requires as its inputs (i) a plausible guess of the system's single-time statistics and (ii) a choice of the dynamically relevant observables or variables of the system. The Rayleigh-Ritz method is essentially an extension of the standard method of moment-closure approximation, already widely used in the theory of multiscale statistical dynamics, e.g. turbulence and phase-ordering processes.

### A.3.2 Exact Calculation of Gradients

The problem we addressed computing gradients is the computation of gradients on finite storage machines. The explosive growth in both on-line computer memory and remote storage requirements of large-scale assimilation studies can be overwhelming and this is a major hurdle in the use of variational methods for data assimilation. Variational data assimilation is a least-squares technique for assimilation in which it is assumed that the optimal state of the system is an extrema of a carefully chosen objective function. When the model is linear (and the statistics stationary processes) it is easily shown that the variational methods is equivalent to the Kalman-Bucy approach and that these are optimal. Provided that an adjoint model is available, the required model gradient can be computed by integrating the model forward and its adjoint backwards. The gradient is then used to extremize the cost function with a suitable iterative or conjugate gradient solver.

The storage problem imposes a severe physical limitation on the size of assimilation studies, even on the largest of computers. Using a recursive strategy, a schedule can be constructed which enables the forward/adjoint model runs to be performed in such a way that storage requirements can be traded for longer computational times. This generally-applicable strategy enables data assimilation studies on significantly larger domains than would otherwise be possible given particular hardware constraints. We show that this trade-off is indeed viable and that when the schedule is optimized, the storage and computational times grow at most logarithmically. This work will be described in detail in an extended paper. This work is a collaboration with G. Leaf, ANL, A. Griewank of the University of Dresden.

### A.3.3 The Path Integral Method

One problem that the mean field approach has (in addition to not being suitable for large problems) is that it requires a great deal of effort in its implementation. We have thus abandoned this type of method and are currently favoring Bayesian ensemble approaches: these will readily accept an existing model (legacy code) and will operate as a black box. A promising approach is the Hybrid Monte Carlo sampling technique as applied to a path integral approach to data assimilation. The path integral approach allows us again to consider linear as well as nonlinear problems, Gaussian as well as non Gaussian problems. The covariance matrix need not be stored. The Hybrid Monte Carlo cleverly uses gradient information in the search for samples of the desired Bayesian distribution, i.e. the distribution conditioned on observations. Our latest idea is to apply a nonlocal matrix preconditioner to speed up the decorrelation times of the samples. The result is a significant speedup.

Our next steps are (1) to develop a black box assimilator, (2) to develop schemes for assimilation in which the observations can be moved to optimize the forecast, (3) to assimilate experimental data from a laboratory experiment (say particles moving in a flow) and model calculations (say the flow itself). The first of these aims has been motivated above. The second one is exploiting the availability of underwater gliding vehicles that can be remotely directed to measure field quantities in a flow. The third one is more of a proof of concept: can one use measured quantities from an experiment to improve computations or vice versa?

### A.3.4 The Diffusion Kernel Method

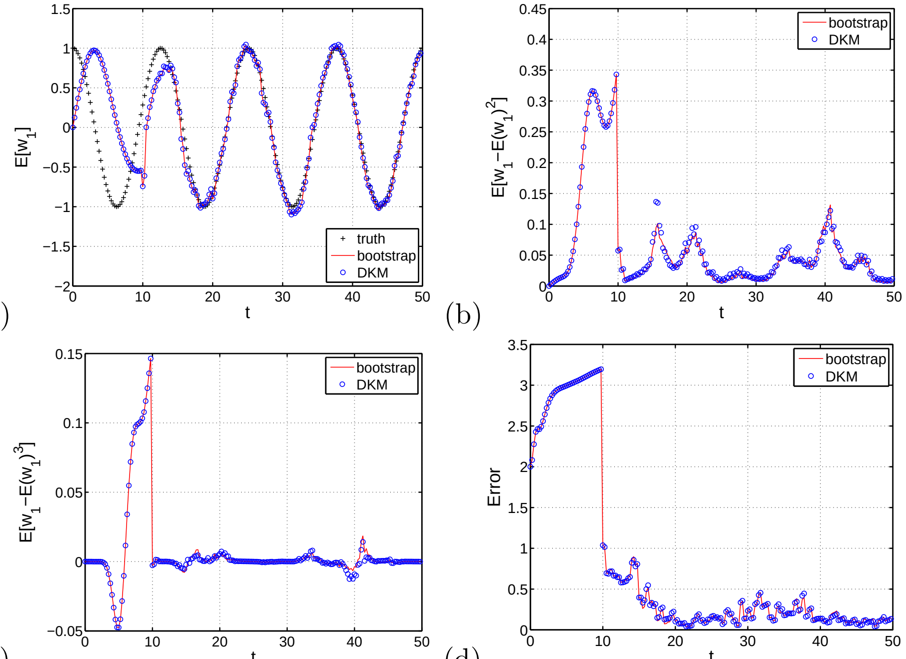
Starting with a general Langevin equation, we can show that the diffusion kernel method has at least two converging statistical moments in a filtering problem involving a model and data.

The general idea is to use the tangent linear model to advance the filter forward to the next filter time step over a small number of branches of prediction. At the filtering time step the Bayesian statement is used to condition the model prediction subject to partial or full data observations. These measurements can have inherent errors. At the new time step we use a fast sampling strategy to produce a population of weighted particles, which are then used to produce a new sample-moment estimate of the full state variable. The most important tool is the use of a functional which can be used to bound the covariance of the branches of predictions and these in turn are used to estimate the number of samples that are required at each time step.

The utility of this methodology is explored in the context of Lagrangian data assimilation, in which fast filtering techniques of fluid trajectories and drifters are generally nonlinear and non-Gaussian and a sub-optimal answer is preferable to the state of the art, which is currently the Extended Kalman Filter (which we can show fails in general). A problem in which the EKF fails is that proposed by Ide, *et al* [45]. Our results are fhown in Figure 18. The bootstrap is the true estimate of the moments. The DKM shows very good agreement with this estimate.

## A.4 Climate Variability

The ocean is the largest heat reservoir on earth and thus of fundamental importance to climate dynamics. Studying how the ocean overturns on advective time scales is essential if we are to understand climatic processes on a global scale. The thermohaline circulation is so called because the two most important components determining the buoyancy of ocean water are its mineral content or salt, and its heat content. Since freshwater inputs from rain, melting ice, river outflow, and precipitation/evaporation, affect the salt concentration in ocean water locally, and since the heat fluxes from the sun and polar ice caps are also spatially nonuniform, the ocean waters tend to sink, move from place to place, and upwell, transporting heat. This transport, of course, is also



(a) (b) (c) (d)

Figure 18: DKM estimate for $w(1,t)$. (a) Mean history, (b) second moment history, (c) third moment history. The red line corresponds to bootstrap moment estimates using the SDE. The blue line, which closely coincides with the bootstrap estimate, is the DKM moment estimations. The black line represents the truth. (d) (Red) boostrap average estimate error, (blue) DKM prediction error.

affected by the Earth's rotation, by oceanic currents, wind forcing, and the blocking and channeling effect of the land masses.

Paleoclimatic studies are suggesting that the thermohaline circulation may have played a causal role in the Dansgaard-Oeschger events and apparently a major role in the major rapid ice sheet collapses that occurred some 10 thousand years ago. Simple box-models of the thermohaline circulation show that several circulation solutions are possible, of which some are oscillatory. One of the most striking of such studies was Marotzke's above-cited work, in which a simple model for the dynamics and a simplified ocean topology are used to show that the strong production of North Atlantic Deep Water, as it is in present day, is one of four possible configurations for oceanic thermal circulation.

We revisited Stommel's box model, which was used to establish the non-unique character of the solutions to the climate equations using a low dimensional/low frequency approximation to the full dynamics. Prior to this work it was thought that waves and other advective effects would have little or no bearing on climate on long scales, as their energy and their coherence over long time scales are small. However, the results from this study showed that the equations are singular in behavior with respect to advective phenomena, such as waves. We incorporate advective effects into the model by means of delay equations and find that the behavior of the Stommel box-model with advection has self-sustaining oscillatory solutions. This behavior is singular, meaning that the oscillations do not vanish if the delay term is sufficiently large (but physical). The advection has the potential to produce self-sustaining oscillations (See Figure 8). When these effects are large enough we show that they can cause a transition in the dynamics of the box-model ocean from a thermally dominated solution to a haline-dominated solution. This work is a collaboration with D. Kurtze (NDSU).

The process of convective adjustment is also being studied in models ranging from simple box-models to fully 3-D ocean general circulation models. 'Convective adjustment' is the algorithmic approach to incorporating fast mixing in the water column of layer models of the primitive equations. The primitive equations are simplified versions of the equations for the large scale flow of the oceans (and with appropriate modifications, of the atmosphere). The crucial simplification is the assumption of hydrostatic momentum balance between the many layers composing the flow. This simplification has a number of consequences on the resulting flow. Among these is that the flow exhibits unrealistic vertical structure and mixing properties. In order to overcome these shortcomings, enhanced parametrizations, combined with convective adjustments, are invoked along the course of the computation. The result is a nominal improvement by the suppression of certain instabilities and the enhancement of viscous effects.

However, Cessi presented compelling evidence that certain aspects of the climate variability observed in large scale general circulation models (particularly in low resolution numerical experiments) are artifacts of the convective adjustment algorithm. In order to fully understand how convective adjustment affects the solutions in we study a low dimensional approximation to the quasi-geostrophic equations which incorporates convective adjustments. The outcome of our analysis is that Stommel-like exchanges (that is, horizontal and vertical convective exchanges), as well as the heat and salt capacity of the lower regions of the flow, can produce dramatically different solutions. In particular, we show that the finiteness of the lower ocean, with which the upper ocean convectively adjusts, leads to oscillations which at most decay in finite time. When the lower boxes of the model are made effectively infinite in capacity the convective adjustment algorithm easily leads to artificial sustained oscillations for certain forcing parameter values.

I am also currently working on an improvement over the convective adjustment algorithm and 'implicit vertical mixing' schemes currently used oceanic global circulation models. It is envisioned that improving the parameterization of the convective process, and incorporating fractional grid cell convection in low resolution climate models will, when implemented in an algorithmically efficient way, lead to significant improvements in both the locations in which convection occurs and the deep ocean tracer properties in current ocean general circulation models. This work is a collaboration with S. Peacock (LANL) and Douglas Kurtze (St. John).

### A.4.1 Carbon Cycle, Glacial/Interglacial Dynamics

During the last glacial era, the partial pressure of atmospheric carbon dioxide ($CO_2$) was around 200 ppmv. This is approximately 80 ppmv less than the preindustrial value of atmospheric $CO_2$. The ocean is the only reservoir large enough to cause such a dramatic change over those timescales. The ocean is able to store large amounts of $CO_2$ because it reacts with water to form an equilibrium with carbonate and bicarbonate ions. The distribution of total $CO_2$ (dissolved $CO_2$, carbonate and bicarbonate) throughout the ocean in controlled by air-sea exchange, the strength of the thermohaline flow, mixing between the surface and the deep water, and by the particulate flux of organic matter sinking to the bottom of the ocean. There is debate over the relative importance of the high and low latitude oceans in the storage of $CO_2$. Simple box models of the $CO_2$ cycle suggest that conditions in the high latitude oceans determine the amount of $CO_2$ the ocean is able to store. However, general circulation models (GCMs), indicate that the low latitude oceans also influence $CO_2$ storage. We have developed a box model which is shown to be consistent with the fundamental fluid and thermodynamic equations governing this flow. In fact, this aspect of consistency is amiss in the existing box models. Using this model, in conjunction with realistic parameter values, we show that both glacial and interglacial solutions may be achieved while conserving total carbon dioxide by changing the forcing of the model to reflect the climate. Our box model thus settles important aspects of the controversy. Since it simple mathematically, it provides a very convenient framework to study $CO_2$ dynamics in the ocean/atmosphere on grand scales.

## A.5 Solitary Waves in a Two-Fluid System with Surface Tension

Benjamin formulated an equation that models a new kind of solitary wave. This solitary wave is a solution of an equation that governs approximately waves on the interface of a two-fluid system in which surface tension effects cannot be ignored. The equation is

$$u_t + u_x + 2uu_x - \alpha L u_x - \beta u_{xxx} = 0, \tag{1}$$

where $\alpha > 0$ and $\beta \geq 0$, and $\alpha \ll \beta$ is the physically relevant range. The operator $L = H\partial_x$ is the composition of the Hilbert transform $H$ and the spatial derivative; $L$ is a Fourier multiplier operator with symbol $|\kappa|$ is essentially the Korteweg-de Vries equation however the fact that $\beta > 0$ endows its solutions with properties that are qualitatively different from the KdV-equation solutions.

We established the existence and stability of this new kind of solitary wave. The waves in question are symmetric about their crests, but unlike the classical Korteweg-de Vries solitary waves, they feature oscillatory tails. Computer-generated approximations of these waves reveal detailed aspects of their structure.

In a current study a numerical integrator is used to study time-dependent solutions. In particular, we find that fairly arbitrary data leads to bound state solutions. The interesting thing about these is that we see these types of solutions in other equations in which there is competition of dispersive effects, in addition to the usual quadratic nonlinearity. We also study the collisions of the solutions and from them assess their stability to nonlinear perturbations. This is work in collaboration with T. B. Benjamin, Oxford, J. L. Bona, UIC, and J. Albert, University of Oklahoma, and J. Hyman, LANL.

In a separate study we are used a pseudo-spectral and time-adaptive code to conduct a large series of numerical experiments which explore the rich behavior of orbitally-stable and unstable solutions to the generalized Benjamin-Bona-Mahony equation

$$u_t + \alpha u_x + (u^p)_x - u_{xxt} = 0, \tag{2}$$

where $u(x,t)$ is a real-valued function, $p \geq 2$ is an integer, and $\alpha \geq 0$ is a constant parameter. This equation has been the subject of intense analytical scrutiny. Bona *et al.* established the stability and instability of solitary waves for the KdV-type equations with polynomial dispersion, following a similar program to that established by Grillakis *et al.* with regards to the existence, uniqueness, stability, and continuous dependence of solution to initial conditions. The equation is rich in mathematical structure, and its study has yielded several important analytical tools that are useful in the analysis of related equations. The equation is also important because (for $p = 2$ and $p = 3$) it models waves in plasmas, ion-acoustic media, and water.

Souganidis and Strauss investigated the orbital stability of solutions to BBM-type equations for any $p$. S&S showed that solitary wave solutions of Eq. (2) are always orbitally stable if $\alpha = 0$. Further, except for $p > p_0 = 5$ and $0 < \lambda < c_0 \leq c$ solitary waves with speed $c$ are always stable. The solitary wave $\phi$ is *Z-stable* if for every $\varepsilon > 0$ there exists a $\delta > 0$ such that if $\|u_0 - \phi\|_Z < \epsilon$ then Eq. (2) has a unique solution in $C([0,\infty); Z)$, with $u(\cdot, 0) = u_0$, such that

$$\sup_{0 \leq t < \infty} \inf_{-\infty < s < \infty} \|u(\cdot, t) - \tau_s \phi\|_Z < \delta,$$

where $Z$ is a Banach space contained in the Sobolev space $H^1(\mathbf{R})$, and $\tau_s$ denotes the translation operator $(\tau_s f)(x) = f(x+s)$.

The experiments confirm the previously-derived theoretical stability estimates and, more importantly, yield insights into their behavior. We have found, among other things, that an initially small and hence slow soliton which is unstable will move to the stable regime by growing and speeding up, possibly shedding another soliton and/or a dispersive tail. Perhaps the most important result is that we show that arbitrary initial data will resolve itself into a train of solitary-waves. This is important because the resolution of solitary-waves is occurring in an equation that is clearly non-integrable. This work is in collaboration with W. McKinney, North Carolina State, and Jerry L. Bona, UIC.

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