Dynamics and Lagrangian Coherent Structures in the Ocean and their Uncertainties

Pierre F.J. Lermusiaux and Francois Lekien

Division of Engineering and Applied Sciences, Harvard University

Mechanical and Aerospace Engineering, Princeton University

Main collaborators on this topic

AOSN2-MURI: **N. Leonard, J. Marsden, A.R. Robinson, J. Belligham, Y. Chao, S. Majumdar**

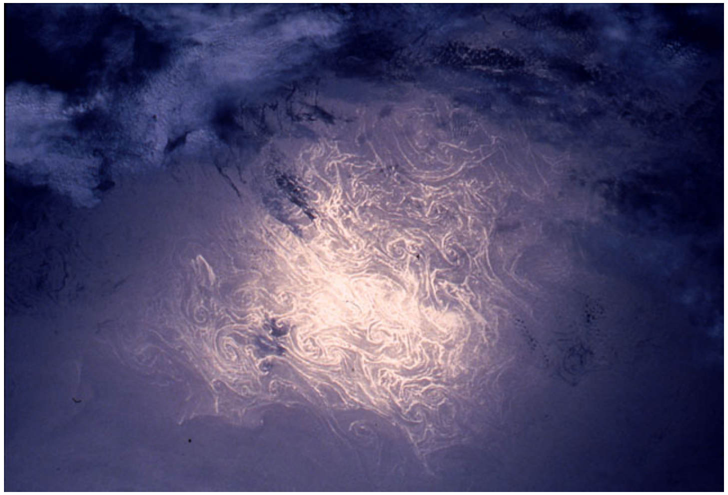
HU: **P.J. Haley, W.G. Leslie, O. Logoutov and X.S. Liang**

http://www.deas.harvard.edu/~pierrel
http://www.lekien.com

---

1. **Introduction and Concepts: Coherent Structures in the Ocean and Uncertainties**
2. **Dynamical and Uncertainty equations**
3. **Uncertainty Algorithms and Computational Systems: HOPS, ESSE, MANGEN**
4. **Results: Uncertainty predictions for 3 dynamical events in the Monterey Bay region**
5. **Conclusions**

Evidence of ‘Coherent’ Structures in the Ocean: Shuttle Photographs



Gulf Stream, Spiral Eddies

Spiral eddies (12 to 18 kms in diameter) in the Gulf Stream (1984) highlighted in Sun glitter. When spiral eddies were first observed in the Gulf of Oman (first shuttle mission, 1981), some thought that sub-mesoscale eddies were perhaps unique to that region.

Greek Island, Spiral Eddies and Wakes

Eastern end of Crete and some of the smaller Greek islands. Extensive spiral eddy field in the Sun glitter in the center of the frame, as well as island wakes — a phenomenon created where islands interrupt the flow pattern or ocean water.

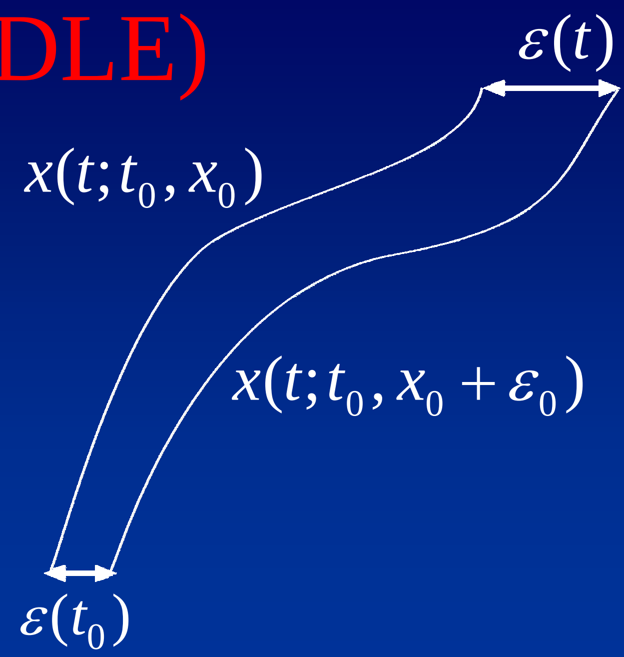
Gulf Stream, Seasonal Plankton Bloom

Gulf Stream shear zone and associated cold core eddies (1985).

Discovery of "coherent structures" in turbulent fluid flow has been one of the most prominent advances in fluid mechanics in last 30 years.

A "coherent structure" may be thought of as a shape or form in a turbulent fluid flow that persists a long time relative to it's own period of internal circulation.

Direct Lyapunov Exponent (DLE)



The finite-time Lyapunov exponent is the maximum exponential growth about a trajectory:

$$\sigma_T(t_0,\mathbf{x}_0) = \frac{1}{T}\ln \max_{\epsilon(t_0)} \left\{ \frac{\epsilon(t)}{\epsilon(t_0)} \right\}$$

More precisely:

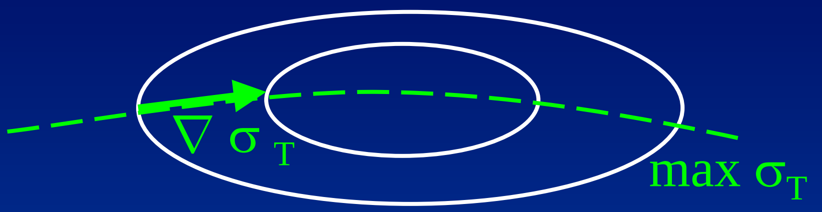
$$\sigma_T = \frac{1}{T}\ln \lambda_{\max} \left\{ \frac{\partial \mathbf{x}(\mathbf{t_0{+}T}, \mathbf{t}_0, \mathbf{x}_0)}{\partial \mathbf{x}_0}^{\top} \frac{\partial \mathbf{x}(\mathbf{t_0{+}T}; \mathbf{t}_0, \mathbf{x}_0)}{\partial \mathbf{x}_0} \right\}$$

The DLE, **Haller (2001)**, is the finite-time LE computed *directly*, using a set of particles released for duration T in a numerical simulation, fluid flow, etc.

The (D)-LE is also the normalized log of the maximum singular value of the finite time strain tensor dx/dx_0. Of course, $x \in R^2$ here!

Lagrangian Coherent Structures

LCS is defined as a ridge of σ_T



1. LCS is parallel to $\nabla \sigma_T$
2. On the LCS, Hessian $\Sigma_T = \nabla^2 \sigma_T$ is negative and minimum in the direction normal to the LCS (i.e., maximum curvature).

Lagrangian coherent structures indicate high stretching and the presence of hyperbolic trajectories (i.e., trajectories with stable and unstable manifolds),

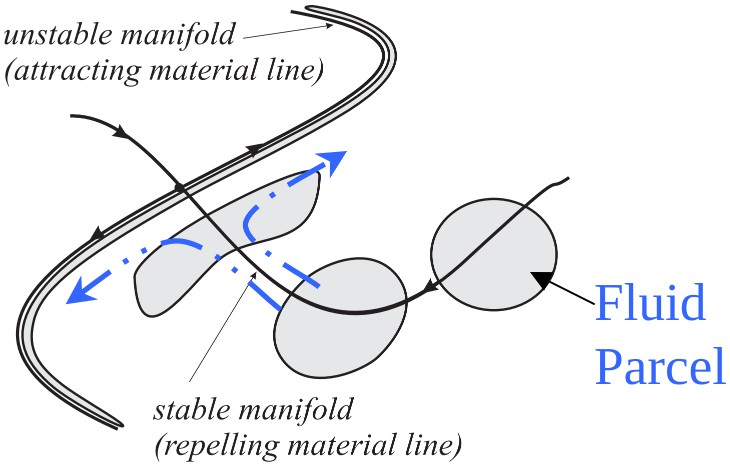
[Haller 2001]

Lagrangian coherent structures are almost invariant manifolds, hence they are a "good approximation" of stable and unstable manifolds.

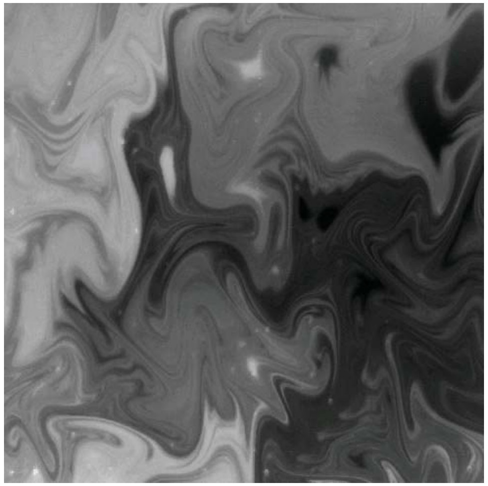
[Shadden, Lekien and Marsden 2001]

Evidence of LCS transport

We refer to a stable manifold as a Repelling Material Line since it would tend to stretch a parcel of Lagrangian particles placed about it, whereas the unstable manifold is deemed an Attracting Material Line since the parcel would get attracted to it as shown to the right.



Mixing of colored dyes.



Left: Picture of fluid with dye (lab experiment)

Right: DLE contour (computed from u,v data) superimposed. Ridges of high DLE are shown in red.

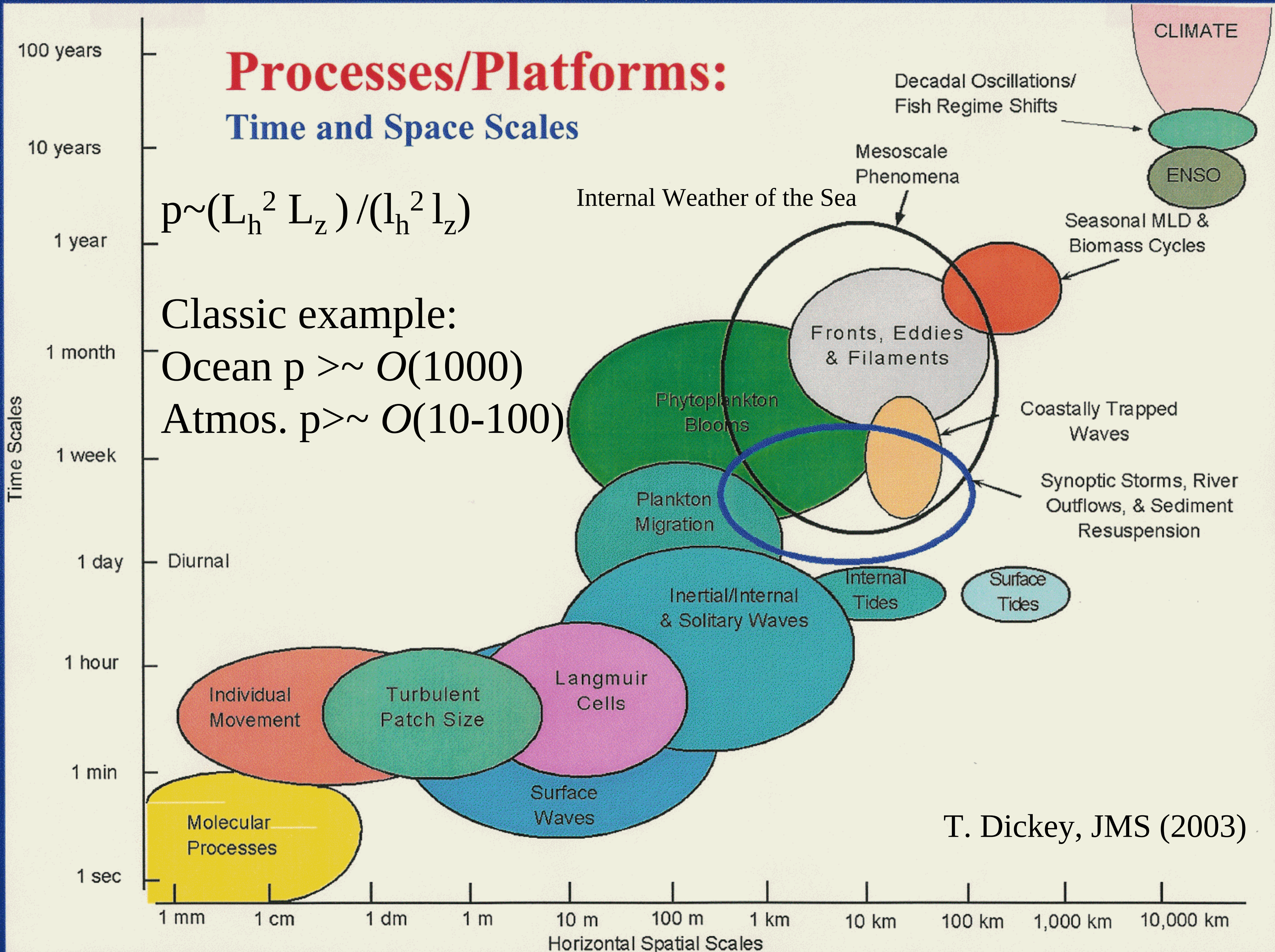
Voth, Haller, & Gollub [PRL 18 (2002)

Processes/Platforms:

Time and Space Scales

$$p \sim (L_h^2 L_z)/(l_h^2 l_z)$$

Classic example:
Ocean p >~ O(1000)
Atmos. p>~ O(10-100)



T. Dickey, JMS (2003)

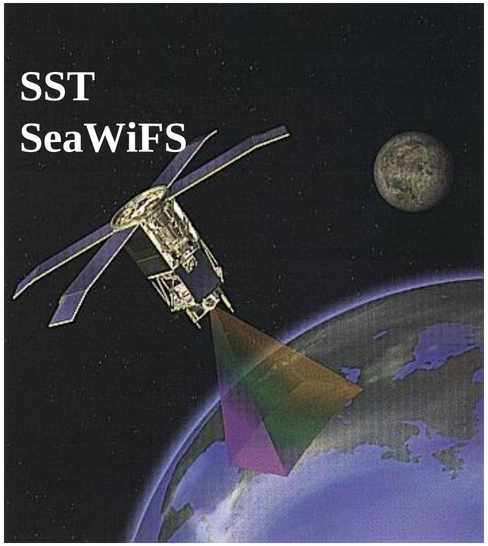
Physical and Multidisciplinary Observations

AUV

Aircraft

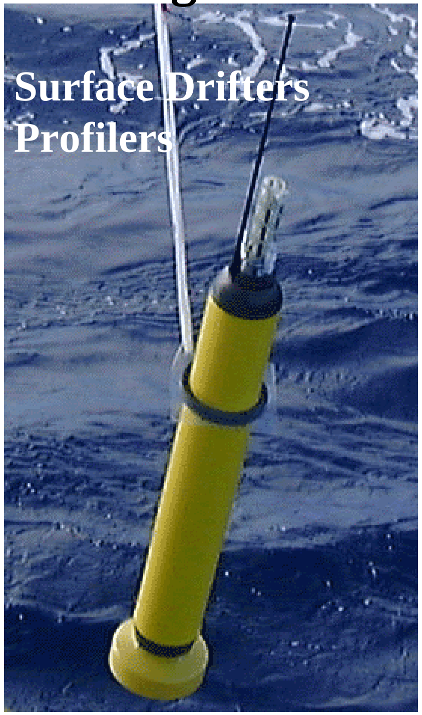
Ships

Satellite



Moored/Fixed

Drifting



Geophysical Fluid Dynamics (GFD)

Study of geophysical flows and dynamics (Earth atmosphere, ocean, etc)

Fundamental equations are Navier-Stokes in rotating frame of reference

Additional practical assumptions limit the range of modeled scales in time and space:

1. Boussinesq fluid (small variations of density about a state of reference)
2. Turbulent flow reduced to scale window of interest, here:
    - Sub-mesoscale, mesoscale to large-scale ocean processes
    - Processes outside this window are averaged and their effects parameterized (turbulent closures)
3. Thinness approximation ($H/L \ll 1$)

Result: the so-called **Primitive-Equations of Ocean Dynamics**

Models of (Interdisciplinary) Ocean Dynamics Utilized

- **Physical model:** **Primitive-Equation (PDE, x, y, z, t: HOPS)**

Horiz. Mom.	$\frac{D\mathbf{u_h}}{Dt} + f\,\mathbf{e}_3 \wedge \mathbf{u}_h = -\frac{1}{\rho_0}\nabla_h\, p_w + \nabla_h \cdot (A_h \nabla_h \mathbf{u}_h) + \frac{\partial\; A_v\, \partial \mathbf{u}_h / \partial z}{\partial z}$	**(1-2)**
Vert. Mom.	$\rho g + \frac{\partial p_w}{\partial z} = 0$	**(3)**
Thermal en.	$\frac{DT}{Dt} = \nabla_h \cdot (K_h \nabla_h T) + \frac{\partial\; K_v\, \partial T/\partial z}{\partial z}$	**(4)**
Cons. of salt	$\frac{DS}{Dt} = \nabla_h \cdot (K_h \nabla_h S) + \frac{\partial\; K_v\, \partial S/\partial z}{\partial z}$	**(5)**
Cons. of mass	$\nabla \cdot \mathbf{u} = 0$	**(6)**
Eqn. of state	$\rho(\mathbf{r}, z, t) = \rho(T, S, p_w)$	**(7)**

- **Biogeochemical model:** **Generic ADR equation (PDE, x, y, z, t)**

$$\frac{\partial \phi_i}{\partial t} + \mathbf{u} \cdot \nabla \phi_i - \nabla_h (A_i \nabla_h \phi_i) - \frac{\partial\; K_i\, \partial \phi_i / \partial z}{\partial z} = \mathcal{B}_i(\phi_1, \ldots, \phi_i, \ldots, \phi_7) \qquad \mathbf{(8-14)}$$

$i =$ NO3, P_{NO3}, ZOO, NH4, DET, CHL, P_{NH4}

DEFINITION AND REPRESENTATION OF UNCERTAINTY

- $\boldsymbol{x}$ = estimate of some quantity (measured, predicted, calculated)

- $\boldsymbol{x}^t$ = actual value (unknown true nature)

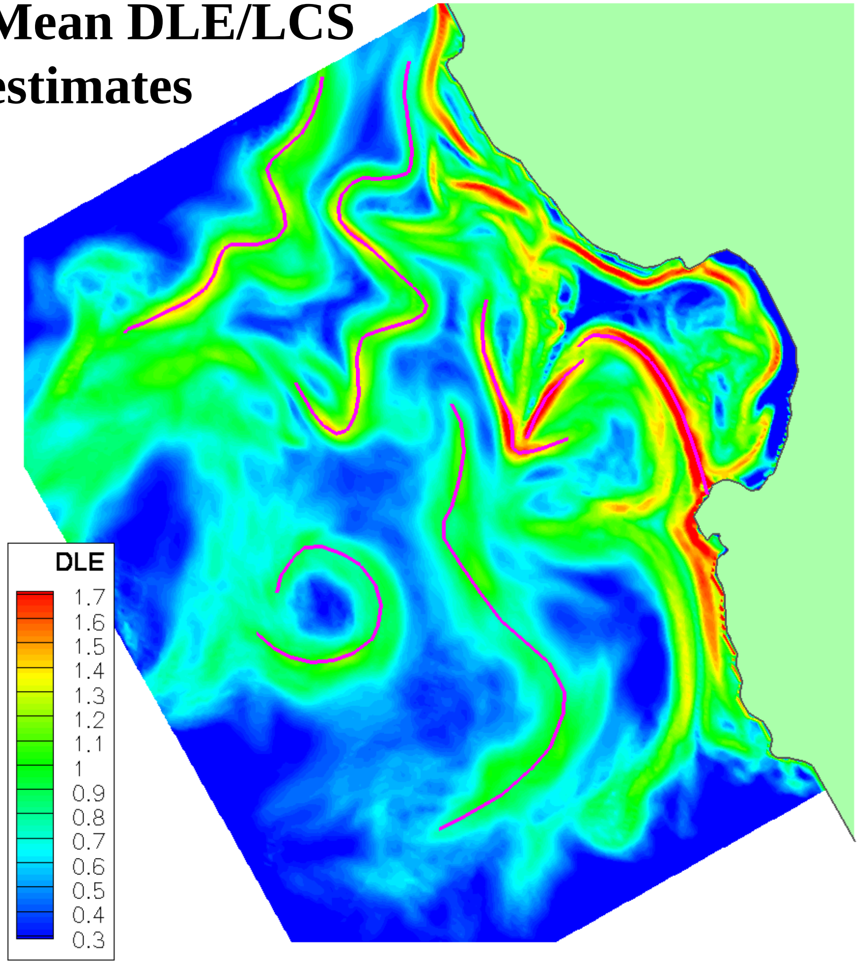
- $\boldsymbol{e} = \boldsymbol{x} - \boldsymbol{x}^t$ (unknown error)

Uncertainty in ***x*** is a representation of the error estimate ***e***
e.g. probability distribution function of ***e***

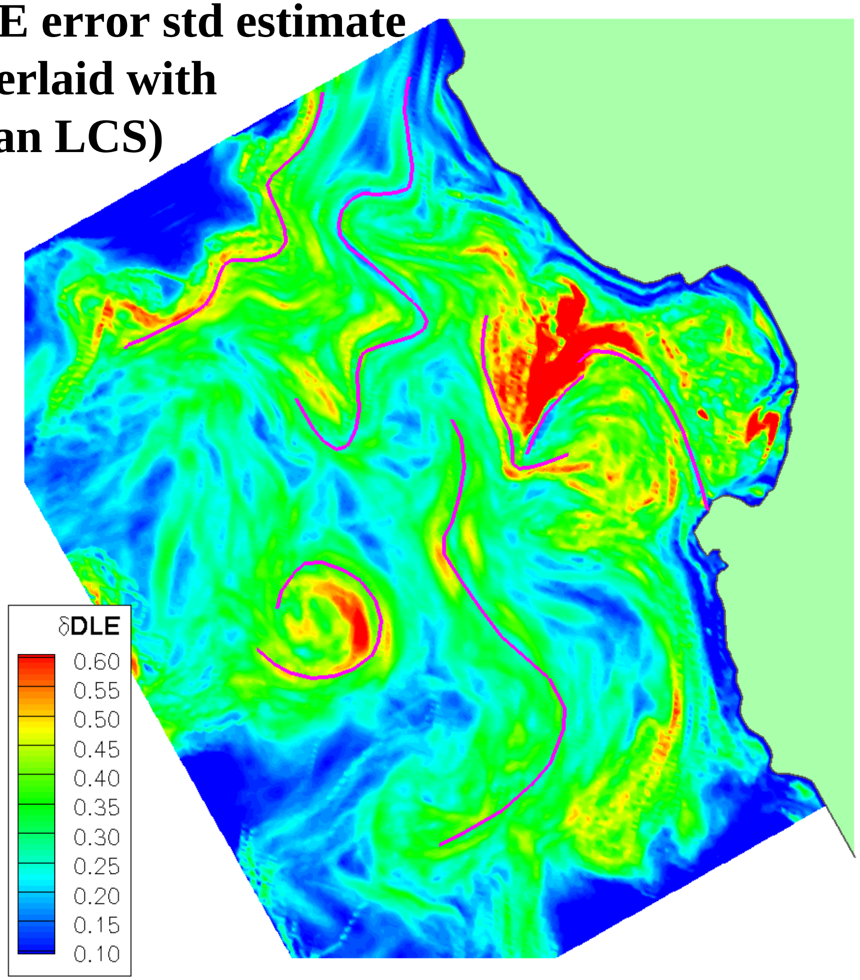
- Variability in ***x*** vs. Uncertainty in ***x***
- Uncertainties in general have structures, in time and in space: They can be represented as fields

One of Main Goals here:
Estimate and Study Uncertainties of LCS

Mean DLE/LCS estimates



DLE error std estimate (overlaid with mean LCS)



How to compute such uncertainty fields?

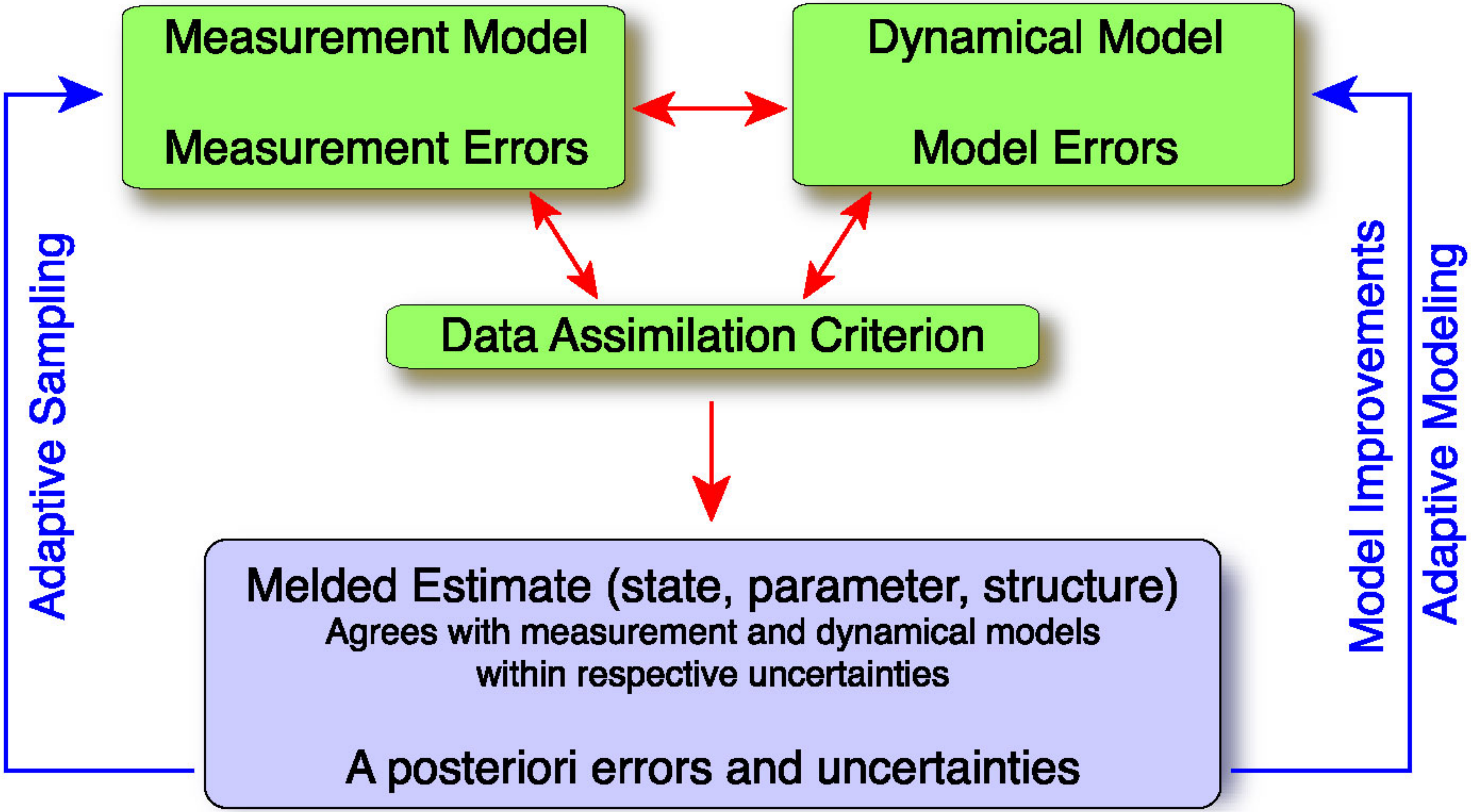
MAIN SOURCES OF UNCERTAINTIES IN MODERN OCEAN SCIENCE

- **Ocean Physics model uncertainties**
  - Bathymetry
  - Initial conditions
  - BCs: surface atmospheric, coastal-estuary and open-boundary fluxes
  - Parameterized processes: sub-grid-scales, turbulence closures, un-resolved processes
    - e.g. tides and internal tides, internal waves and solitons, microstructure and turbulence
  - Numerical errors: steep topographies/pressure gradient, non-convergence

- **Measurement uncertainties**
  - Sensor errors (random and bias/drift)
  - Environmental noise (processes measured but not of interest, e.g. of scales outside of studied scale window)
  - Equation(s) linking model variables to measured variables

WHAT IS DATA ASSIMILATION?

A Melded Estimate of Data and Dynamics



e.g. Robinson A.R., P.F.J. Lermusiaux and N.Q. Sloan, III (1998). *Data Assimilation*. The Sea, Vol. 10.

Robinson A.R. and P.F.J. Lermusiaux (2002). *DA for physical-biological interactions*. The Sea, Vol.12.

Generic Data Assimilation Problem

Dynamical models:

$$d\phi_i + \mathbf{u}\cdot\nabla\phi_i dt - \nabla(K_i\nabla\phi_i)dt = B_i(\phi_1,\ldots,\phi_i,\ldots,\phi_n)dt + d\eta_i \qquad (i = 1,\cdots,n)$$

e.g. i= u, v, T, $\cdots$, ZOO, $\cdots$, p

Parameter equations:

$$dP_\ell = C_\ell(\phi_1,\ldots,\phi_i,\ldots,\phi_n)dt + d\zeta_\ell \qquad (\ell = 1,\cdots,p)$$

e.g. $P_\ell = \{\ K_i,\ R_i,\ \cdots\}$

Measurement models:

$$y_j = \mathcal{H}_j(\phi_1,\cdots,\phi_i,\cdots,\phi_n) + \epsilon_j \qquad (j = 1,\cdots,m)$$

e.g. $y_j = \{\ XBT_j,\ Fluo_j,\ SSH_j,\ CODAR_j\}$

Assimilation criterion:

$$\min_{\phi_i, P_\ell} \quad J(d\eta_i\ ,\ d\zeta_\ell\ ,\ \epsilon_j\ ,\ q_\eta\ ,\ q_\zeta\ ,\ q_\epsilon)$$

CLASSES OF DATA ASSIMILATION SCHEMES

	Error Evol.	Criterion
• **Estimation Theory (Filtering and Smoothing)**		
1. Direct Insertion, Blending, Nudging	- Linear	
2. Optimal interpolation	- Linear	LS
3. Kalman filter/smoother	- Linear	LS
4. Bayesian estimation (Fokker-Plank equations)	- Non-lin.	Non-LS
5. Ensemble/Monte-Carlo methods	- Non-lin.	LS/Non-LS
6. Error-subspace/Reduced-order methods: Square-root filters, e.g. SEEK	- (Non)-Lin.	LS
7. Error Subspace Statistical Estimation (ESSE): 5 and 6	-Non-lin.	LS/Non-LS
• **Control Theory/Calculus of Variations (Smoothing)**		
1. "Adjoint methods" (+ descent)	- Linear	LS
2. Generalized inverse (e.g. Representer method + descent)	- Linear	LS
• **Optimization Theory (Direct local/global smoothing)**		
1. Descent methods (Conjugate gradient, Quasi-Newton, etc)	- Lin	LS/Non-LS
2. Simulated annealing, Genetic algorithms	- Non-lin.	LS/Non-LS

- **Hybrid Schemes**
  - Combinations of the above

Continuous Problem

Ocean Dynamical Model $d\phi_i + \mathbf{u}.\nabla\phi_i dt = \nabla(K_i \nabla\phi_i)dt + d\eta_i \quad (\phi_i = u, v, \psi, T, S)$

Measurement Model $y_j = \mathcal{H}_j(\phi_1, \cdots, \phi_i, \cdots, \phi_n) + \epsilon_j \quad (y_j = T_j, S_j)$

Assimilation Criterion $\min_{\phi_i} \quad J(d\eta_i\,,\ d\zeta_\ell\,,\ \epsilon_j\,,\ q_\eta\,,\ q_\zeta\,,\ q_\epsilon)$

Particles Trajectory $d\mathbf{x} = \mathbf{v}(\mathbf{x}, t; \eta_i, \epsilon_j)\ dt$

DLE/LCS computation LCS is defined as a ridge of σ_T(x,y,z,t)

Continuous-Discrete Problem

$\mathbf{x} = (\mathbf{u}, \mathbf{v}, \psi, \mathbf{T}, \mathbf{S})$ on discrete grid of ocean model **M**

$$d\mathbf{x} = \mathrm{M}(\mathbf{x}, x, y, z, t)dt + d\eta(z) \qquad \eta \sim \mathcal{N}(0, \mathbf{Q})$$

$$\mathbf{y} = \mathrm{H}_j(\mathbf{x}, x, y, z, t)dt + \epsilon(z) \qquad \epsilon \sim \mathcal{N}(0, \mathbf{R})$$

$$d\chi = \mathbf{v}(x, y, z, t)dt$$

Evolution of PDF Equations:

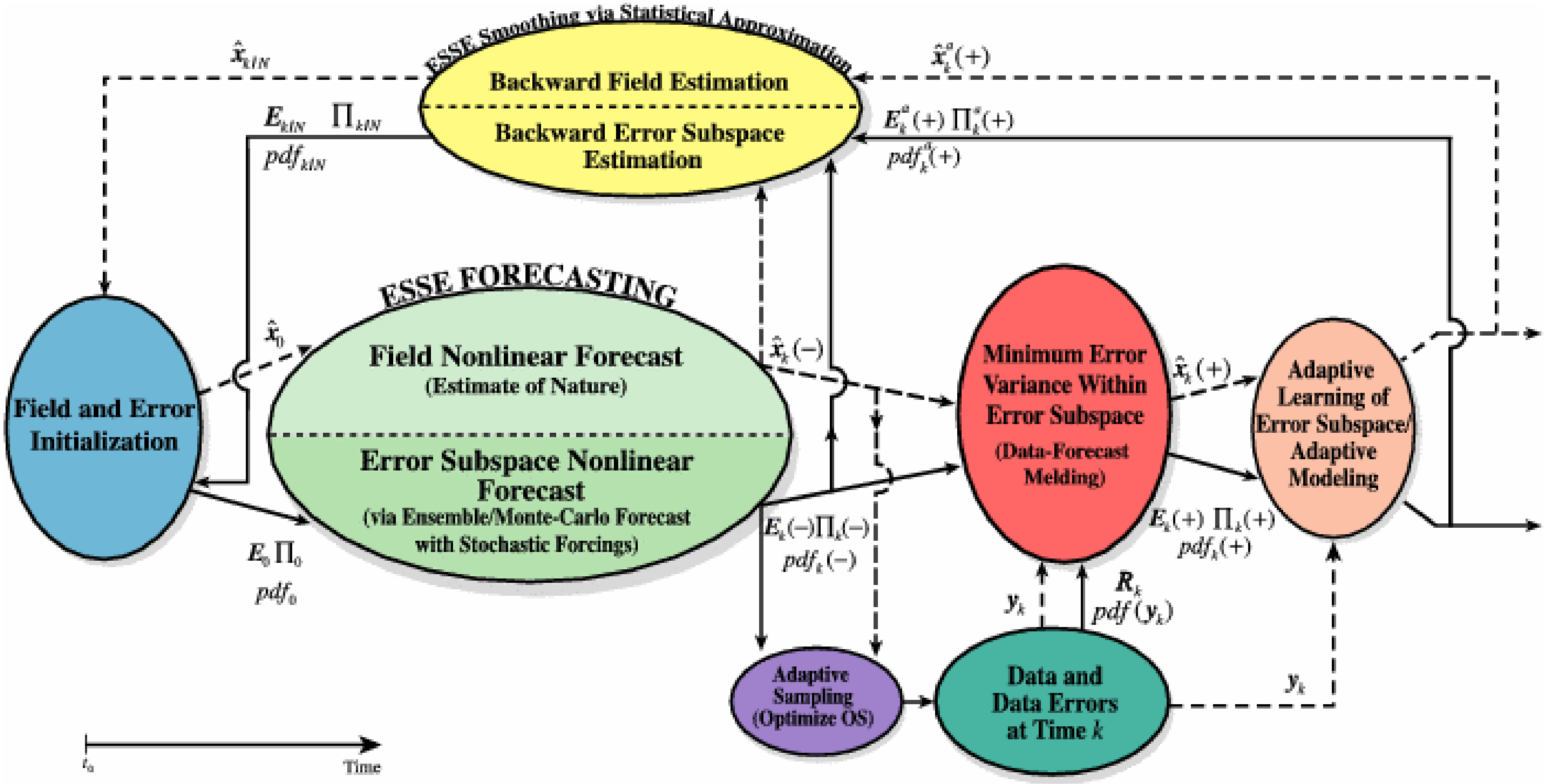
- Fokker-Planck equation (prediction)
- Sources/Sinks of uncertainties are the:
    1. Initial Conditions
    2. Stochastic forcings, and
    3. Nonlinear terms in the Nav.Stok. (PE) equations, basically what sets the dynamical properties of the system.
    4. Effects of data assimilation: data type, locations and uncertainties (Zakai eqn)

4 Uncertainty problems:

1. Prediction problem (from real-time or hindcast)
2. Re-analysis and full assimilation (filtering and smoothing) close to stationnary errors if observation system well chosen/adapted
3. Predictability limit problem/estimation (entropy on/of LCS) error growth
4. Full state space trajectories

Solved by ensemble ESSE approach: 1 DLE/LCS for each ensemble member

Error Subspace Statistical Estimation (ESSE)



- Uncertainty forecasts (with dynamic error subspace, error learning)
- Ensemble-based (with nonlinear and stochastic primitive eq. model (HOPS)
- Multivariate, non-homogeneous and non-isotropic Data Assimilation (DA)
- Consistent DA and adaptive sampling schemes
- Software: not tied to any model, but specifics currently tailored to HOPS

Data Assimilation via ESSE

Table 1. Filtering/Smoothing via ESSE: Continuous-Discrete Problem Statement

Dynamical Model:	$d\widehat{\mathbf{x}} = \mathcal{M}(\widehat{\mathbf{x}})\, dt + d\widehat{\boldsymbol{\eta}}\,, \;\text{with}\; \widehat{\mathbf{x}}(\mathbf{r}_0, t_0) = \widehat{\mathbf{x}}_0 + \widehat{\mathbf{n}}(0)\,.$
Measurement Model:	$\mathbf{y}_k^{\text{o}} = \mathcal{H}(\mathbf{x}_k) + \widehat{\boldsymbol{\epsilon}}_k\,.$
Estimation Criterion:	
Estimate Error Subpace:	$\left\{\text{Find } \mathbf{P}_k^p = \mathbf{E}_k \boldsymbol{\Pi}_k \mathbf{E}_k^T \text{ with } \operatorname{rank}(\mathbf{E}_k) = p \;\middle|\; \min_{\boldsymbol{\Pi}_k, \mathbf{E}_k} \lVert \mathbf{P}_k - \mathbf{P}_k^p \rVert \right\}$
Estimate State by Min. Err. Var. in ES:	$\left\{\text{Find } \widehat{\mathbf{x}}_k \;\middle|\; \min_{\widehat{\mathbf{x}}_k} J_k = \operatorname{tr}\left[\mathbf{P}_k^p(+)\right] \text{ using } [\mathbf{y}_0^{\text{o}}, \ldots, \mathbf{y}_k^{\text{o}}/\mathbf{y}_N^{\text{o}}]\right\}$

- **Optimal error space reduction and Min. Err. Var. combined:**

"Estimate the ocean evolution by minimizing the largest (most energetic) expected errors, in agreement with the full dynamical model and measurement model (data) constraints, and their respective uncertainties."

- Linked to POD/Polynomial Chaos, but with time-varying error Karhunen-Loeve basis:

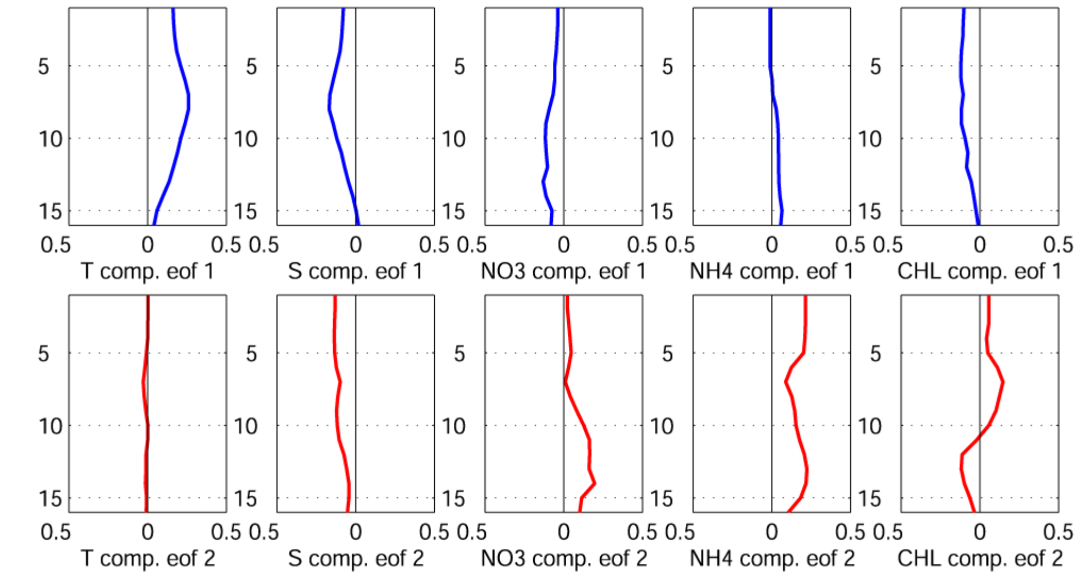
$$\mathbf{x}(x,t,\theta) = \bar{\mathbf{x}}(x,t) + \sum_{i=1}^{M} \sqrt{\lambda_i}\;\; \phi_u^s(\mathbf{x},t)\; \zeta_i(\theta)$$

Initialization of the Dominant Error Covariance Decomposition

- Dominant uncertainties: missing or uncertain variability in IC, e.g. smaller mesoscale variability

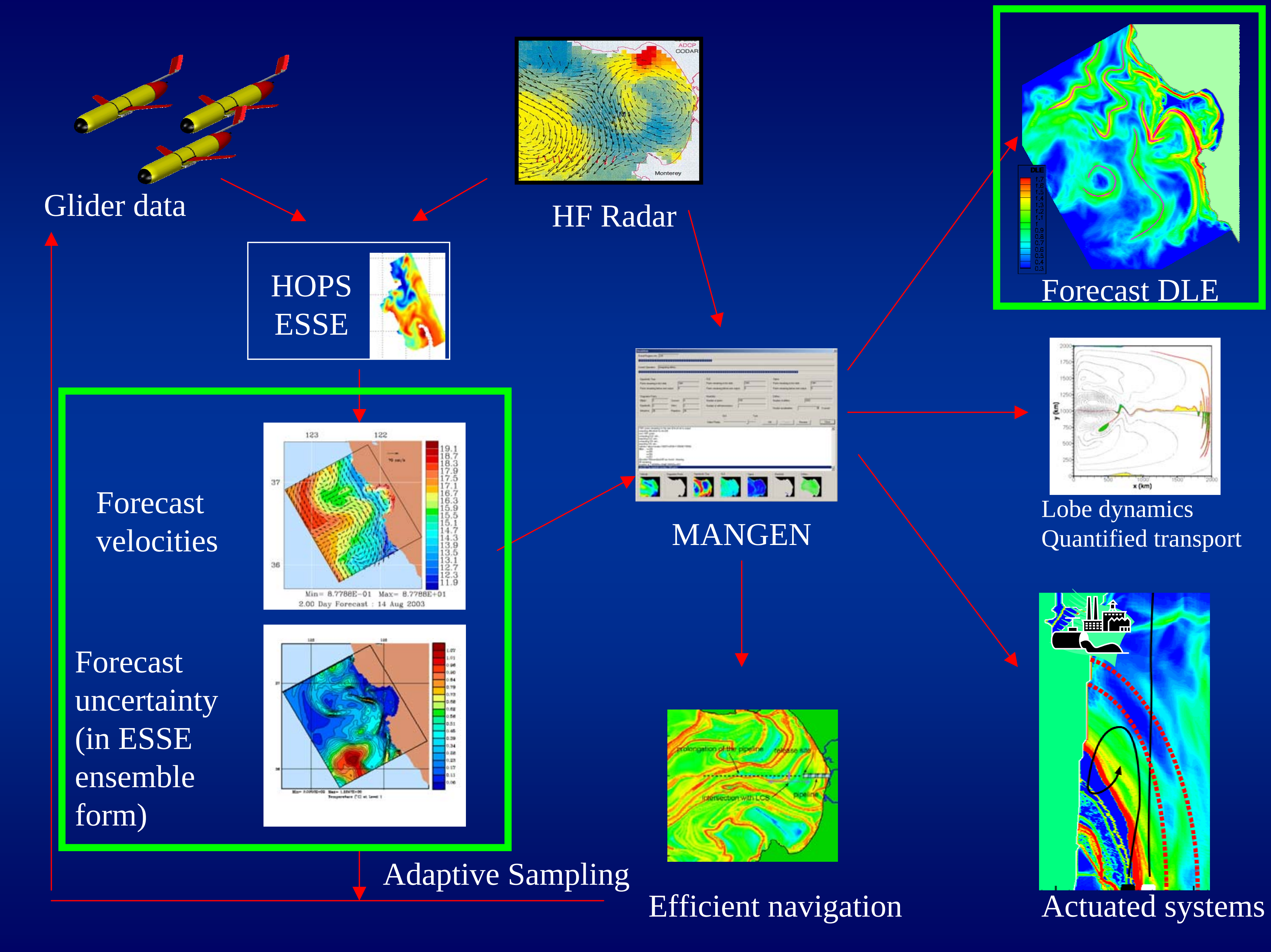
- Approach: Multi-variate, 3D, Multi-scale

``Observed'' portions:
directly specified and eigendecomposed from differences between the initial state and data, and/or from a statistical model fit to these differences



``Non-observed'' portions:
Keep ``observed'' portions fixed and compute ``non-observed'' portions from ensemble of numerical (stochastic) dynamical simulations

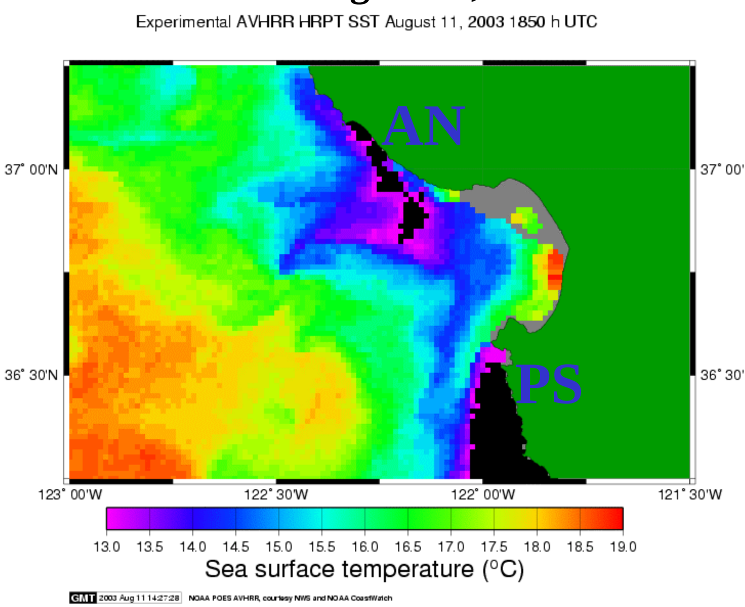
See: Lermusiaux et al (QJRMS, 2000) and Lermusiaux (JAOT, 2002)

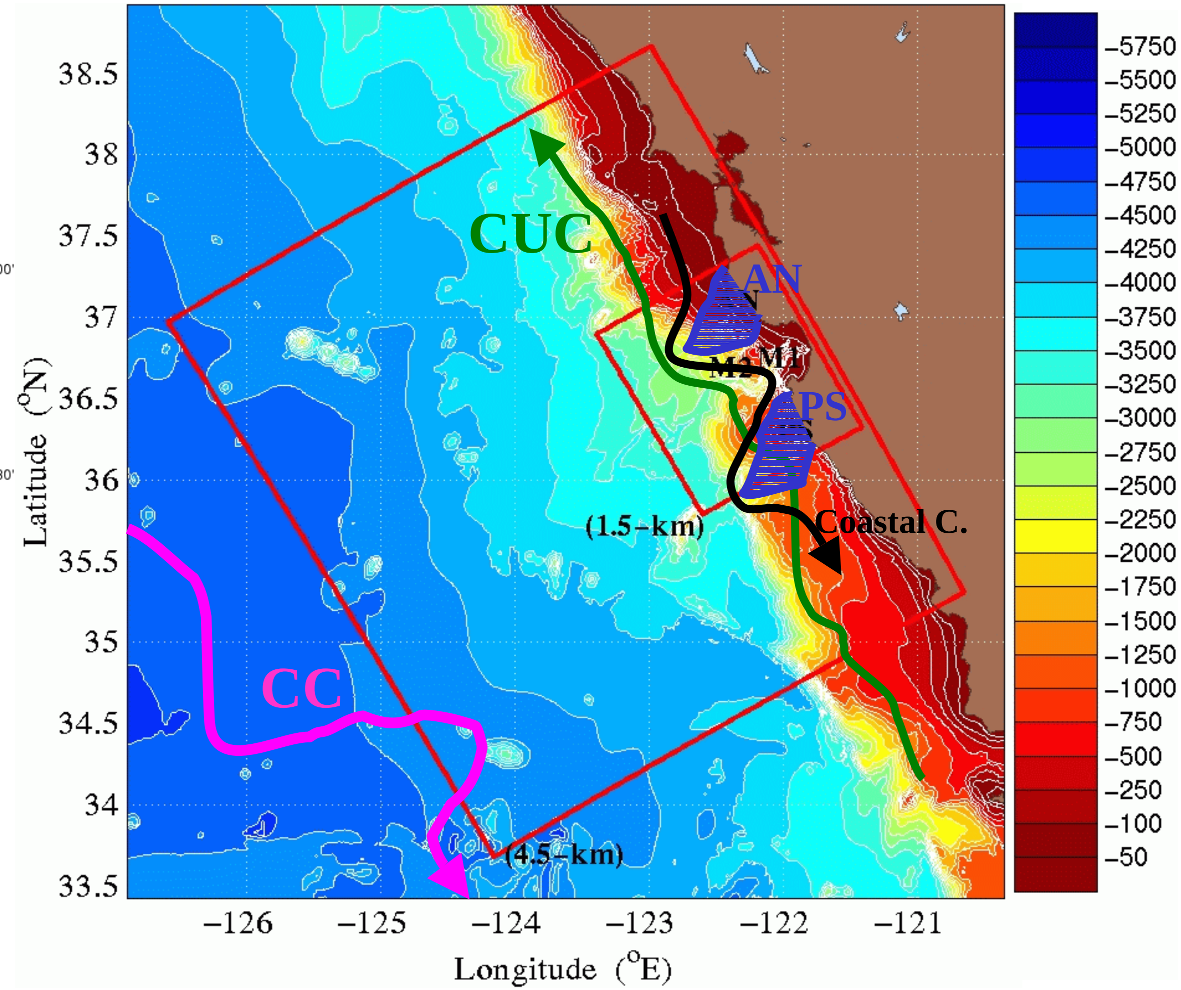


Glider data
ADCP
CODAR
Monterey
HF Radar
HOPS
ESSE
Forecast velocities
Min= 8.7788E-01 Max= 8.7788E+01
2.00 Day Forecast : 14 Aug 2003
Forecast uncertainty (in ESSE ensemble form)
MANGEN
Forecast DLE
Lobe dynamics
Quantified transport
Adaptive Sampling
prolongation of the pipeline
release site
intersection with LCS
pipeline
Efficient navigation
Actuated systems

REGIONAL FEATURES of Monterey Bay and California Current System and Real-time Modeling Domains (AOSN2, 4 Aug. – 3 Sep., 2003)

SST on August 11, 2003

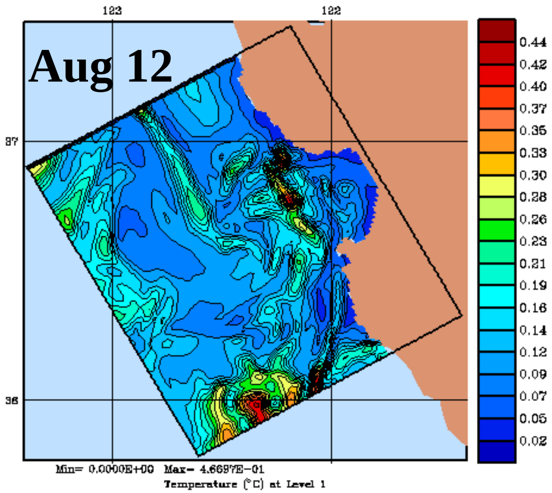




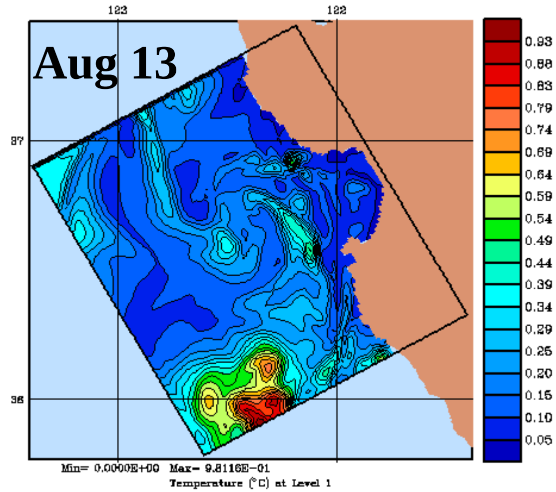
REGIONAL FEATURES

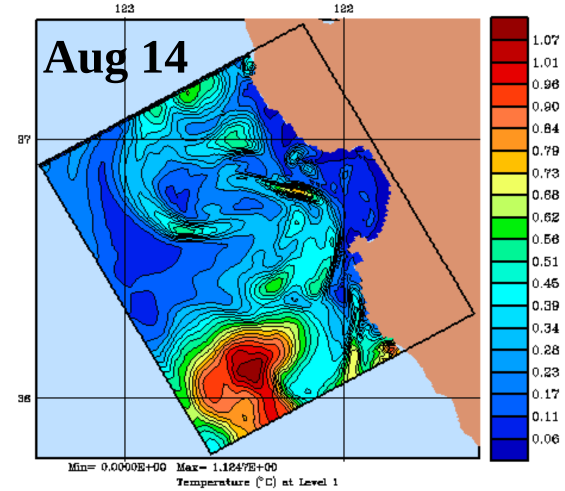
- **Upwelling centers at Pt AN/ Pt Sur:**…………Upwelled water advected equatorward and seaward
- **Coastal current, eddies, squirts, filam., etc:**….Upwelling-induced jets and high (sub)-mesoscale var. in CTZ
- **California Undercurrent (CUC):**……………..Poleward flow/jet, 10-100km offshore, 50-300m depth
- **California Current (CC):**……………………Broad southward flow, 100-1350km offshore, 0-500m depth

ESSE Surface Temperature Error Standard Deviation Forecasts

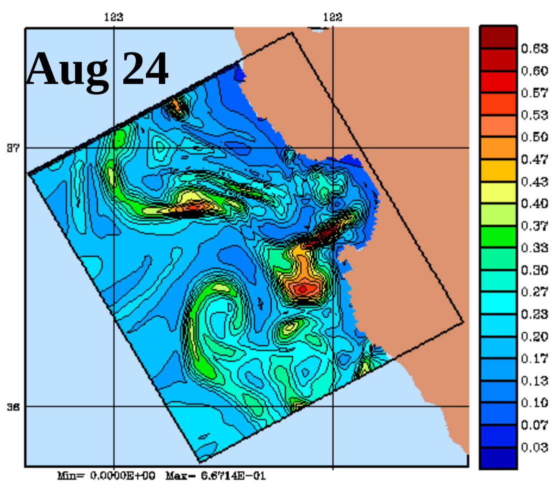


Start of Upwelling

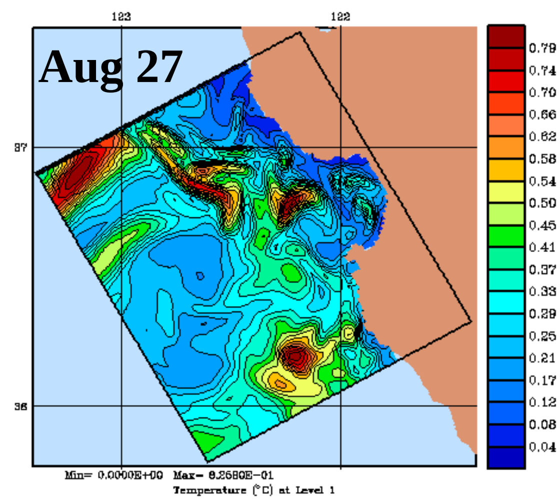


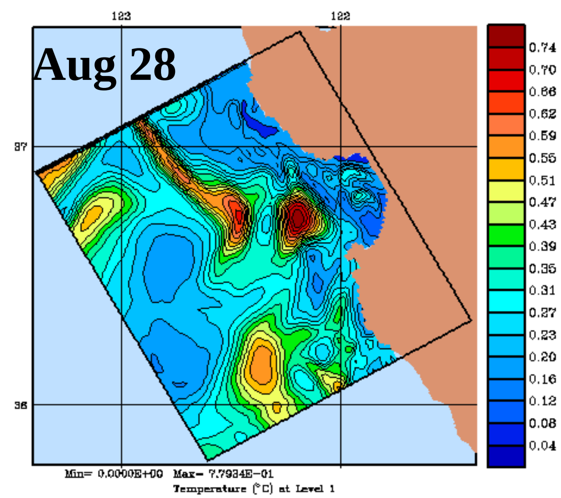


First Upwelling period



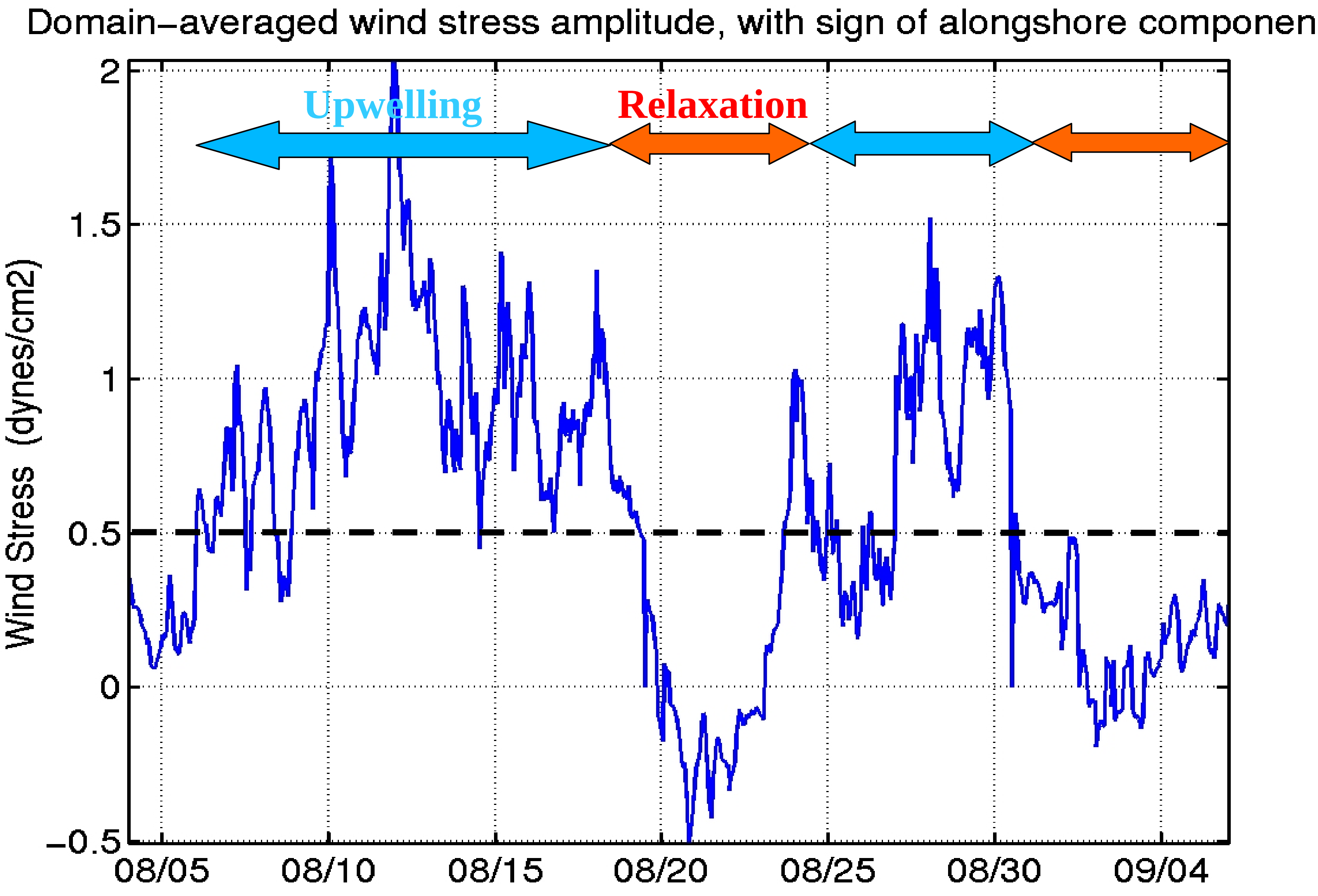
End of Relaxation





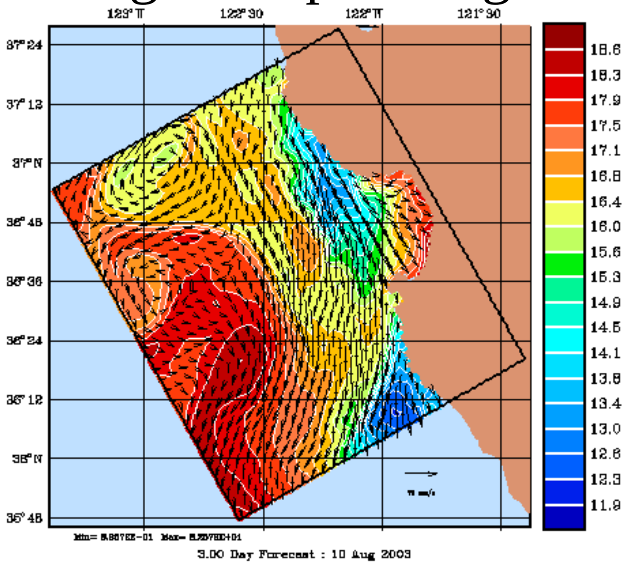
Second Upwelling period

Oceanic responses and atmospheric forcings during August 2003

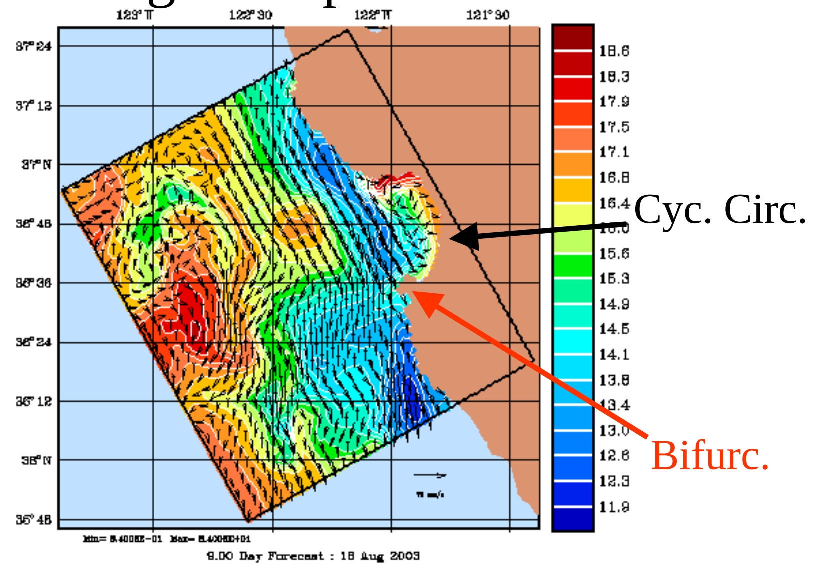


Oceanic responses and atmospheric forcings during August 2003

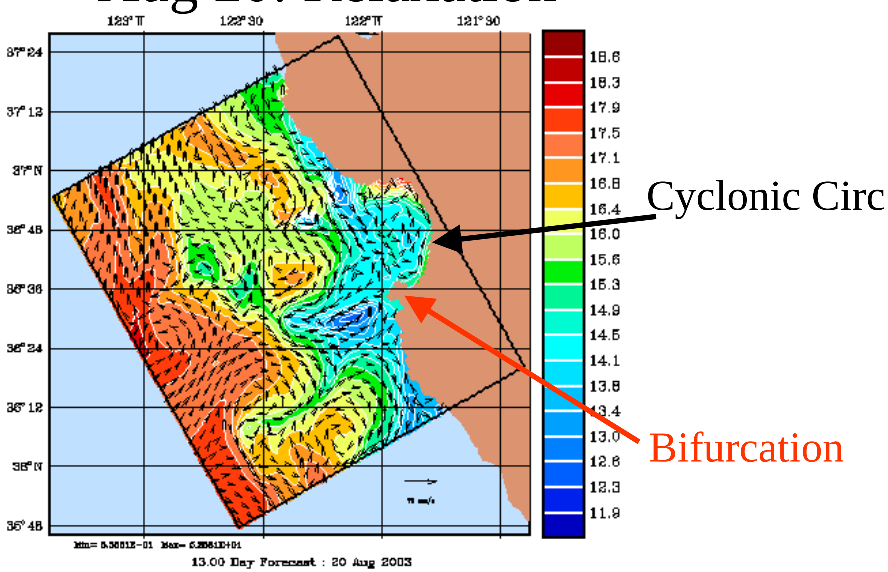
Aug 10: Upwelling



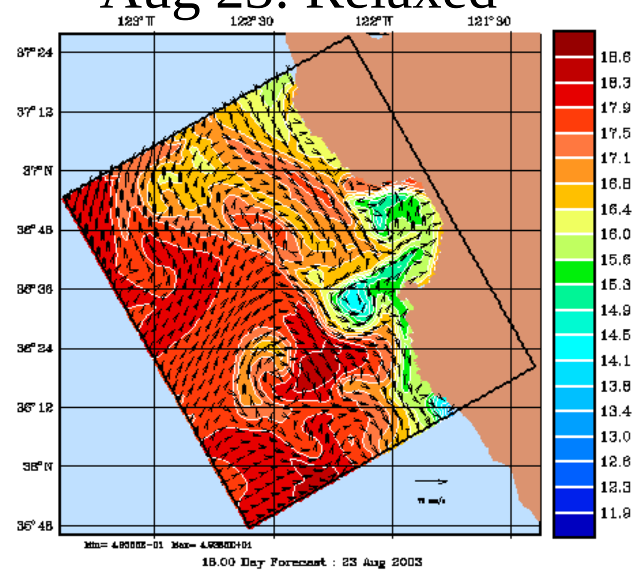
Aug 16: Upwelled



Aug 20: Relaxation



Aug 23: Relaxed



Upwelling: Aug 26 - 29

Predicted Surface Temp. overlaid with velocity vectors

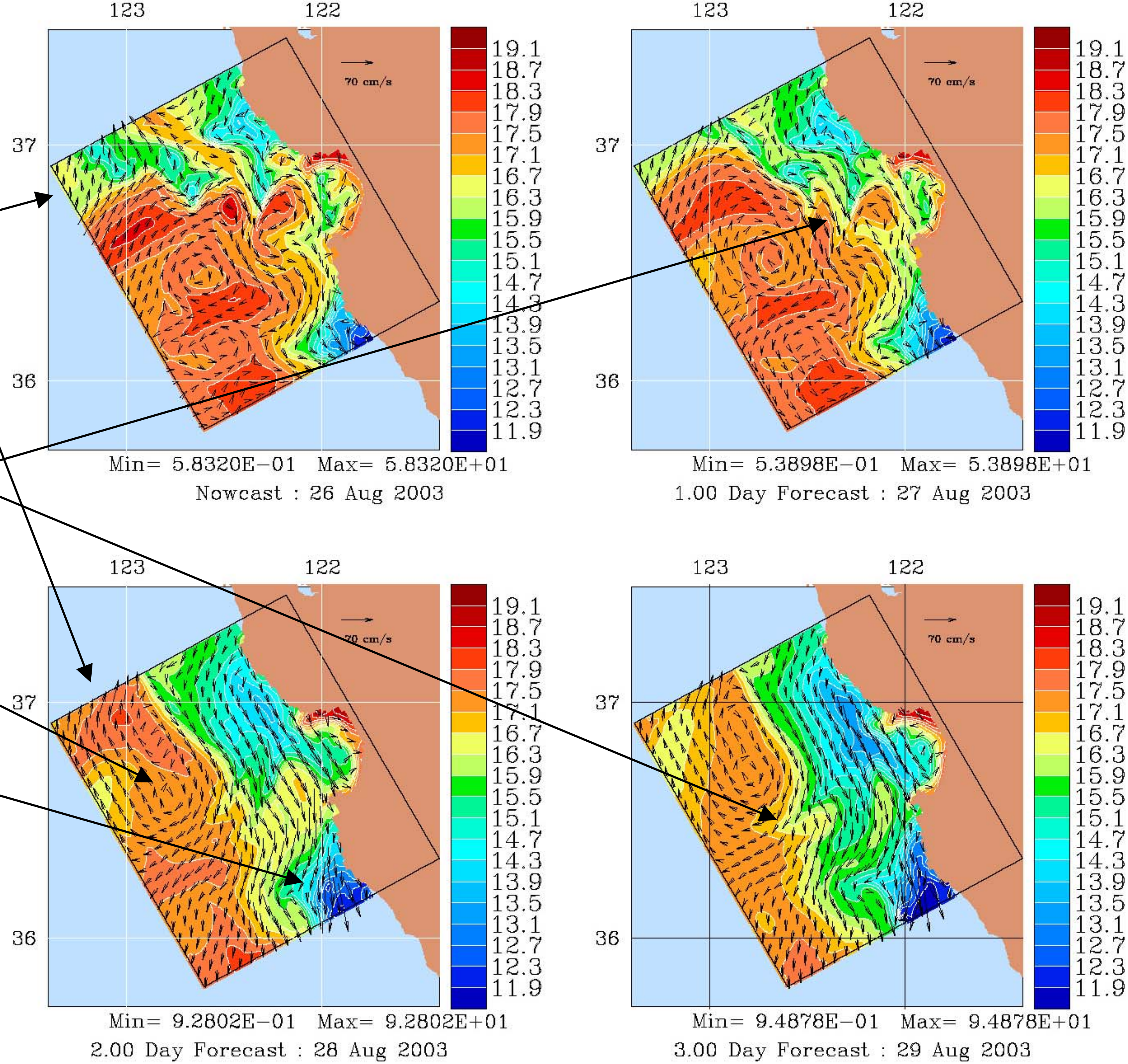
Northward advection of cold eddy field

Pt AN Upwelling Plume/Squirt

Offshore eddy

Pt Sur upwelling and fronts/eddying

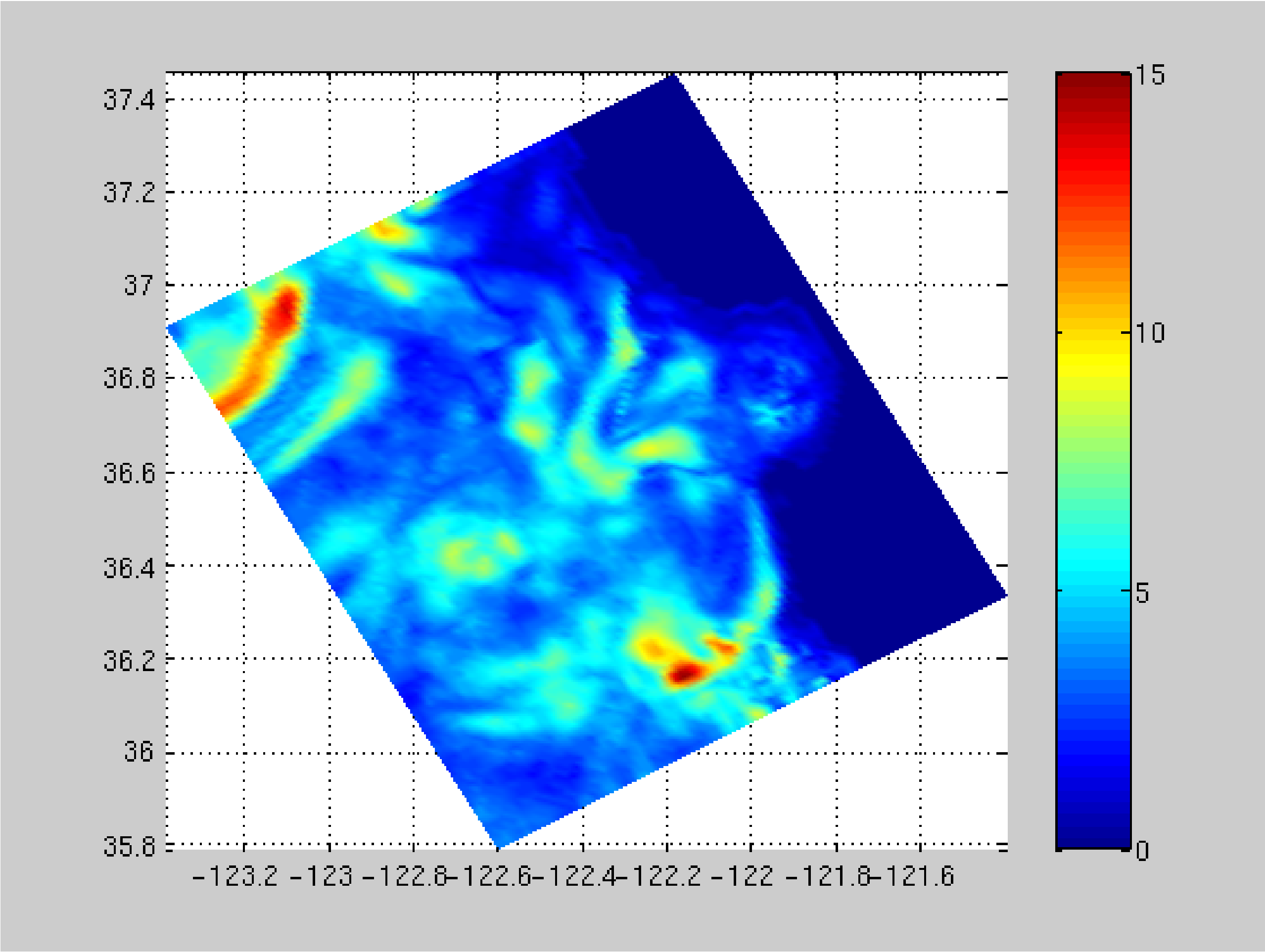
Daily cycles and wind-driven responses



Upwelling (Aug 26-Aug 29): |u| error Std. estimate

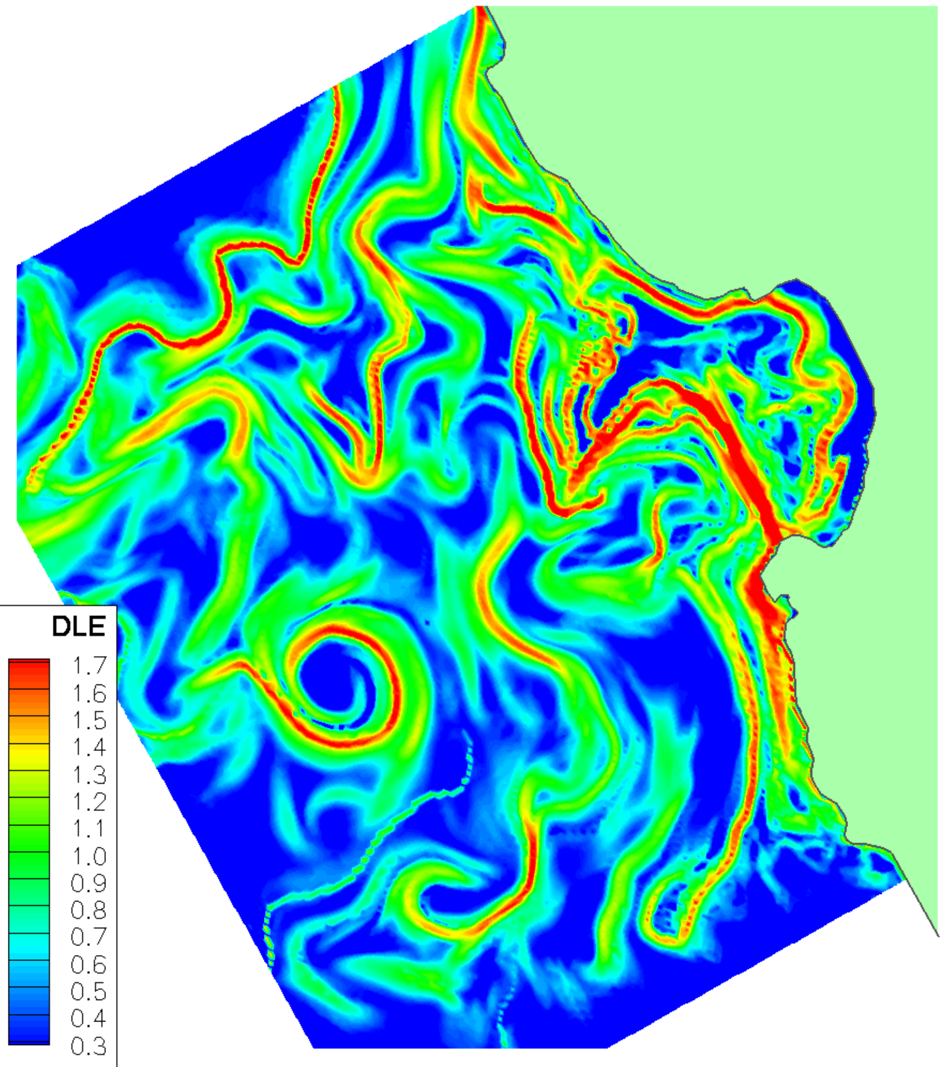
Main features (from north to south)

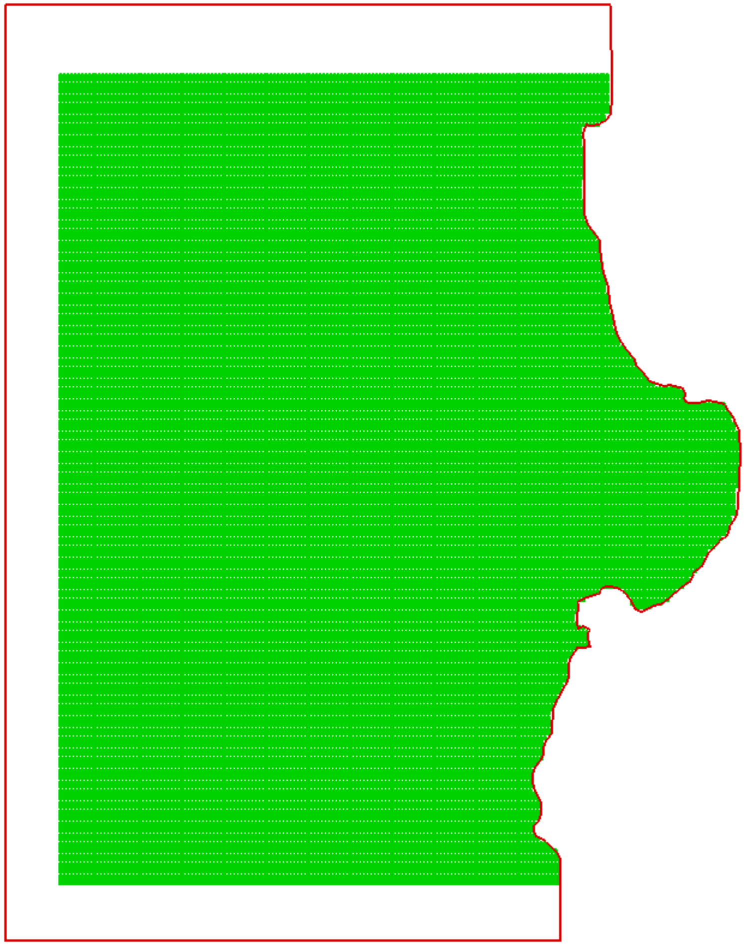
- Uncertainty ICs:
  - -a function of past dynamics and of past measurement types/locations
- Northward advection of cold eddy field
- Pt AN Upwelling Plume/Squirts formation, position and instabilities
- Offshore eddy
- Pt Sur upwelling frontal position and instabilities
- Daily cycles and wind-driven uncertainty reduction/burst



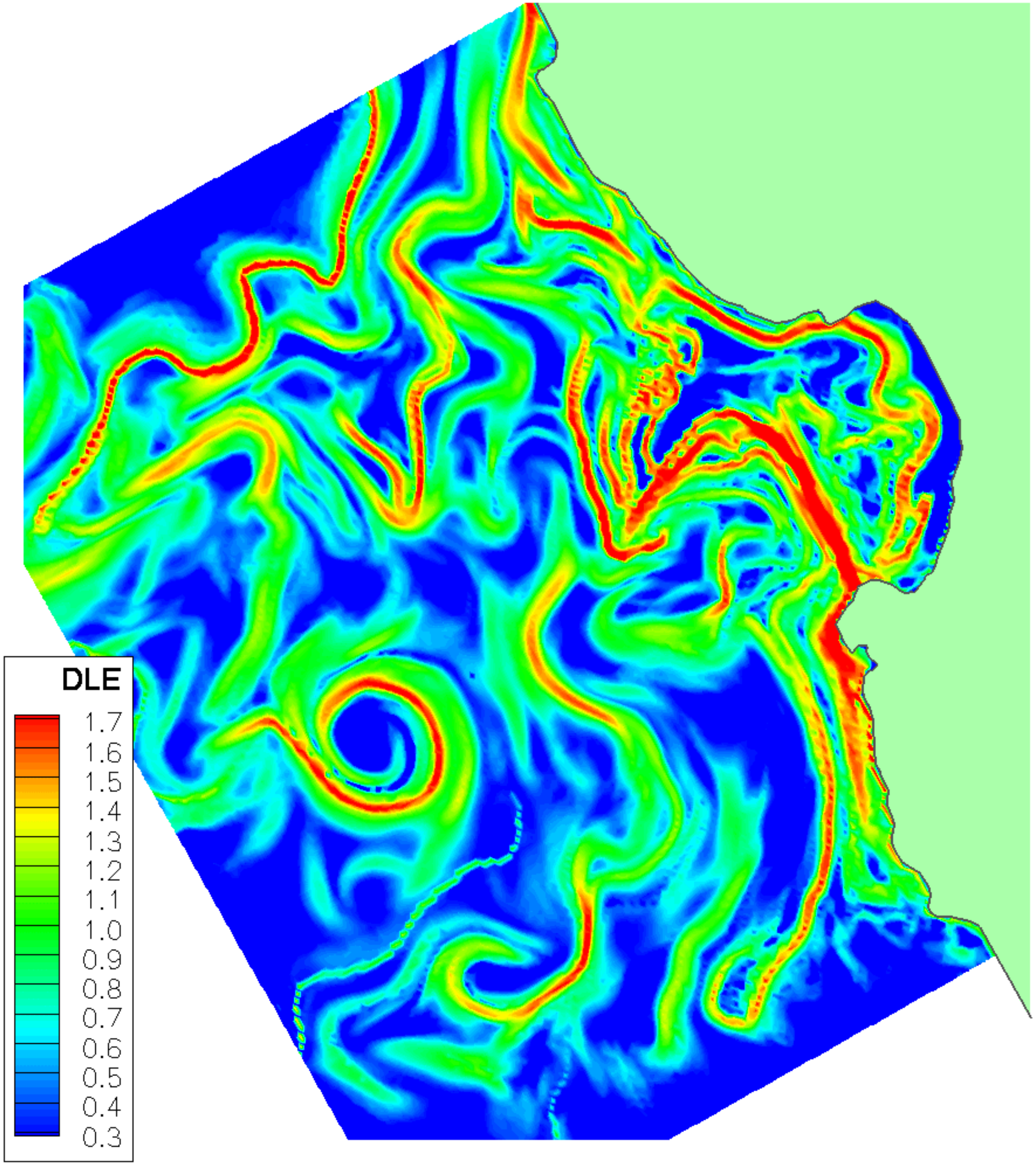
Ocean Realization #1 (hindcast)

Flow field evolution (right) and its DLE for T= 3 days (below)



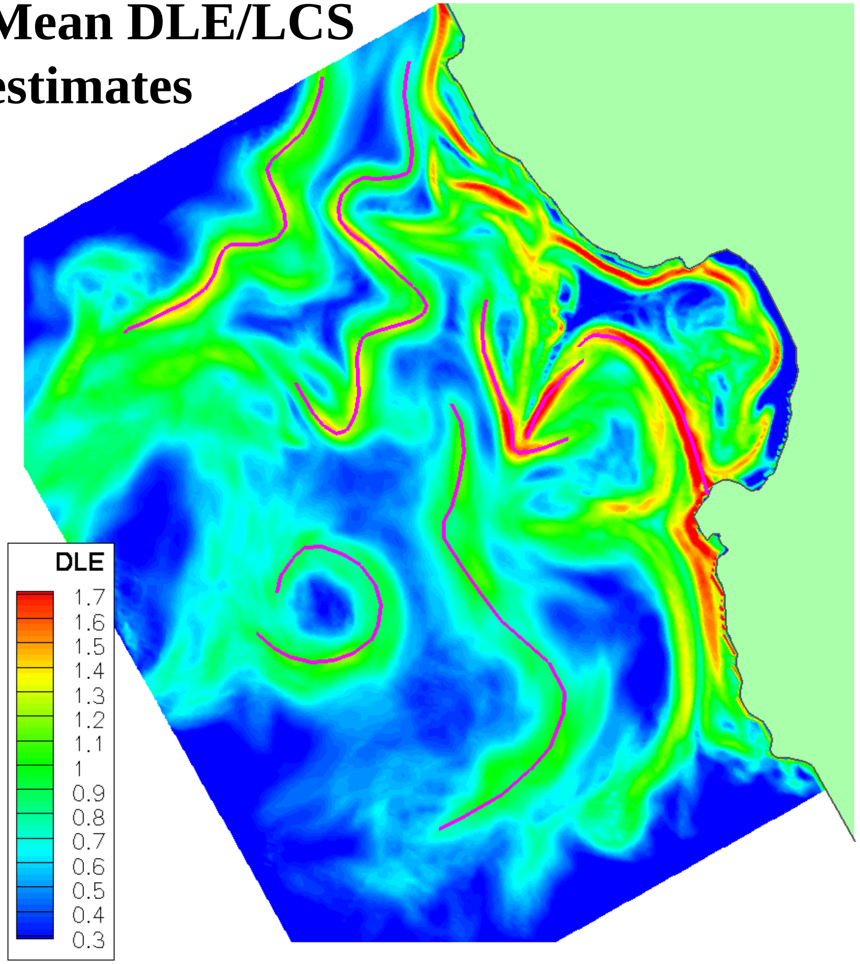


DLE
Realizations #1-26

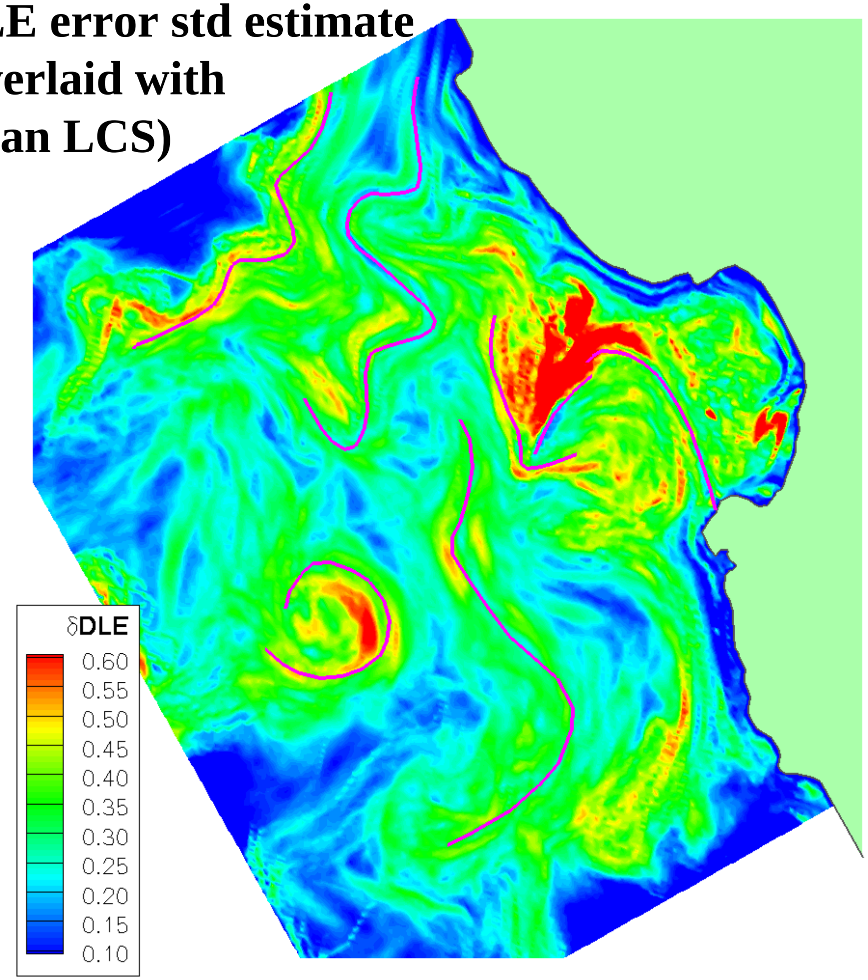


Uncertainties of DLE/LCS

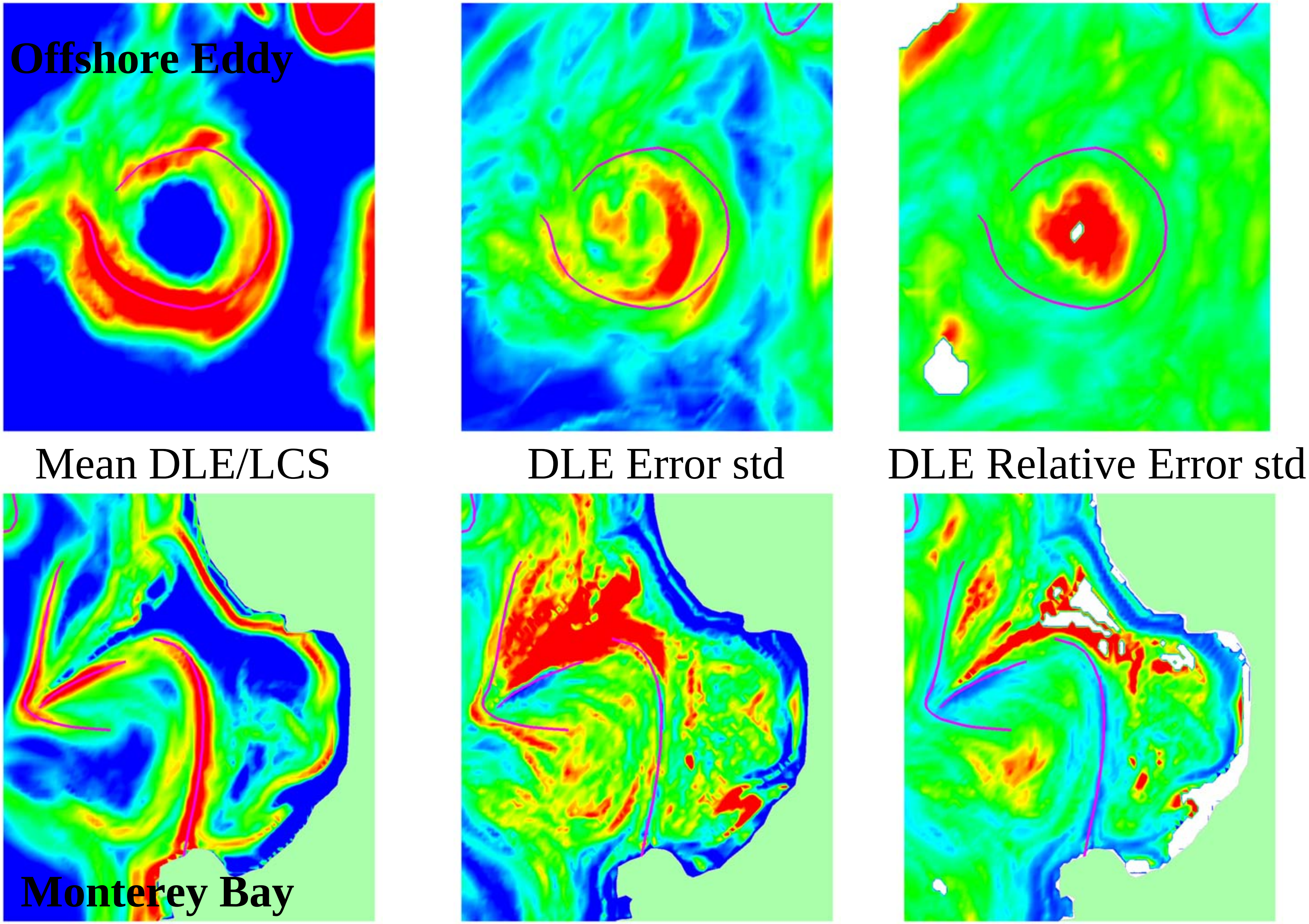
Mean DLE/LCS estimates



DLE error std estimate (overlaid with mean LCS)



Focus on 2 structures: Offshore Eddy and Monterey Bay

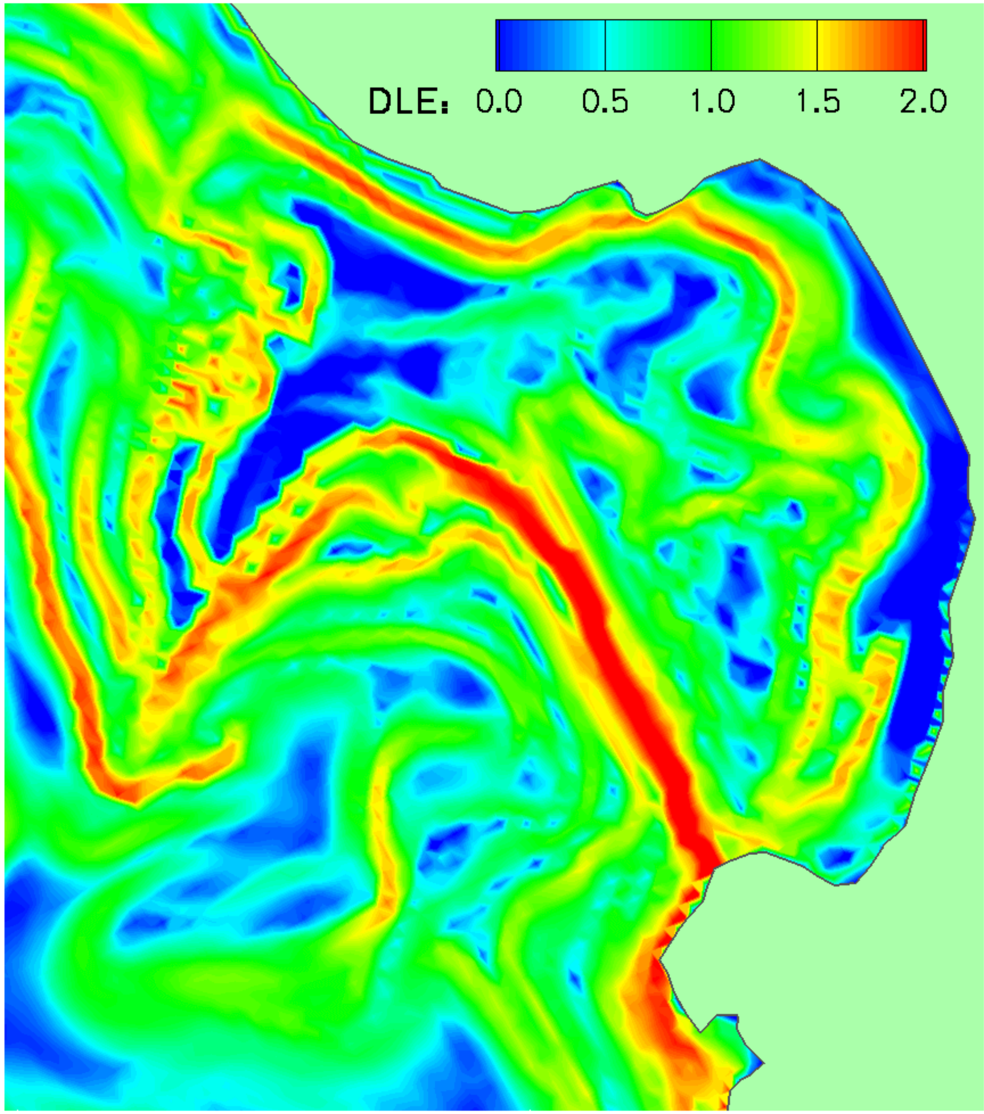


DLE

Realizations #1-26

Zoom over

Monterey Bay region



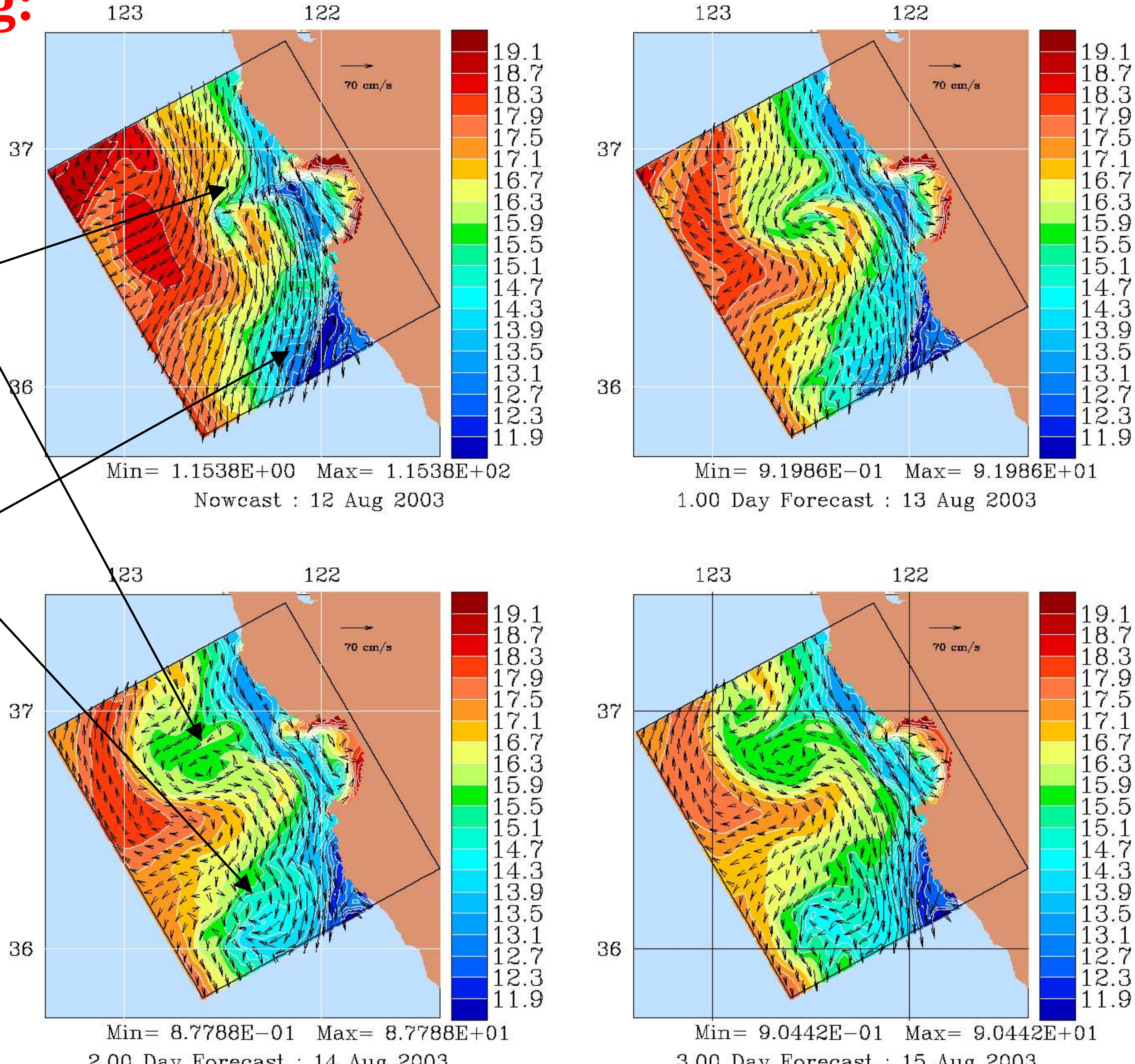
1st Upwelling: Aug 12 - 15

Predicted Surface Temp. overlaid with velocity vectors

Pt AN Upwelling Plume/Squirt and eddying

Pt Sur upwelling and fronts/eddying

Strongly wind-driven regime of surface currents

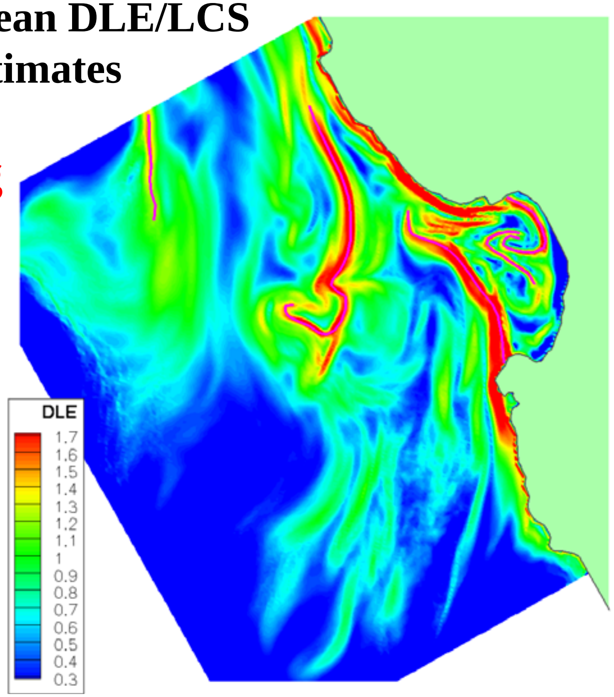


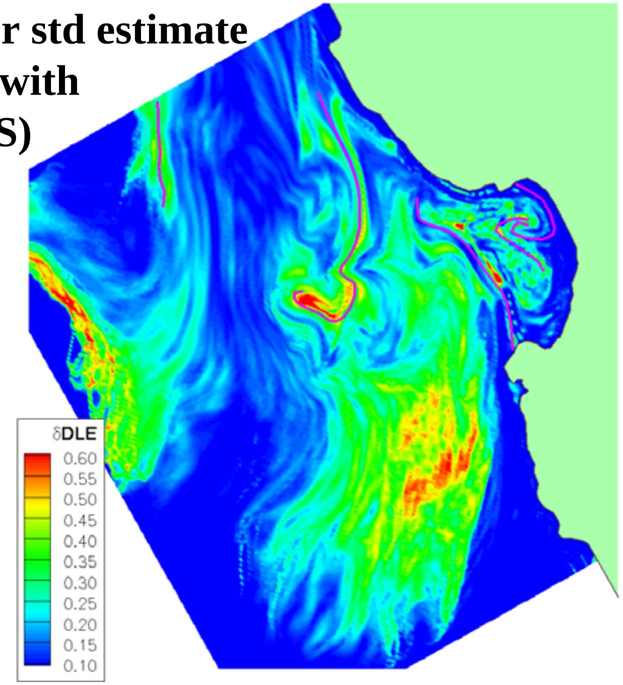
Mean DLE/LCS estimates

DLE error std estimate (overlaid with mean LCS)

1st Upwelling
Aug 7-18

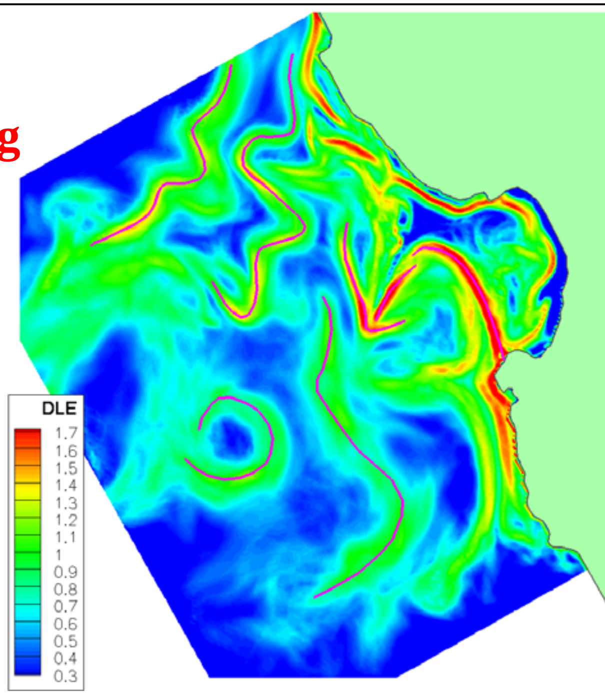
Our 3 days (Aug 12-15) are within Sustained Up. period

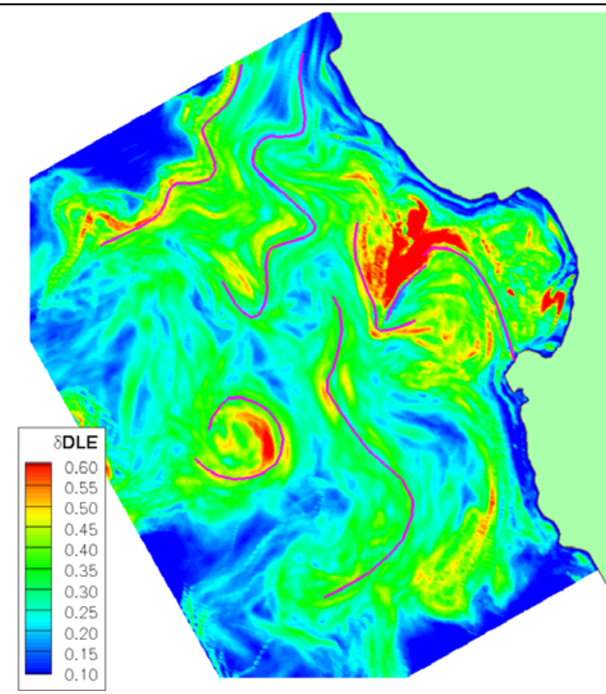




2nd Upwelling
Aug 26-30

Our 3 days (Aug 26-29) are within Up. formation period



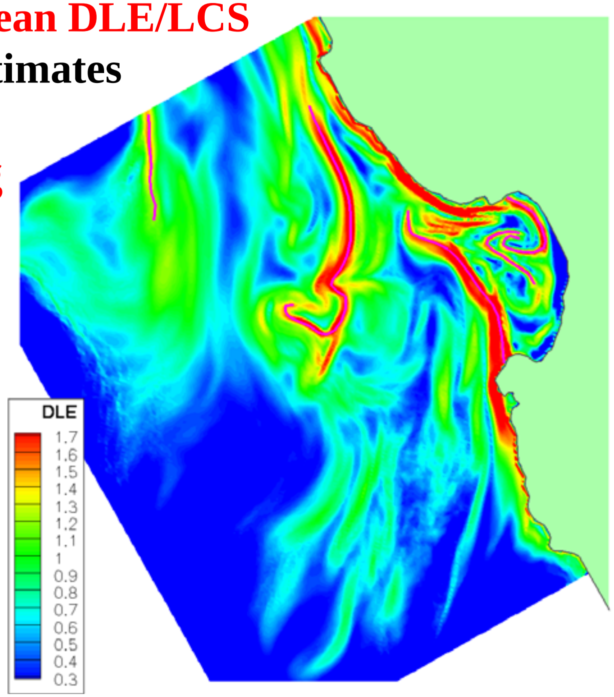


Mean DLE/LCS estimates

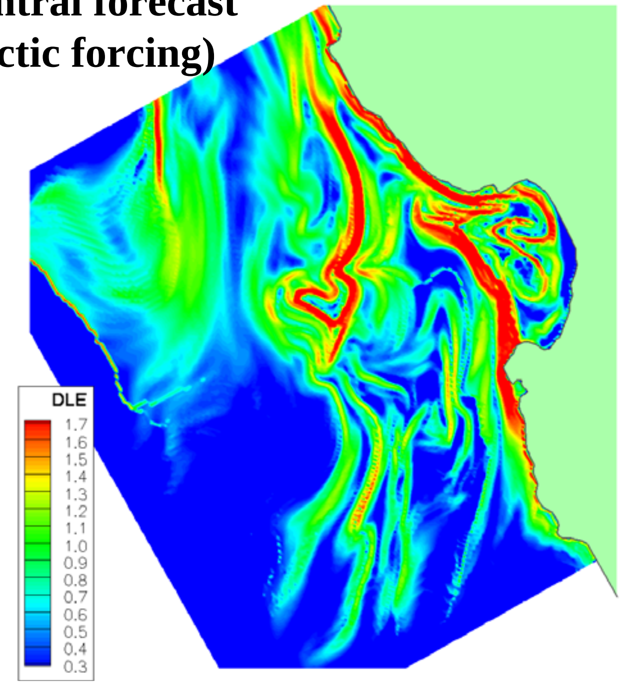
DLE of central forecast (no stochactic forcing)

1st Upwelling Aug 7-18

Our 3 days (Aug 12-15) are within Sustained Up. period

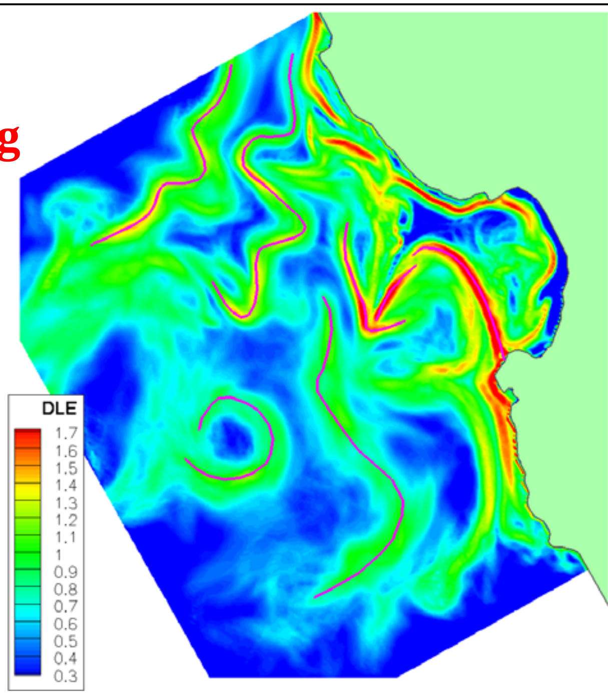


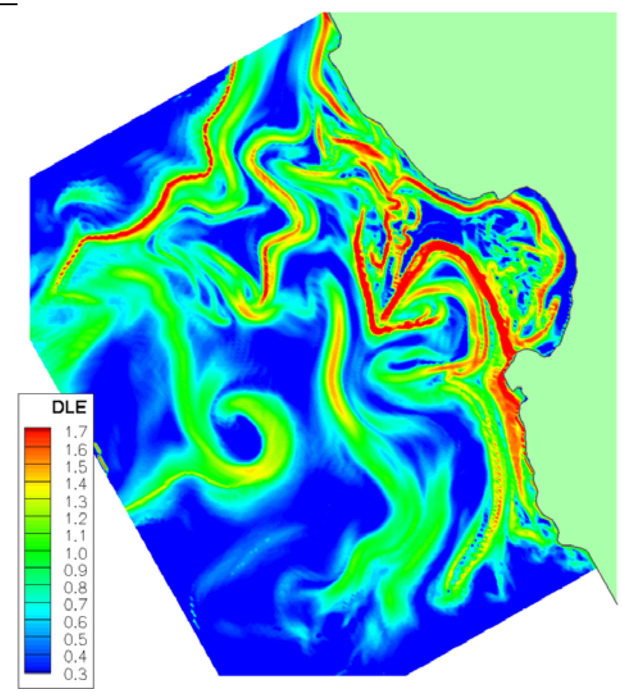
Proxi for DLE of the mean



2nd Upwelling Aug 26-30

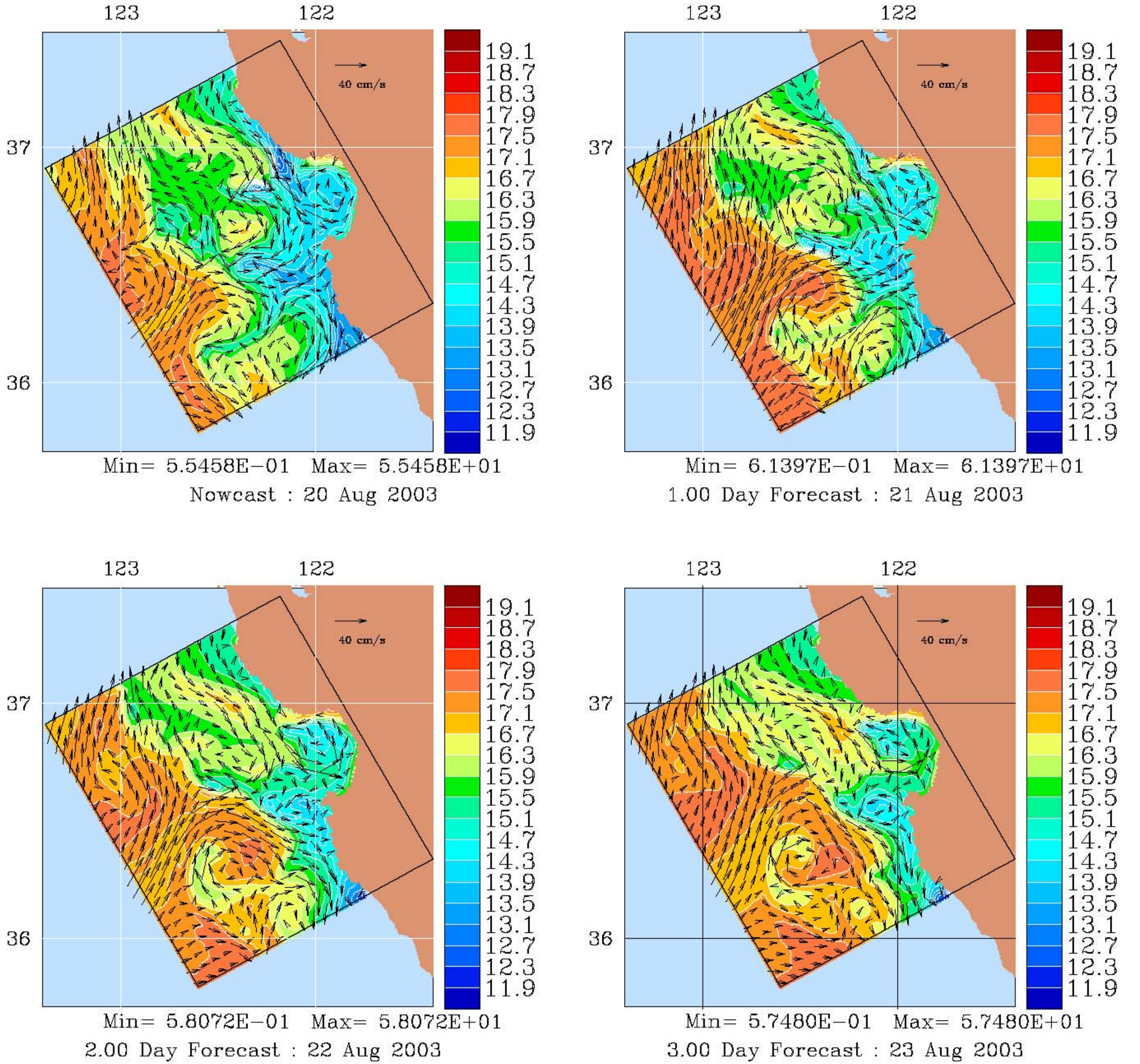
Our 3 days (Aug 26-29) are within Up. formation period



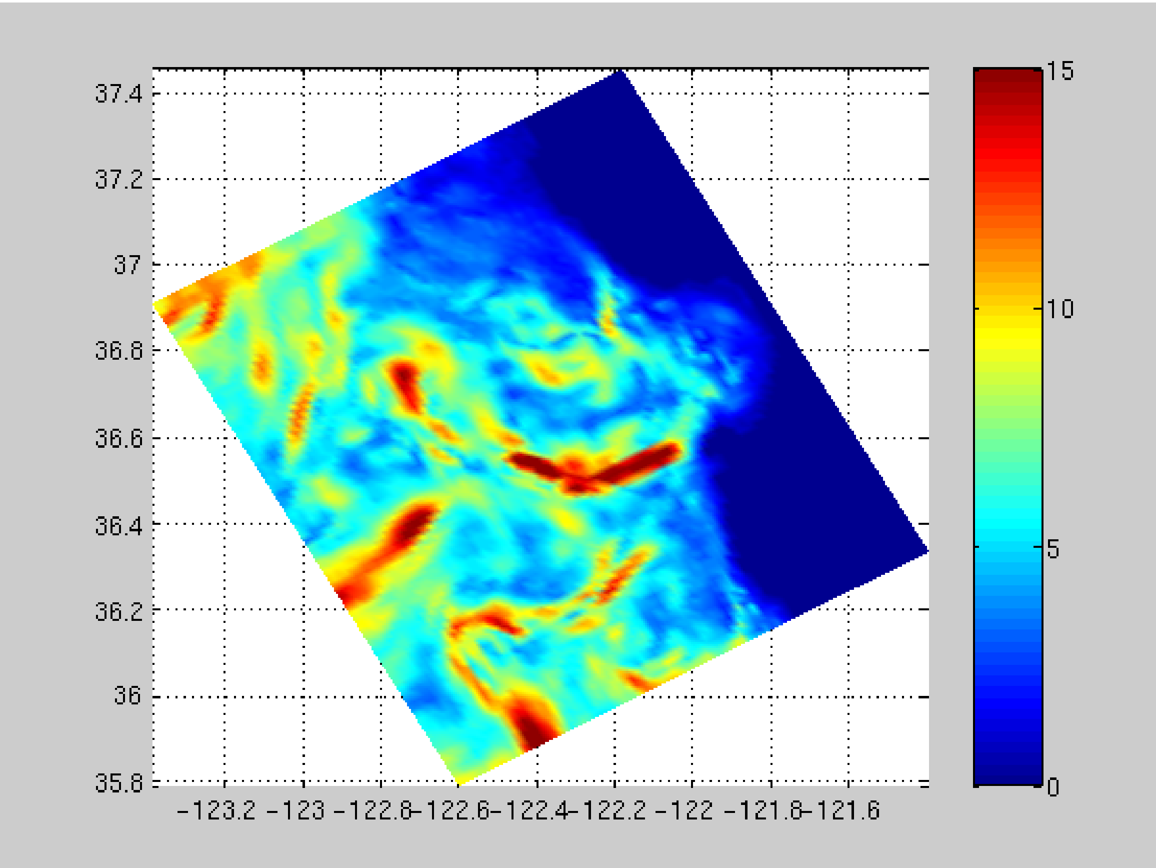


Relaxation Aug 19-25

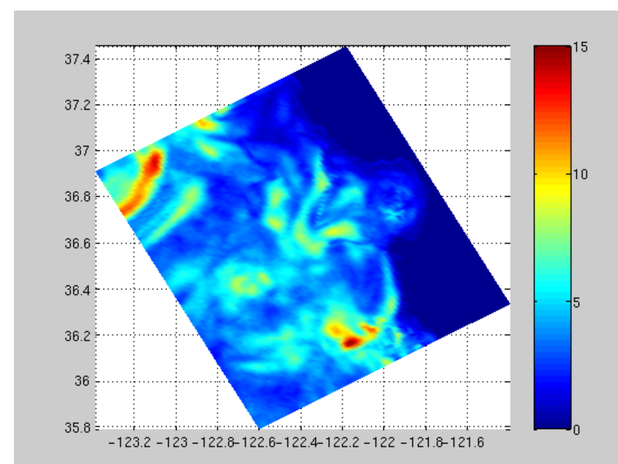
- Wind-forcing subsides
- Larger-scale atmos. control eliminated
- Transfer of kinetic energy to internal ocean dynamics
- Mesoscale and sub-mesocale instabilities and eddies



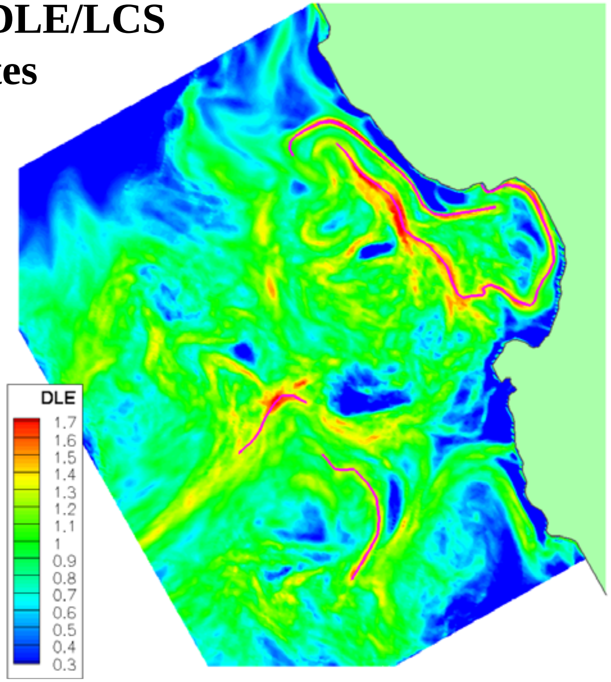
Relaxation (Aug 20-Aug 23): |u| error Std. estimate



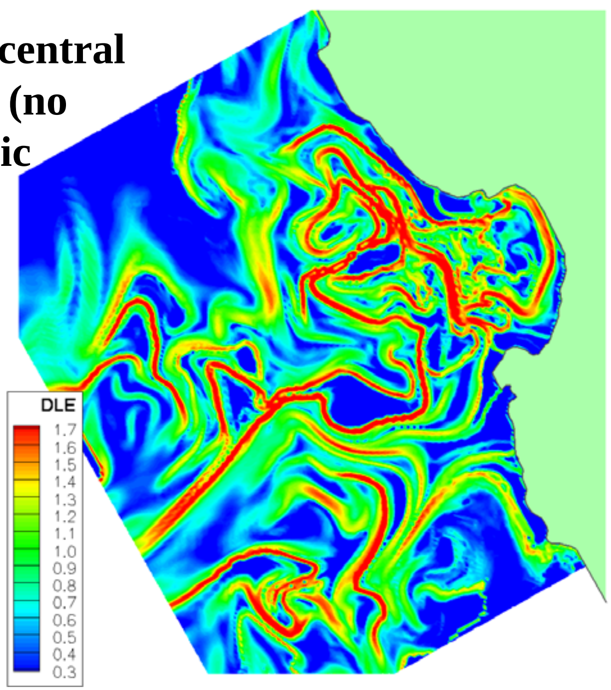
Reminder: Upwelling



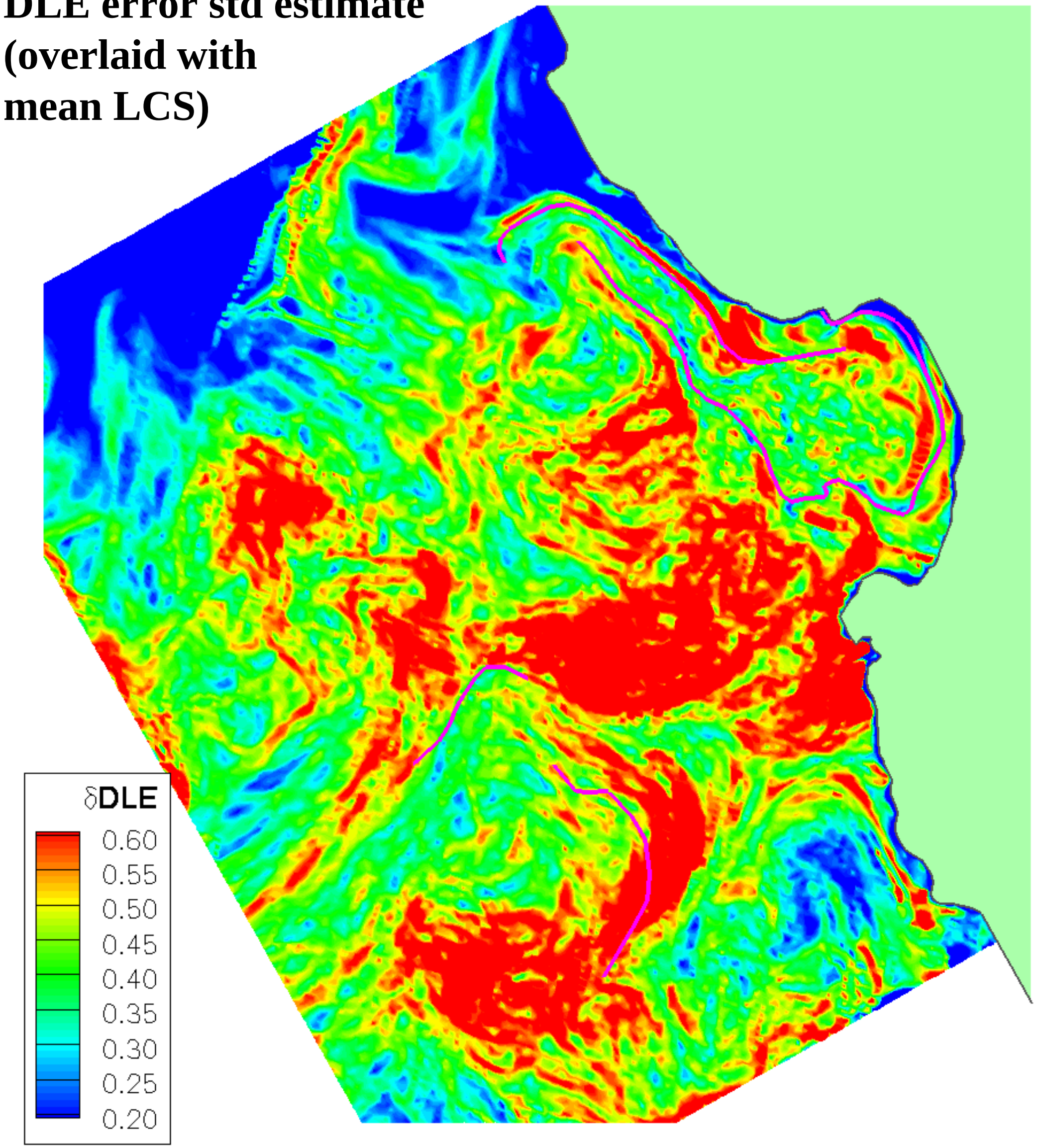
Mean DLE/LCS estimates



DLE of central forecast (no stochastic forcing)

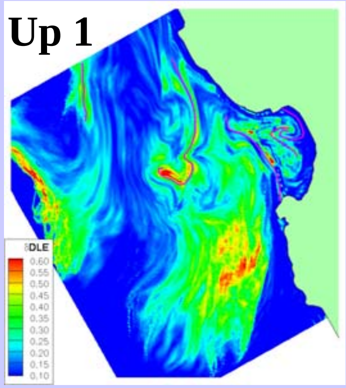


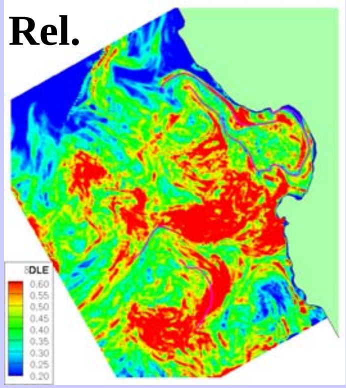
DLE error std estimate (overlaid with mean LCS)

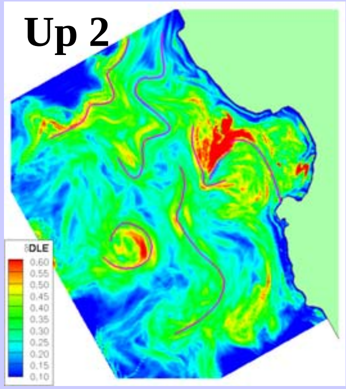


CONCLUSIONS

DLE error std estimate (overlaid with mean LCS) for 3 dynamical events







- HOPS/ESSE and MANGEN combined for useful nonlinear scheme for interdisciplinary estimation of oceanic LCS and their uncertainties via multivariate ocean data assimilation

- Uncertainty from ensemble of ocean field estimates transferred to ensemble of LCS estimates for 3 prediction problems in the Monterey Bay region: 2 upwelling events and 1 relaxation event

- Main results:
  - Uncertainty estimates allow to identify most robust LCS
  - More intense DLE ridge are usually relatively more certain
  - Different oceanic regimes have different LCS uncertainty fields and properties

- Work is in progress and future work include:
  - Larger ensemble sizes and evaluations of convergence tests
  - Statistical studies of LCS uncertainties: histograms for pdf estimate, pdf properties, higher moments, etc
  - Studies in LCS space: pdf along LCS arc, assign pdf to each LCS, etc
  - Physical-Biological LCS and uncertainties
  - LCS data assimilation