Uncertainty Prediction and Intelligent Sampling for Ocean Estimation

Pierre F.J. Lermusiaux

T. Sapsis, P.J. Haley, M. Ueckermann, T. Sondergaard, K. Yigit, W.G. Leslie, O. Logutov, A. Agarwal and J. Xu

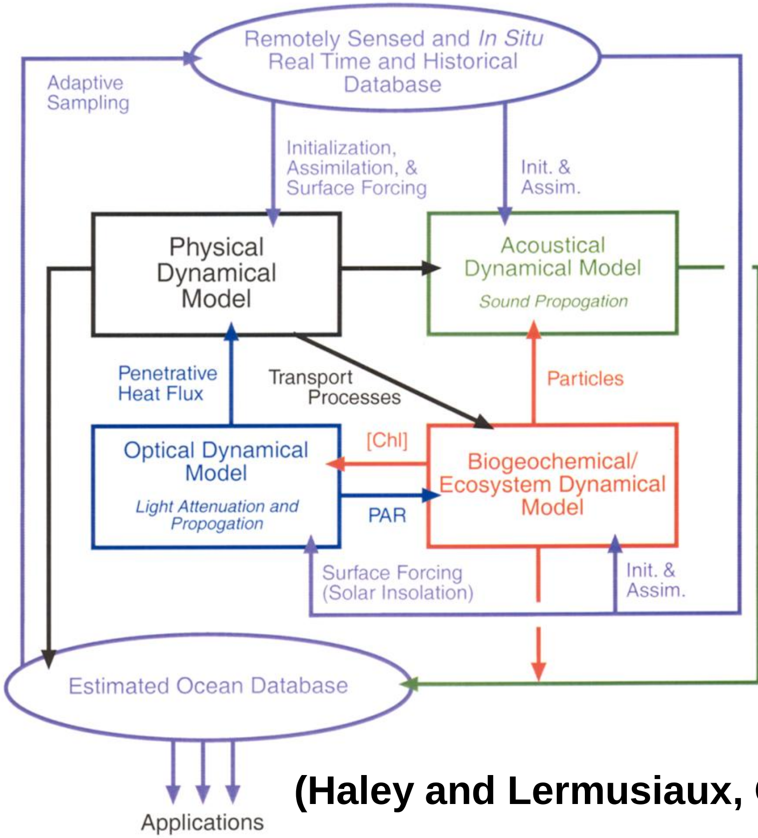
Mechanical Engineering, MIT

Multidisciplinary Simulation, Estimation and Assimilation Systems (MSEAS)
http://mseas.mit.edu/

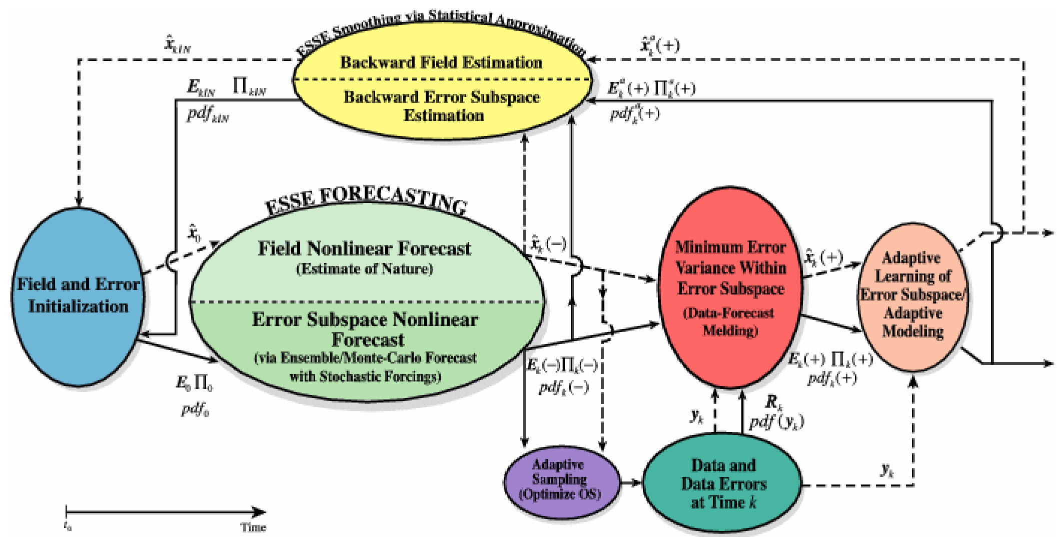
- **Introduction**
- **Two Grand Challenges in Ocean/Earth-System Sciences & Engineering**
  - **Prognostic Equations for Stochastic Fields of Large-Dimension**
  - **Intelligent Adaptive Sampling: the Science of Autonomy**
- **Conclusions**

Thanks to MIT, ONR and NSF (and many collaborators including C. Wunsch, N. Patrikalakis and H. Schmidt)

MIT Multidisciplinary Simulation Estimation and Assimilation System (MSEAS)



(Haley and Lermusiaux, OD-2010)



(Lermusiaux, PhysD-2007)

Stochastic Ocean Modeling Systems

Free-surface PE, Generalized Biological models, Coupled to acoustic models, XML schemes to check configuration, Unstructured grid models (Ueckermann et al)

Error Subspace Statistical Estimation

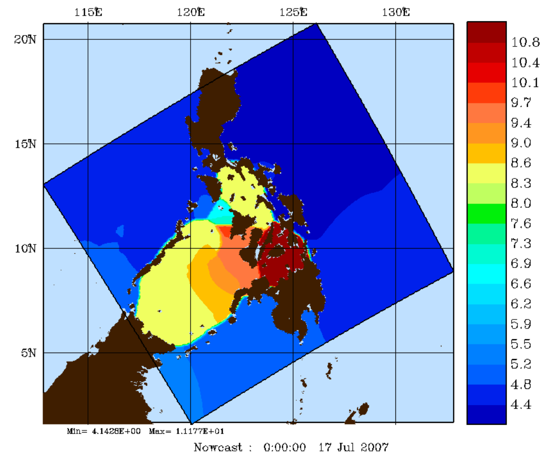
Uncertainty forecasts, Ensemble-based, Multivariate DA, Adaptive sampling, Adaptive modeling, Towards multi-model estimates

New MSEAS Methods and Codes

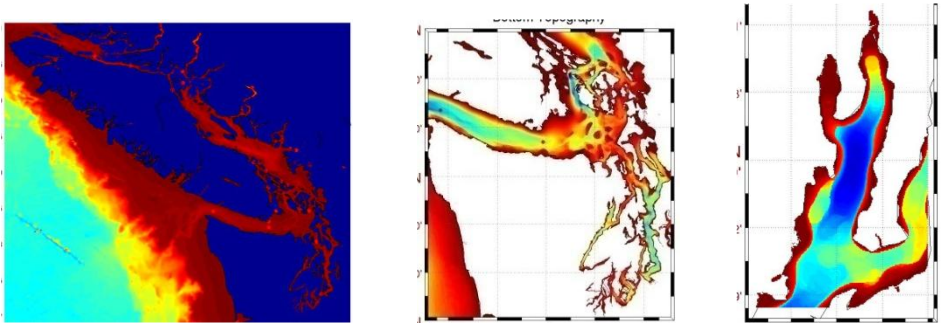
- **Two new OA schemes to remove correlations across ground but introduce 3D effects** (*Agarwal and Lermusiaux, 2008, in prep.*) based on:

  1. Fast Marching Method or Level Sets Method
  2. Numerical Diffusion Equation

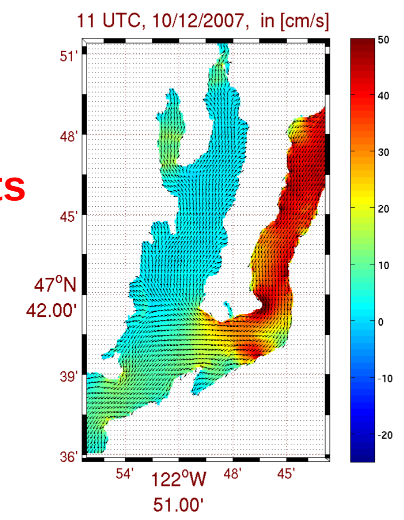
OA of T at 1000m in Philippines Strait



- **New Nested Barotropic Tidal Prediction and Inversion** (*Logutov and Lermusiaux, Ocean Mod.-2008; Logutov, Ocean Dyn.-2008*)



Tidal Currents [cm/s]



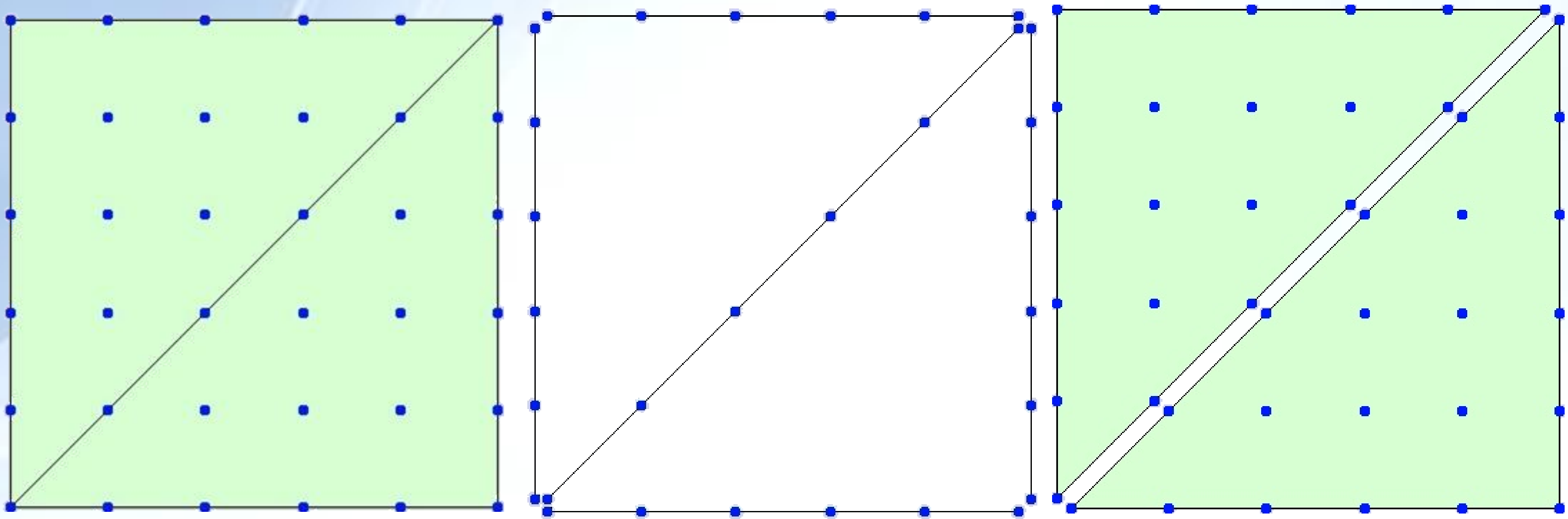
- **Uncertainty Estimation and Bayesian Fusion of Multi-Model Estimates** (*Logutov 2007 and Logutov et al, 2008, Lermusiaux et al, HOPS-ROMS-NCOM, In prep*):

Next-Generation Ocean Models

MIT Workshop August 2010, see: http://mseas.mit.edu/IMUM2010/

- Ocean Codes: Complex, based on 20-30 years old schemes
- Goal: Develop Multiscale Next-Generation Codes using new Technology

Continuous Galerkin | Hybrid Discontinuous Galerkin (HDG) | Discontinuous Galerkin

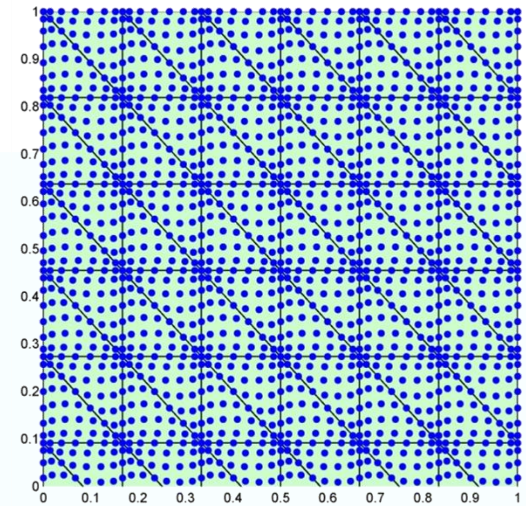


No duplication of DOF | Duplication at corners, but no interior DOFs! | Duplication at edges, too many DOFs

HDG Basics: if boundary value of element is known, the element is solved, Cockburn et al (2009)

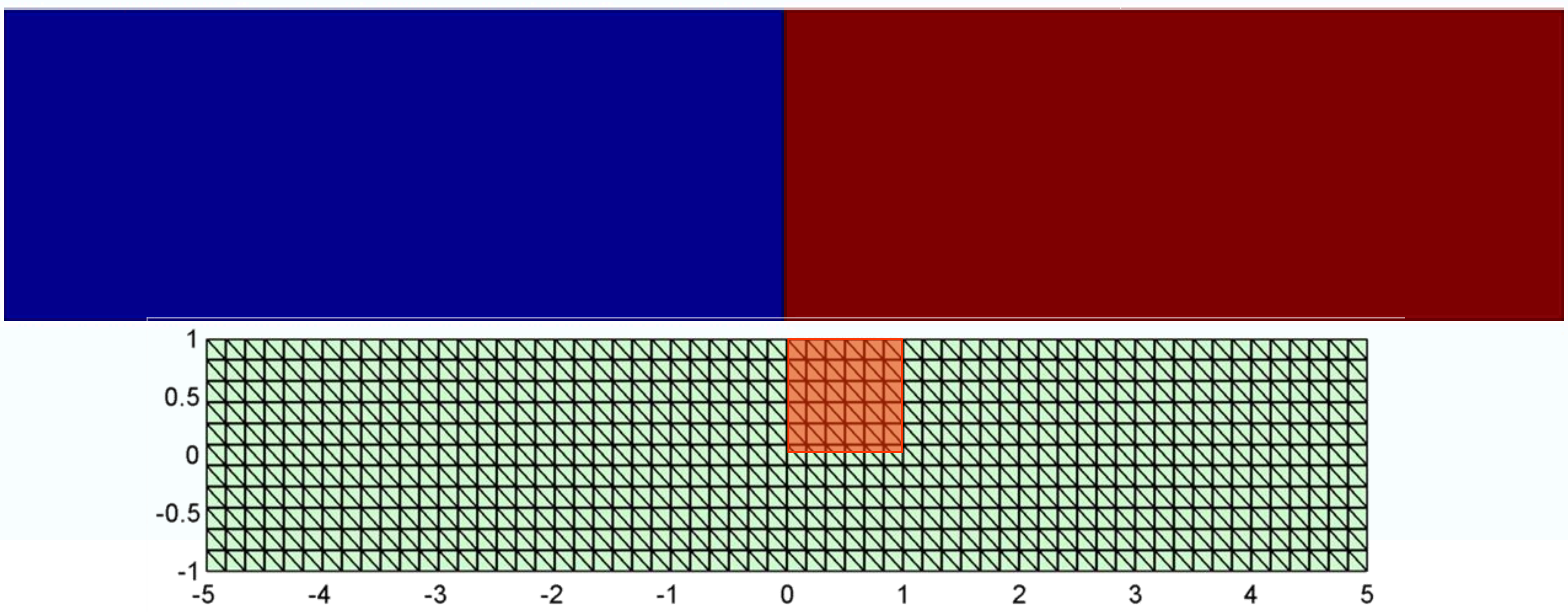
Ueckermann, MIT-SM-2009; Ueckermann and Lermusiaux, OD-2010, OM-2010)

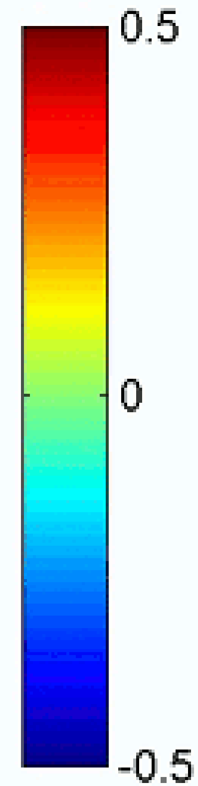
- 37,000 DOF, 14,000 HDG unknowns
- 13.5 hrs
- 1320 Elements
- *p*=6
- Gr = 1.25×10^6, Sc=0.71



time: 0

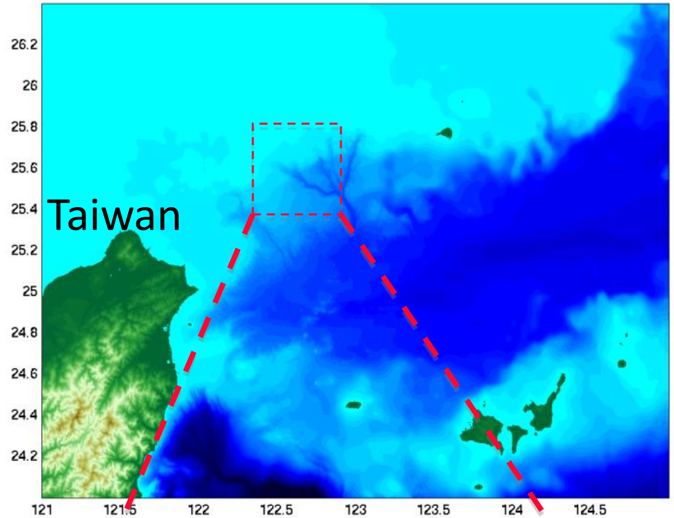
ρ



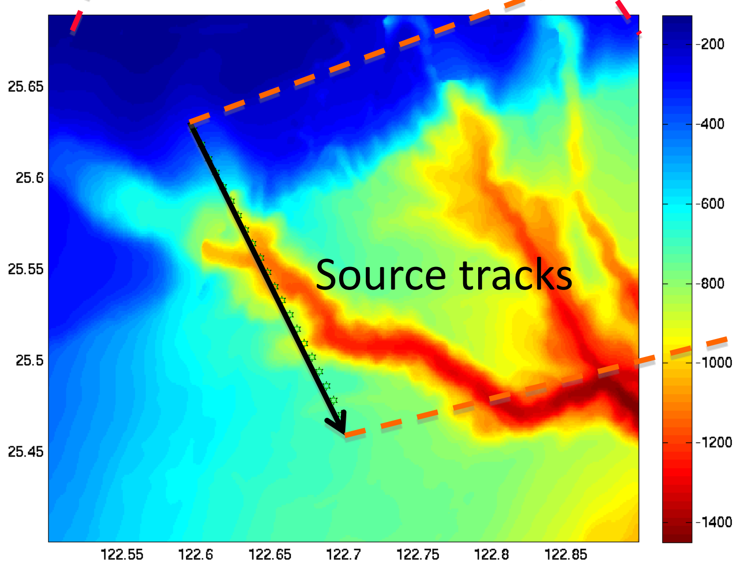


4. Hartel, C., Meinburg, E., and Freider, N. (2000). *Analysis and direct numerical simulations of the flow at a gravity-current head. Part 1. Flow topology and front speed for slip and no-slip boundaries.* J. Fluid. Mech, 418:189-212.

Quantifying, Predicting and Exploiting Uncertainty DRI: Canyon Acoustics - Xu and Lermusiaux, JOE-2010, JASA-2010

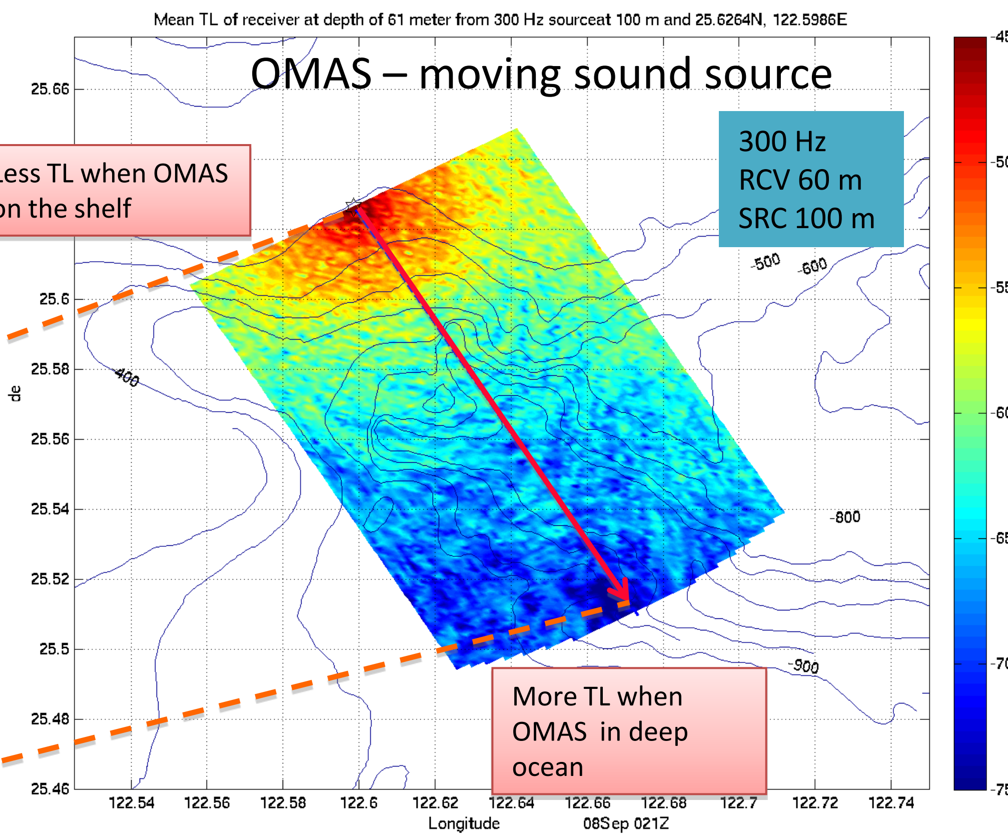


Bathymetry



Bathymetry of Mien Hua Canyon

Predict full sonified field in 3D environmental region and guide the locations of source and receiver deployment

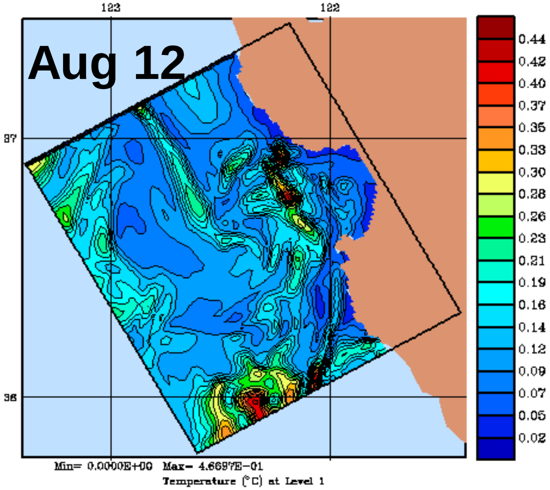


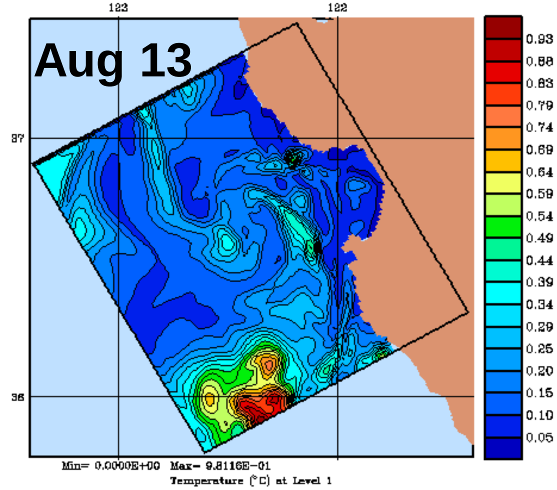
Nx2D (RAM) 15km propagation – 0.2 degree resolutions in 360 degree:

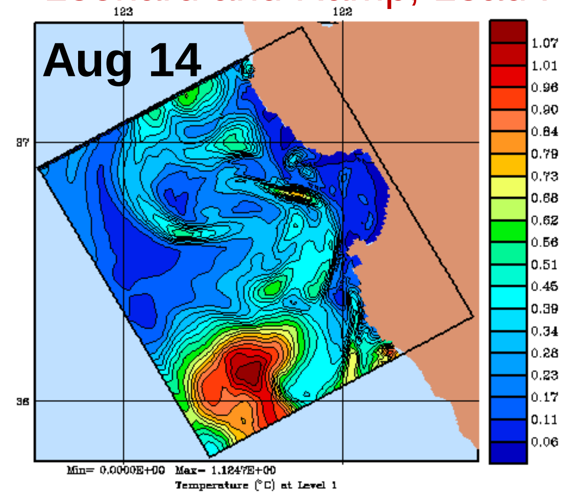
1800 (directions) X 15 locations

ESSE Surf. Temp. Error Standard Deviation Forecasts for AOSN-II

Leonard and Ramp, Lead PIs

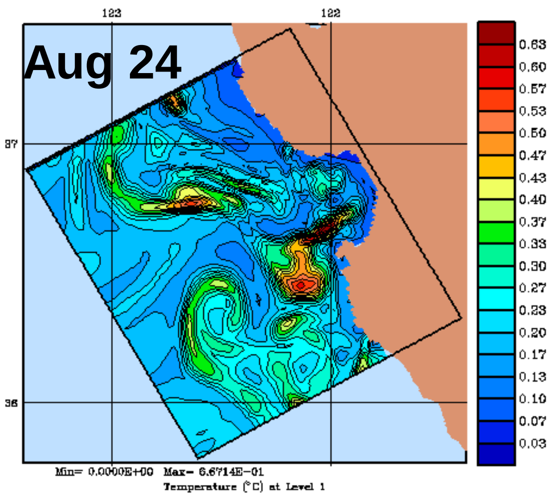


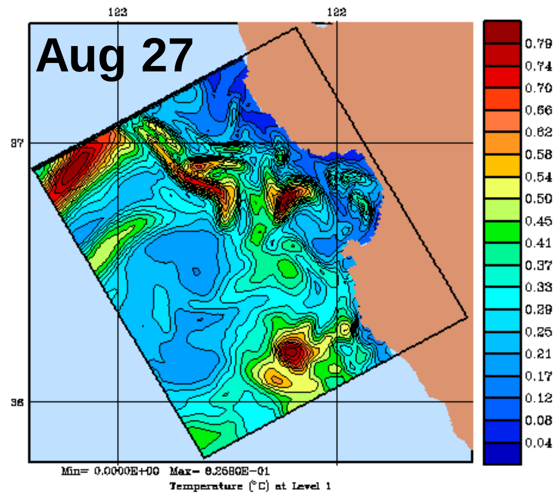


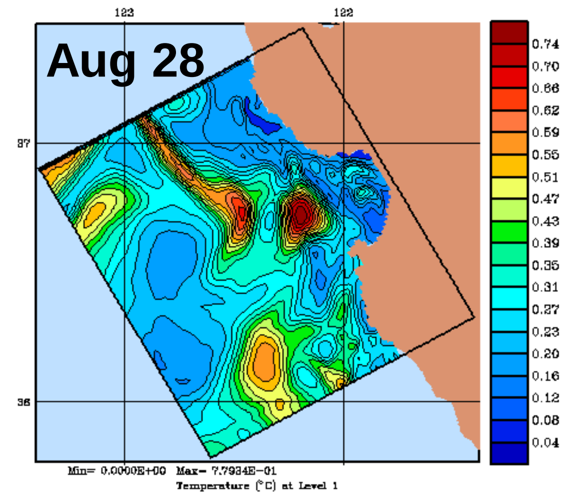


Start of Upwelling

First Upwelling period







End of Relaxation

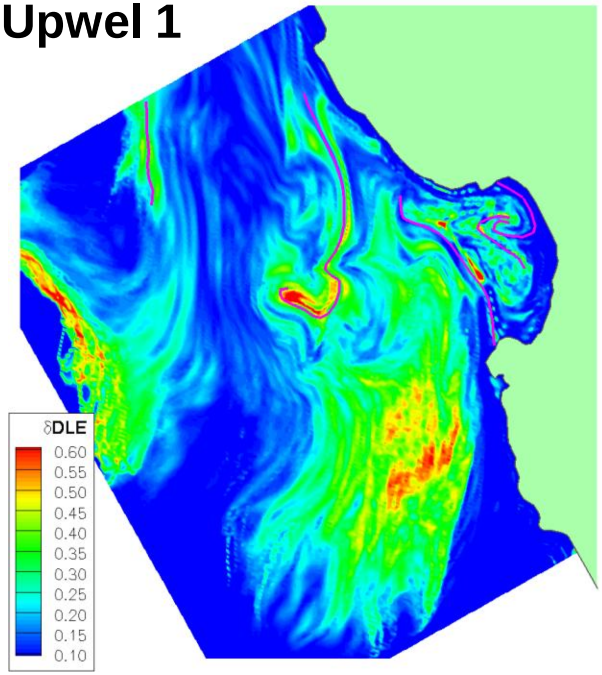
Second Upwelling period

- **Real-time consistent error forecasting, data assimilation and adaptive sampling (1 month)**
- **ESSE results described in details and posted on the Web daily**

Flow Skeletons and Uncertainties:
Mean LCS overlaid on DLE error std estimate for 3 dynamical events

- Two upwellings and one relaxation (**about 1 week apart each**)
- Uncertainty estimates allow to identify most robust LCS (more intense DLE ridges are usually relatively more certain)
- Different oceanic regimes have different LCS uncertainty fields and properties

Upwel 1

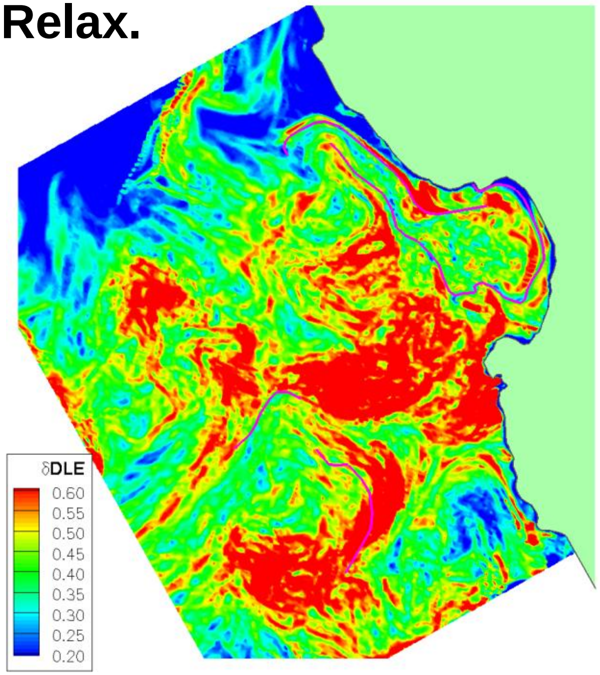


[Lermusiaux and Lekien, 2005. and In Prep, 2010

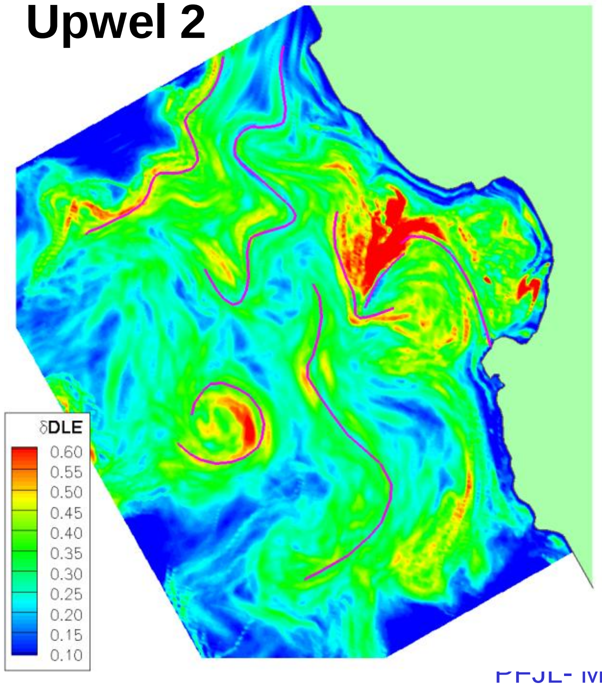
Lermusiaux, JCP-2006

Lermusiaux, Ocean.-2006]

Relax.



Upwel 2



A Grand challenge in Large Nonlinear Systems

Quantitatively estimate the accuracy of predictions

Computational challenges for the deterministic (ocean) problem

- Large dimensionality of the problem, un-stationary statistics
- Wide range of temporal and spatial scales (turbulent to climate)
- Multiple instabilities internal to the system
- Very limited observations

Need for stochastic modeling …

- Approximations in deterministic models including parametric uncertainties
- Initial and Boundary conditions uncertainties
- Measurement models

Need for data assimilation …

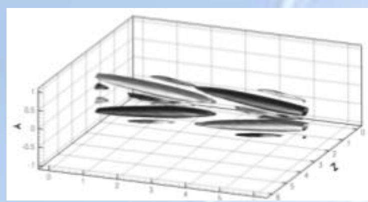
- Evolve the nonlinear, i.e. non-Gaussian, correlation structures
- Nonlinear Bayesian Estimation

Overview of Uncertainty Predictions Schemes

$$\boxed{\boldsymbol{u}(\boldsymbol{x},t;\omega)} = \bar{\boldsymbol{u}}(\boldsymbol{x},t) + \sum_{i=1}^{s} \boxed{Y_i(t;\omega)}\,\boxed{\boldsymbol{u}_i(\boldsymbol{x},t)}$$

Uncertainty propagation via POD method

[C. Rowley, Oberwolfach, 2008]



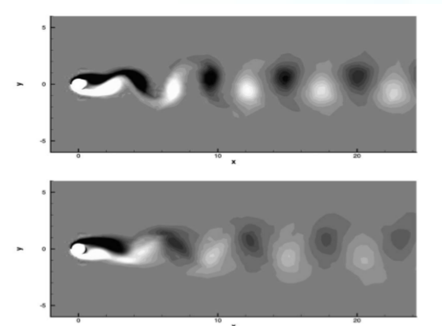
According to Lumley (Stochastic tools in Turbulence, 1971) it was introduced independently by numerous people at different times, including Kosambi (1943), Loeve (1945), Karhunen (1946), Pougachev (1953), Obukhov (1954).

Uncertainty propagation via generalized Polynomial-Chaos Method

Xiu & Karniadakis, J. Comp. Physics, 2002

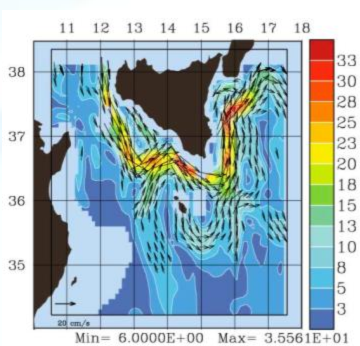
Knio & Le Maitre, Fluid Dyn. Research, 2006

Meecham & Siegel, Phys. Fluids, 1964



[Xiu & Karniadakis, J. Comp. Physics, 2002]

[Lermusiaux & Robinson, Deep Sea Research, 2001]



Uncertainty propagation via Monte Carlo method restricted to an "evolving uncertainty subspace"

(Error Subspace Statistical Estimation - ESSE)

Lermusiaux & Robinson, MWR-1999, Deep Sea Research-2001

Lermusiaux, J. Comp. Phys., 2006

B. Ganapathysubramanian & N. Zabaras, J. Comp. Phys., (under review)

Problem Setup

Statement of the problem: A Stochastic PDE

$$\frac{\partial \boldsymbol{u}(\boldsymbol{x},t;\omega)}{\partial t} = \mathcal{L}\left[\boldsymbol{u}(\boldsymbol{x},t;\omega);\omega\right] \qquad \boldsymbol{x} \in \boldsymbol{D}$$

$$\boldsymbol{u}(\boldsymbol{x},t_0;\omega) = \boldsymbol{u}_0(\boldsymbol{x};\omega) \qquad \boldsymbol{x} \in \boldsymbol{D} \qquad \mathcal{B}\left[\boldsymbol{u}|_{\partial \boldsymbol{D}}\right] = h(\partial \boldsymbol{D};\omega)$$

$\mathcal{L}(\bullet;\omega)$	Nonlinear differential operator (possibly with stochastic coefficients)
$\boldsymbol{u}_0(\boldsymbol{x};\omega)$	Stochastic initial conditions (given full probabilistic information)
$h(\partial \boldsymbol{D};\omega)$	Stochastic boundary conditions (given full probabilistic information)

Goal: Evolve the full probabilistic information describing $\boldsymbol{u}(\boldsymbol{x},t;\omega)$

An important representation property for the solution: Compactness

$$\boldsymbol{u}(\boldsymbol{x},t;\omega) = \bar{\boldsymbol{u}}(\boldsymbol{x},t) + \sum_{i=1}^{s} Y_i(t;\omega)\,\boldsymbol{u}_i(\boldsymbol{x},t)$$

Advantage: Finite Dimension Evolving Subspace

Disadvantage: Redundancy of representation

Evolving the full representation

Major Challenge : Redundancy

$$\boldsymbol{u}(\boldsymbol{x},t;\omega)=\bar{\boldsymbol{u}}(\boldsymbol{x},t)+\sum_{i=1}^{s}Y_i(t;\omega)\,\boldsymbol{u}_i(\boldsymbol{x},t)$$

First Step (easy): Separate deterministic from stochastic/error subspace

Commonly used approach: Assume that $\overline{Y_i(t;\omega)}=0$

Second step (tricky): Evolving the finite dimensional subspace $\mathcal{V}_S$

A separation of roles: What can $\dfrac{dY_i(t;\omega)}{dt}$ tell us ?

***Only** how the stochasticity evolves inside $\mathcal{V}_S$*

source of redundancy

A separation of roles: What can $\dfrac{\partial \boldsymbol{u}_i(\boldsymbol{x},t)}{\partial t}$ tell us ?

*How the stochasticity evolves **both** inside and normal to $\mathcal{V}_S$*

Natural constraint to overcome redundancy

Restrict "evolution of $\mathcal{V}_S$" to be "normal to $\mathcal{V}_S$" i.e.

$$\int \frac{\partial \boldsymbol{u}_i(\boldsymbol{x},t)}{\partial t}\,\boldsymbol{u}_j(\boldsymbol{x},t)\,d\boldsymbol{x}=0 \qquad \text{for all} \quad i=1,\dots,s \quad \text{and} \quad j=1,\dots,s$$

Dynamically Orthogonal Evolution Equations

Theorem 1: For a stochastic field described by the evolution equation

$$\frac{\partial \boldsymbol{u}(\boldsymbol{x},t;\omega)}{\partial t} = \mathcal{L}\left[\boldsymbol{u}(\boldsymbol{x},t;\omega);\omega\right], \quad \boldsymbol{x} \in \boldsymbol{D}$$

$$\boldsymbol{u}(\boldsymbol{x},t_0;\omega) = \boldsymbol{u}_0(\boldsymbol{x};\omega), \quad \boldsymbol{x} \in \boldsymbol{D} \qquad \mathcal{B}\left[\boldsymbol{u}(\boldsymbol{\xi},t;\omega)\right] = h(\boldsymbol{\xi},t;\omega), \quad \boldsymbol{\xi} \in \partial\boldsymbol{D}$$

assuming a response of the form $\boldsymbol{u}(\boldsymbol{x},t;\omega) = \bar{\boldsymbol{u}}(\boldsymbol{x},t) + \sum_{i=1}^{s} Y_i(t;\omega)\,\boldsymbol{u}_i(\boldsymbol{x},t)$

we obtain the following evolution equations

SDE describing evolution of stochasticity inside V_s

$$\frac{dY_j(t;\omega)}{dt} = \int_{\boldsymbol{D}} \mathcal{L}\left[\boldsymbol{u}(\boldsymbol{y},t;\omega)\right] - E^{\omega}\left[\mathcal{L}\left[\boldsymbol{u}(\boldsymbol{y},t;\omega)\right]\right] \boldsymbol{u}_j(\boldsymbol{y},t)\, d\boldsymbol{y}$$

Family of PDEs describing evolution of stochastic subspace V_s

$$\frac{\partial \boldsymbol{u}_j(\boldsymbol{x},t)}{\partial t} = E^{\omega}\left[Y_i(t;\omega)\,\mathcal{L}\left[\boldsymbol{u}(\boldsymbol{x},t;\omega)\right]\right]\boldsymbol{C}^{-1}_{Y_iY_j} - E^{\omega}\left[\int_{\boldsymbol{D}} \boldsymbol{u}_k(\boldsymbol{y},t)\, Y_i(t;\omega)\,\mathcal{L}\left[\boldsymbol{u}(\boldsymbol{y},t;\omega)\right] d\boldsymbol{y}\right]\boldsymbol{C}^{-1}_{Y_iY_j}\boldsymbol{u}_k(\boldsymbol{x},t)$$

$$\mathcal{B}\left[\boldsymbol{u}_j(\boldsymbol{\xi},t;\omega)\right] = E^{\omega}\left[Y_i(t;\omega)\, h(\boldsymbol{\xi},t_0;\omega)\right]\boldsymbol{C}^{-1}_{Y_iY_j}, \quad \boldsymbol{\xi} \in \partial\boldsymbol{D}$$

PDE describing evolution of mean field

$$\frac{\partial \bar{\boldsymbol{u}}(\boldsymbol{x},t)}{\partial t} = E^{\omega}\left[\mathcal{L}\left[\boldsymbol{u}(\boldsymbol{x},t;\omega)\right]\right], \ \boldsymbol{x} \in \boldsymbol{D} \qquad \mathcal{B}\left[\bar{\boldsymbol{u}}(\boldsymbol{\xi},t;\omega)\right] = E^{\omega}\left[h(\boldsymbol{\xi},t;\omega)\right], \ \boldsymbol{\xi} \in \partial\boldsymbol{D}$$

Sapsis and Lermusiaux, Physica D (2009)

POD & PC methods from DO equations

SDE describing evolution of stochasticity inside V_s

$$\frac{dY_j\;\;t;\omega}{dt} = \int_D \mathcal{L}\left[\boldsymbol{u}\;\;\boldsymbol{y},t;\omega\;\;\right] - E^{\omega}\left[\mathcal{L}\left[\boldsymbol{u}\;\;\boldsymbol{y},t;\omega\;\;\right]\right]\,\boldsymbol{u}_j\;\;\boldsymbol{y},t\;\;d\boldsymbol{y}$$

Family of PDEs describing evolution of stochastic subspace V_s

$$\frac{\partial \boldsymbol{u}_j\;\;\boldsymbol{x},t}{\partial t} = E^{\omega}\left[Y_i\;\;t;\omega\;\;\mathcal{L}\left[\boldsymbol{u}\;\;\boldsymbol{x},t;\omega\;\;\right]\right]\boldsymbol{C}^{-1}_{Y_iY_j} - E^{\omega}\left[\int_D \boldsymbol{u}_k\;\;\boldsymbol{y},t\;\;Y_i\;\;t;\omega\;\;\mathcal{L}\left[\boldsymbol{u}\;\;\boldsymbol{y},t;\omega\;\;\right]d\boldsymbol{y}\right]\boldsymbol{C}^{-1}_{Y_iY_j}\boldsymbol{u}_k\;\;\boldsymbol{x},t$$

$$\mathcal{B}\left[\boldsymbol{u}_j\;\;\boldsymbol{\xi},t;\omega\;\;\right] = E^{\omega}\left[Y_i\;\;t;\omega\;\;h\;\;\boldsymbol{\xi},t_0;\omega\;\;\right]\boldsymbol{C}^{-1}_{Y_iY_j},\;\; \boldsymbol{\xi}\in\partial\boldsymbol{D}$$

PDE describing evolution of mean field

$$\frac{\partial \bar{\boldsymbol{u}}\;\;\boldsymbol{x},t}{\partial t} = E^{\omega}\left[\mathcal{L}\left[\boldsymbol{u}\;\;\boldsymbol{x},t;\omega\;\;\right]\right],\;\; \boldsymbol{x}\in\boldsymbol{D} \qquad \mathcal{B}\left[\bar{\boldsymbol{u}}\;\;\boldsymbol{\xi},t;\omega\;\;\right] = E^{\omega}\left[h\;\;\boldsymbol{\xi},t;\omega\;\;\right],\;\; \boldsymbol{\xi}\in\partial\boldsymbol{D}$$

Choosing a priori the stochastic subspace V_s using POD methodology we recover POD equations.

Choosing a priori the statistical characteristics of the stochastic coefficients $Y_j\;\;t;\omega$ we recover the PC equations.

Formulation of Initial Conditions

Stochastic initial conditions

$$\boldsymbol{u}(\boldsymbol{x},t_0;\omega)=\boldsymbol{u}_0(\boldsymbol{x};\omega) \qquad \boldsymbol{x}\in\boldsymbol{D}$$

Formulation in stochastic subspace terms

Initial condition for the mean field equation

$$\bar{\boldsymbol{u}}(\boldsymbol{x},t_0;\omega)=E^{\omega}\left[\boldsymbol{u}_0(\boldsymbol{x};\omega)\right]$$

Initial condition for the basis of the error subspace

$$\boldsymbol{C}_{\boldsymbol{uu}}(\boldsymbol{x},\boldsymbol{y})=E^{\omega}\left[\left(\boldsymbol{u}_0(\boldsymbol{x};\omega)-\bar{\boldsymbol{u}}_0(\boldsymbol{x};\omega)\right)\left(\boldsymbol{u}_0(\boldsymbol{y};\omega)-\bar{\boldsymbol{u}}_0(\boldsymbol{y};\omega)\right)^T\right]$$

$$\int \boldsymbol{C}_{\boldsymbol{uu}}(\boldsymbol{x},\boldsymbol{y})\,\boldsymbol{u}_i(\boldsymbol{x})\,d\boldsymbol{x}=\lambda_i^2\boldsymbol{u}_i(\boldsymbol{y})$$

Computation of eigenvalues/eigenvectors

$$V_s(\sigma_{cr})=span\{\boldsymbol{u}_i(\boldsymbol{x})\,|\,\lambda_i>\sigma_{cr}\}$$

Selection of Error Subspace dimensionality

Lermusiaux et al, *Q.J.R. Meteorol. Soc.-1999*; Lermusiaux, JAOT-2001 Miller and Ehret, MWR-2002

Initial condition for the stochastic coefficients

$$Y_i(t;\omega)=\int_{\boldsymbol{D}}\left[\boldsymbol{u}_0(\boldsymbol{y};\omega)-\bar{\boldsymbol{u}}_0(\boldsymbol{y};\omega)\right]\boldsymbol{u}_i(\boldsymbol{y},t)\,d\boldsymbol{y}$$

Application I : Navier-Stokes in a cavity

2D viscous flow with stochastic initial conditions and no stochastic excitation

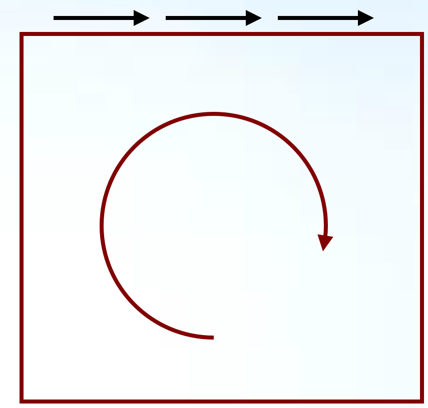
$$\frac{\partial u}{\partial t}+\frac{\partial P}{\partial x}=\frac{1}{\mathrm{Re}}\Delta u-\frac{\partial\; u^2}{\partial x}-\frac{\partial\; uv}{\partial y}$$

$$\frac{\partial v}{\partial t}+\frac{\partial P}{\partial y}=\frac{1}{\mathrm{Re}}\Delta v-\frac{\partial\; uv}{\partial x}-\frac{\partial\; v^2}{\partial y}$$

$$\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}=0$$

$u=U, v=0$

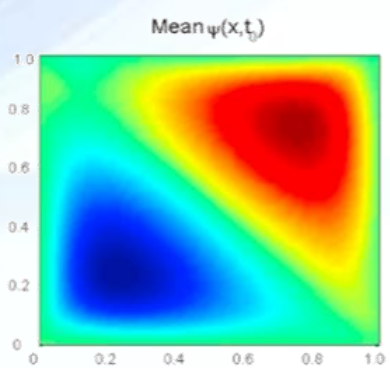
$u=0$ $\quad v=0$



$u=0$ $\quad v=0$

$u=0, v=0$

Initial mean flow



Streamfunction

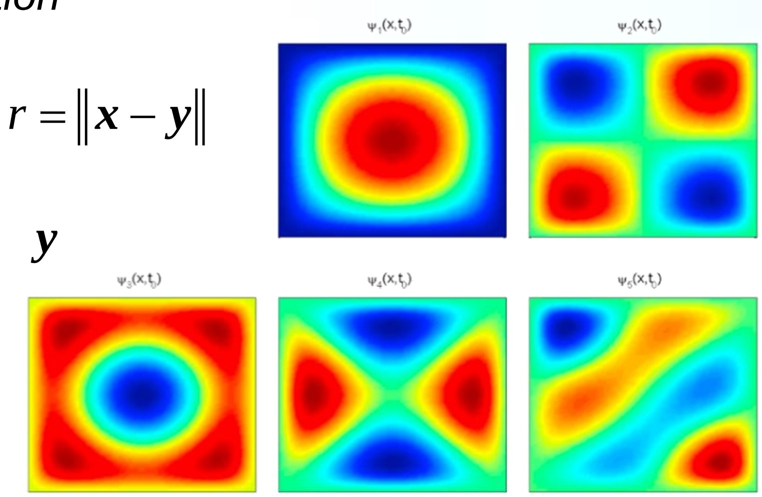
Initial Covariance function

$$C\;\; r\;\; =\left(1+br+\frac{b^2r^2}{3}\right)e^{-br} \qquad r=\left\|\boldsymbol{x}-\boldsymbol{y}\right\|$$

$$\int \boldsymbol{C}\;\; \left\|\boldsymbol{x}-\boldsymbol{y}\right\|\;\; \hat{\boldsymbol{u}}_i\;\; \boldsymbol{x}\;\; d\boldsymbol{x}=\lambda_i^2\hat{\boldsymbol{u}}_i\;\; \boldsymbol{y}$$

$$\boldsymbol{u}_{0,i}\;\; \boldsymbol{x}\;\; =\hat{\boldsymbol{u}}_i\;\; \boldsymbol{x}$$

$$Y_i\;\; t_0;\omega\;\; \sim\mathcal{N}\;\; 0,\lambda_i$$



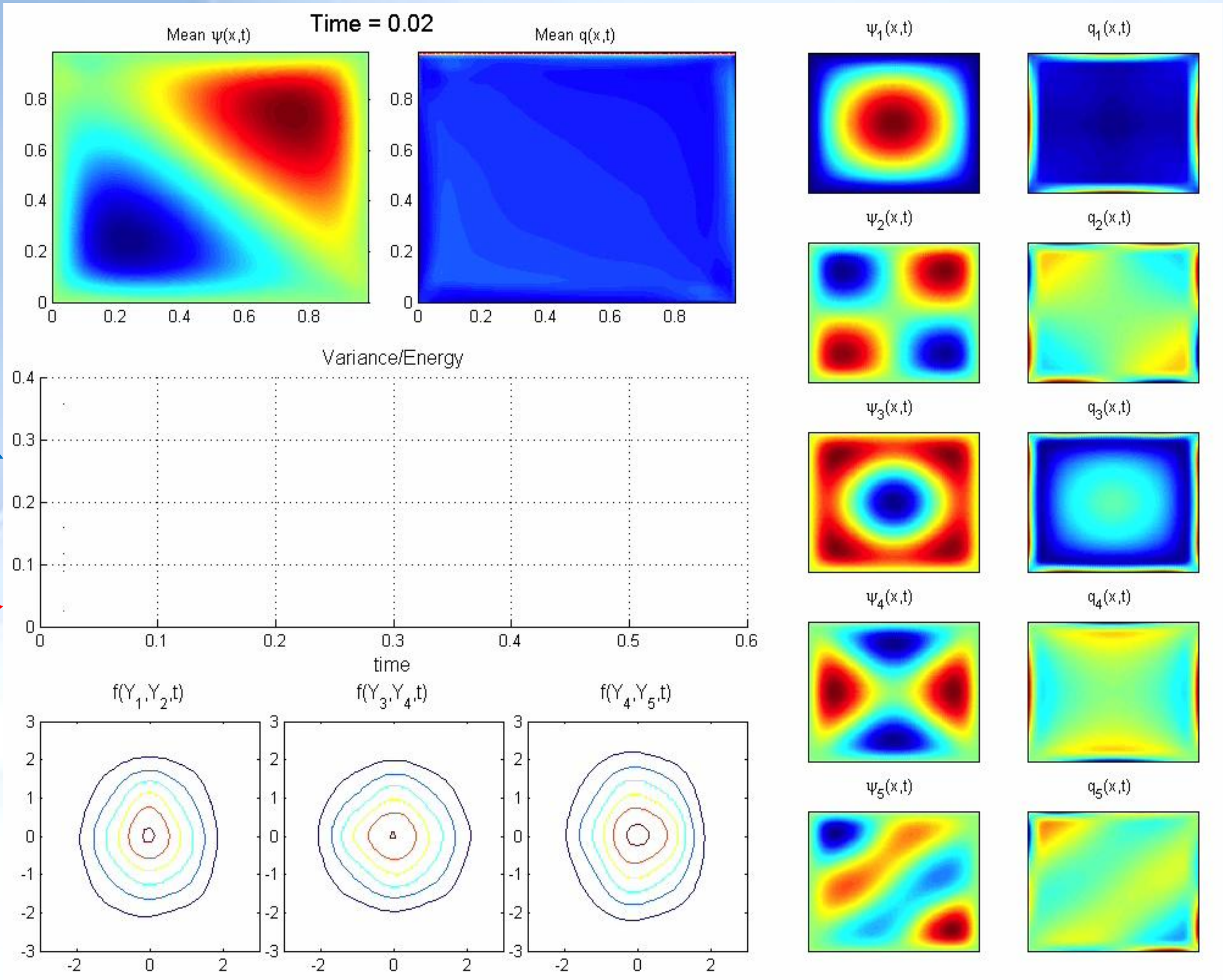
PDE Numerics: C-grid, upwind [M. Griebel et al., 1998] SDE Numerics: here, s-dimensional Monte-Carlo

Application I : Navier-Stokes in a cavity

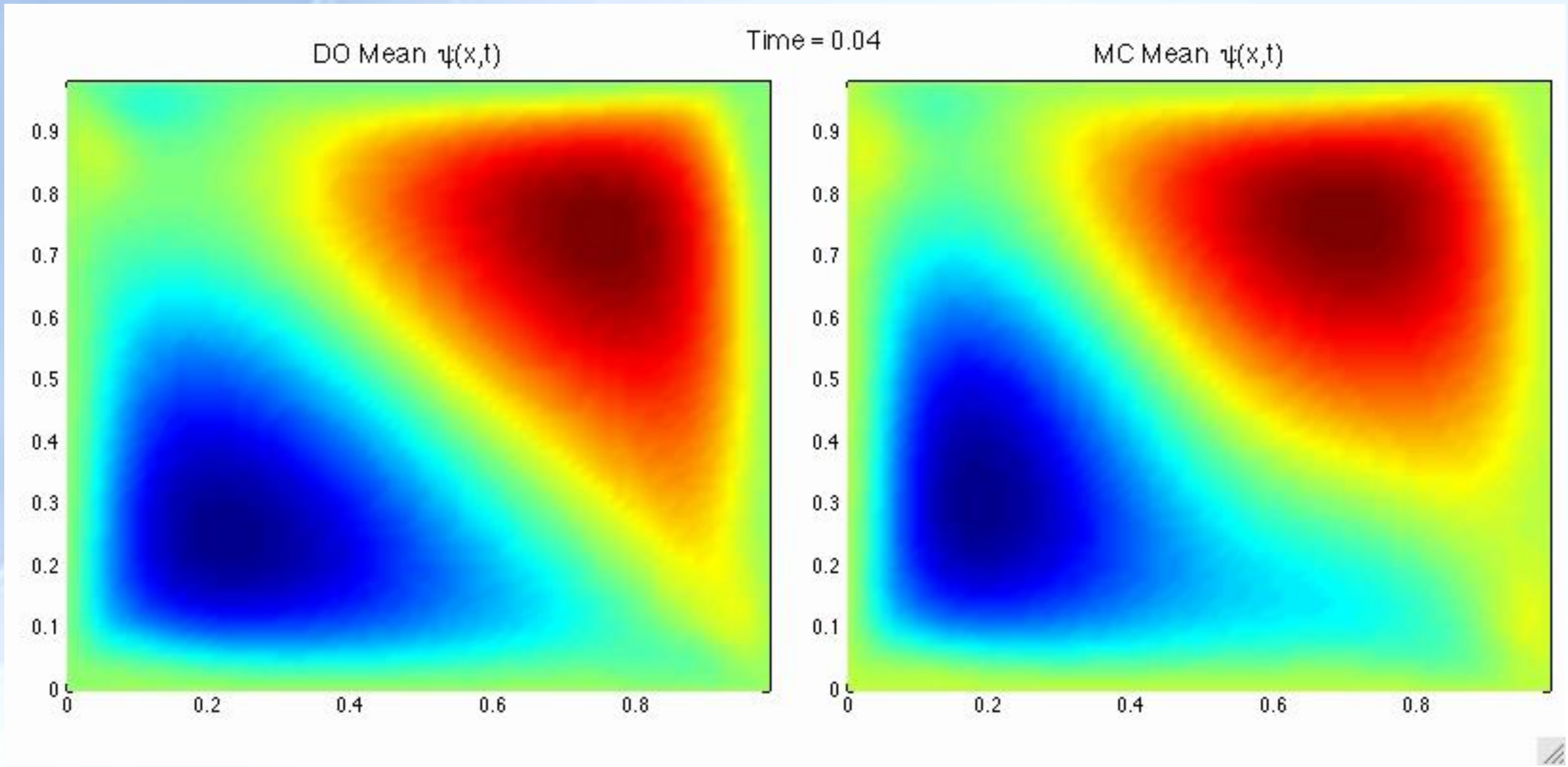
Re = 1000

Variances of each mode

Energy of mean flow



Comparison with Monte-Carlo

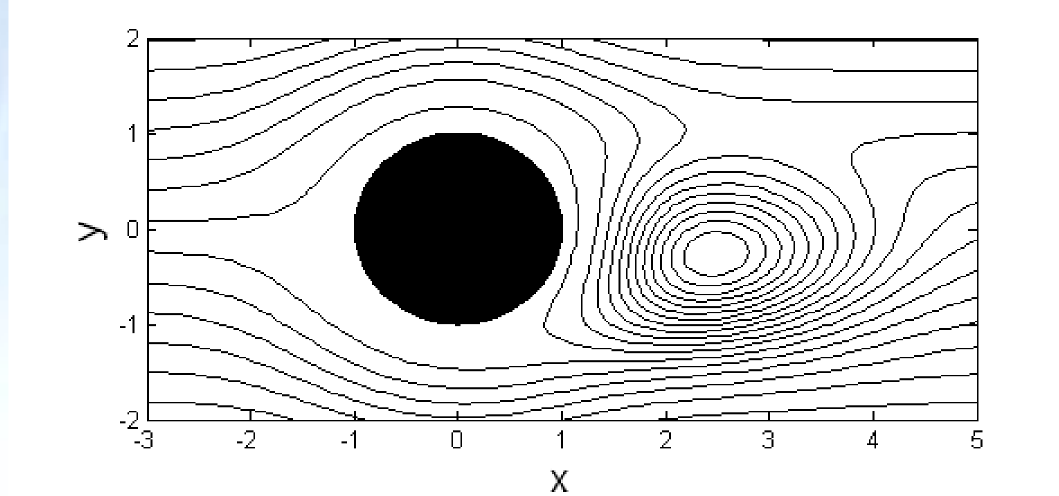


Comp. time: 11min (4000 samples) 12,3h (300 samples)

Application: Navier-Stokes behind a cylinder

von – Kármán vortex street behind a cylinder

Re = 100



Stochastic Initial Conditions

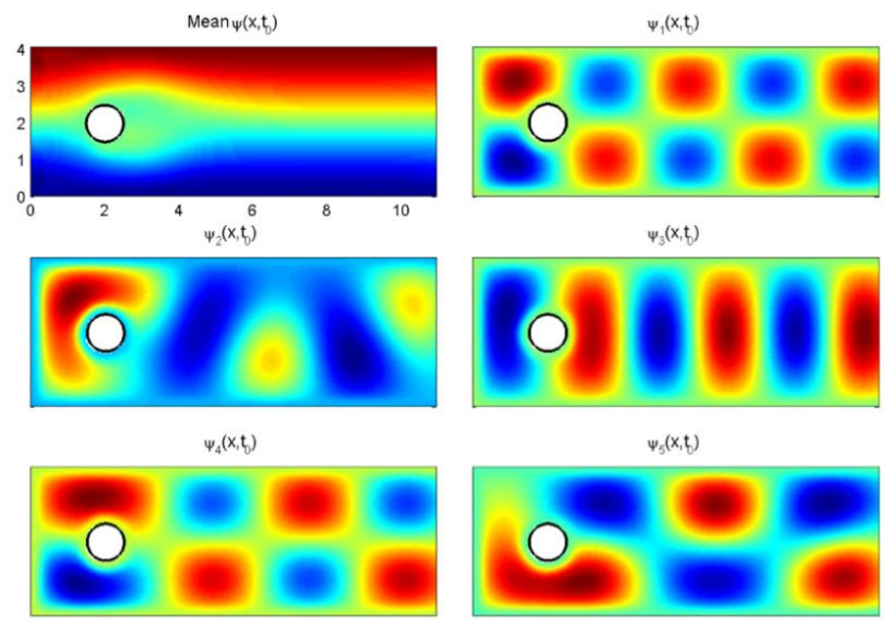
Gaussian Distribution

$$C\ \ r\ \ = \left(1+br+\frac{b^2r^2}{3}\right)e^{-br} \qquad r = \|\mathbf{x}-\mathbf{y}\|$$

$$\int \mathbf{C}\ \ \|\mathbf{x}-\mathbf{y}\|\ \ \hat{\mathbf{u}}_i\ \ \mathbf{x}\ \ d\mathbf{x} = \lambda_i^2 \hat{\mathbf{u}}_i\ \ \mathbf{y}$$

$$\mathbf{u}_{0,i}\ \ \mathbf{x}\ \ = \hat{\mathbf{u}}_i\ \ \mathbf{x}$$

$$Y_i\ \ t_0;\omega\ \ \sim \mathcal{N}\ \ 0,\lambda_i$$

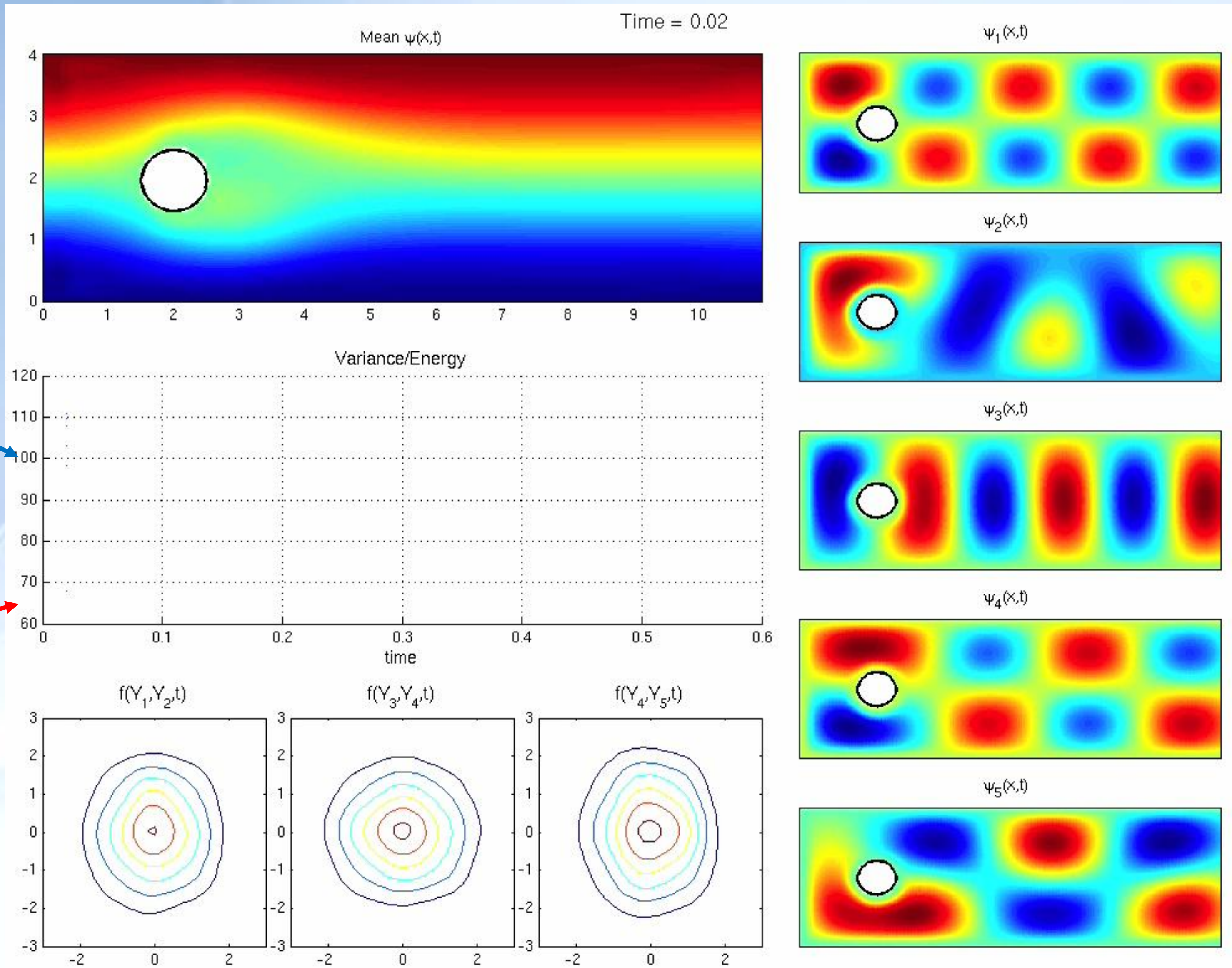


Application II: Navier-Stokes behind a cylinder

Re = 100

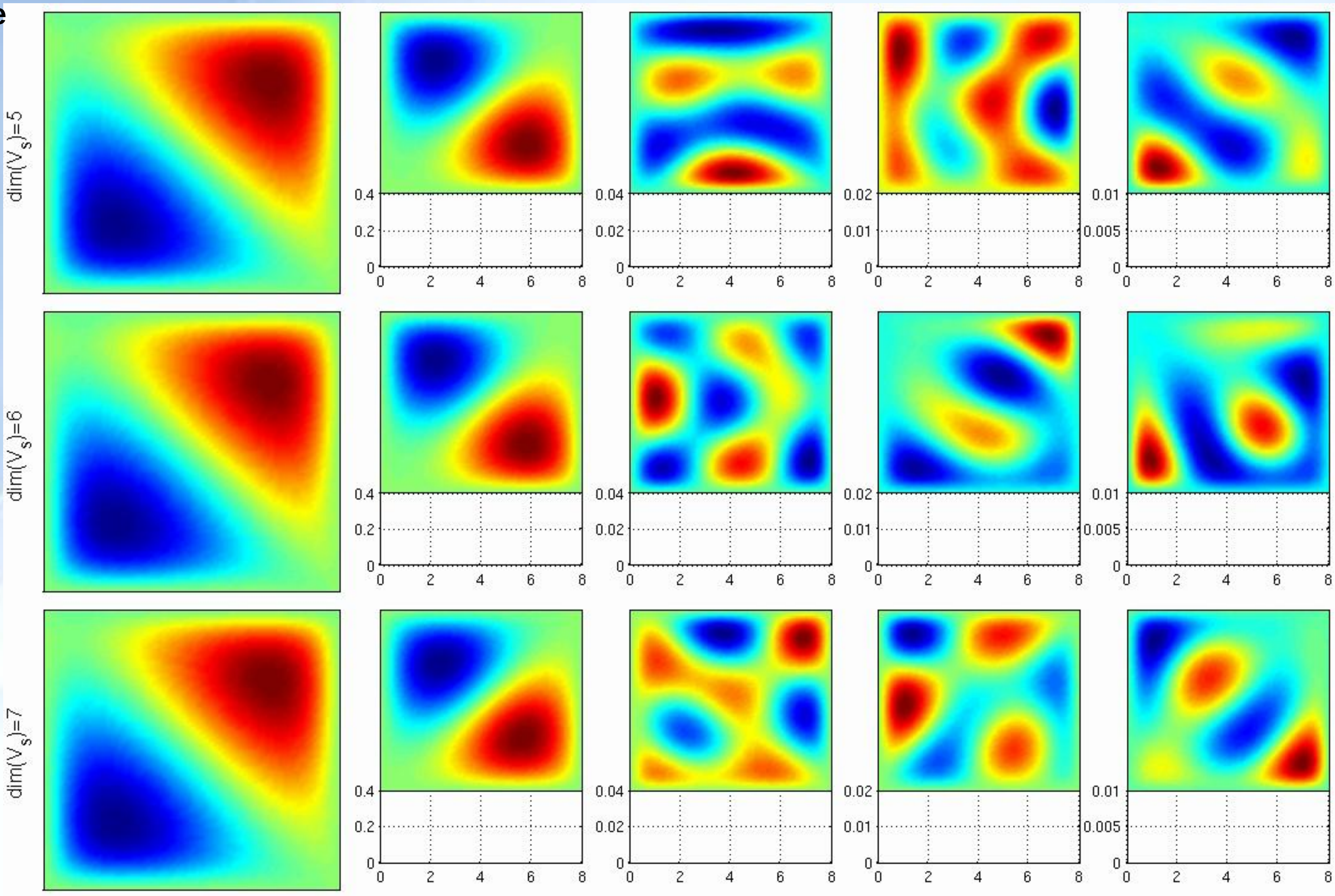
Variances of each mode

Energy of mean flow

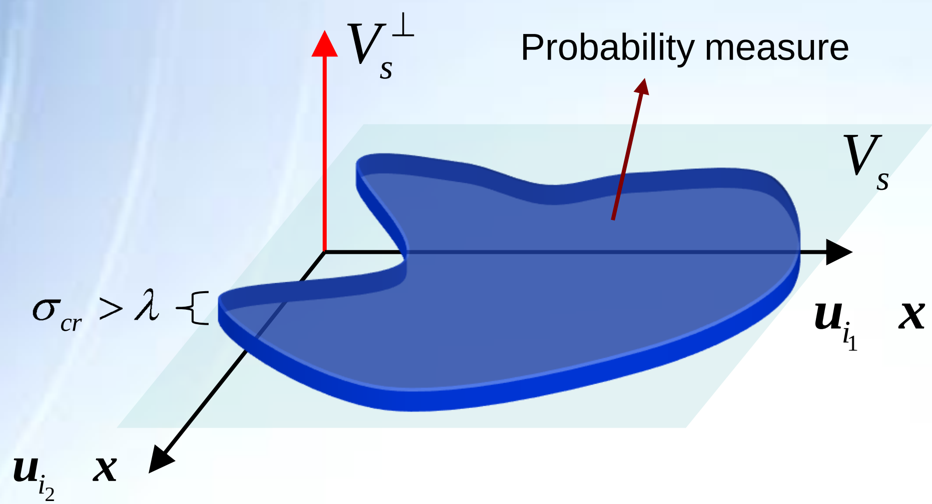


Example of Convergence Study

Subspace Size:	Mean	Mode 1	Mode 2	Mode 3	Mode 4
5					
6					
7					



Adapt the stochastic subspace dimension



- In the context of DO equations so far the size of the stochastic subspace V_s remained invariant.
- For intermittent or transient phenomena the dimension of the stochastic subspace may vary significantly with time. This is accounted for by ESSE.

We need criteria to evolve the dimensionality of the stochastic subspace

This is a particularly important issue for stochastic systems with deterministic initial conditions

Criteria for dimension reduction / increase

Dimension Reduction

Comparison of the minimum eigenvalue of the correlation matrix $\boldsymbol{C}_{Y_iY_j}$.

$$\lambda_{\min}\left[\boldsymbol{C}_{Y_iY_j}\right] < \sigma_{cr} \longrightarrow \text{pre-defined value}$$

Removal of the corresponding direction from the stochastic subspace.

Dimension Increase

Comparison of the minimum eigenvalue of the correlation matrix $\boldsymbol{C}_{Y_iY_j}$.

$$\lambda_{\min}\left[\boldsymbol{C}_{Y_iY_j}\right] > \Sigma_{cr} \longrightarrow \text{pre-defined value}$$

Addition of a new direction $\boldsymbol{u}_i \;\; \boldsymbol{x}, t$ in the stochastic subspace V_s.

How do we choose this new direction ?

Same problem when we start with deterministic initial condition
(dimension of stochastic subspace is zero)

Analytical criteria for selection of new directions

Theorem 2: For a stochastic field described by the evolution equation

$$\frac{\partial \mathbf{u}(\mathbf{x},t;\omega)}{\partial t} = \mathcal{L}\left[\mathbf{u}(\mathbf{x},t;\omega);\omega\right], \qquad \mathbf{x}\in \mathbf{D}$$

and with current state at $t = t_c$ described by

$$\mathbf{u}(\mathbf{x},t_c;\omega) = \bar{\mathbf{u}}(\mathbf{x},t_c) + \sum_{i=1}^{s} Y_i(t_c;\omega)\,\mathbf{u}_i(\mathbf{x},t_c)$$

the maximum variance growth rate of a stochastic perturbation in $V_s^{\perp}$ will be given by

Frechet Derivative

$$\rho\left[t_c;\mathbf{u}(\mathbf{x},t;\omega)\right] = \max_k \lambda_k\left[\frac{A_{ij}+A_{ji}}{2}\right], \qquad A_{ij} \equiv \int_{\mathbf{D}} \vartheta_j(\mathbf{y},t)\,\frac{\delta\mathcal{L}\left[\mathbf{u}(\bullet,t;\omega)\right]}{\delta\mathbf{u}}\left[\vartheta_i(\mathbf{y},t)\right]d\mathbf{y}$$

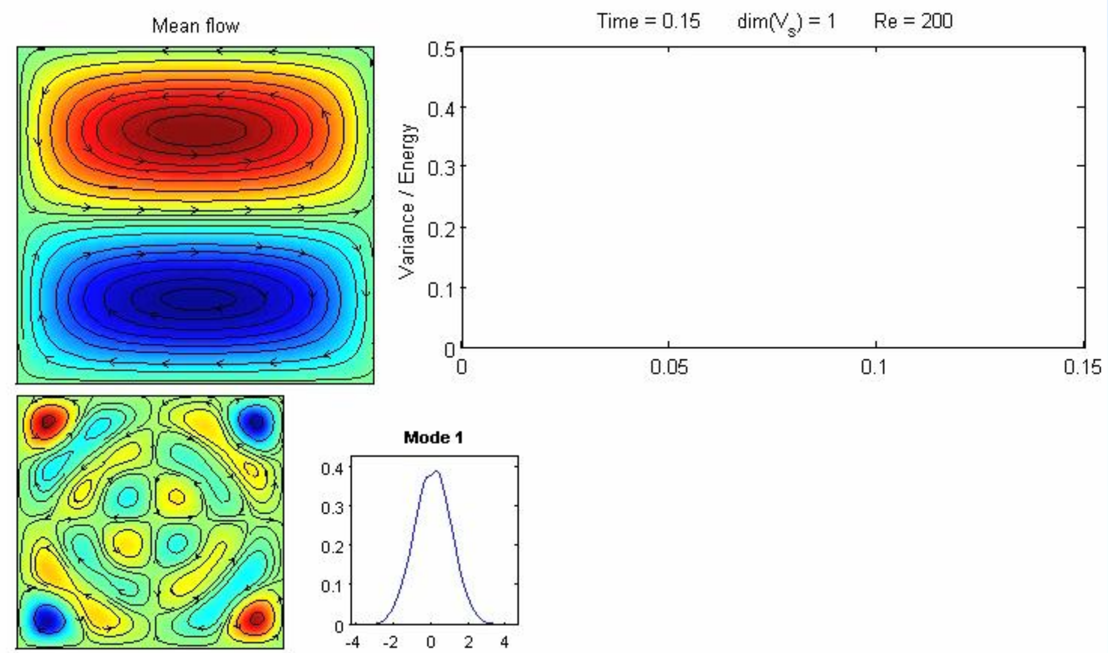
where $\vartheta_i(\mathbf{y},t),\ \ i=1,\dots,m$ is a finite basis that approximates $V_s^{\perp}$.

The corresponding direction of maximum growth is given by

$$\vartheta(\mathbf{x},t) = \sum_{i=1}^{m} v_i\,\vartheta_i(\mathbf{x},t)$$

where $v_i,\ \ i=1,\dots,m$ is the eigenvector associated with ρ.

Example: Double Gyre look-alike, Re=200



Deterministic
Initial Conditions

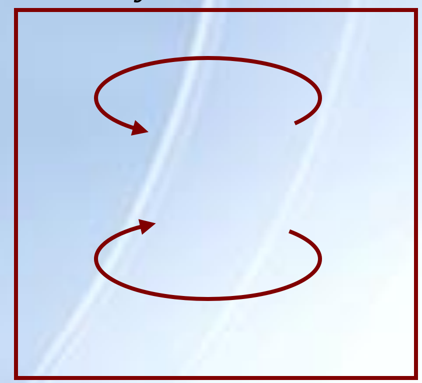
Stochastic behaviour of an idealized wind-driven ocean circulation model

Barotropic, single – layer quasi-geostrophic model (Simmonet and Dijkstra, 2002)

$$\frac{\partial u}{\partial y} = 0, v = 0$$

$u = 0$

$v = 0$



$u = 0$

$v = 0$

$$\frac{\partial u}{\partial y} = 0, v = 0$$

$$\frac{\partial u}{\partial t} + \frac{\partial P}{\partial x} = \frac{1}{\mathrm{Re}} \Delta u - \frac{\partial u^2}{\partial x} - \frac{\partial uv}{\partial y} + fv - \frac{a}{2\pi} \cos 2\pi y$$

$$\frac{\partial v}{\partial t} + \frac{\partial P}{\partial y} = \frac{1}{\mathrm{Re}} \Delta v - \frac{\partial uv}{\partial x} - \frac{\partial v^2}{\partial y} - fu$$

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \qquad f = f_0 + \beta_0 y$$

$$\boxed{\mathrm{Re} = \frac{UL}{A_H}; \quad a = \frac{\tau_0 L}{\rho d U^2}; \quad \beta = \frac{\beta_0 L^2}{U}}$$

- *Realistic parameters*
- *Zero initial conditions*
- *Small stochastic initial disturbance – Gaussian characteristics*
- *Adaptive number of modes*

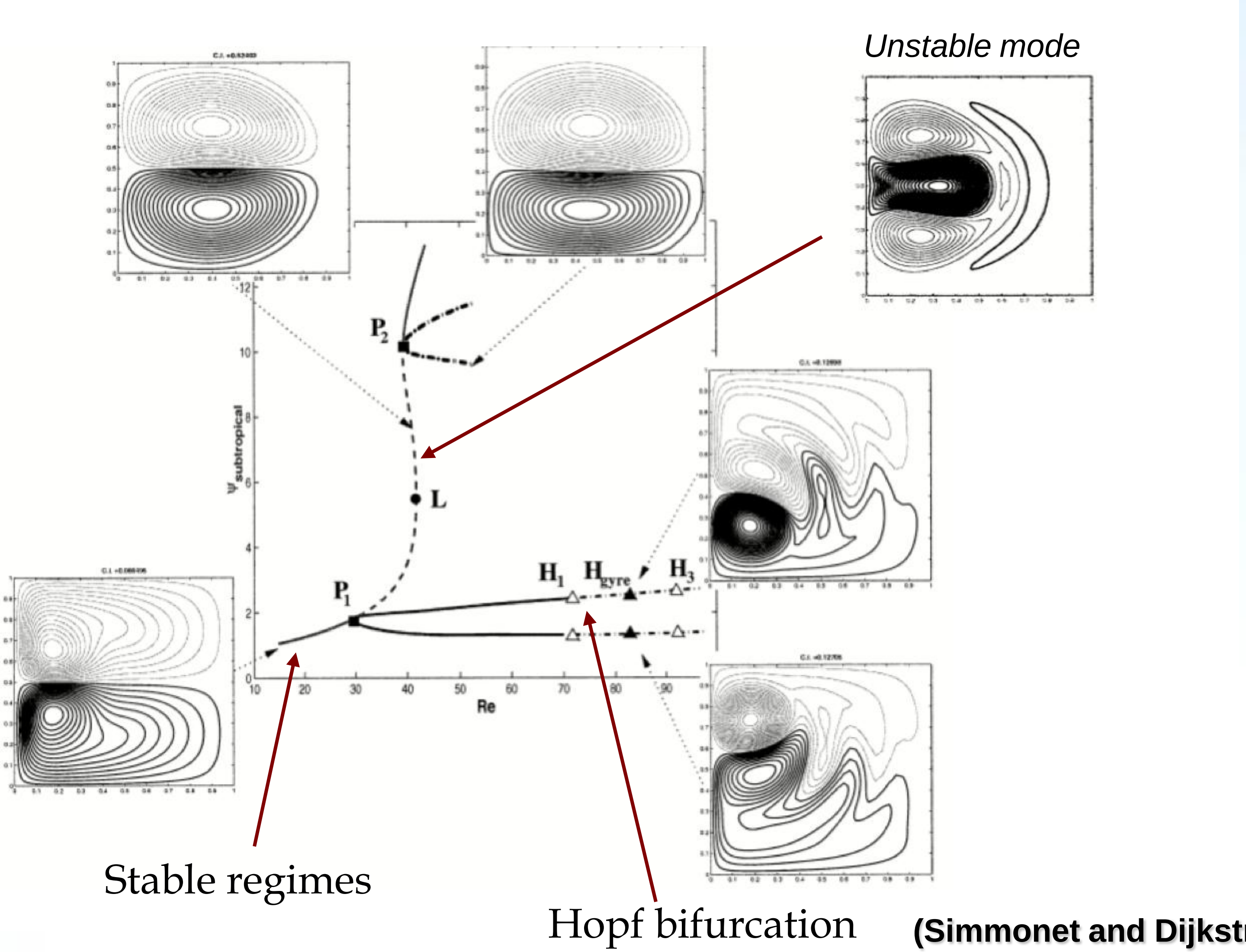
Dimensional parameters

Parameter	Value	Parameter	Value
U	$7.1 \times 10^{-3} m.s^{-1}$	L	$1.0 \times 10^6 m$
L/U	$4.46 yr$	D	$2500 m$
τ_0	$1.26 \times 10^{-1} Pa$	β_0	$7.1 \times 10^{-12} (m.s)^{-1}$
ρ	$10^3 Kg.m^{-3}$	f_0	$5.0 \times 10^{-5} s^{-1}$

Non - dimensional parameters

Parameter	Value	Parameter	Value
a	1000	β	10^3
F	0	μ	0

Bifurcation diagram

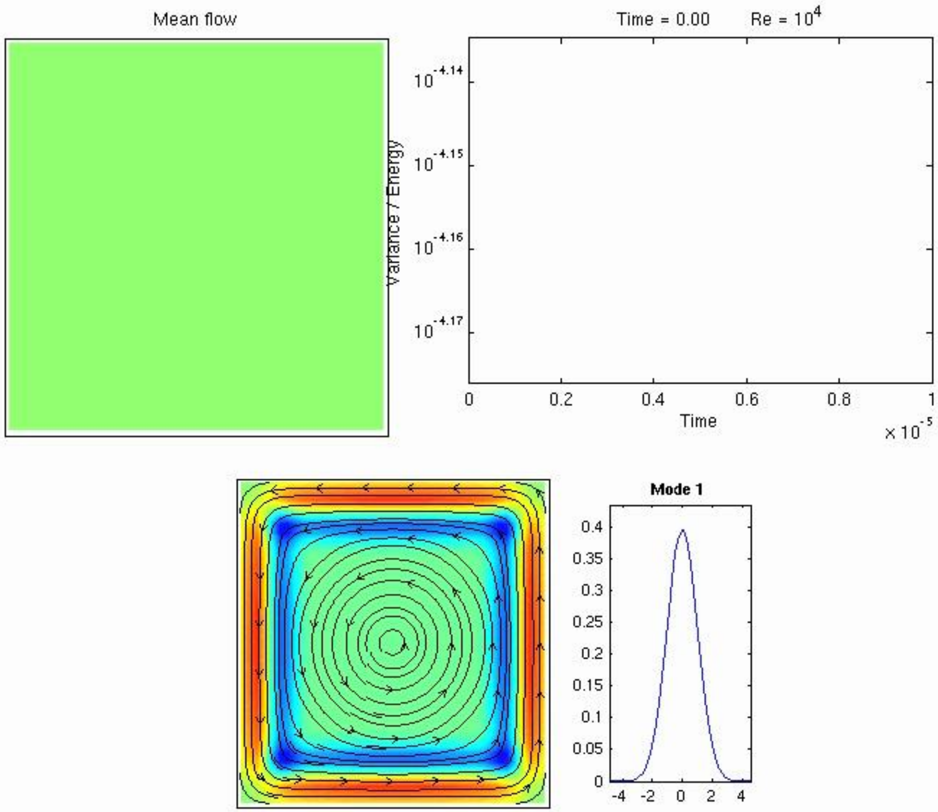


(Simmonet and Dijkstra, 2002)

Stochastic response for larger Reynolds/excitation

$$\frac{\partial u}{\partial t}+\frac{\partial P}{\partial x}=\boxed{\frac{1}{\mathrm{Re}}}\Delta u-\frac{\partial\, u^2}{\partial x}-\frac{\partial\, uv}{\partial y}+fv+\boxed{\frac{a}{2\pi}}\cos 2\pi y$$

$$\frac{\partial v}{\partial t}+\frac{\partial P}{\partial y}=\boxed{\frac{1}{\mathrm{Re}}}\Delta v-\frac{\partial\, uv}{\partial x}-\frac{\partial\, v^2}{\partial y}-fu \qquad f=f_0+\beta_0 y$$



Re = 1500, a = 3000

Re = 30000, a = 30000

- Mean flow reach, temporarily, a steady state regime.
- Modes variance is initially increasing monotonically through periodic oscillations.
- Subsequently variance is varying chaotically. At this point both the modes and the mean preserve their symmetry properties.
- Mean flow loses its stability and oscillations begin to occur, while the modes lose their symmetry.

- Detachment of the double gyre from the left boundary.
- Exponential growth of variance through periodic oscillations.
- Minor deformation of the mean flow from the modes.
- Periodic oscillations of the DO modes with two periods of oscillations.
- Both the modes and the mean preserve their symmetry properties.

- Mean flow forms a jet.
- DO modes consist of very small scale structures.
- Jet penetrates inside the basin up until the variance becomes comparable with the energy of the mean.
- For these ICs, Gaussian statistics are very robust although the variance is completely unsteady.
- Mean flow lose its structure.
- Transition to completely chaotic state.

Grand challenge II in Large Nonlinear Systems

Optimally sense the (ocean) system with large numbers of heterogeneous and autonomous vehicles that are smart

Smart Sensing Vehicle Swarms

- Knowledgeable about the predicted (ocean) system and its uncertainties
- Knowledgeable about the predicted effects of their sensing on future estimates

Our collaborative experience …

- Adaptive sampling via ESSE with non-linear predictions of error reductions
- Mixed Integer Linear Programming (MILP) for path planning
- Nonlinear path planning using Genetic algorithms
- Dynamic programming and onboard routing for path planning
- Command and control of vehicles over the Web, directly from model instructions

Our General Autonomy Problem Statement

Consider the spatially-discretized dynamical stochastic prediction (SPDEs) of the ocean state ***x*** and the data $\mathbf{y}_k$ collected by a spatially-discretized sampling ***H*** of a swarm of underwater vehicles:

$$d\mathbf{x} = \mathbf{M}(\mathbf{x}, t) + d\boldsymbol{\eta} \qquad (1)$$

$$\mathbf{y}_k = \mathbf{H}(\mathbf{x}_k, t_k) + \varepsilon_k \qquad (2)$$

Consider optimum estimate of **x** knowing $\mathbf{y}_k$ that is a function of the conditional probability p(**x**, t | $\mathbf{y}_k$) which is itself governed between observations by a Fokker–Planck equation (Lermusiaux, JCP-2006).

<u>General problem statement</u>: Predict and evolve ***H*** such that an objective function *J*, that is a function of the optimal estimate of **x** and of the evolving sensing plans **H(t),** is maximum.

J represents properties to be optimized by evolving swarming plans **H**: (uncertainties, hot-spots, coverage)

<u>Progress in ocean/weather prediction (ESSE/ETKF etc, Bishop, Majumdar)</u>
<u>New ocean aspects</u>: swarms, multi-scale, nonlinear (ESSE – DO equations)

Remarks on General Problem Statement

- Our autonomy problem is more than learning from data only (based on eqn. (2) only), which is often referred to as onboard routing with or without communications among vehicles
- Also more than classic robotics problems such as obstacle avoidance by swarms of vehicles or path planning that minimize energy utilization using the flow field. In these cases, the optimum estimation of the ocean state (based on fluid SDEs) is not used
- Also more than using dynamical system theory to steer groups of agents (also not coupled with ocean estimation itself)
- <u>Our Plan: combine schemes so that ocean prediction, learning and swarming are all part of single problem, with all feedbacks</u>
- Theoretical work generic and applicable to varied domains where the fields to be sensed are dynamic and of large-dimensions. However, applications focus on marine operations

Ocean Autonomy and Adaptive Sampling: Multiple Facets

Foci	- Optimal science & applications (Physics, Acoustics and Biology) - Demonstration of adaptive sampling value, etc.
Objective Functions	i. Maintain synoptic accuracy (e.g. regional coverage) ii. Minimize uncertainties (e.g. uncertain ocean estimates), or iii. Maximize sampling of expected events (meander, eddy, filament) Multidisciplinary or not - Local, regional or global, etc.
Time and Space Scales	i. Tactical scales (e.g. minutes-to-hours adaptation by each vehicle) ii. Strategic scales (e.g. hours-to-days adaptation for cluster/swarm) iii. Experiment scales
Assumptions	- Fixed or variable environment (w.r.t. asset speeds) - Objective function depends on the predicted data values or not - With/without constraints (operational, time and cost).
Methods	Control, Bayesian-based, Nonlinear programming, (Mixed)-integer programming, Simulated Annealing, Genetic algorithms, Neural networks, Fuzzy logics, Artificial intelligence, etc

Choices set the type of Autonomy research

a) Adaptive sampling via ESSE

[Lermusiaux, DAO-1999;
Lermusiaux, Physica D-2007;
Lermusiaux and Majumdar, In prep.]

- Objective: Minimize predicted trace of error covariance (T,S,U,V error std Dev).
- Scales: Strategic/Experiment. Day to week.
- Assumptions: Small number of pre-selected tracks/regions (based on quick look on error forecast and constrained by operation)
- Example of Problem solved: e.g. Compute today, the tracks/regions to sample tomorrow, that will most reduce uncertainties the day after tomorrow.

- Objective field changes during computation and is affected by data to-be-collected
- Model errors ***Q*** can account for coverage term

Dynamics: $dx = M(x)dt + d\eta \qquad \eta \sim N(0, Q)$

Measurement: $y = H(x) + \varepsilon \qquad \varepsilon \sim N(0, R)$

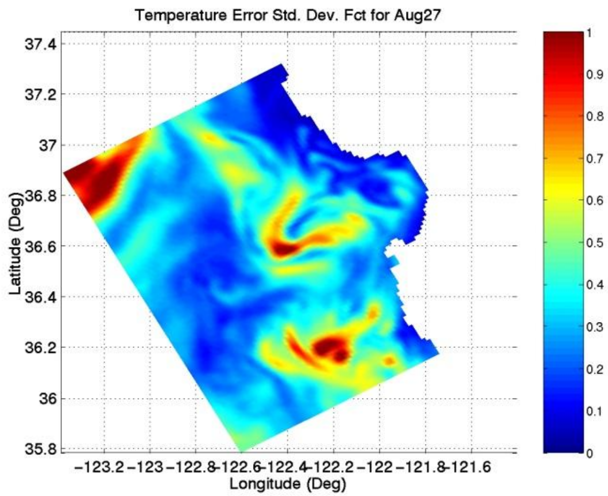
Non-lin. Err. Cov.:

$$dP/dt = <(x - \hat{x})(M(x) - M(\hat{x}))^T> + <(M(x) - M(\hat{x})(x - \hat{x})^T> + Q$$

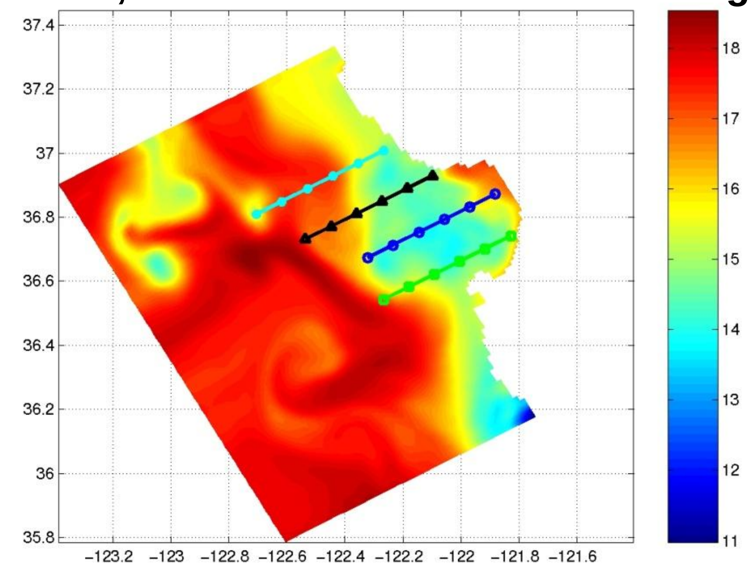
Metric or Cost function: e.g. Find future H_i and R_i such that

$$\underset{Hi,Ri}{Min} \quad tr(P(t_f)) \qquad or \qquad \underset{Hi,Ri}{Min} \int_{t_0}^{t_f} tr(P(t))\, dt$$

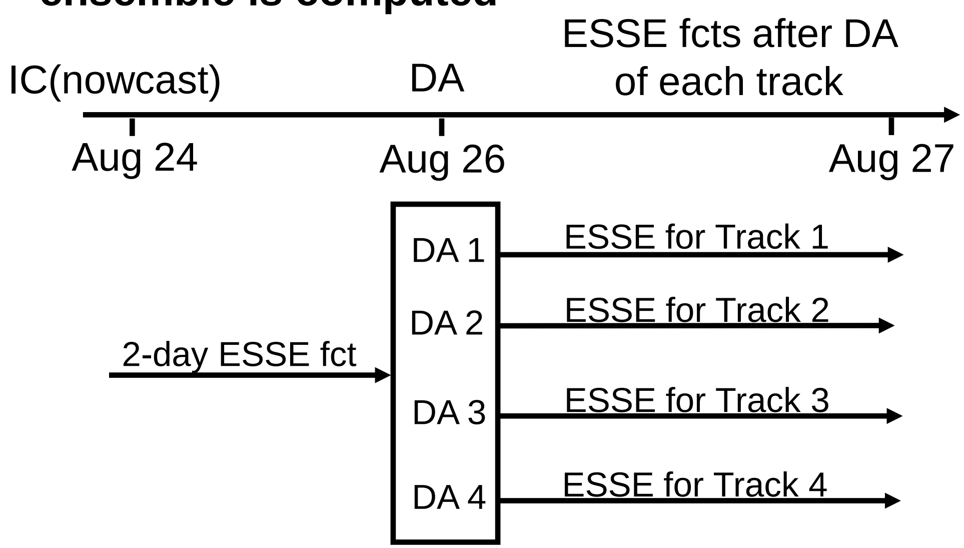
Which sampling on Aug 26 optimally reduces uncertainties on Aug 27?



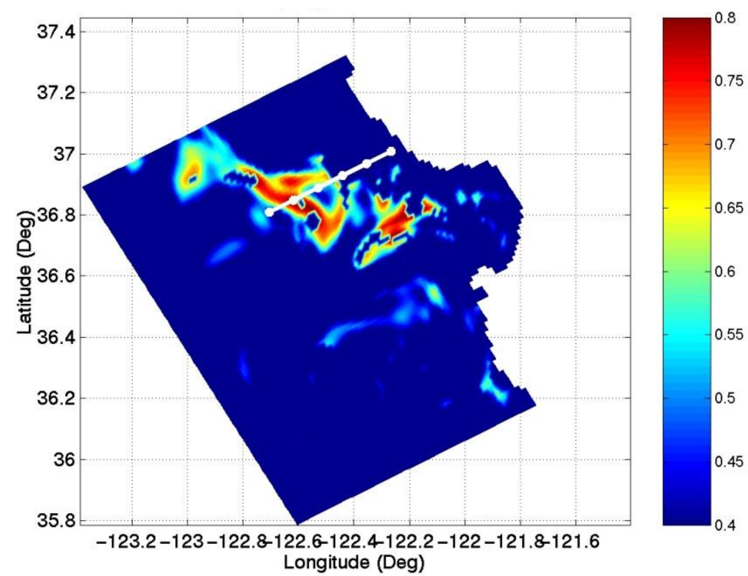
4 candidate tracks, overlaid on surface T fct for Aug 26



- **Based on nonlinear error covariance evolution**
- **For every choice of adaptive strategy, an ensemble is computed**



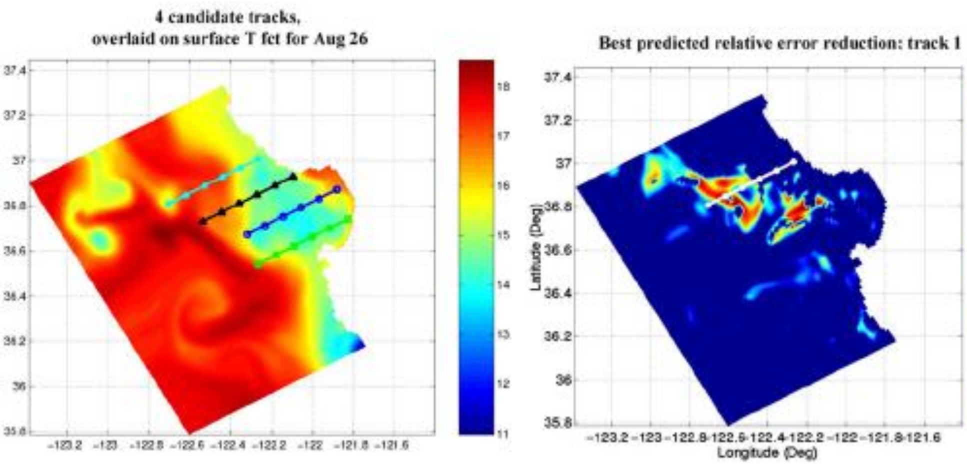
Best predicted relative error reduction: track 1



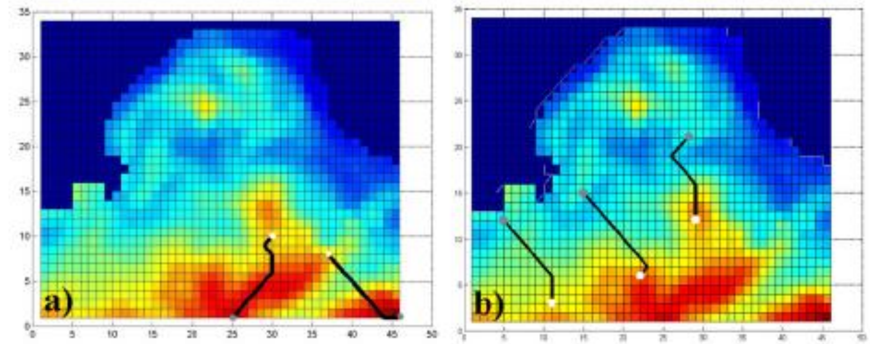
MIT

Adaptive Sampling Methodologies for Smart Robotic Swarms

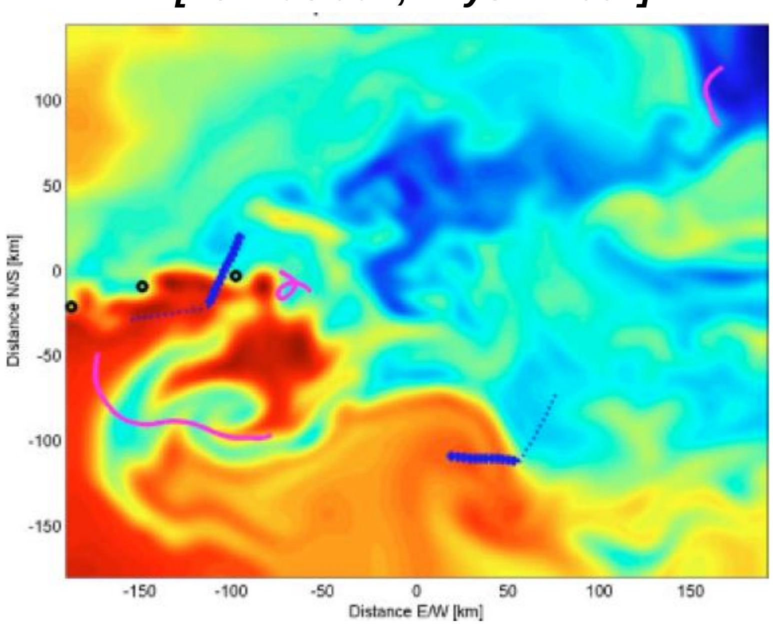
Lermusiaux et al



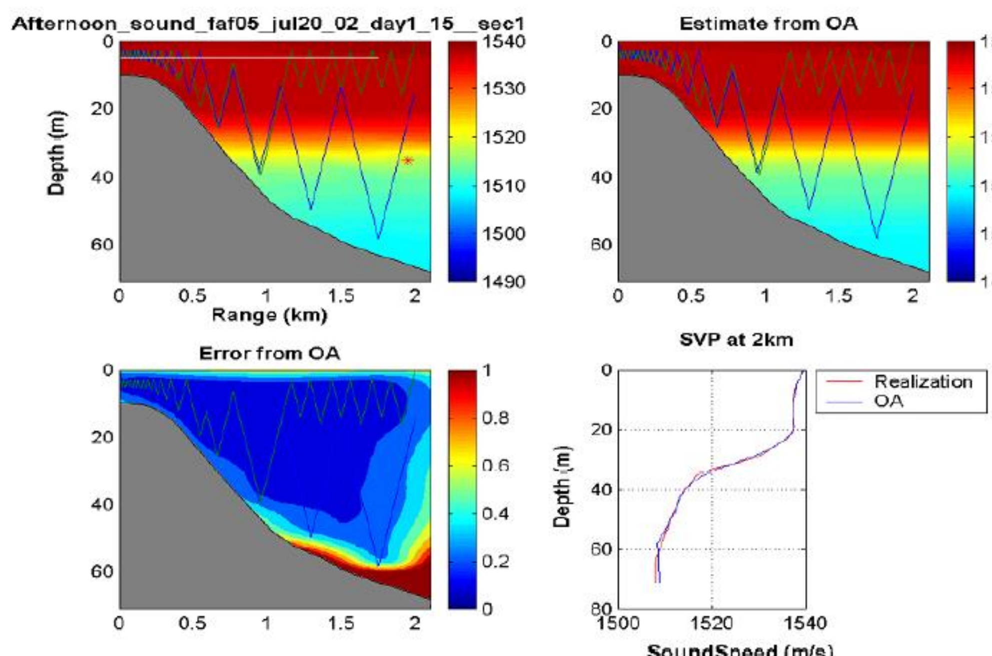
Adaptive Sampling via ESSE
[Lermusiaux, Phys.D-2007]



Optimal Path generation w/ 'fixed' objective field
[Yilmaz et al, OE-2008; Lermusiaux, et al 2007]



Genetic Algorithm
[Heaney et al., JFR-2007, OSSE OM-2010]



Path Planning based on Dynamic Programming
[Wang et al., Proc. IEEE-2006, JMS-2009]

Optimal Path Generation for a "Variable" Objective Field

[Yilmaz and Lermusiaux, Ocean Modeling, 2010-to-be-submitted]

Combines MILP path planning optimization
with ESSE-data-assimilation and adaptive sampling

- Extends MILP-scheme of Yilmaz et al.(IEEE-Oceans-2006; IEEE Trans.-JOE-2008) which assumed fixed and 2D objective field
- Uses the ESSE prediction of the uncertainty reduction by the sampling paths
- n-days look-ahead, assimilates forecast mean data (idealized POMDPS)
- Hiearchical multigrid approach (computes paths on averaged coarse grid first, then refines the paths)
- 3D paths included by vertical integration over key ocean layers, then solving smaller set of 2D problems, then back to 3D

Advantages:

- Objective field (error stand. dev.) set piecewise-linear: solved *exactly* by MILP
- Possible paths defined on discrete grid: set of possible path is thus finite
- Multiple constraints imposed on vehicle displacements for meaningful paths:
    - Ship, communications, separation distance, etc.

Disadvantages: Ignores ocean currents (and not based on SPDEs)

Optimal Path Generation for a "Variable" Objective Field

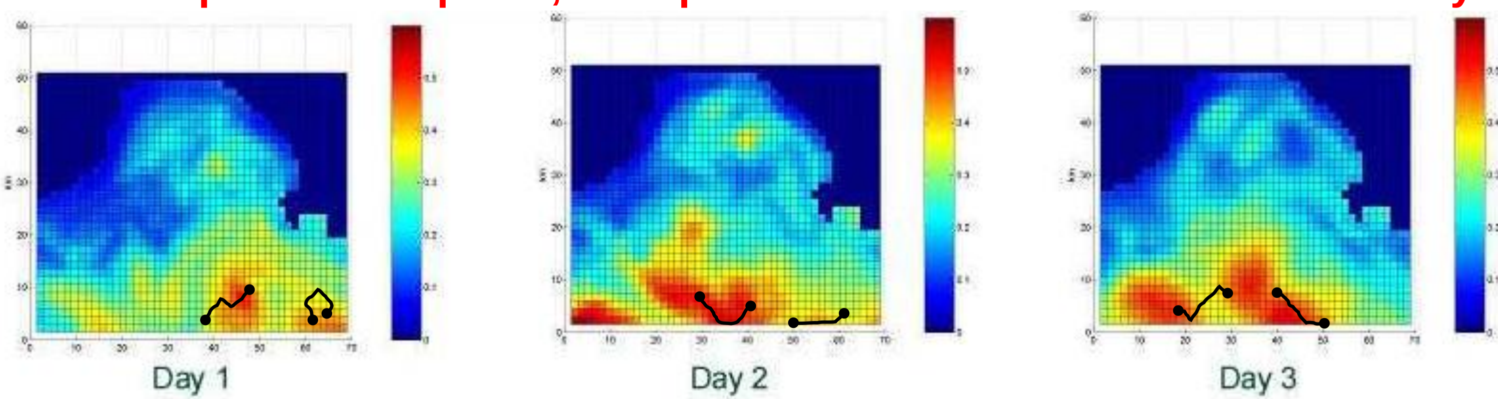
[Yilmaz and Lermusiaux, Ocean Modeling, 2010-to-be-submitted]

- **MILP computes optimal paths for *n* days using ESSE forecast uncertainties**
- **ESSE assimilates forecast data for day 1, updates forecast errors for days 2 to n**
- **MILP re-computes paths for days 2 to n based on updated ESSE forecast**
- **ESSE assimilates forecast data for day 2, updates errors for days 3 to n, …, etc**

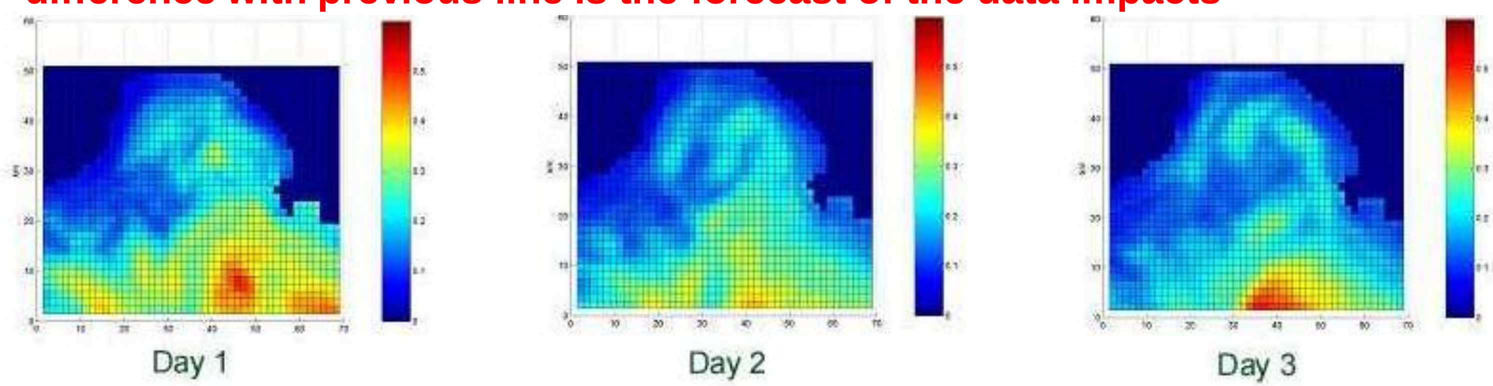
Example: Two Vehicles, n=3 days of forecast optimal paths

- **MILP computes paths that samples largest ESSE forecast errors for the next 3 days**
- **ESSE assimilates the unknown forecast data for day 1, new ESSE errors are predicted for days 2 and 3, and a new MILP search is done for the last 2 days**
- **ESSE assimilates the forecast data for day 2, predicts a new error for day 3 and a final MILP search is done for this final day 3**
- **Result: predicted optimal paths for 3 days**

Result: Optimal AUV paths, on top of Prior ESSE error forecast for 3 days

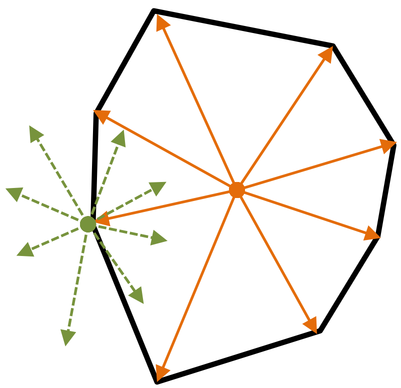


Posterior ESSE error forecast for 3 days (after DA of forecast optimal AUVs): difference with previous line is the forecast of the data impacts



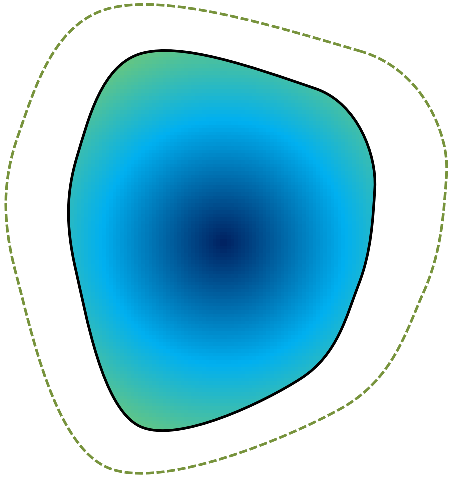
Level Set Representation for Optimal Path Planning for Swarms in (strong) Currents

Advance many vehicles in many directions



OR

Represent vehicles 'front' with a level set



- Can lead to poorly defined curves
    - Only have to solve for 1D curve
- What to do with multiple vehicles?
- Exponential increase in cost

- Continuous representation
    - Need so solve 2D field
- Easily deals with multiple vehicles
- Front propagates normal to itself

Time 1

Time 2

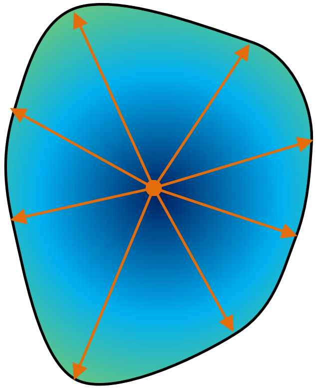
Level Set Representation for Optimal Path Planning for Swarms in Currents

Continuous Equations

$$\frac{\partial \varphi}{\partial t} + \mathbf{u} \cdot \nabla \varphi = 0$$

$$\mathbf{u} = \mathbf{u}_{LS} + \mathbf{u}_{FF}$$

$$\mathbf{u}_{LS} = F \frac{\nabla \varphi}{|\nabla \varphi|}$$



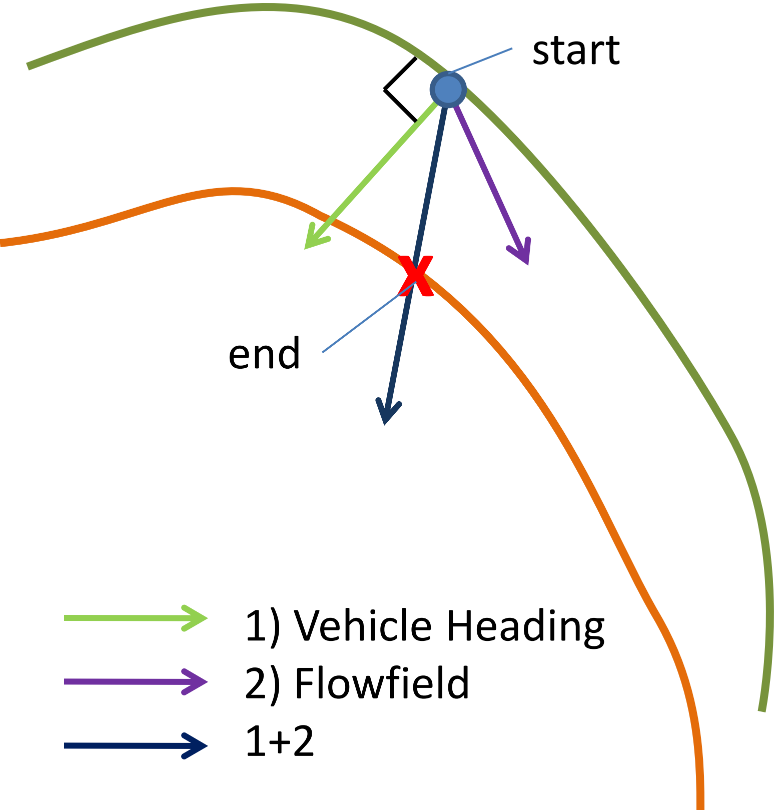
Numerically: Fractional Step PDE scheme

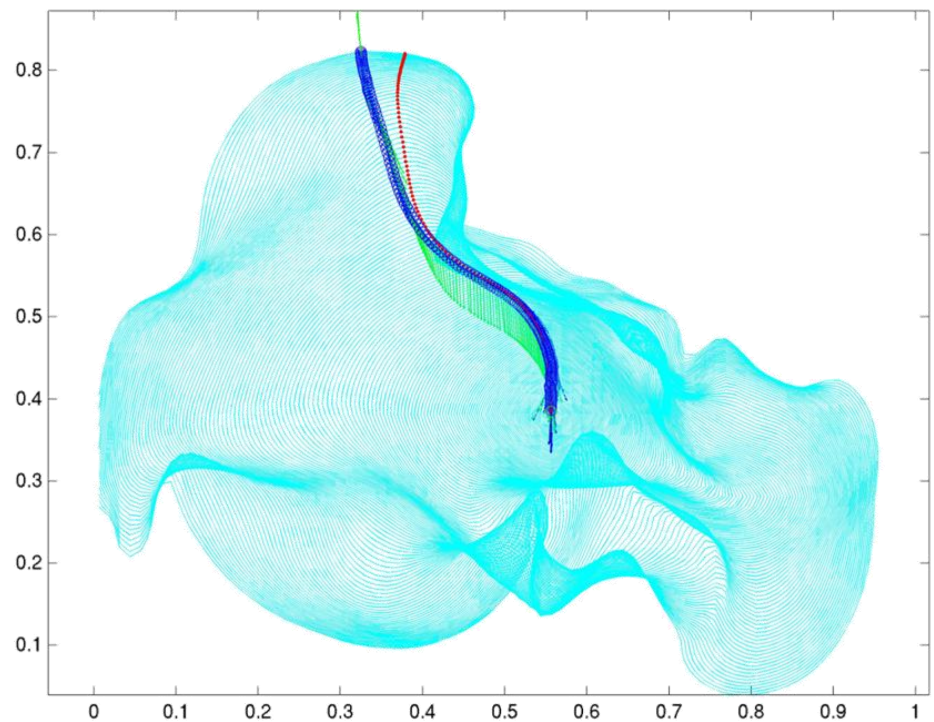
$$\begin{aligned}
\tilde{\varphi} &= \varphi^k + \frac{\Delta t}{2} \mathbf{u}_{LS} \cdot \nabla \varphi^k \\
&= \varphi^k + \frac{\Delta t}{2} F \frac{\nabla \varphi}{|\nabla \varphi|} \cdot \nabla \varphi^k \\
&= \varphi^k + \frac{\Delta t}{2} F |\nabla \varphi| \\
\varphi^* &= \tilde{\varphi} + (\Delta t) \mathbf{u}_{FF}^{k+1} \cdot \nabla \tilde{\varphi} \\
\varphi^{k+1} &= \varphi^* + \frac{\Delta t}{2} F |\nabla \varphi|
\end{aligned}$$

Level Set Representation – Optimal Path Construction

Once Level sets are constructed, we need to reconstruct the optimal path or AUV headings

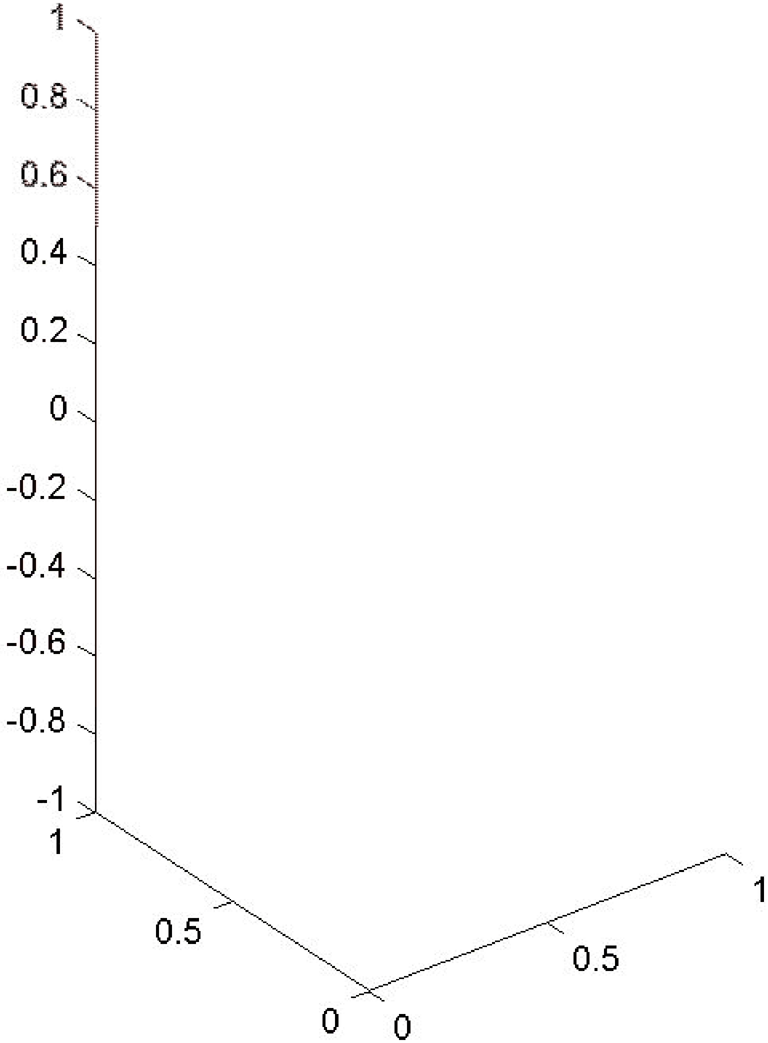
- Save Level Set curves and flowfield at each point on Level Set
- Integrate backwards from point of interest (go back from Lagrangian to Eulerian reference frame, used in the proof of optimality)

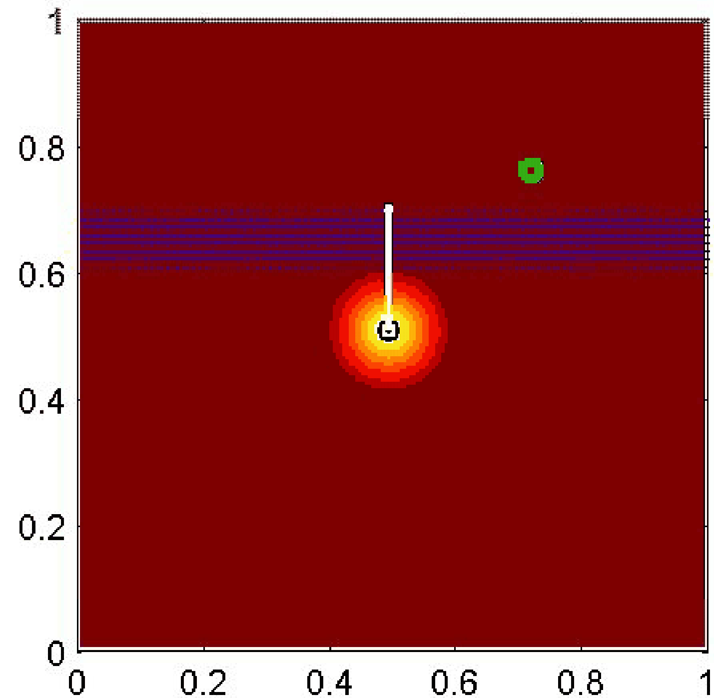




Level Set Path Planning – Examples

Crossing a Jet



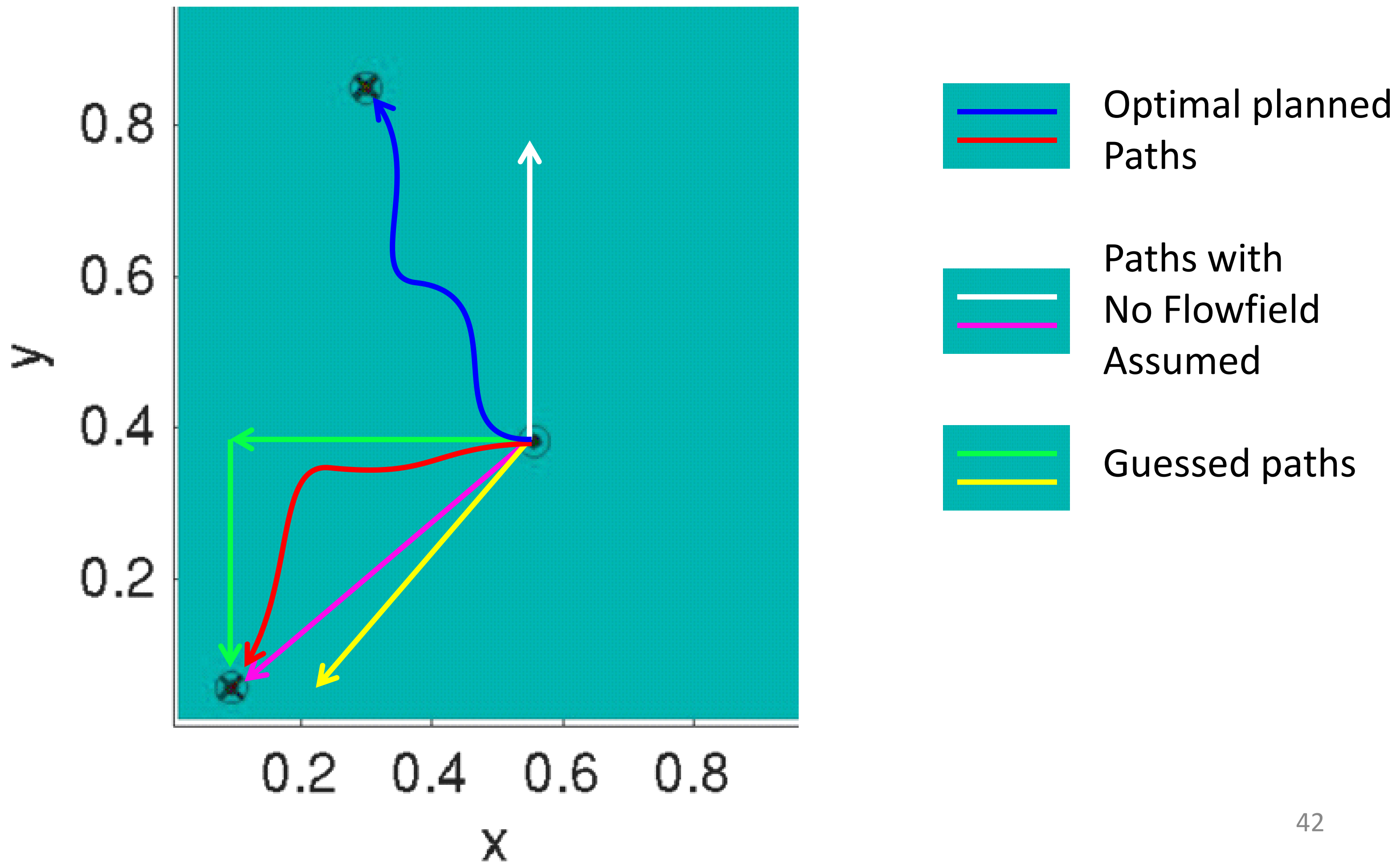


Other examples tested:
-Getting in/out of an eddy
-Meanders
-Wavy field, etc

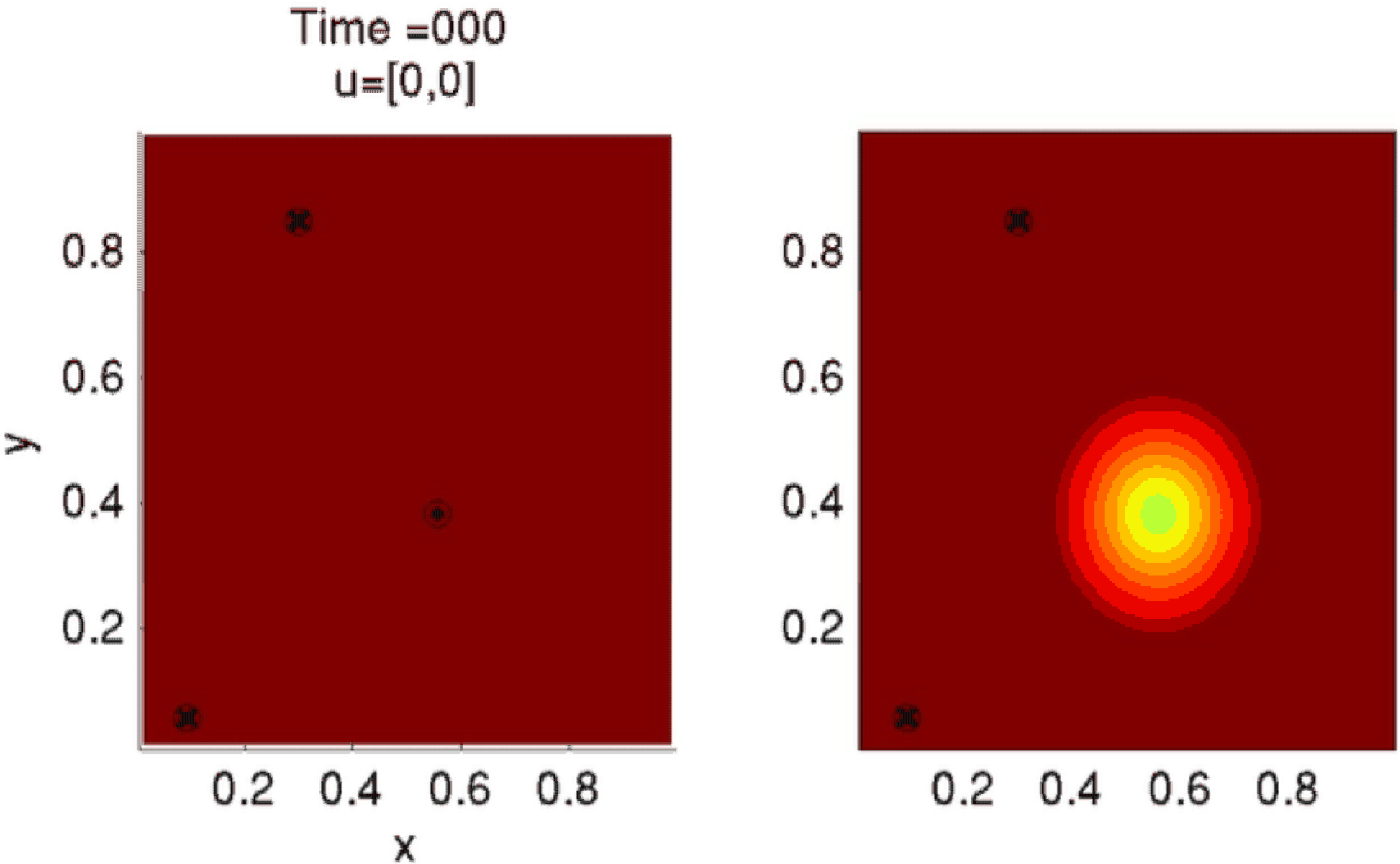
Level Set Path Planning – Examples

Complex Flowfield with strong currents, Multiple vehicles

- 1 vehicle wishes to sample South-West Corner
- 1 vehicle wishes to sample as North as possible

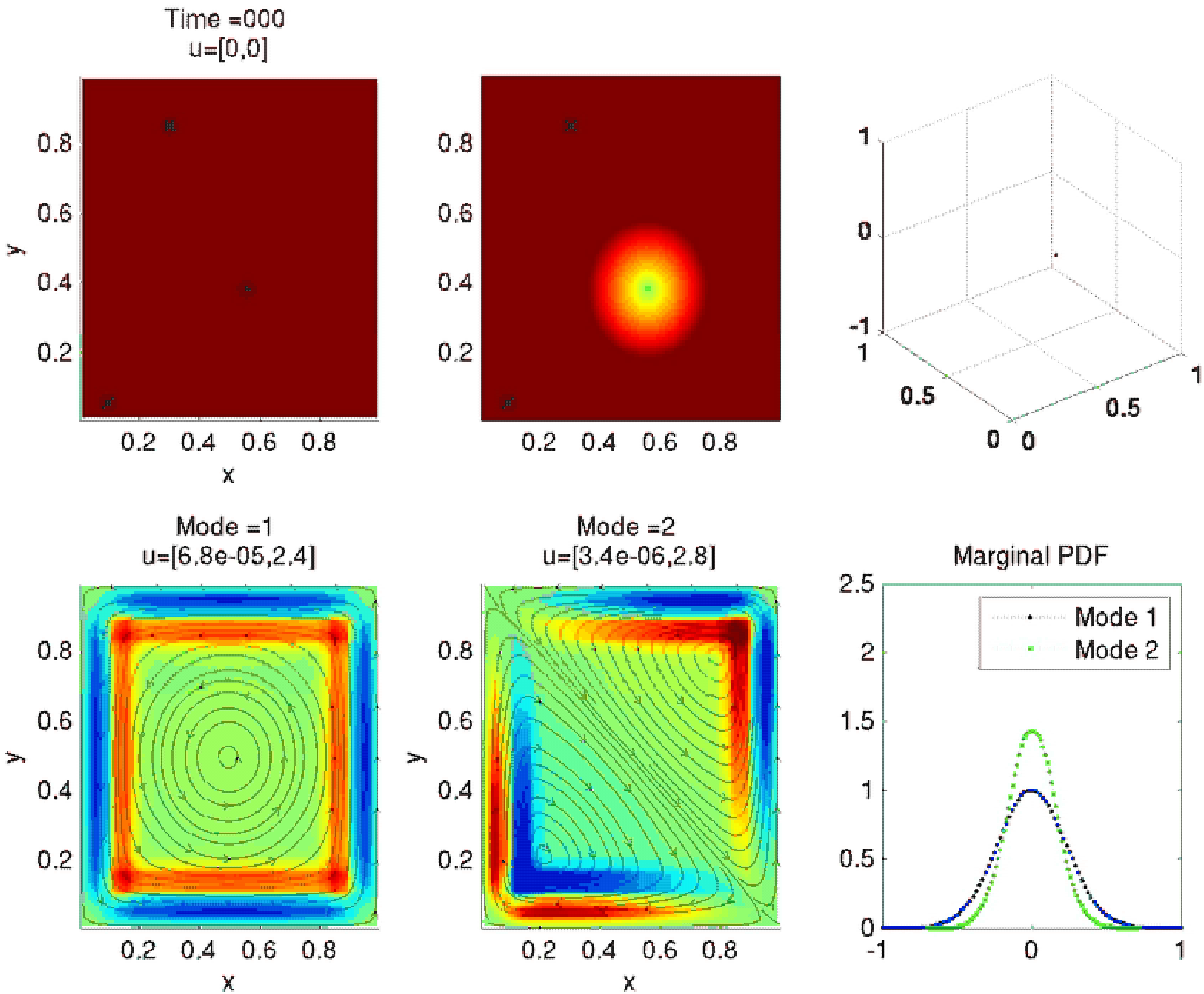


Level Set Path Planning – Examples
Uses a 2D-wind-driven ocean circulation



Level Set Planning: Ongoing Work on Uncertainty - DA

1) Utilize Uncertainty on Level Sets and/or 2) Uncertain level sets



Combine Partially Observable MDPs (POMDPs) with DO/ESSE equations for Adaptive Sampling

Key Idea: Steer UAVs using hierarchical “Partially Observable Markov Decision Processes”

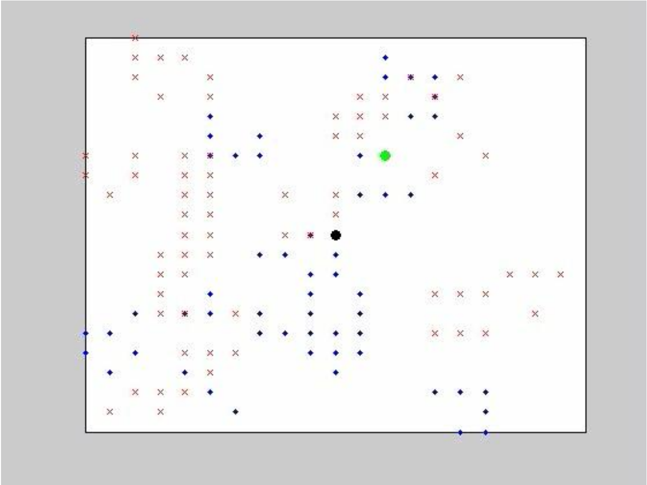
Examples of *global* goals may be:

- Track region / ocean feature
- Mimic swarming scheme
- Investigate region of large predicted uncertainties
- Combinations of the above

Goal: Maximize utility (Bellman Optimality Equation): $U_\infty(b) = \gamma \max_a \left[r(b,a) + \int U_\infty(b')\, p(b' | b,a)\, db' \right]$

Initial Simple Test Case: Game of Life.

- One AUV (**black circle**).
- One *global* goal (**green circle**).
- Many *local* goals:
  - “Good” cells (**blue dots**).
  - “Bad” cells (**red x’s**).
- Multiple uncertainties:
  - observations and actions.



M. Gardner, *The fantastic combinations of John Conway’s new solitaire game “life”*, Scientific American 223 (October 1970): 120-123.

DO equations and ESSE data assimilation

Data Assimilation (by Kalman update, combining DO uncertainty predictions with ESSE):

- Generate realizations:

$$\{u_r(x,t_o)\}_1^N = \bar{u}(x,t_o) + \{Y_i(t_o;\omega)\}_1^N u_i(x,t_o)$$

- Calculate Kalman Gain:

$$K = BH^T\left(R + HBH^T\right)^{-1}$$

- Perform Kalman update:

$$\{u_r^+(x,t_o)\}_1^N = \{u_r(x,t_o)\}_1^N + K\left(y(x,t_o) - H\bar{u}(x,t_o)\right)$$

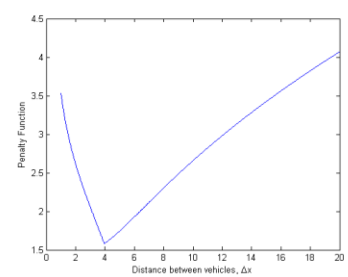
- Project back into D.O. framework:

$$u_i(x,t_o) = \phi_i(x,t_o)\ ;\ Y_i = \left\langle \{u_r^+(x,t_o)\}_1^N, u_i(x,t_o) \right\rangle$$

Inter-vehicle communication/potential:

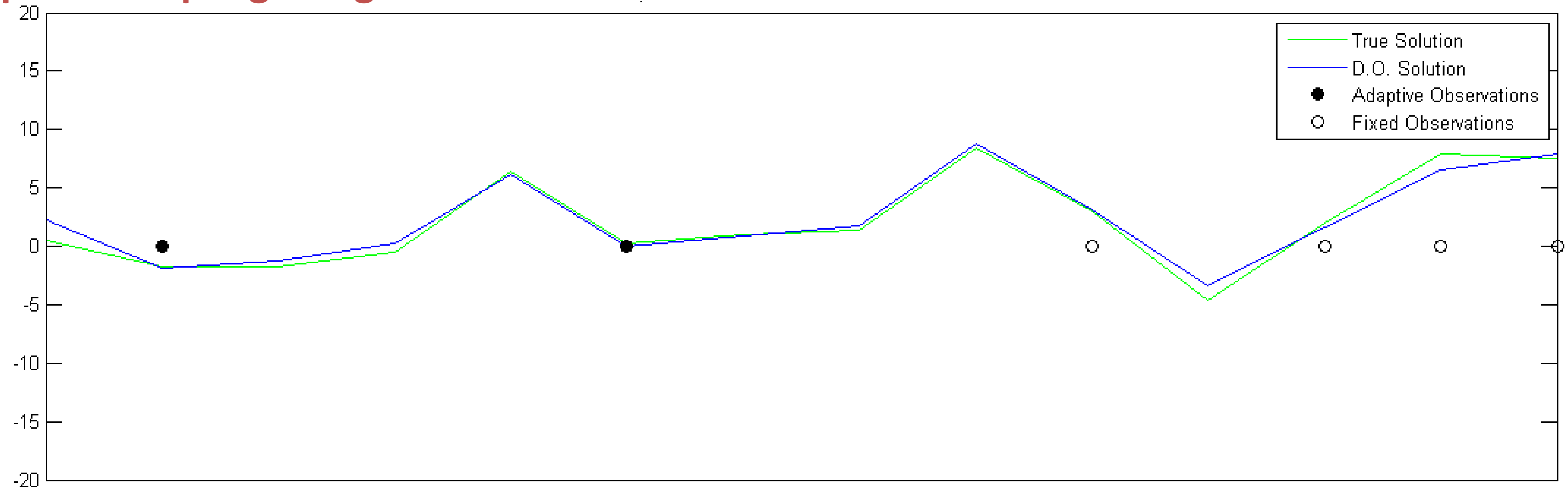
- Add penalty term to POMDP reward function:

$$Penalty = k\sqrt{\left|\Delta x - x_0\right| + 10/\left|\Delta x\right|}$$



Example: Lorenz-95

Adaptive Sampling using POMDP-like scheme:



Lorenz-95 Equation (with added diffusion):

$$\frac{du_i}{dt} = \underbrace{u_{i-1}\;\; u_{i+1} - u_{i-2}}_{\textit{advection}} + \underbrace{k\;\; u_{i+1} - 2u_i + u_{i-1}}_{\textit{diffusion}} \overbrace{-u_i}^{\textit{dissipation}} + \underbrace{f}_{\textit{forcing}}$$

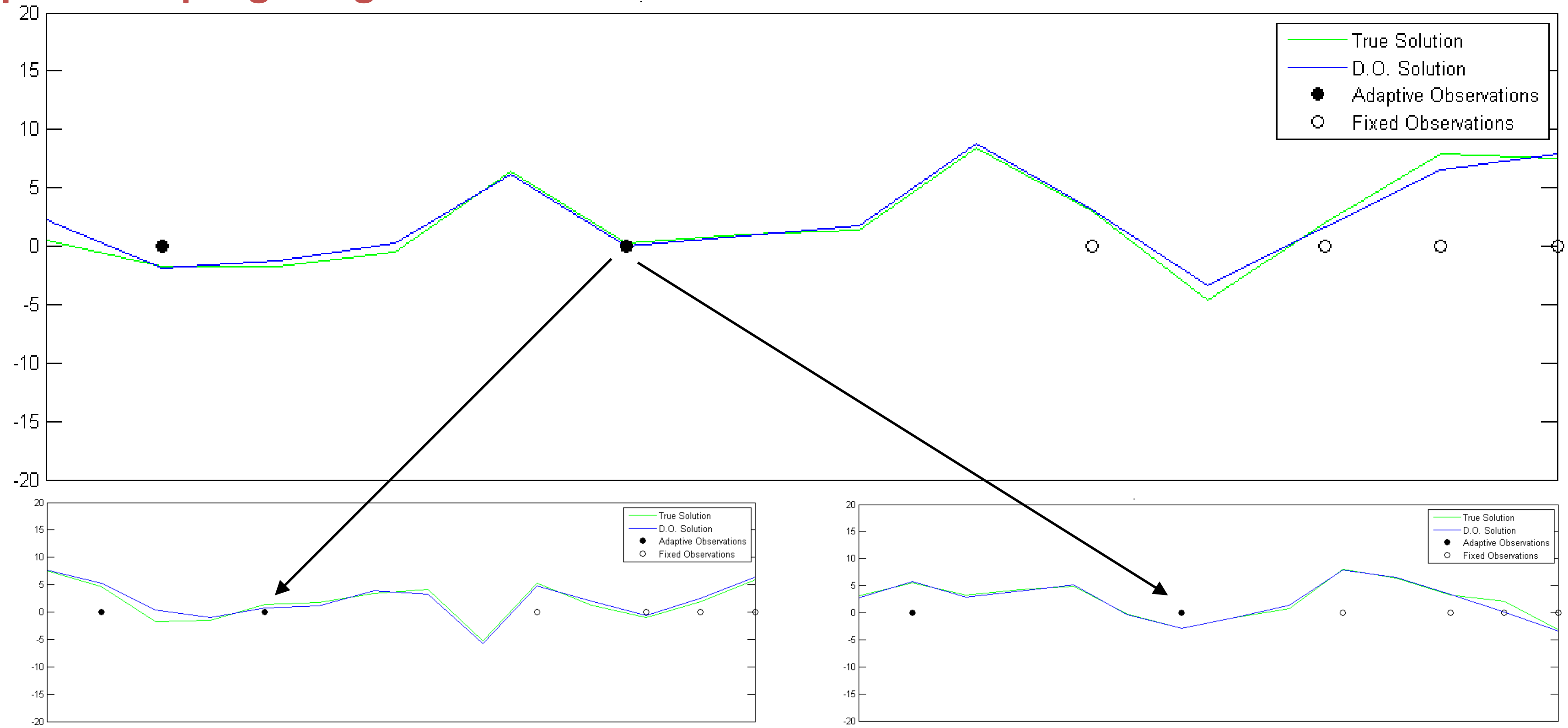
"40 ODEs: represent an atmospheric quantity at 40 sites spaced equally about a latitude circle.."

Where to make supplementary observations?

E.N. Lorenz & K.A. Emanuel, *Journal of the Atmospheric Sciences, 1998, Vol: 55, Iss: 3.*

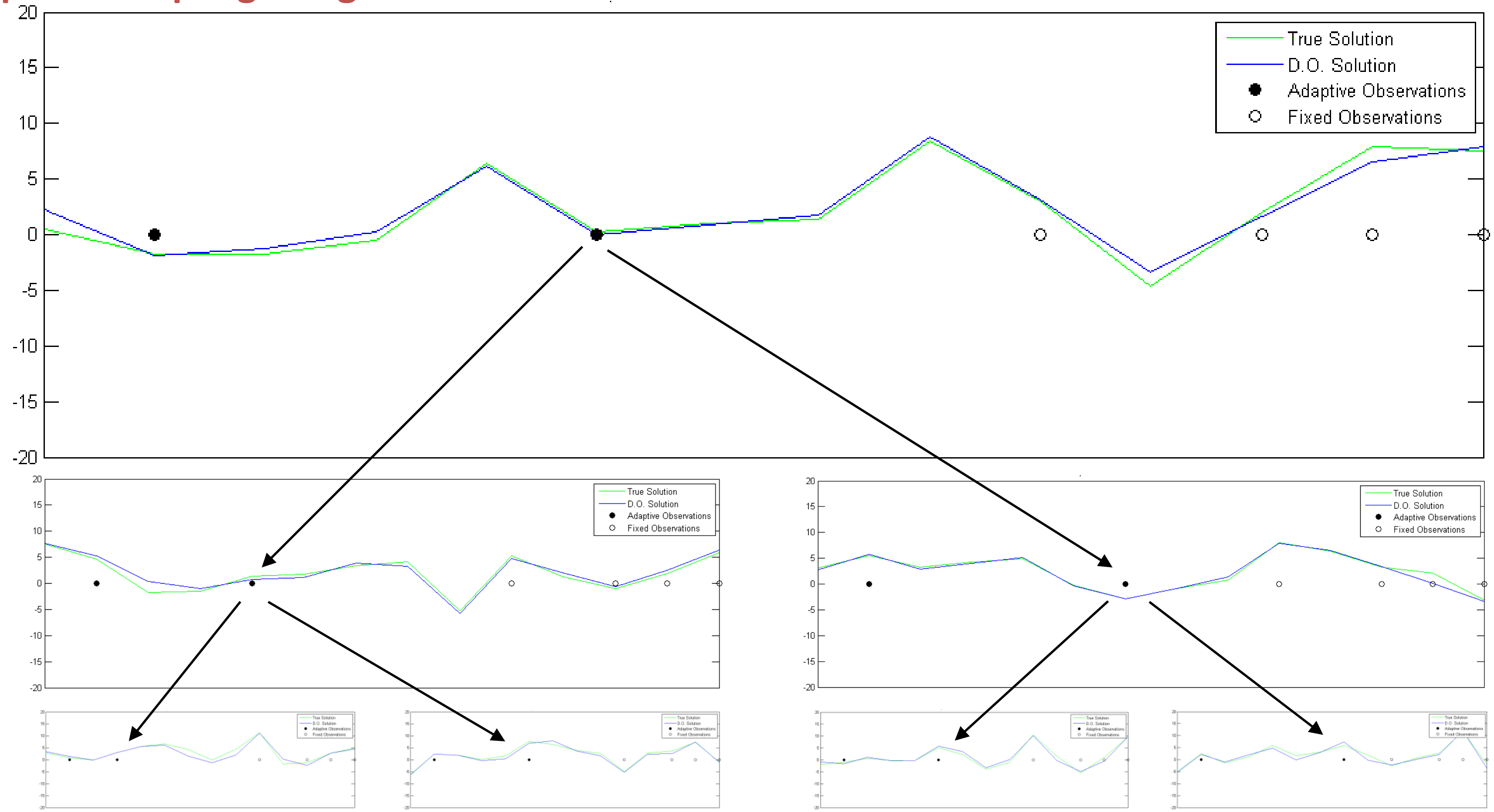
Example: Lorenz-95

Adaptive Sampling using POMDP-like scheme:



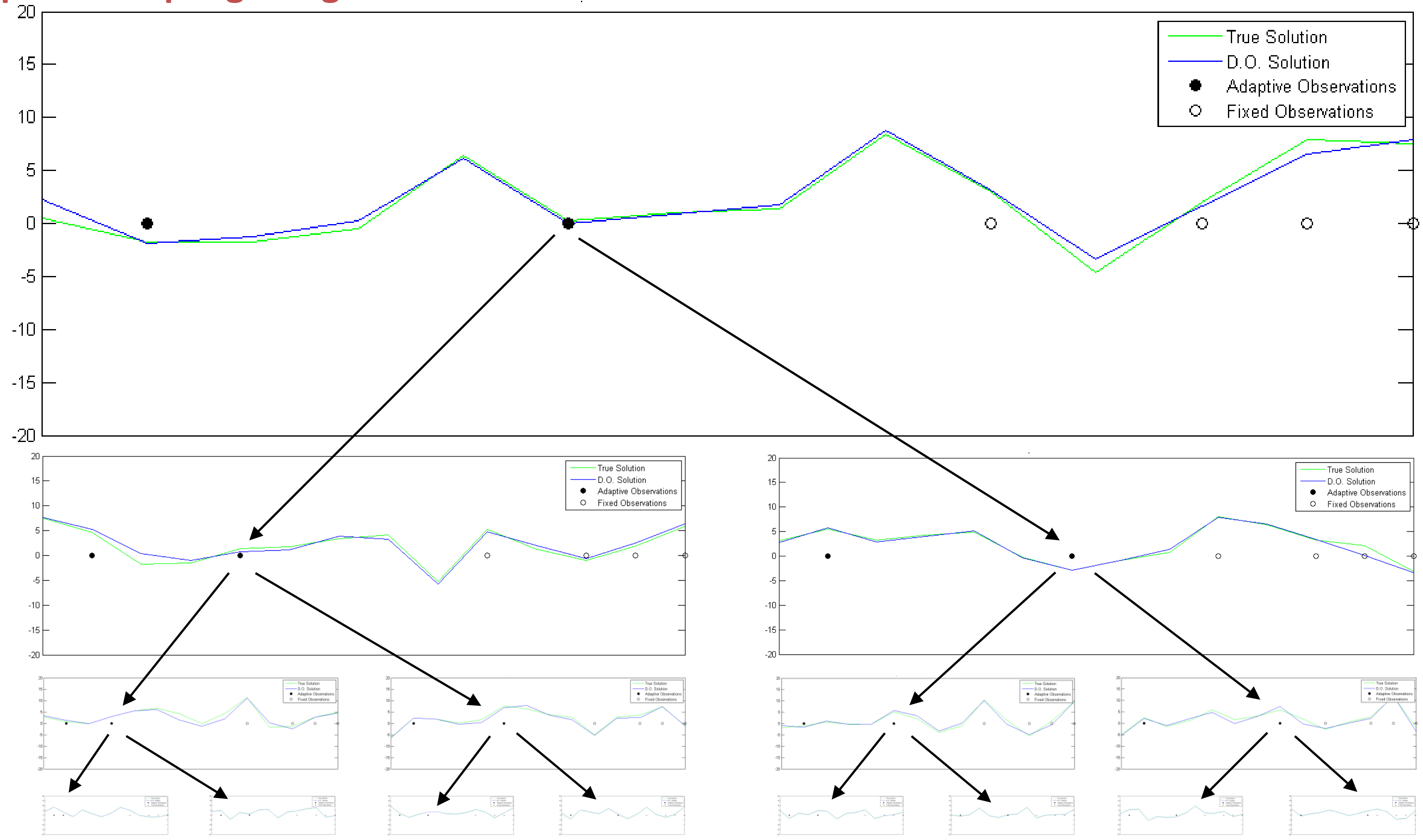
Example: Lorenz-95

Adaptive Sampling using POMDP-like scheme:



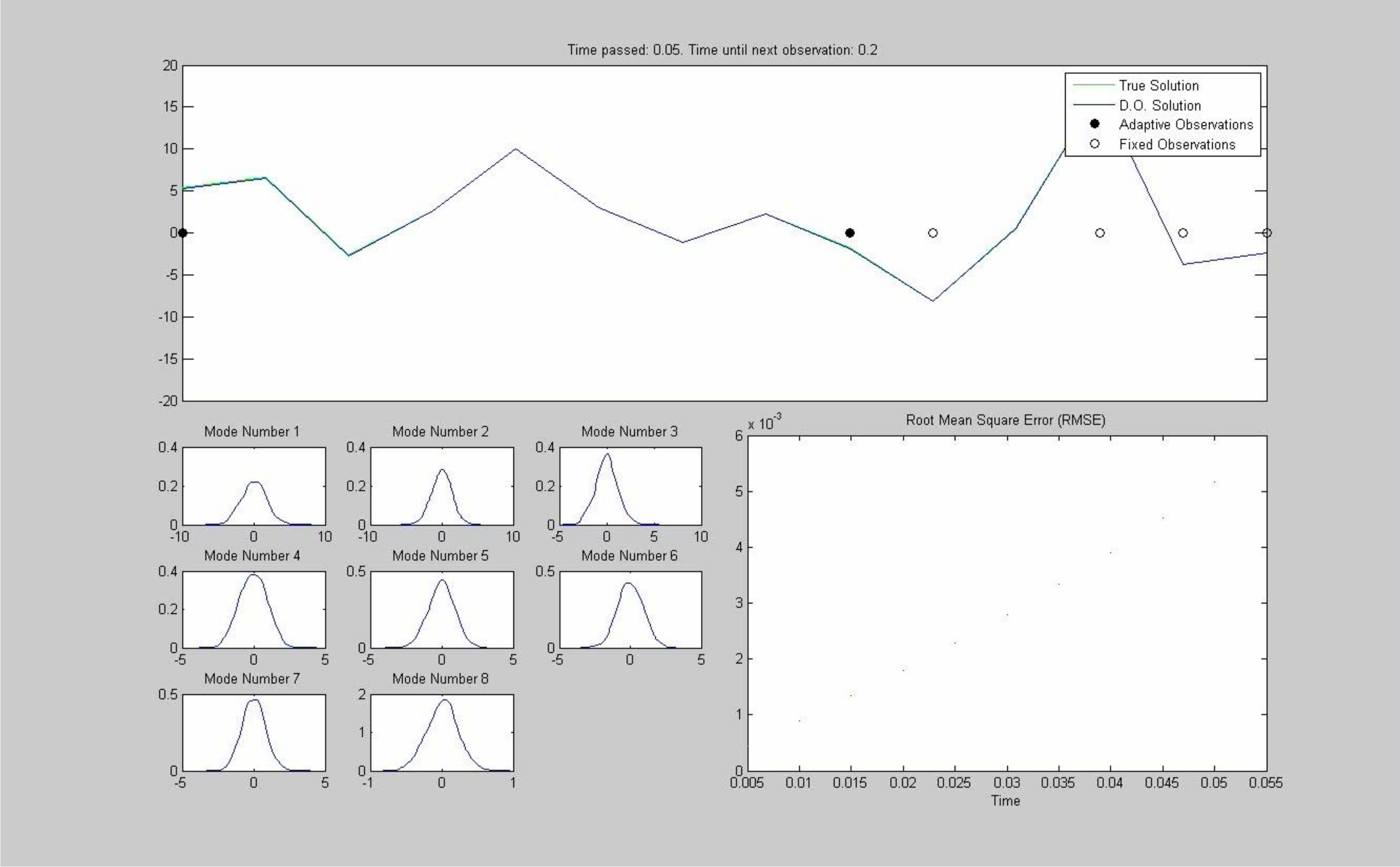
Example: Lorenz-95

Adaptive Sampling using POMDP-like scheme:



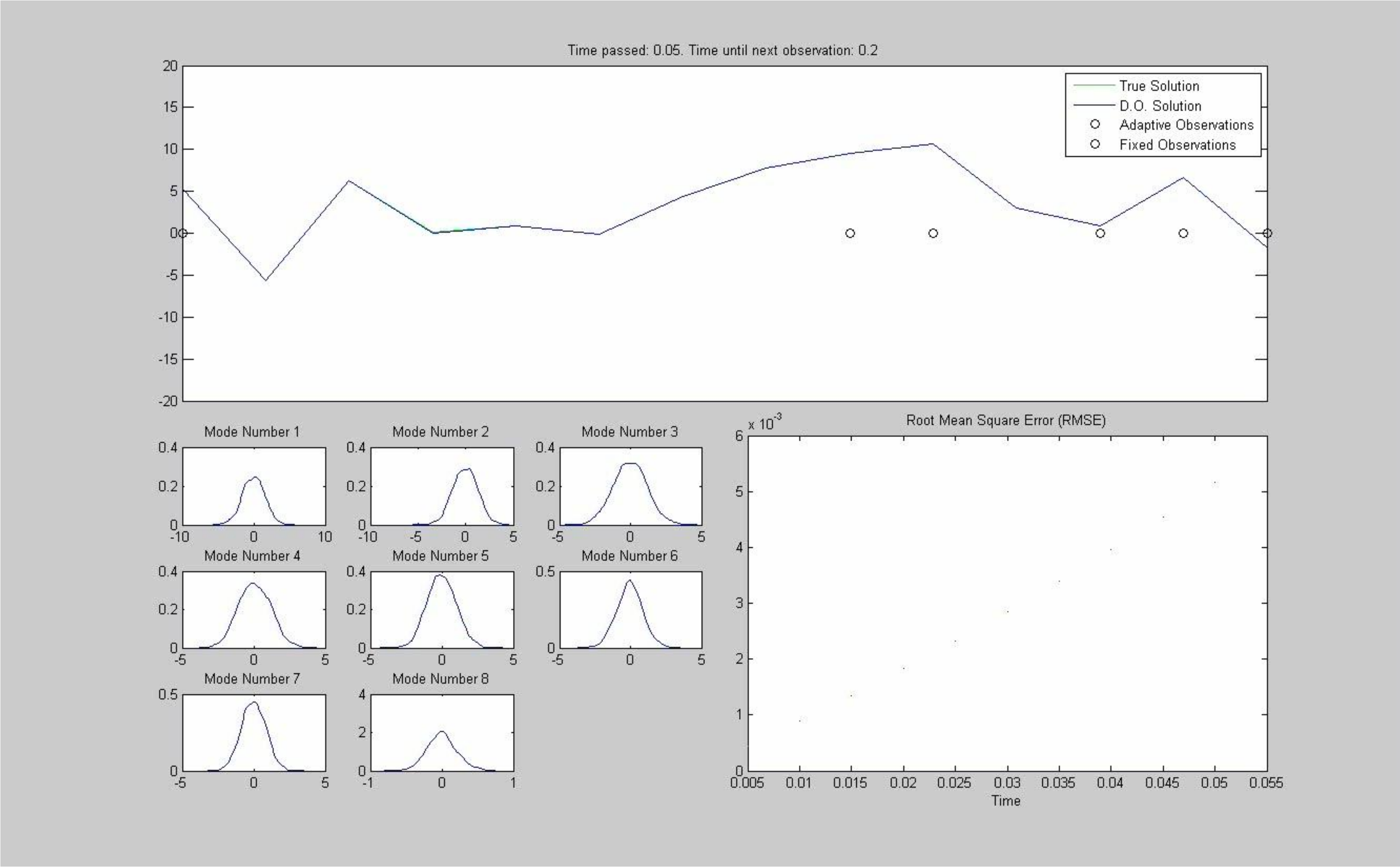
Example: Lorenz-95

- Adaptive Observations -



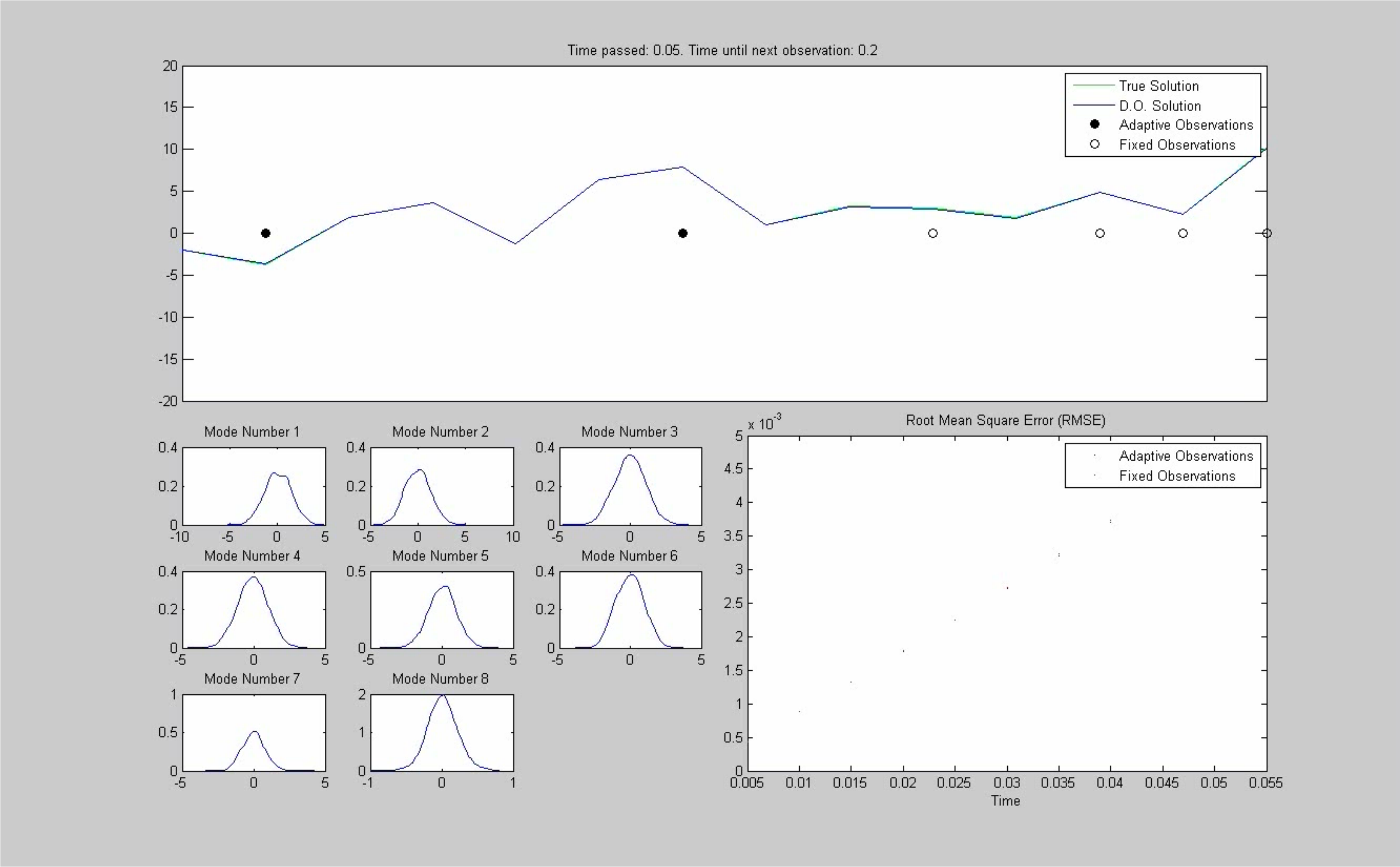
Example: Lorenz-95

- Fixed Observations -



Example: Lorenz-95

- Adaptive Observations (overlaid on Fixed observations)-



Information Theory with DO-ESSE

Key Idea: The D.O. equations provide an accurate probabilistic description of current and future states of the ocean field. When making intelligent decisions, we wish to move beyond simple metrics defined in terms of second order statistics only.

Useful Information Theoretic Measures:

- Differential Entropy: $h_p(X) = -\int p(x) \log p(x)\, dx$
- Mutual Information: $I(X;Y) = h(X) - h(X|Y)$

Key Concept: The "Information matrix",

$$\mathbf{I} = \begin{bmatrix} I(X_1;Y_1) & \cdots & I(X_1;Y_n) \\ \vdots & I(X_i;Y_j) & \vdots \\ I(X_n;Y_1) & \cdots & I(X_n;Y_n) \end{bmatrix}$$

Goal:

$$Y_j = \underset{j \in (1,\ldots,n)}{\arg\max} \left(\sum_{i=1}^{n} I(X_i, Y_j) \right)$$

CONCLUSIONS – DO equations

- **Prognostic Equations for Stochastic Fields**
  - Derived new closed DO field equations (applied to several 2D NS/cases)
  - Adapted the size of the subspace (as in ESSE)
- **Ongoing Research:**
  - Idealized Climate – MOC (Cessi and Young, 1992, Ganopolski and Rahmstorf, 2002)
  - Evolve the subspace based on data (learning as in ESSE)
  - DO Data Assimilation (ESSE+Bayesian)
  - Complete "DO Numerics" manuscripts
    - Direct cost of DO eqns:

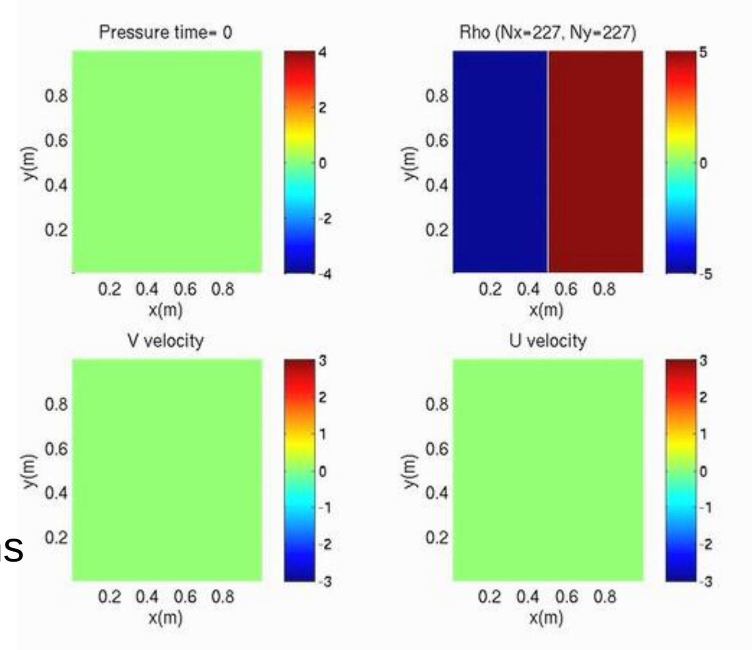
$$O(s^2) \times (\text{Cost of Determ. PDE})$$

    - With projection methods, cost reduces to:

$$O(s) \times (\text{Cost of Determ. PDE})$$

Impose all modes to be incompressible and solve for pseudo-pressures that contain all cross-pressure terms

Note: looking into non-intrusive methods too



CONCLUSIONS – Smart Sampling

- **Intelligent Adaptive Sampling: the Science of Autonomy**
  - Developed and utilized varied Adaptive Sampling schemes
  - Path Planning for Sensing Swarms using Level Set Methods
  - Merging adaptive DO equations, ESSE-Data-Assimilation and POMDPs for Smart Adaptive Sampling in 1D
- **Ongoing Research:**
  - Continue combination of "ESSE+DO + Level Set + Information theory" for Collaborative Sampling Swarms
  - Optimal control and dynamical systems
  - Artificial intelligence and "Noisy Game Theoretic" schemes
  - Bio-inspired and agile sensing