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Sequential and Variational Assimilation for Predicting Loop Current in Gulf of Mexico: Toward Hybrid?

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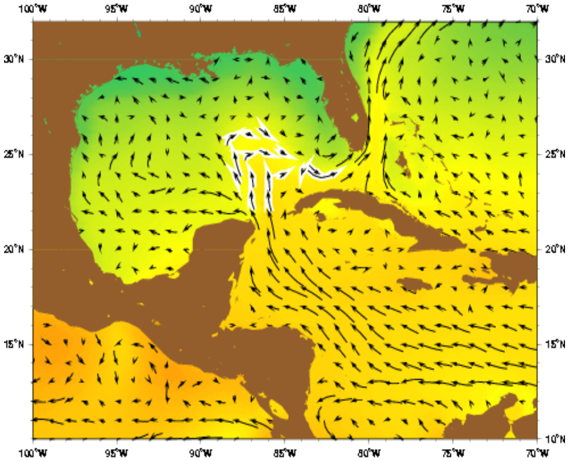
Talk Outline

- Ocean Data Assimilation:
  - Sequential and Variational Approaches
- Predicting Loop Current in Gulf of Mexico
  - EnKF vs. 4DVAR
- Hybrid 4DVAR-EnKF assimilation
- Future Plans for the Saudi Seas



How to Predict the State of the Ocean?

Examples of Red Sea Models at KAUST

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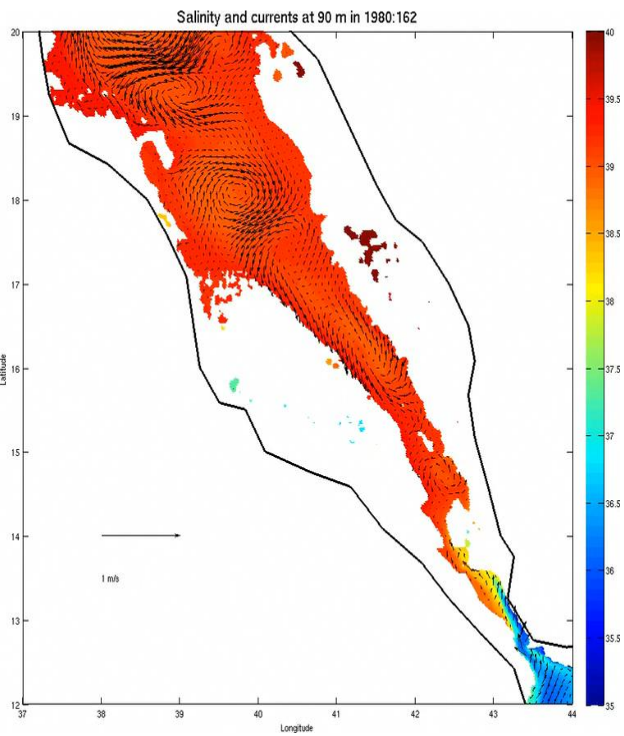
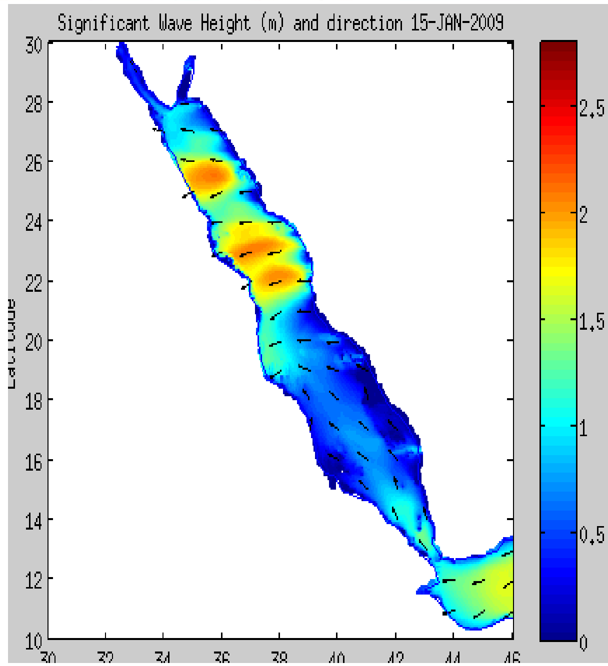
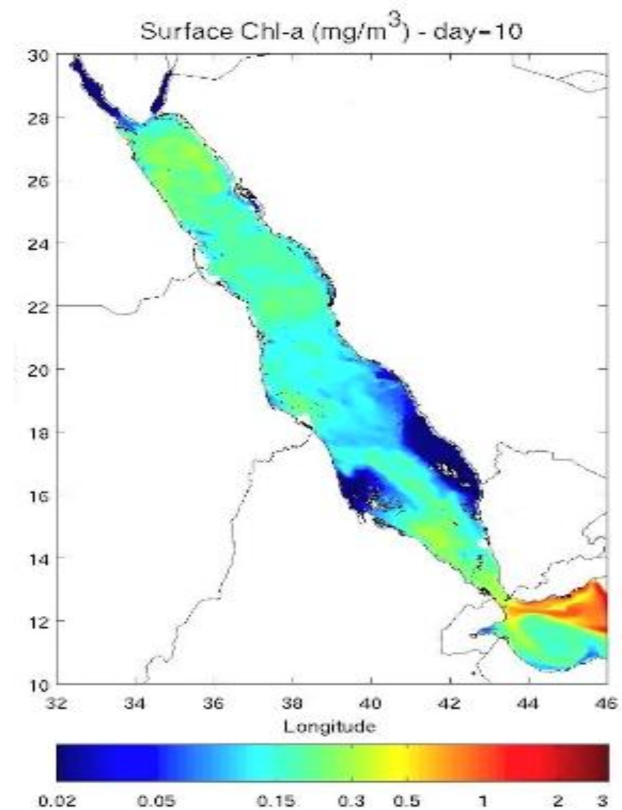




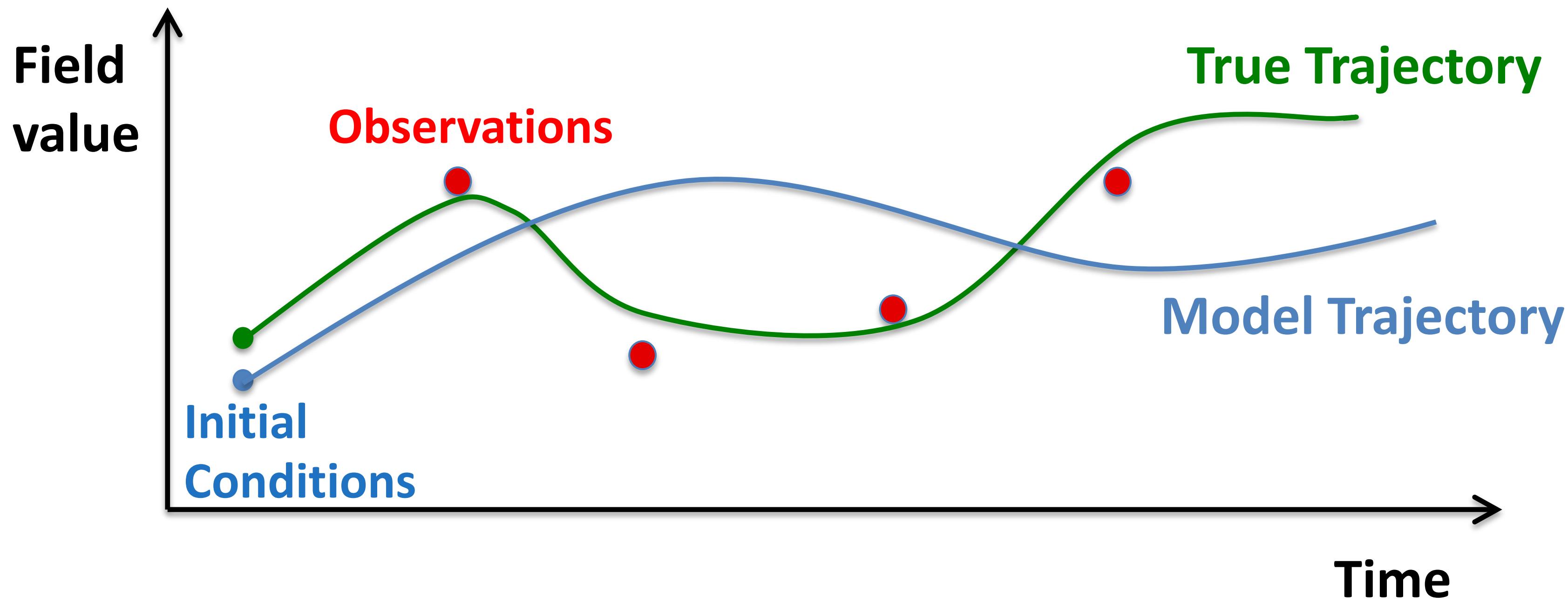


Facts about Ocean Models

- Numerical solution of the discretized PDEs governing the evolution of the ocean variability
- Highly complex, very expensive, strongly nonlinear, and chaotic models
- Subject to many sources of uncertainties: Omitted physics, poorly known parameters, uncertain inputs, numerical errors, etc …

Ocean models are often only crude approximations of the real ocean

Uncertainties in Ocean Models



Data Assimilation

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- **Sources of information:**
  - *Numerical models, but imperfect*
  - *Observations, but too sparse*

- **Data assimilation (5th paradigm):** Combines models and data
  - *Models dynamically interpolate data in space and time*
  - *Data guide model toward the true trajectory*

The goal is to *predict*, *analyze*, *and quantify uncertainties of the ocean state*

- **Difficulties:**
  - *Huge dimension ($10^6 – 10^{10}$)*
  - *Nonlinear, multiphysics, multiscales, very expensive models*
  - *Poorly known statistical properties of uncertainties*

Bayesian Formulation

Compute probability distribution function of the state given available observations

System dynamic and observation equations:

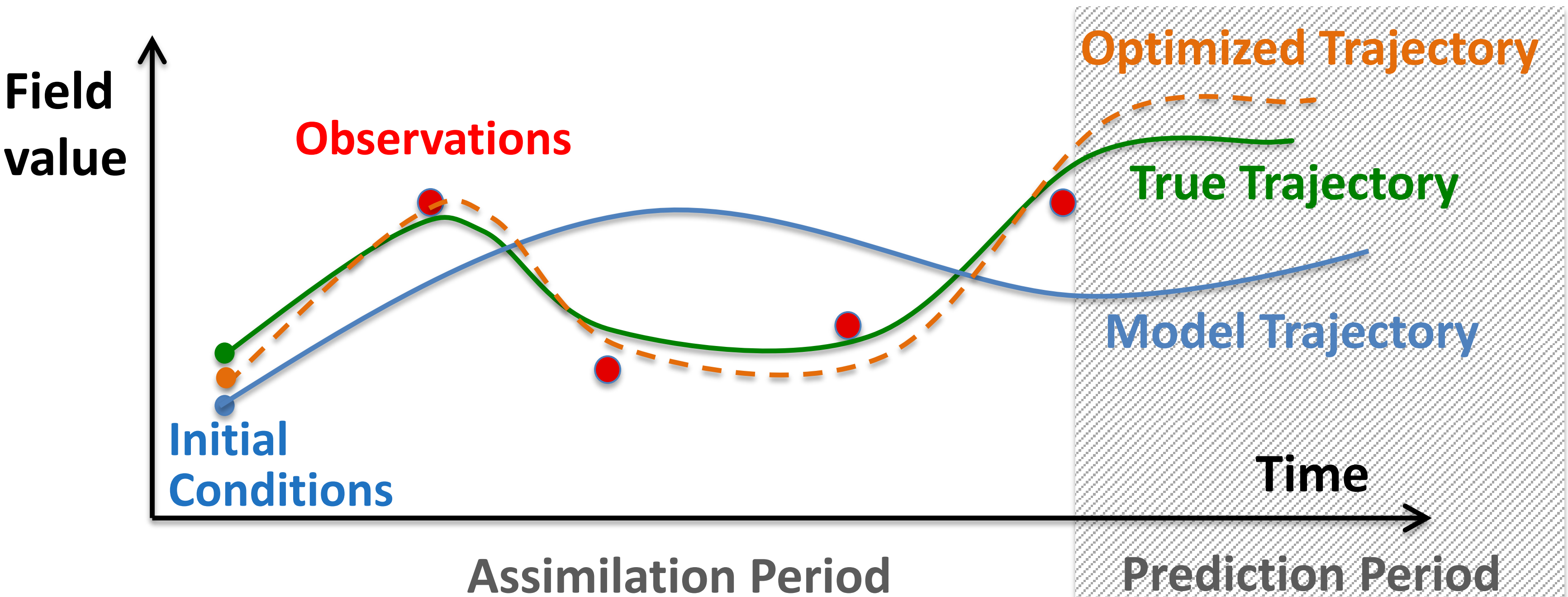
$$\mathbf{x}_k = \mathbf{M}\mathbf{x}_{k-1} + \eta_k \qquad\qquad \mathbf{y}_k = \mathbf{H}\mathbf{x}_k + \epsilon_k$$

Need to estimate: $p\left(\mathbf{x}_0, \mathbf{x}_1, \ldots \mathbf{x}_N | \mathbf{x}^b, \mathbf{y}_0, \mathbf{y}_1, \ldots, \mathbf{y}_N\right)$. Use Bayes rule,

$$\begin{aligned}
p\left(\mathbf{x}_{0:N}|\mathbf{x}^b, \mathbf{y}_{0:N}\right) \quad &\propto \quad p\left(\mathbf{y}_{0:N}|\mathbf{x}^b, \mathbf{x}_{0:N}\right) \cdot p\left(\mathbf{x}_{0:N}|\mathbf{x}^b\right) \\
&= \prod_{k=0}^{N} p\left(\mathbf{y}_k|\mathbf{x}_k\right) \cdot p\left(\mathbf{x}_0|\mathbf{x}^b\right) \cdot p\left(\mathbf{x}_1|\mathbf{x}_0\right) p\left(\mathbf{x}_2|\mathbf{x}_1\right) \cdots p\left(\mathbf{x}_N|\mathbf{x}_{N-1}\right) \\
&= \prod_{k=0}^{N} p\left(\mathbf{y}_k|\mathbf{x}_k\right) \cdot p\left(\mathbf{x}_0|\mathbf{x}^b\right) \cdot \prod_{k=0}^{N} p\left(\mathbf{x}_k|\mathbf{x}_{k-1}\right) \triangleq c1 \cdot \exp\left[-\frac{1}{2}\mathcal{J}\left(\mathbf{x}_{0:N}\right)\right]
\end{aligned}$$

$$\boxed{\begin{aligned}\Rightarrow \text{ Min } \mathcal{J}\left(\mathbf{x}_{0:N}\right) = &\left(\mathbf{x}_0 - \mathbf{x}^b\right)^T \mathbf{B}^{-1}\left(\mathbf{x}_0 - \mathbf{x}^b\right) + \\ &\sum_{k=0}^{N}\left(\mathbf{y}_k - \mathbf{H}\mathbf{x}_k\right)^T \mathbf{R}_k^{-1}\left(\mathbf{y}_k - \mathbf{H}\mathbf{x}_k\right) + \sum_{k=0}^{N}\left(\mathbf{x}_k - \mathbf{M}\mathbf{x}_{k-1}\right)^T \mathbf{Q}_k^{-1}\left(\mathbf{x}_k - \mathbf{M}\mathbf{x}_{k-1}\right)\end{aligned}}$$

Variational Assimilation – 4DVAR



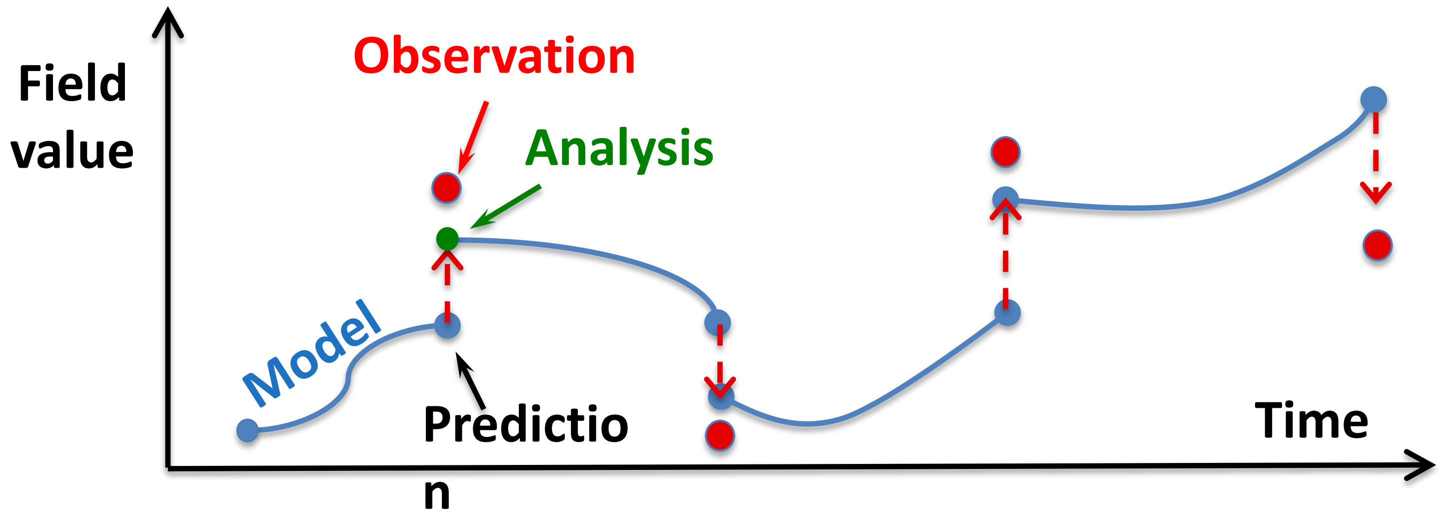
Perfect Model

$$Min\, J(X_0) = \sum_{Time} \left\| X_{Time} - Data_{Time} \right\|^2_{R^{-1}} + \left\| X_0 - Forecast \right\|^2_{B^{-1}}$$

- Data are assimilated over a given period
- *Dynamically consistent solution*
- *Requires an adjoint model and non-convex optimization*

Sequential Assimilation – Filtering

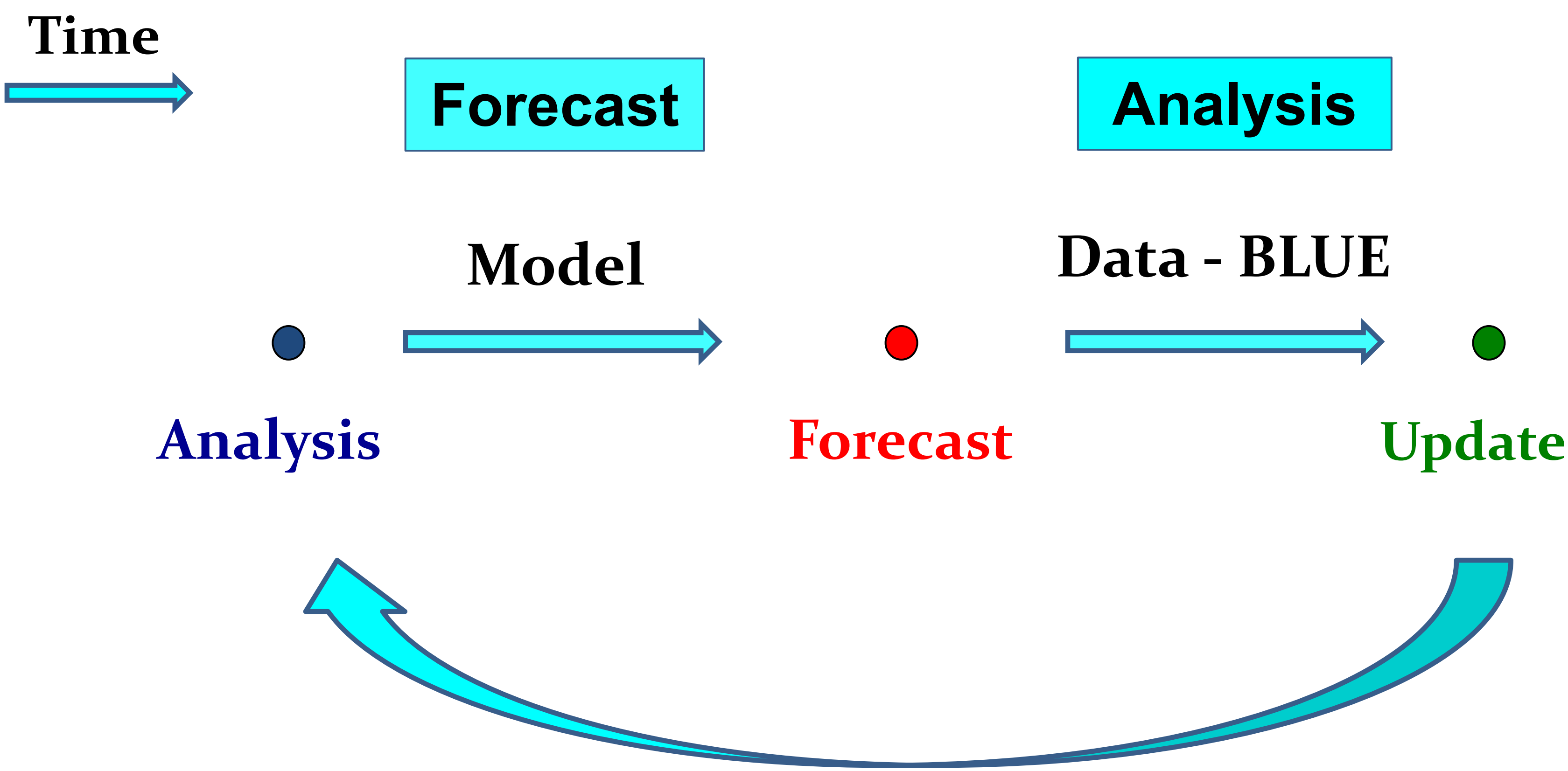
<u>Need to estimate:</u> $p\left(\mathbf{x}_k \middle| \mathbf{y}_{0:k}\right) \propto \underbrace{p\left(\mathbf{y}_k \middle| \mathbf{x}_k, \mathbf{y}_{1:k-1}\right)}_{\text{Analysis}} \cdot \underbrace{p\left(\mathbf{x}_k \middle| \mathbf{y}_{1:k-1}\right)}_{\text{Forecast}}$



Gaussian Update $\quad Min\, J(X) = \left\| X - Data \right\|^2_{R^{-1}} + \left\| X - Forecast \right\|^2_{B^{-1}}$

- Data are assimilated as they become available
- Update background B in time, and dynamically inconsistent solution
- <u>Same solution as 4DVAR at end of assimilation for linear Gaussian systems</u>

Sequential Assimilation – OI (Good Old Days!)



- **No update of the background covariance B**

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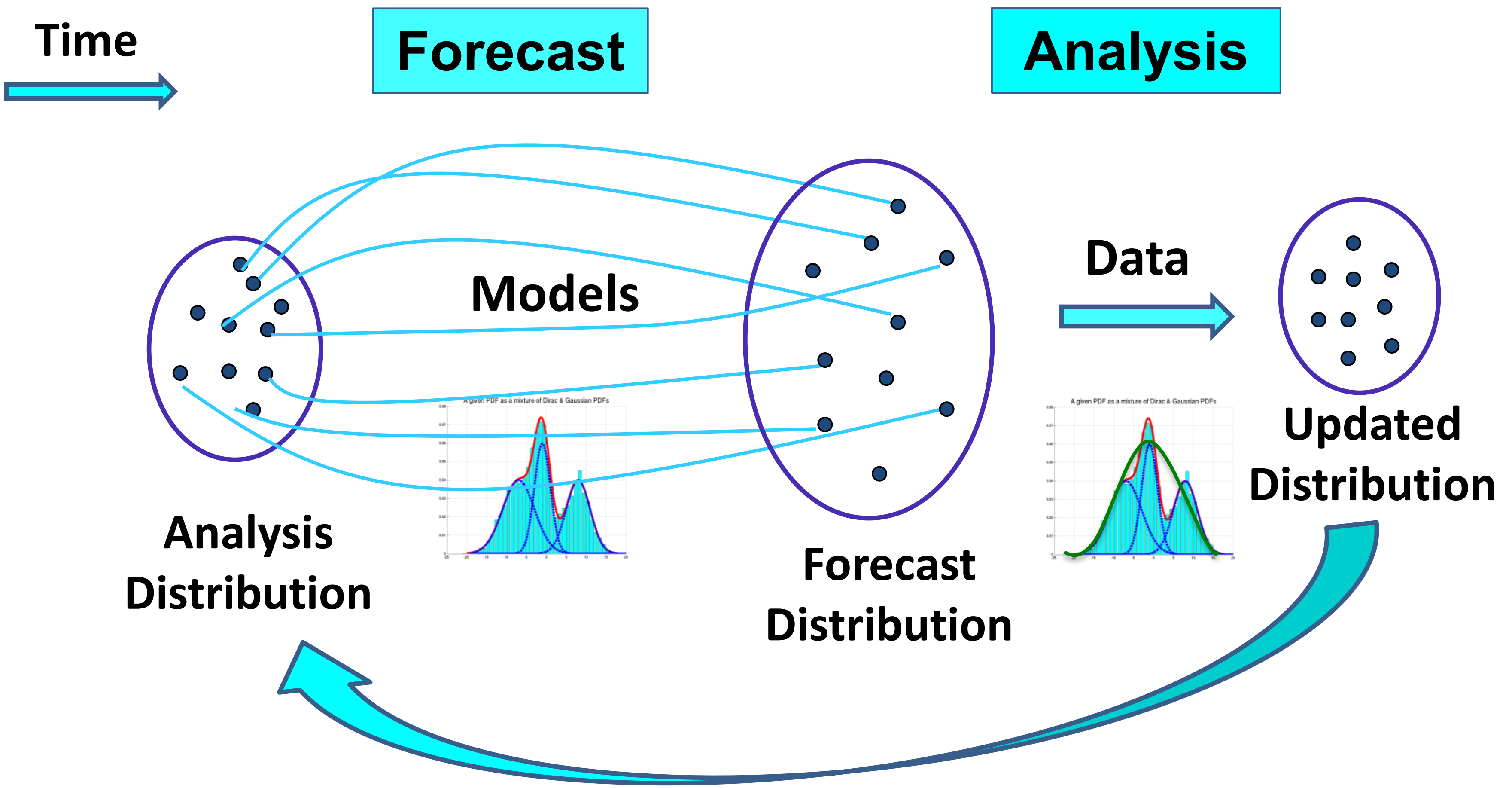
Sequential Assimilation – EnKFs



Distributions → Estimates & Uncertainties (decision making)

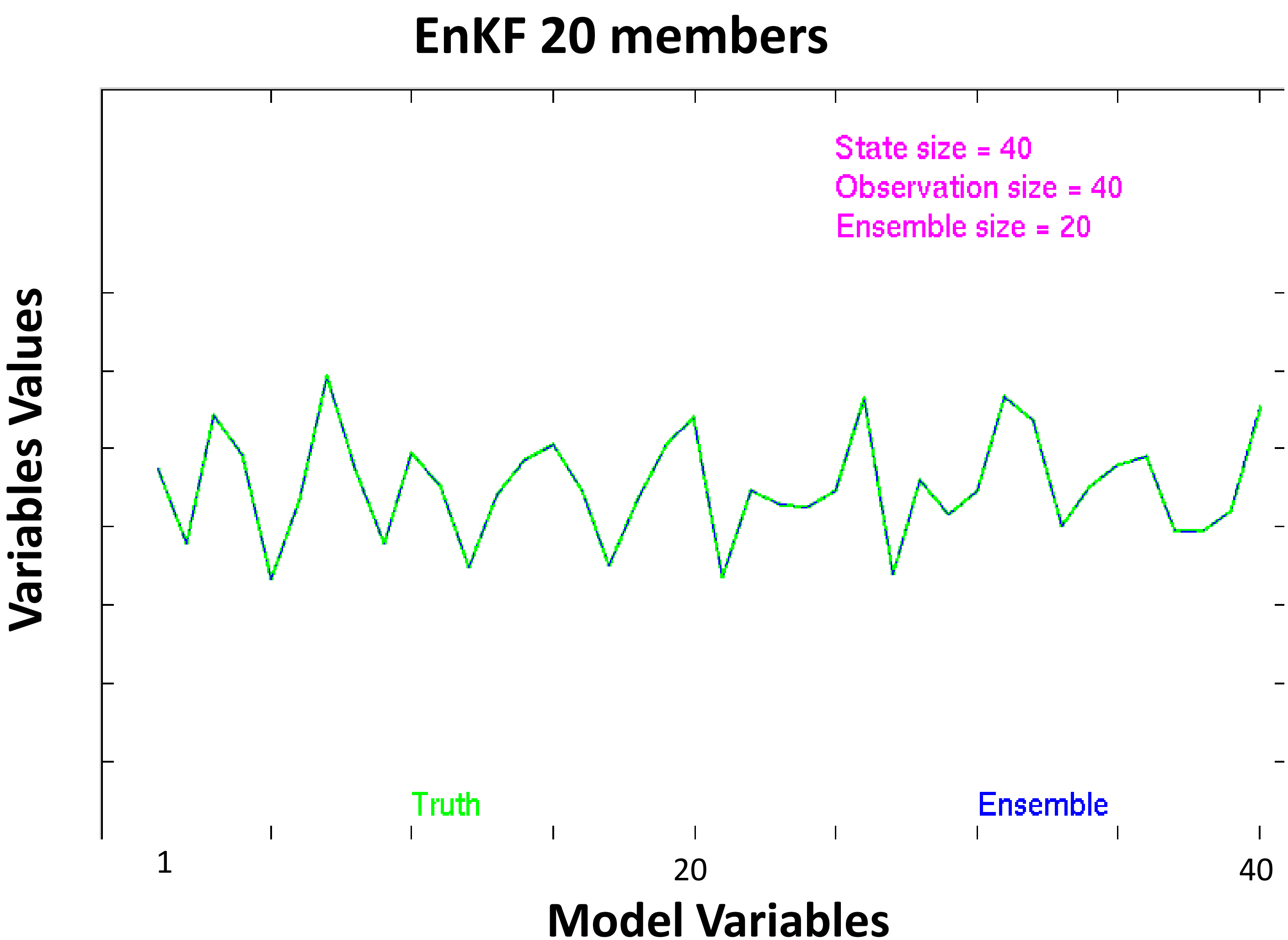
EnKF Showcase – Lorenz-96 Model

- The Lorenz-96 model mimics time evolution of an atmospheric variable

$$\frac{dx_j}{dt} = (x_{j+1} - x_{j-2})x_{j-1} - x_j + F \quad \text{with} \quad \begin{cases} j = 1, \ldots, 40 \\ F = 8 \\ \Delta t = 0.05 \sim 6h \end{cases}$$

- A set of reference states S were retained
- Observations of "odd" variables from $S + \Phi(0;1)$
- Initial *pdf* assumed $\Phi\left(\bar{S}; \mathrm{cov}(S)\right)$

Quantifying & Reducing Uncertainties with EnKF

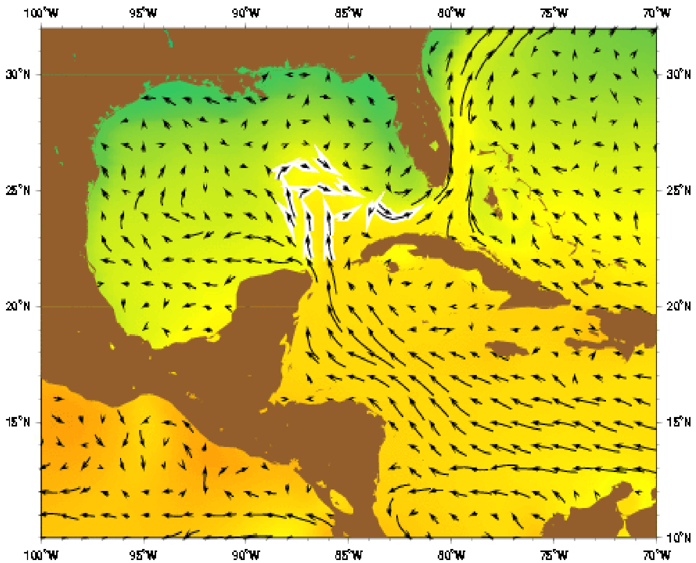


Predicting Loop Current in GoM

- Predict the evolution of the loop current in the Gulf of Mexico to support oil industry

- Funded by BP, in collaboration with Bruce Cornuelle & G. Gopalakrishnan (Scripps), Patrick Heimbach (MIT), Armin Kohl (Hamburg), and Tim Hoar & Jeffrey Anderson (NCAR)

- <u>Prediction System:</u>
    - *MIT general circulation model*
    - *Data: Satellites & Gliders*

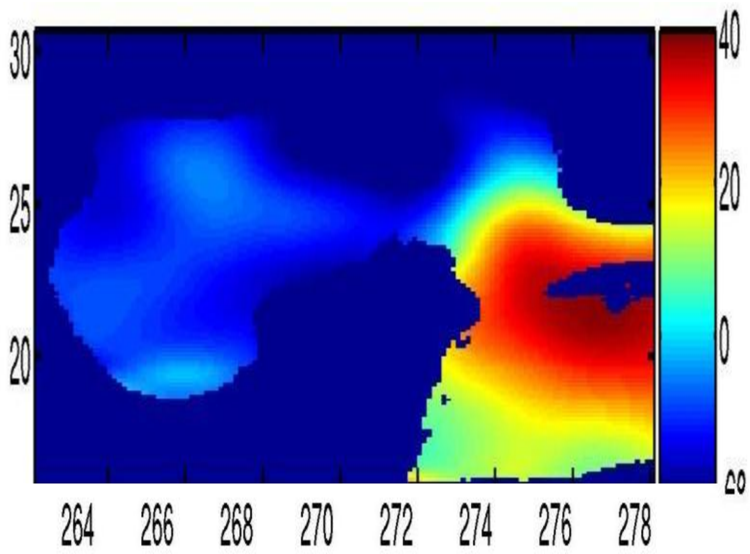


MITgcm – GoM

- 10×10 km horizontal resolution and 50 vertical layers
- Model state variables: U, V, S, T (dim ≈ 2×10^7)
- 6-hourly NCEP atmospheric forcing (winds, heat, precipitation, …)
- Initial conditions and Open boundaries: model nested in $1/12\times1/12$ degree global assimilated HYCOM
- *Monthly NCEP and HYCOM climatology for prediction*

Model vs. Altimetry

Model



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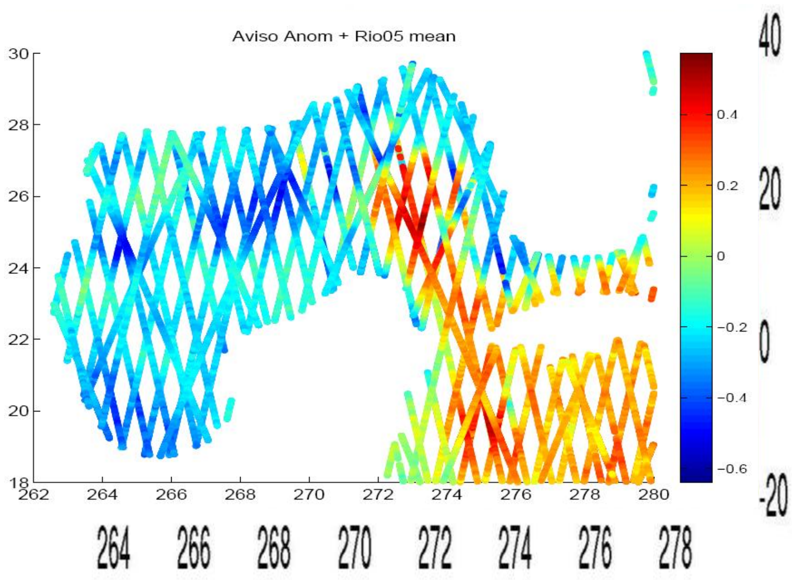
AVISO SSH



Assimilation System

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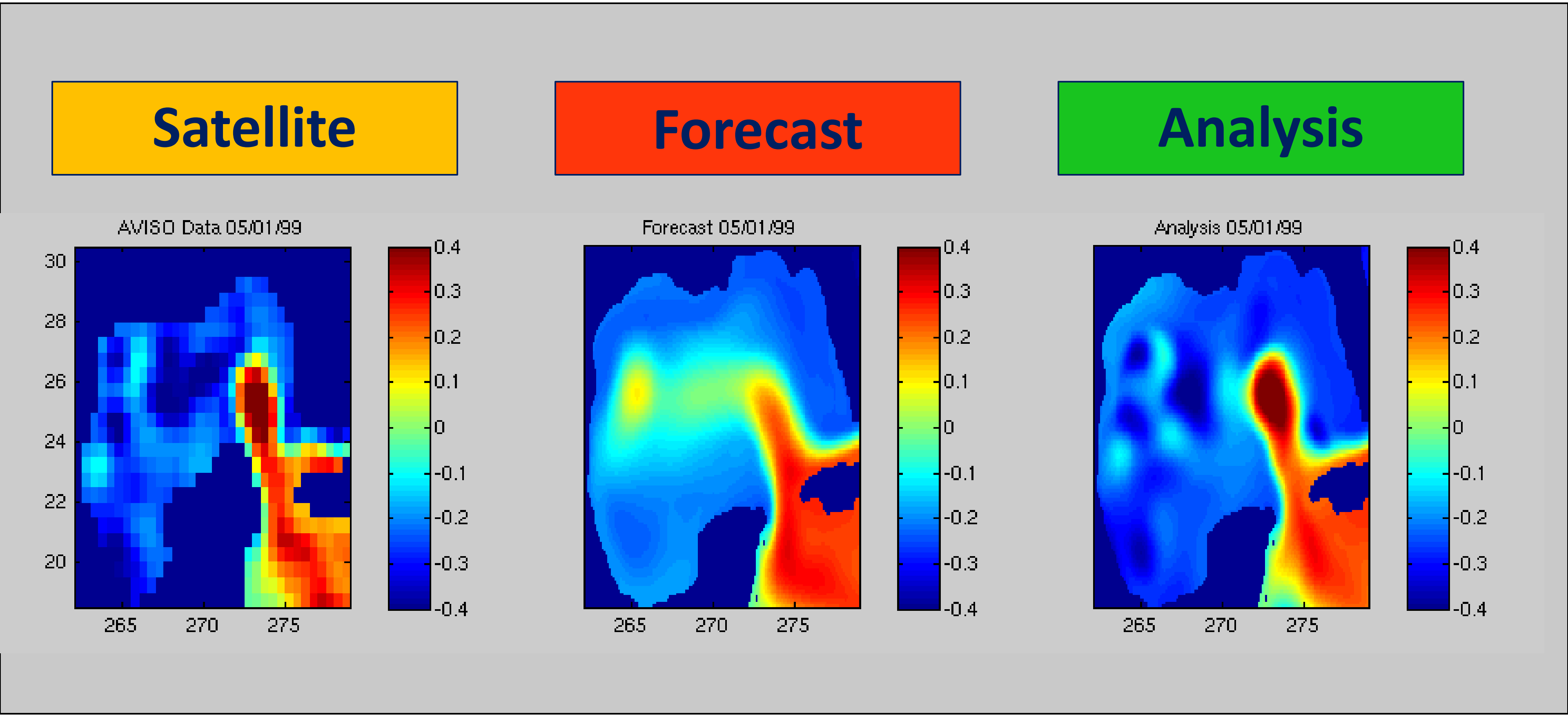
- Variational (15 iterations) and EnKF (50 members) assimilation
- Along tracks satellites SSH data and satellite gridded SST data are assimilated every day
- Assimilation and prediction period:

Assimilation Period
2 months: March - April

Forecast Period
2 months: May - June

- Performance evaluation:
  - *RMSE between analysis/forecast and data*
  - *Comparison with gridded AVISO SSH and TMI SST products*
  - *Evaluation against un-assimilated gliders data and assimilated HYCOM*

Weekly EnKF Forecasts and Analyses



4DVAR vs. EnKF in GoM – AVISO RMSE

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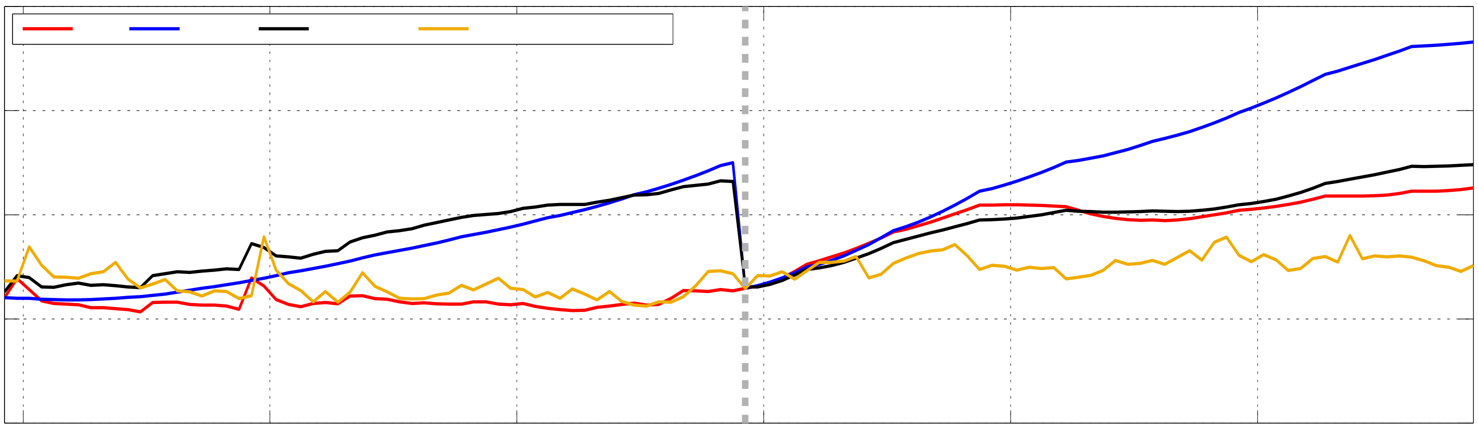
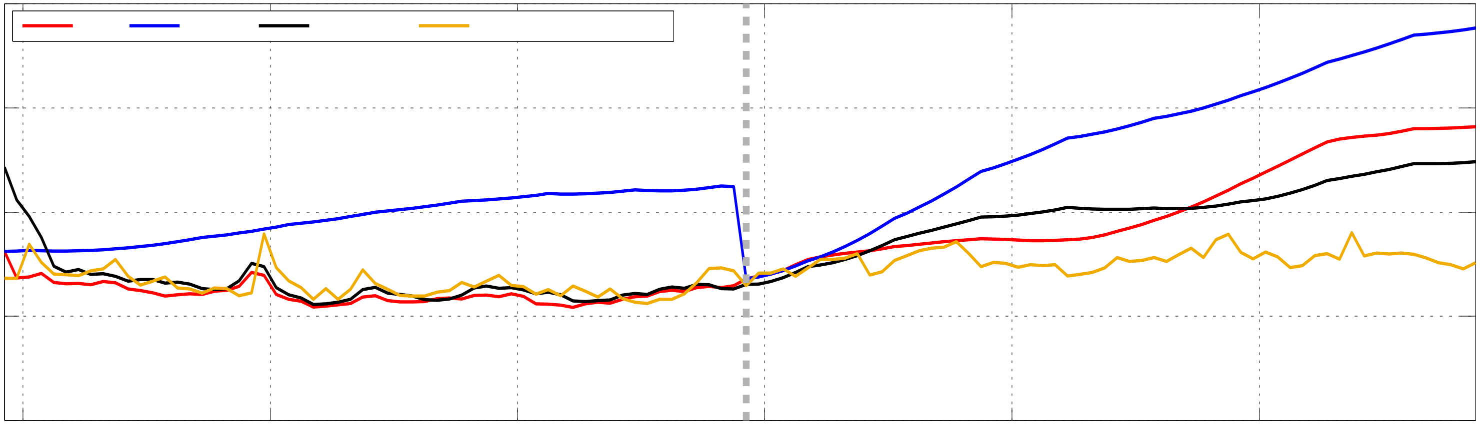


4DVAR
HYCOM
Forecast
Analysis
Persistence



EnKF
HYCOM
Forecast
Analysis
Persistence

4DVAR vs. EnKF in GoM – Forecast SSH

EnKF - mean

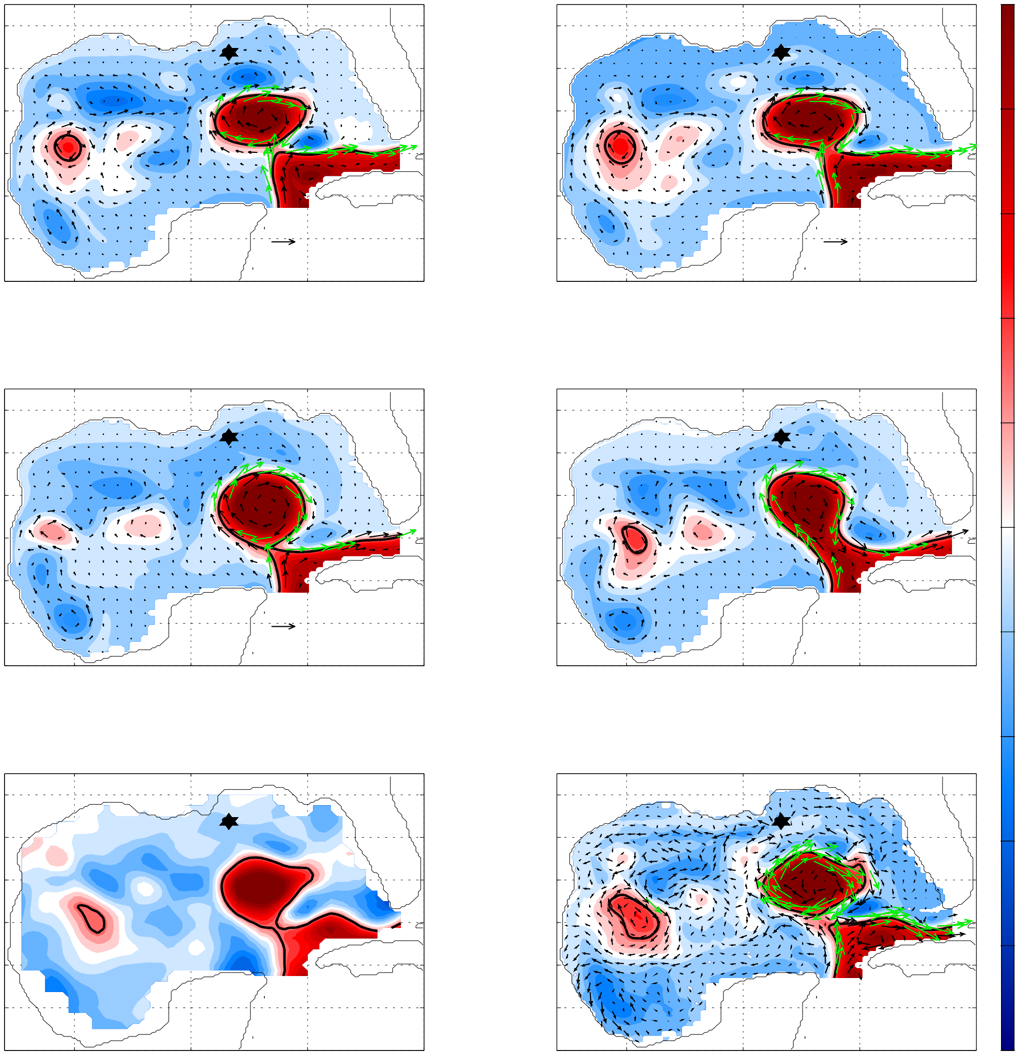
EnKF

4DVAR

MIT – HYCOM IC

AVISO

HYCOM



4DVAR vs. EnKF in GoM – Forecast SST

EnKF - mean

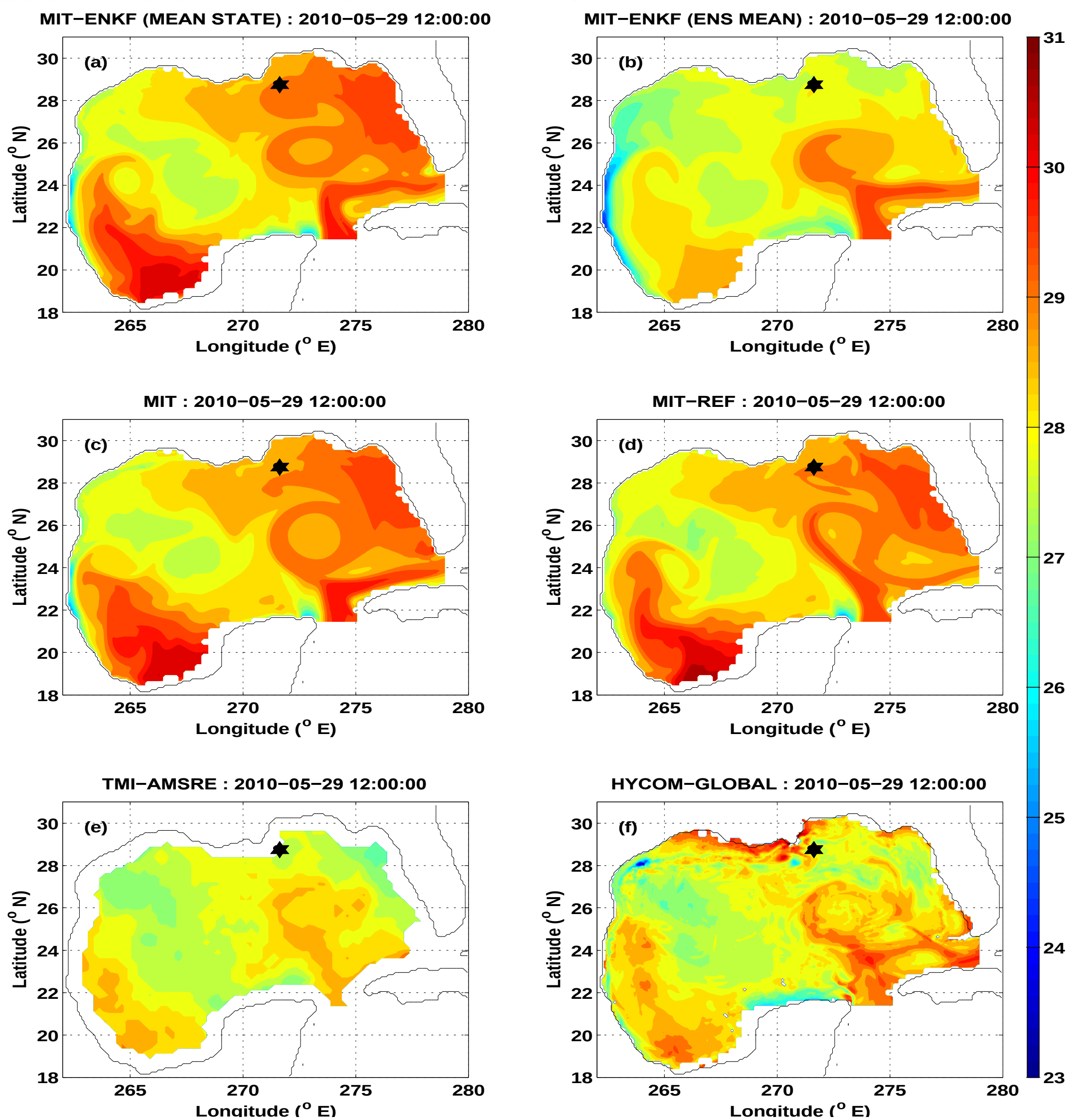
EnKF

4DVAR

MIT – HYCOM IC

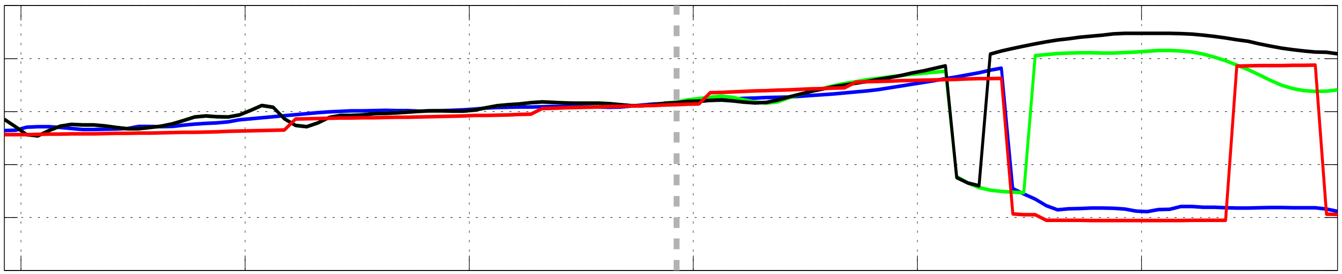
TMI

HYCOM

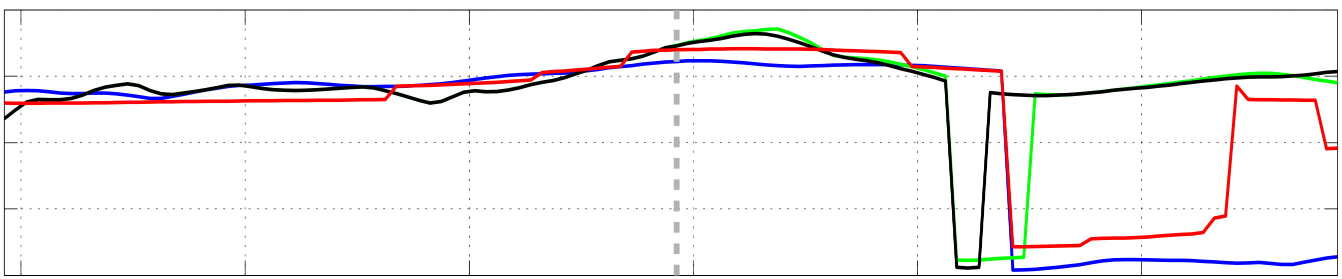


4DVAR vs. EnKF in GoM – Eddy Shedding

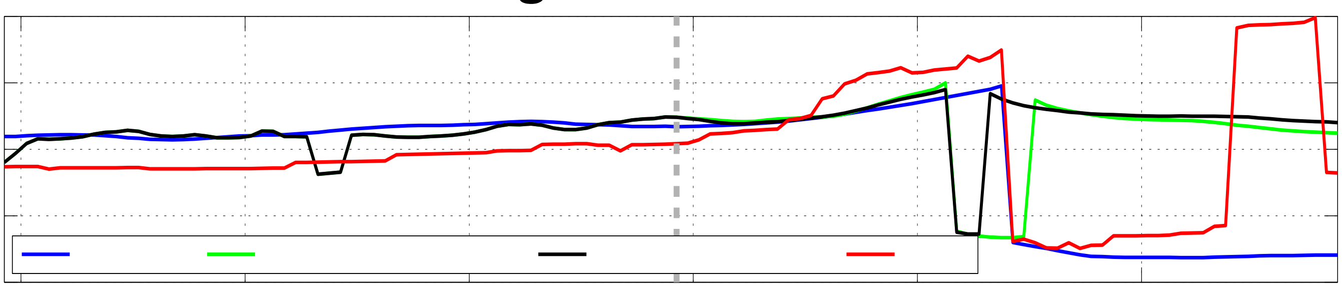
Maximum western extent of LC in ºW



Maximum northern extent of LC in ºN



Length of LC in Km



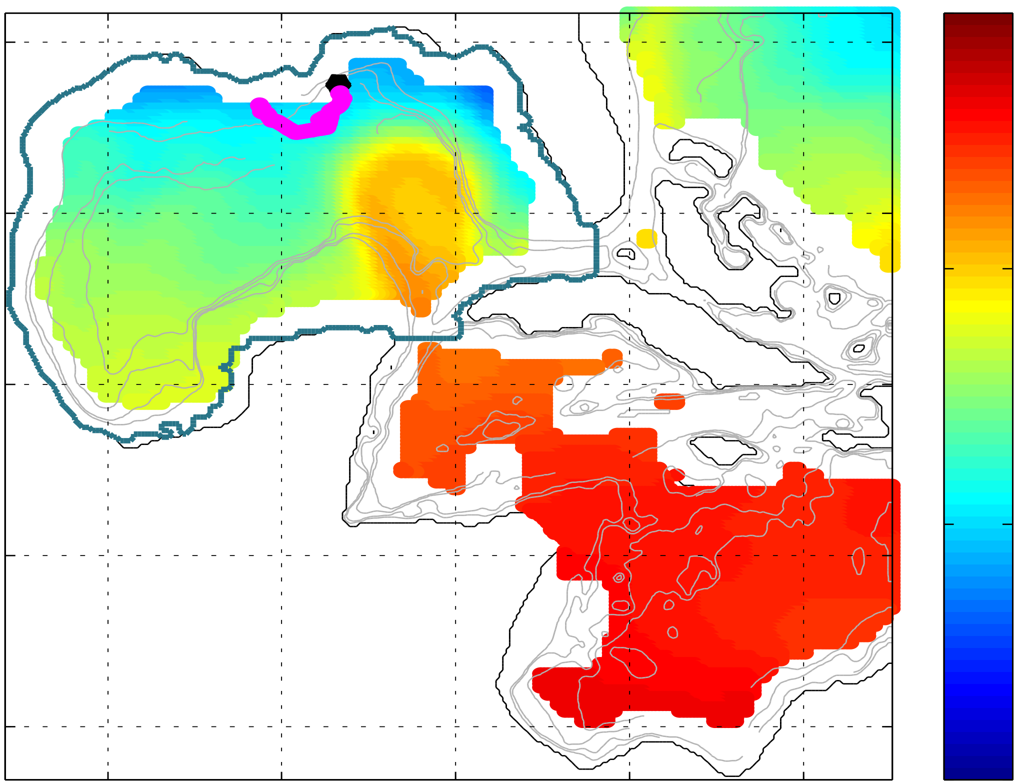
AVISO

4DVAR

EnKF

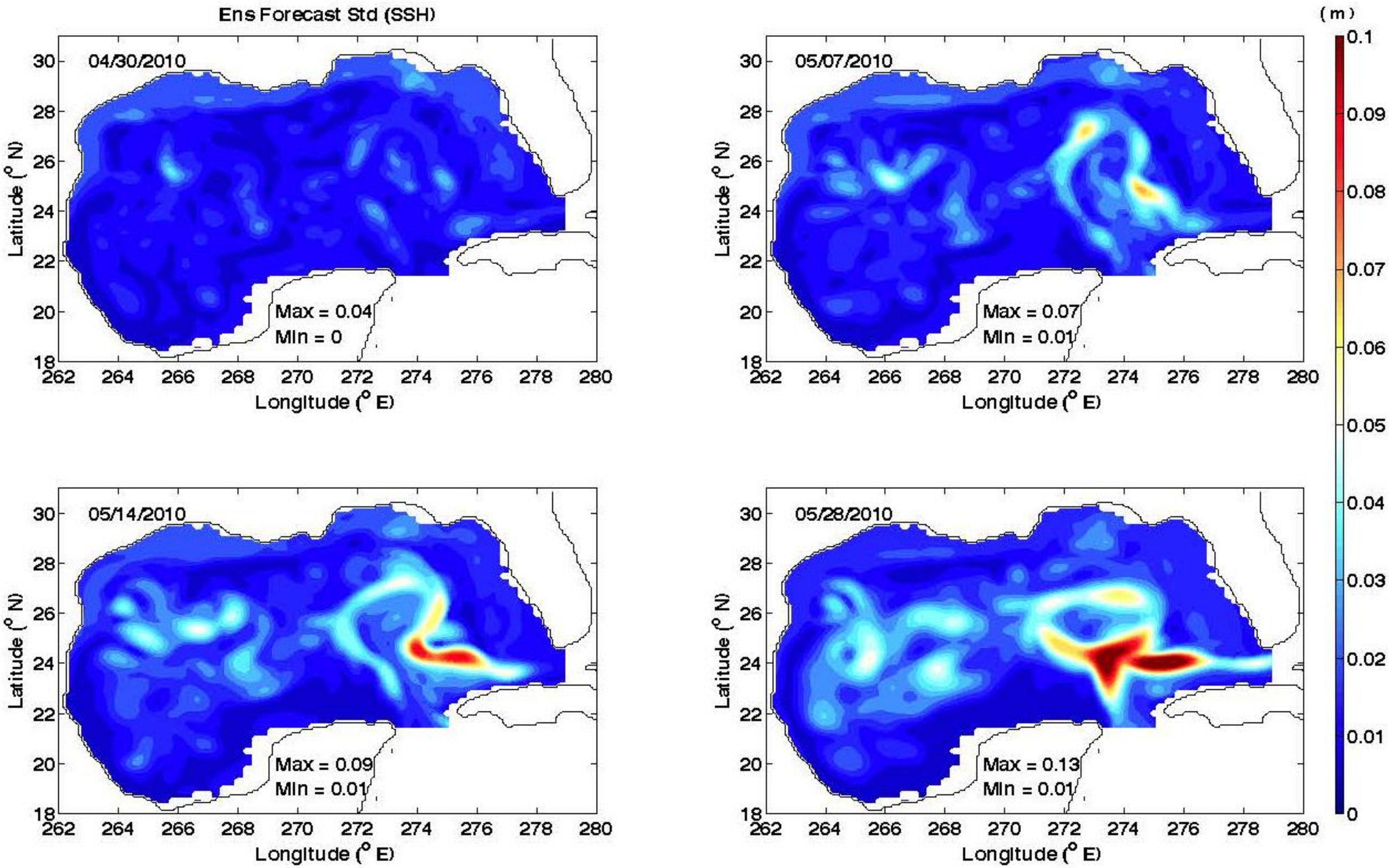
EnKF – mean

4DVAR vs. EnKF in GoM – Glider Salinity

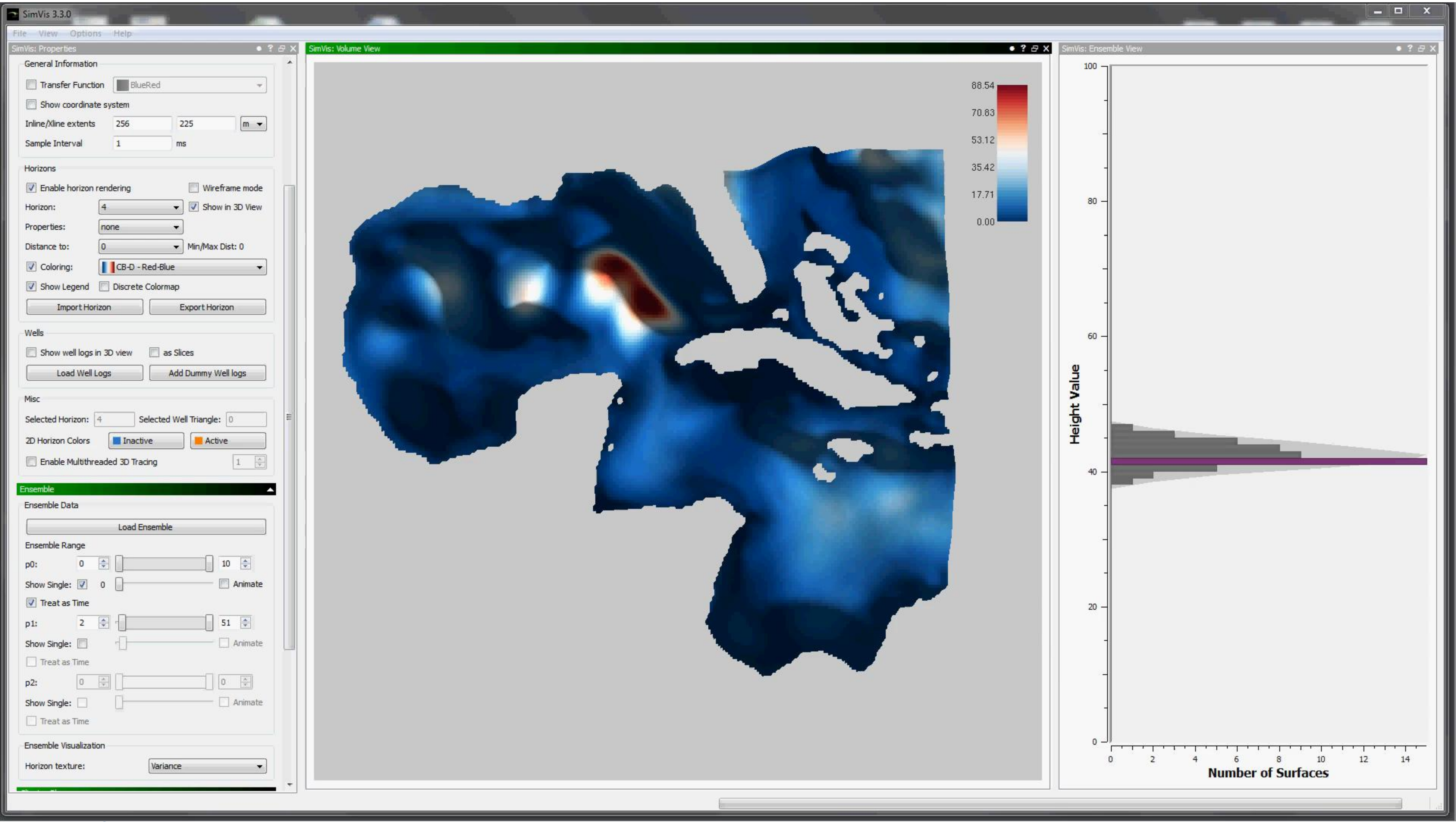


June 2010

Evolution of Forecast Uncertainties in EnKF



Visualizing EnKF Uncertainties



Summary EnKF vs. 4DVAR in GoM

- DA is essential for accurate ocean simulations and predictions
- The MITgcm assimilation system:
  - *Enabled for 4D sequential and variational techniques*
  - *Assimilate all types of ocean data*
- First experience from GoM:
  - *Filtering does better with data fitting and short term predictions, and provides some estimate of uncertainties*
  - *4DVAR provides dynamically more consistent solution, and does better with long term predictions*
- Still room for improvements …

EnKF vs. 4DVAR

4D-VAR	EnKF
Requires an adjoint model	Portable (Monte Carlo approach)
Full-rank	Rank deficient → *localization & inflation*
No efficient method to propagate uncertainties (background)	Update uncertainties (low-rank) → *more suitable for forecasting*
Dynamically consistent solution	No efficient method to impose some dynamical constraints

EnKF Background Limitation

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Accurate description of background covariance is critical

- Accuracy EnKF background covariance is mainly limited by:

  "Small ensembles" & *"Model deficiencies"*

  - *Rank deficiency*: not enough degrees of freedom to fit data
  - *Spurious correlations*: unreliable statistics from small ensemble
  - *Underestimated background* (weak spread)

Mitigating EnKF Background Limitation

- EnKF background is only an approximation of the true background

$$\mathbf{P}^t = \mathbf{P} + \mathbf{B}$$

- Inflation, localization and hybrid are all used to somehow represent estimates of $\mathbf{B}$

- *Hybrid*: Relax a OI/3D-VAR background to the flow-dependent EnKF background

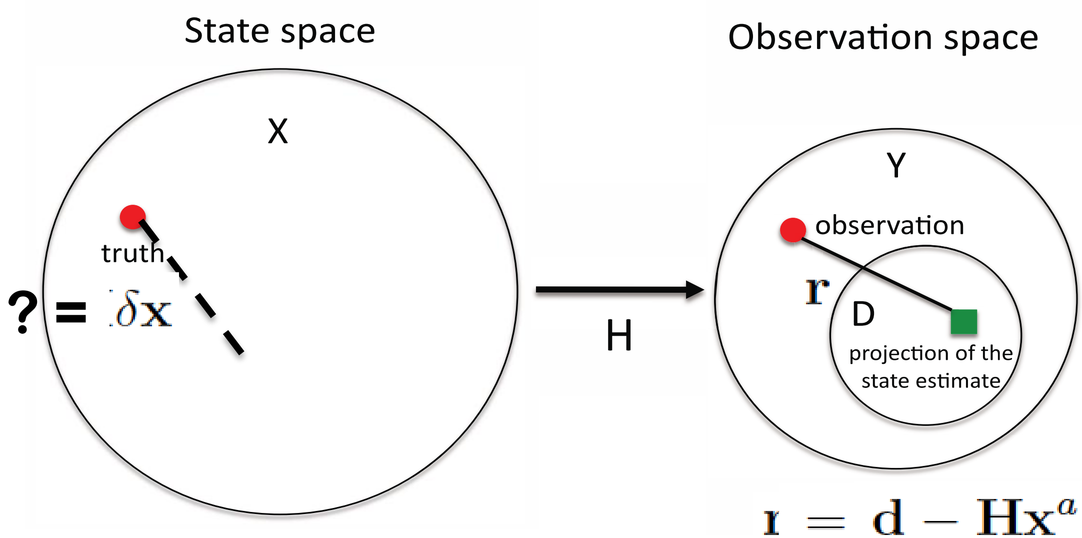
$$\tilde{\mathbf{P}}^t = \alpha\mathbf{P} + (1-\alpha)\mathbf{B}$$

… *or any combination of these*

Adaptive EnKF – AEnKF

- If background is not accurately estimated, analysis errors (residuals) are the result of missing directions in the ensemble
  - *Residuals carry information about EnKF background deficiency*

The idea is to back-project the residuals from the observation space to the state space and use that as new ensemble member(s)



Generating A New Member

- Enrich the EnKF ensemble with new members generated from the ensemble "null" space

- To estimate the new member(s)

$$\mathbf{d} - \mathbf{H}\mathbf{x}^f \quad = \quad \mathbf{H}(\mathbf{x}^a - \mathbf{x}^f) + \mathbf{H}\delta\mathbf{x} + \mathbf{r}^e$$

  which is equivalent to

$$\mathbf{r} \; = \; \mathbf{d} - \mathbf{H}\mathbf{x}^a \quad = \quad \mathbf{H}\delta\mathbf{x} + \mathbf{r}^e$$

- Solves for as an inverse problem with

$$J\left(\delta\mathbf{x}^e\right) \quad = \quad \frac{1}{2}\delta\mathbf{x}^{eT}\mathbf{B}^{-1}\delta\mathbf{x}^e + \frac{1}{2}\left(\mathbf{r} - \mathbf{H}\delta\mathbf{x}^e\right)^T\mathbf{R}^{-1}\left(\mathbf{r} - \mathbf{H}\delta\mathbf{x}^e\right)$$

- A new member is then

$$\boxed{\mathbf{x}^{a,e} \quad = \quad \mathbf{x}^a + \beta\delta\mathbf{x}^e}$$

4D - AEnKF

- 4D-VAR formulation to reduce dependency on B and include more information from model dynamics and data (past residuals)

$$J_{4D}(\delta\mathbf{x}_{i-n}) = \frac{1}{2}\delta\mathbf{x}_{i-n}{}^T\mathbf{B}^{-1}\delta\mathbf{x}_{i-n} + \frac{1}{2}\sum_{j=i-n}^{i}\alpha_j\left(\mathbf{r}_j - \mathbf{G}_j\delta\mathbf{x}_{i-n}\right)^T\mathbf{R}_j^{-1}\left(\mathbf{r}_j - \mathbf{G}_j\delta\mathbf{x}_{i-n}\right)$$

with $\mathbf{G}_j = \mathbf{H}_j\mathbf{M}_{j,i-n},$

- Amounts to integrate the residuals with the adjoint backward in time

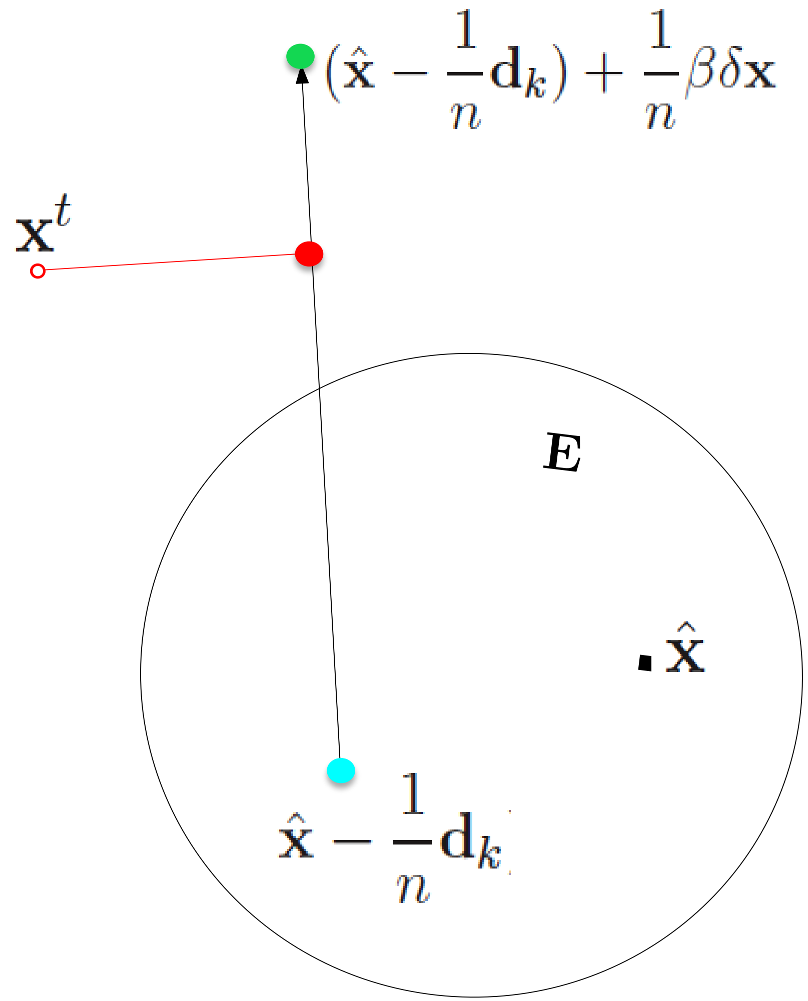
- A new member at t_{i-n} is then

$$\boxed{\mathbf{x}_{i-n}^{a,e} = \mathbf{x}_{i-n}^{a} + \beta\delta\mathbf{x}_{i-n}^{e}}$$

which is integrated forward to obtain a new member at t_i.

New Member(s) – Geometric Interpretation

- In practice, we need to remove members from the EnKF ensemble
- We remove the members that distort the least the EnKF background distribution
- Weighting factor β can be chosen according to an optimum criterion. Here we just set it by trial & error
- More members can be sampled from the estimated distribution of $\mathbf{x}^{a,e}$, or similarly from the descent direction of the optimized cost function



Adaptive vs. Hybrid

- Adaptive limits growth of the ensemble to directions indicated by the residuals but not represented in the ensemble

- Adaptive easier to implement: the “two” assimilation systems are implemented separately

- Technically speaking, however, adaptive does not increase the background rank, so localization may still be needed

Numerical Experiments with Lorenz-96

- $\mathbf{B}$ covariance of free-run (Hamill and Snyder, 2000)
- Assimilation period: "reference" states from 3 years
- Observations from reference states every day of "All" variables, "Half", "Quarter"
- *Model error*: F = 8 in reference model and F = 6 in forecast model
- *Sampling errors*: only 10 ensemble members
- We compare EnKF, 3D-VAR/hybrid, AEnKF, and 4D-AEnKF

Averaged RMS

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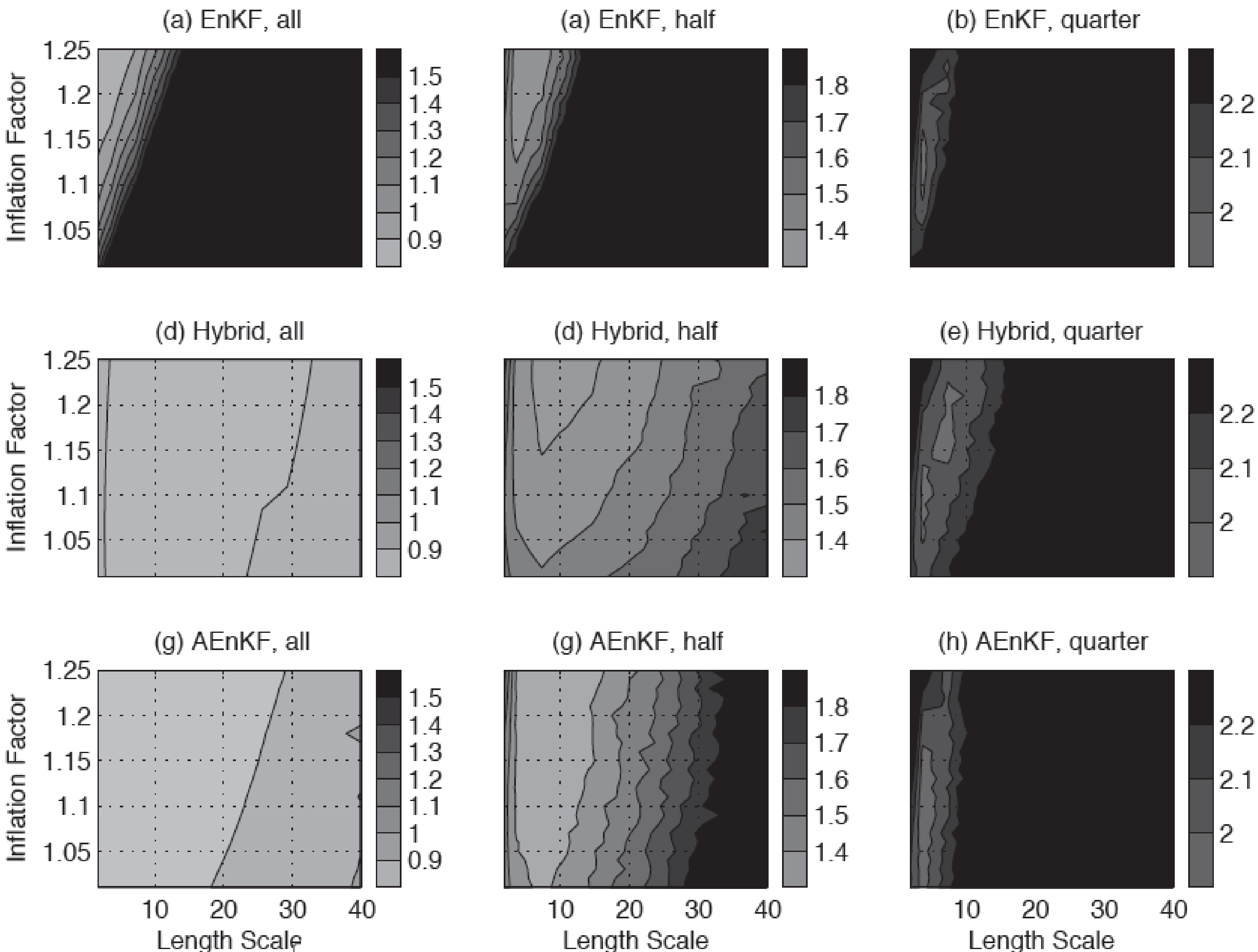
EnKF

Hybrid

AEnKF

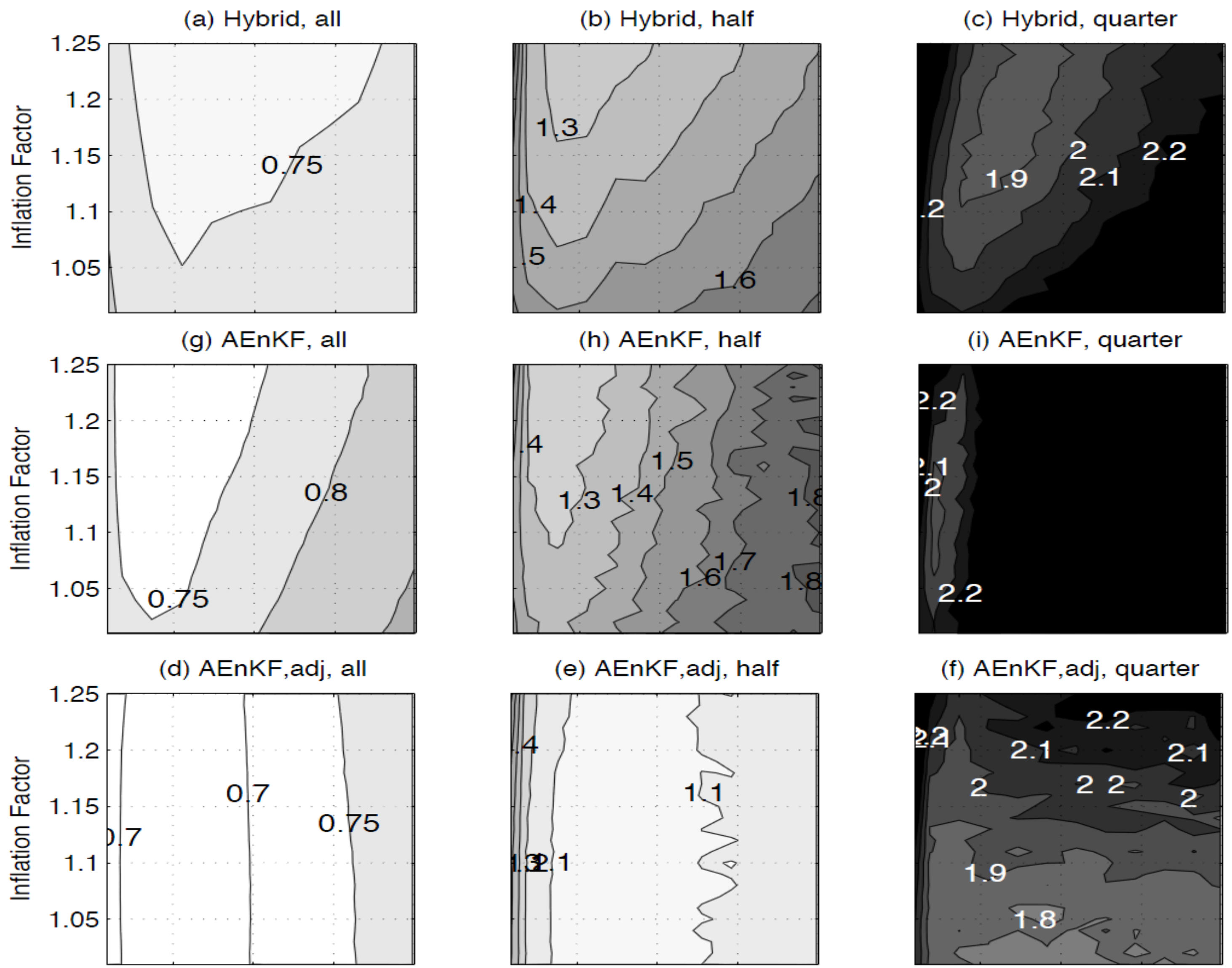


Averaged RMS (B = Identity)

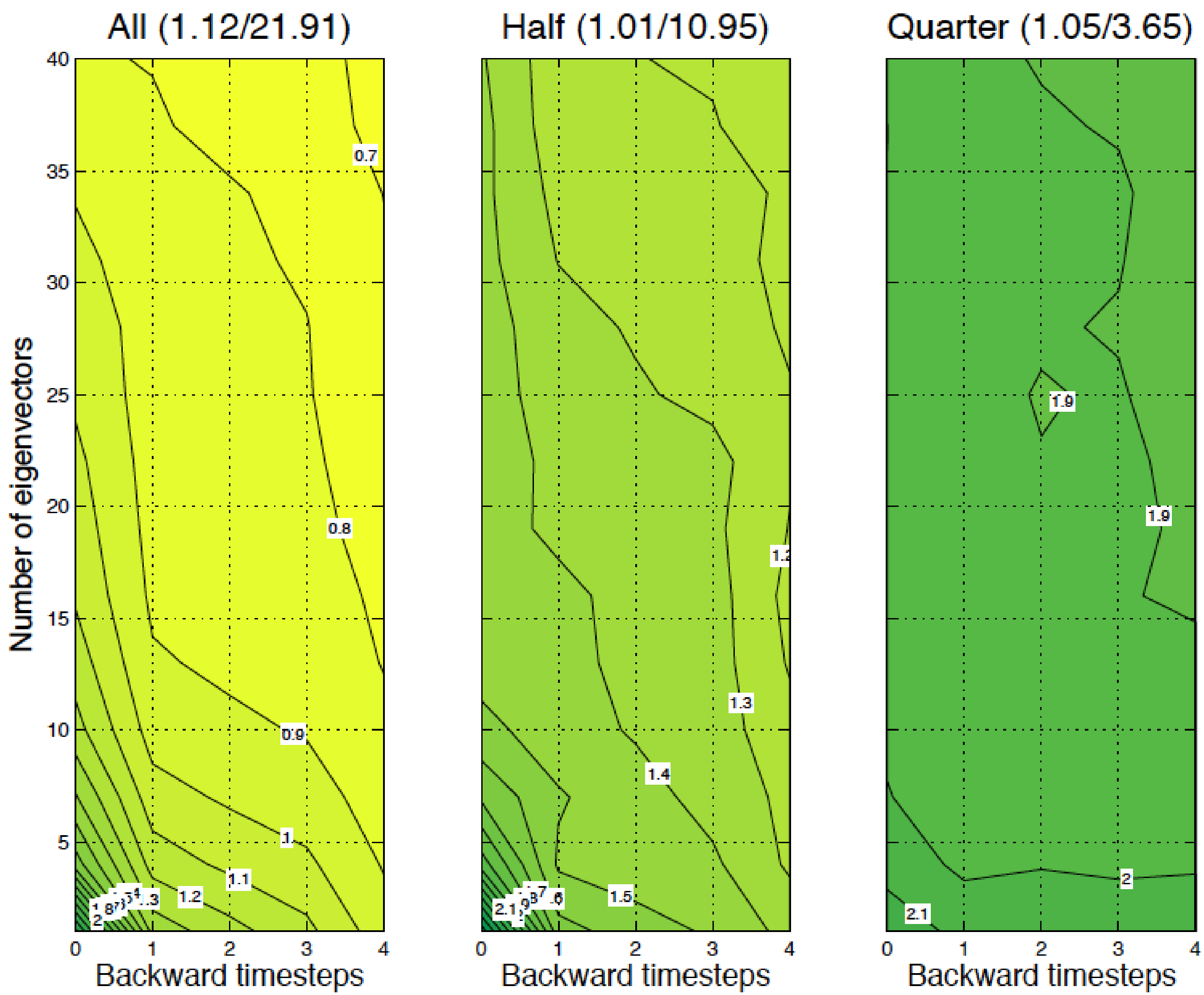
Hybrid

AEnKF

4D-AEnKF



4D-AEnKF as number of adjoint steps



Discussion

- Combining good features of EnKF and 4D-VAR could improve performances

- This however requires implementing the two systems; quite demanding

- Hybrid seems to becoming the method of choice for weather centers

Hybrid methods use EnKF to improve VAR background covariances). Adaptive uses VAR to enrich EnKFs ensembles

References

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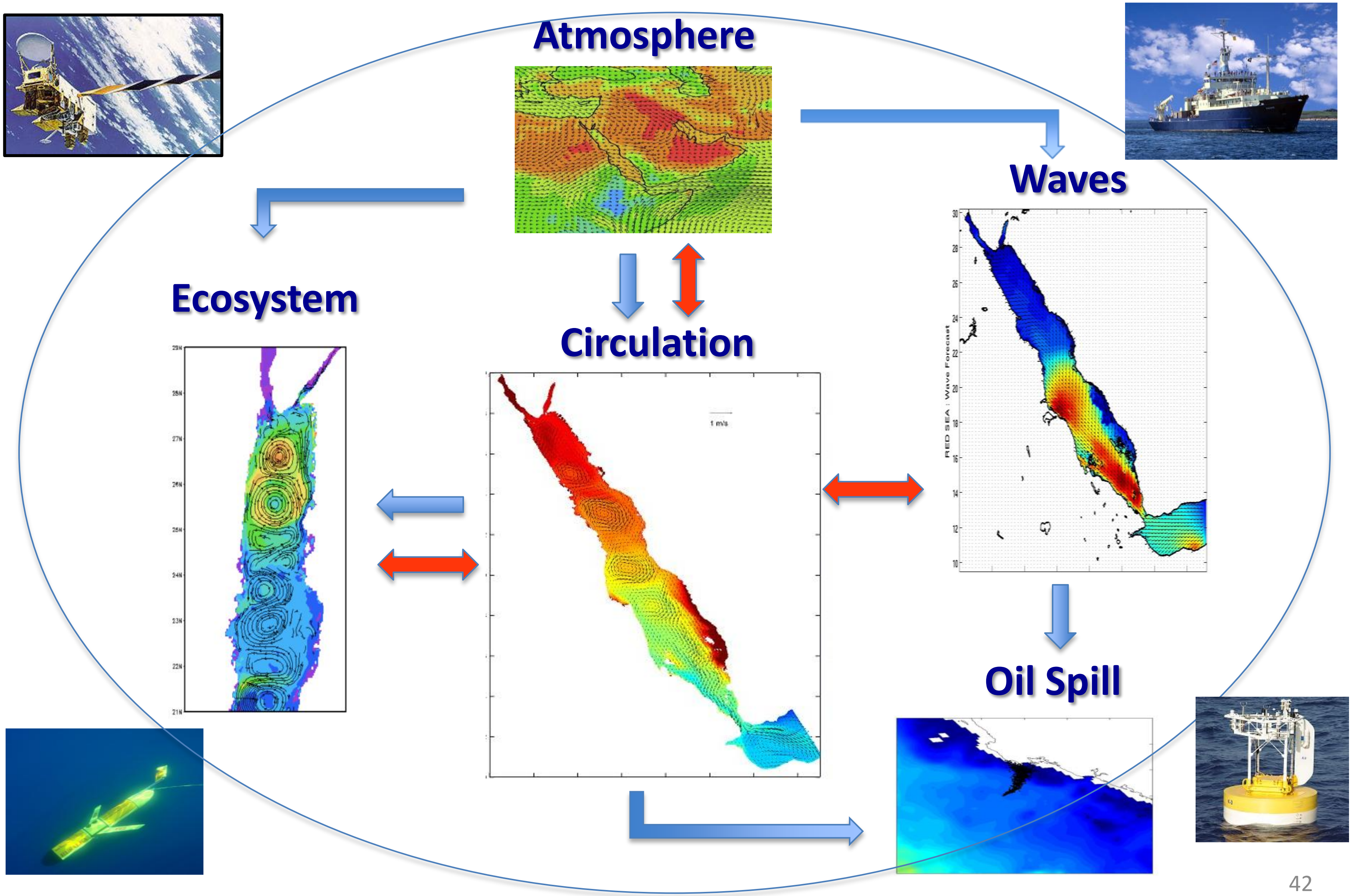
- H. Song, I. Hoteit, B. Cornuelle, X. Luo, and A. Subramanian: *An adaptive adjoint-based ensemble Kalman filter*. MWR, under revision, 2012.

Red Sea ARAMCO Project: One Integrated System



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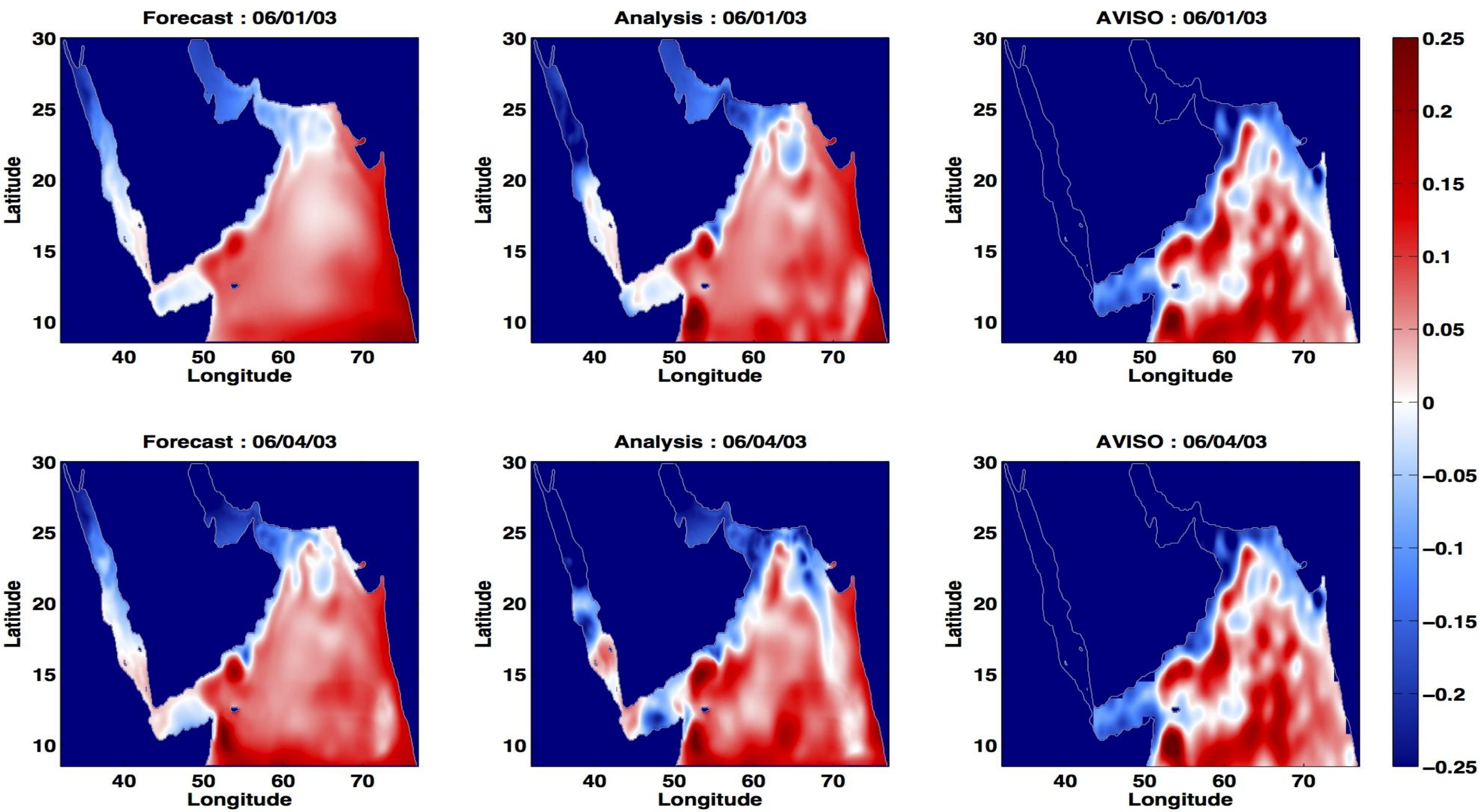
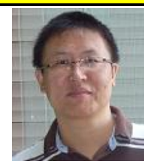
Massively Parallel Saudi Seas Assimilation System

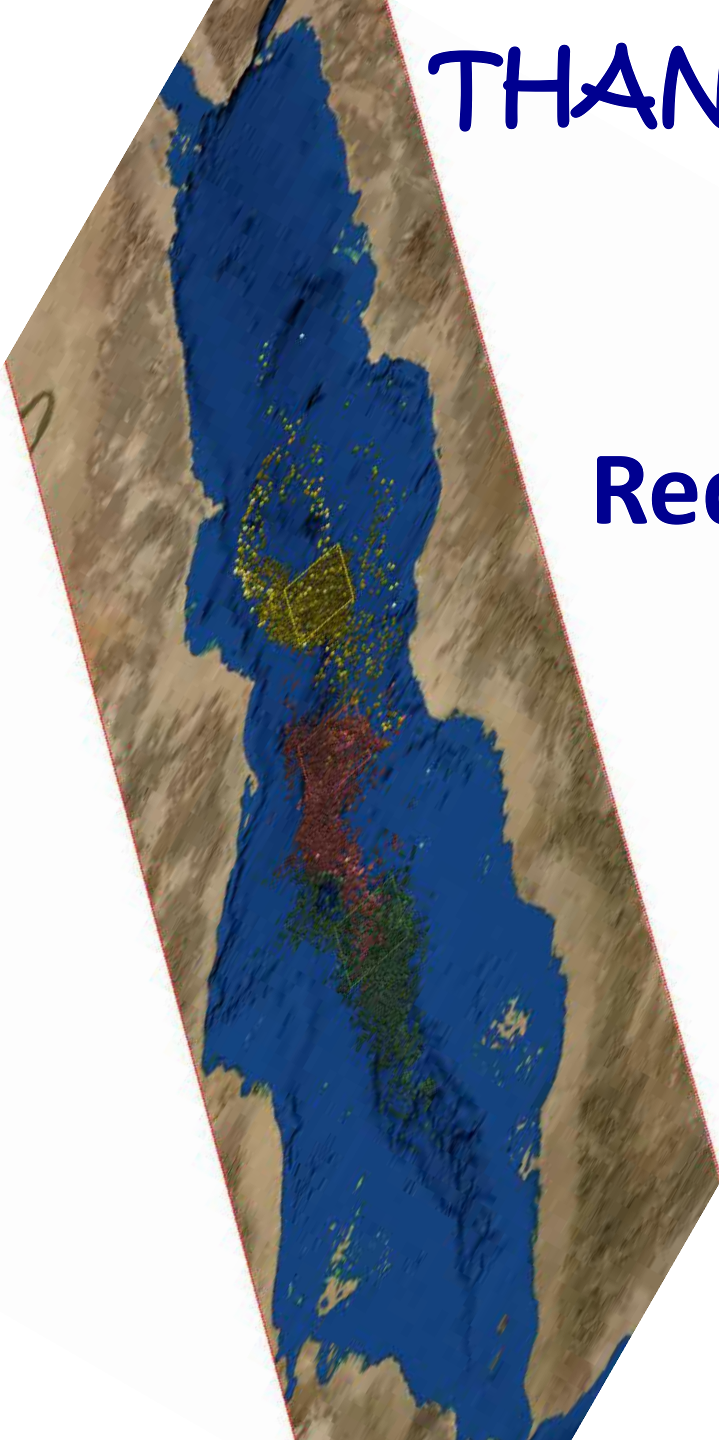
Three-Days Saudi Seas Forecasts and Analyses vs. Altimetry



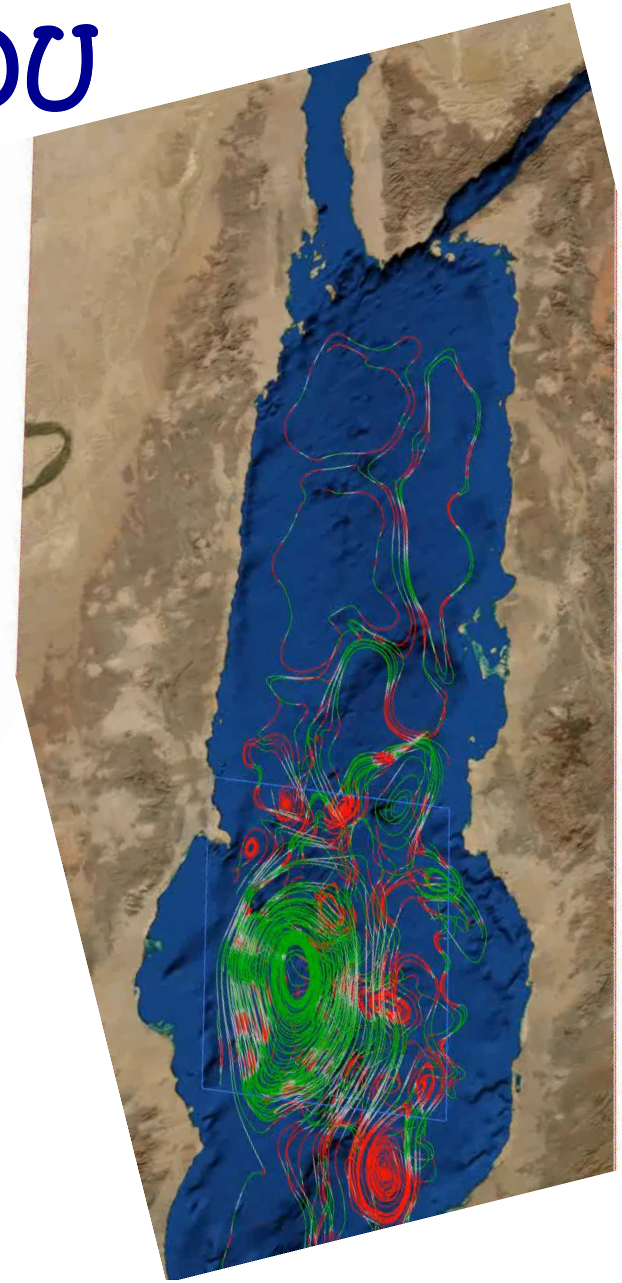
Group Members and Collaborators

Ocean Group Members		Collaborators	
Fengchao Yao Postdoc, ErSE		**Bruce Cornuelle** UCSD, USA	**G. Gopalakrishnan** UCSD, USA
Dionysios Raitsos Postdoc, ErSE		**Patrick Heimbach** MIT, USA	**Larry Pratt** WHOI, USA
V. Yesubabu Postdoc, ErSE		**Jeffrey Anderson** NCAR, USA	**G. Triantafyllou** HCMR, Greece
Peng Zhan PhD, ErSE		**Armin Kohl** Hamburg, Germany	**Charles Jackson** UT-Austin, USA
Sabique Langodan PhD, ErSE		**Burt Jones** KAUST, MarSE	**Y. Abu-Alnaja** KAUST, MarSE

THANK YOU

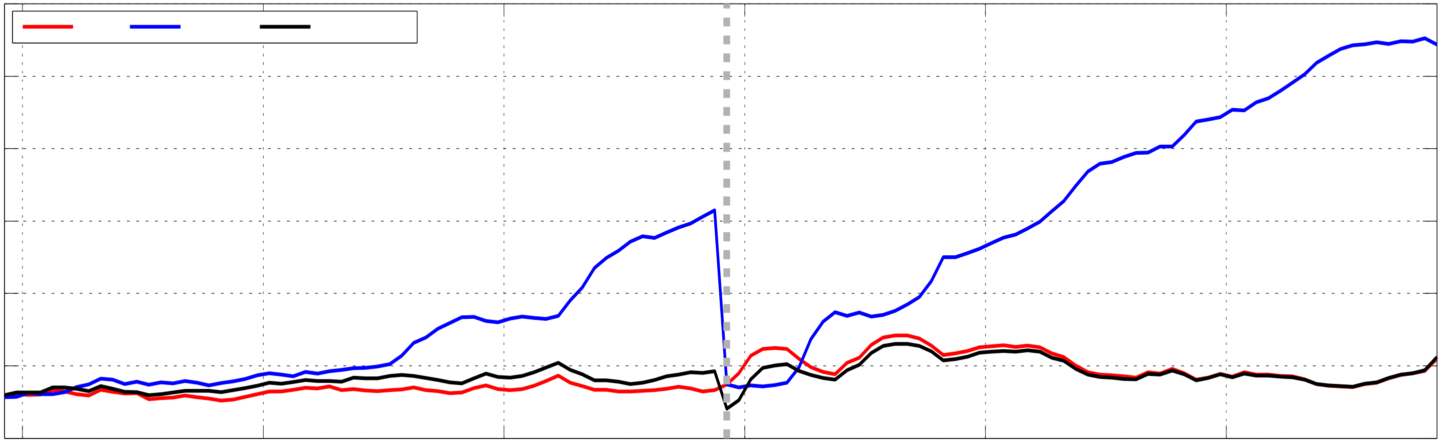


Red Sea



http://assimilation.kaust.edu.sa

4DVAR vs. EnKF in GoM – SST RMSE

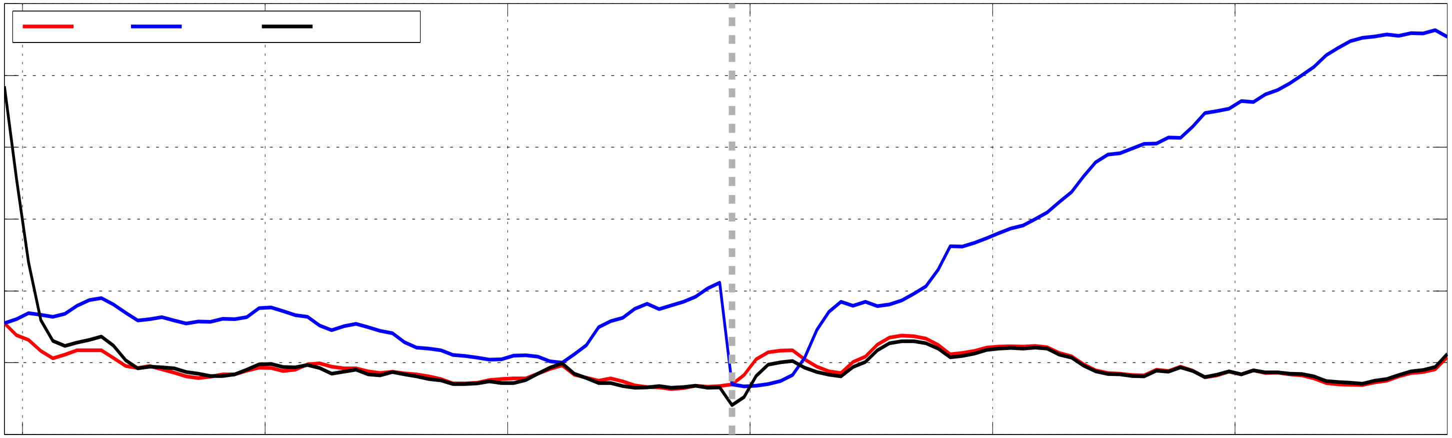


4DVAR

Persistence

Forecast

Analysis



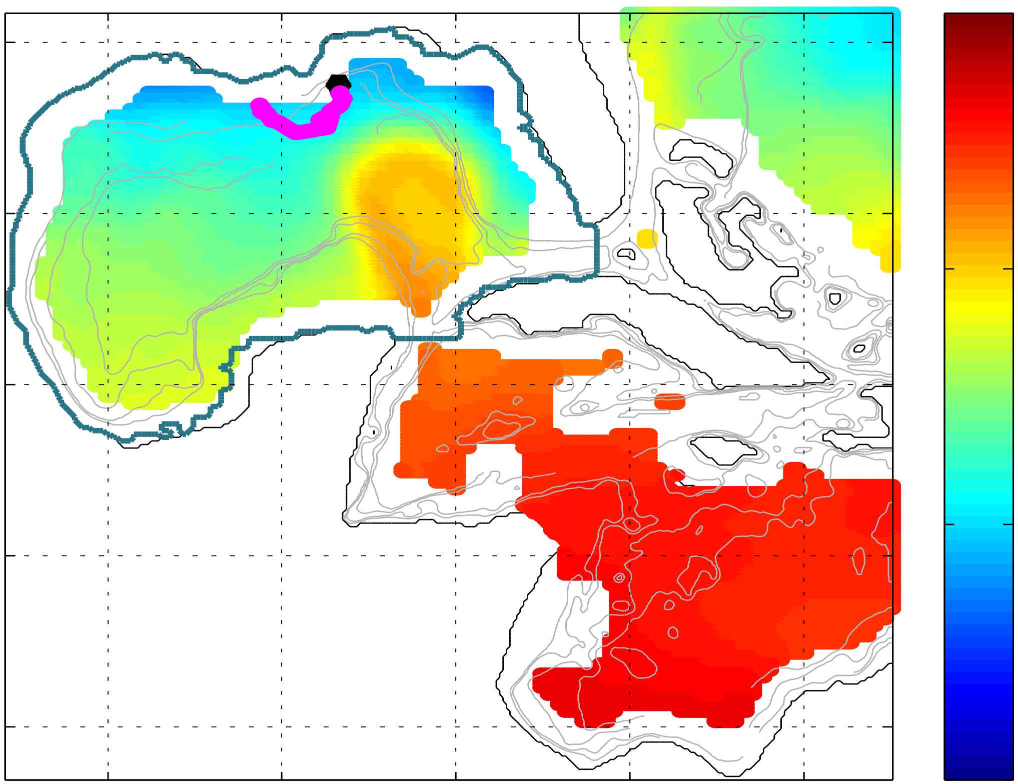
EnKF

Persistence

Forecast

Analysis

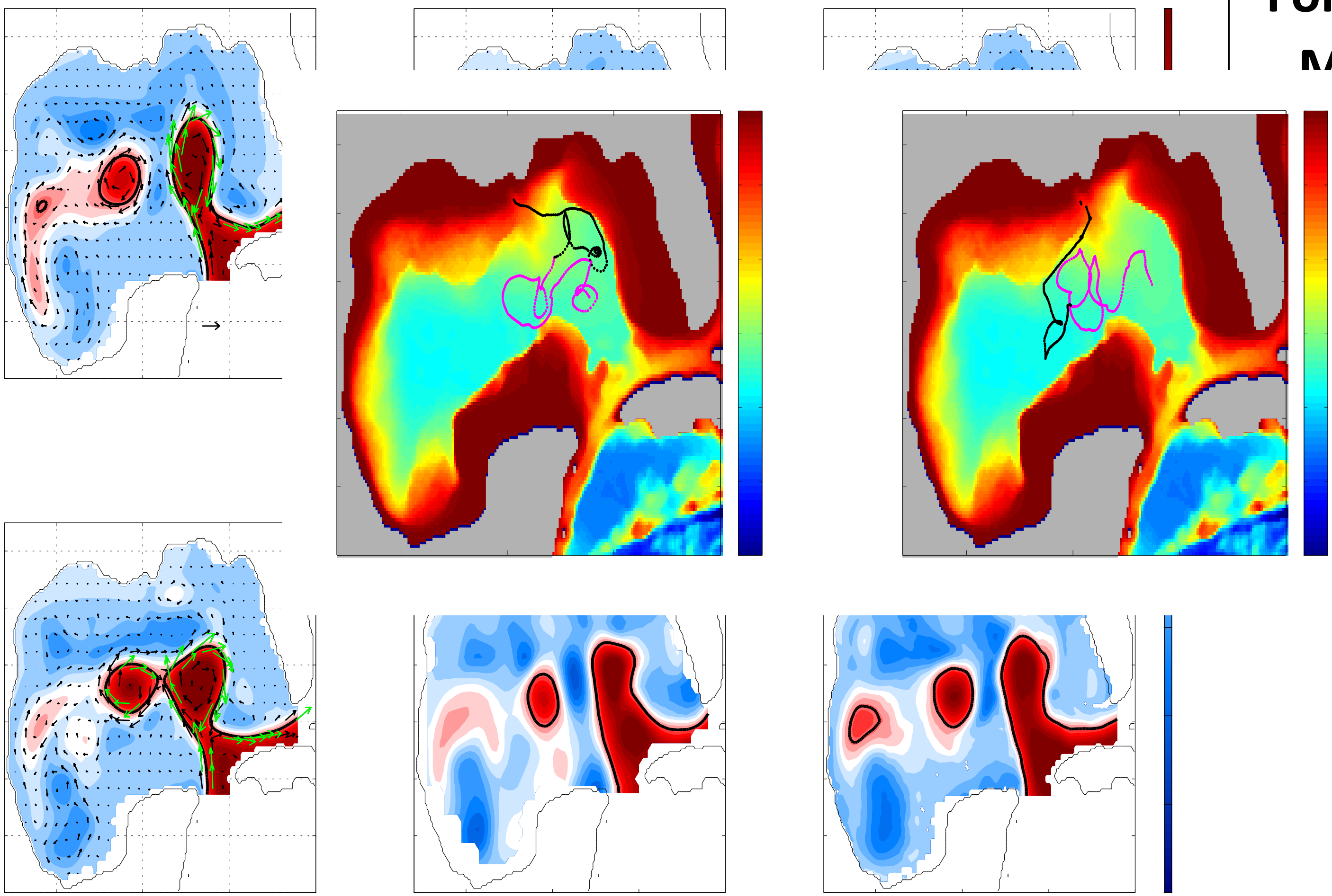
4DVAR vs. EnKF in GoM – Glider Temp



June 2010

Assimilation of Gliders Data in 4DVAR

Forecast - 4 weeks
March 30, 2012



SSH
SSH + 1 Glider
SSH + 2 Gliders

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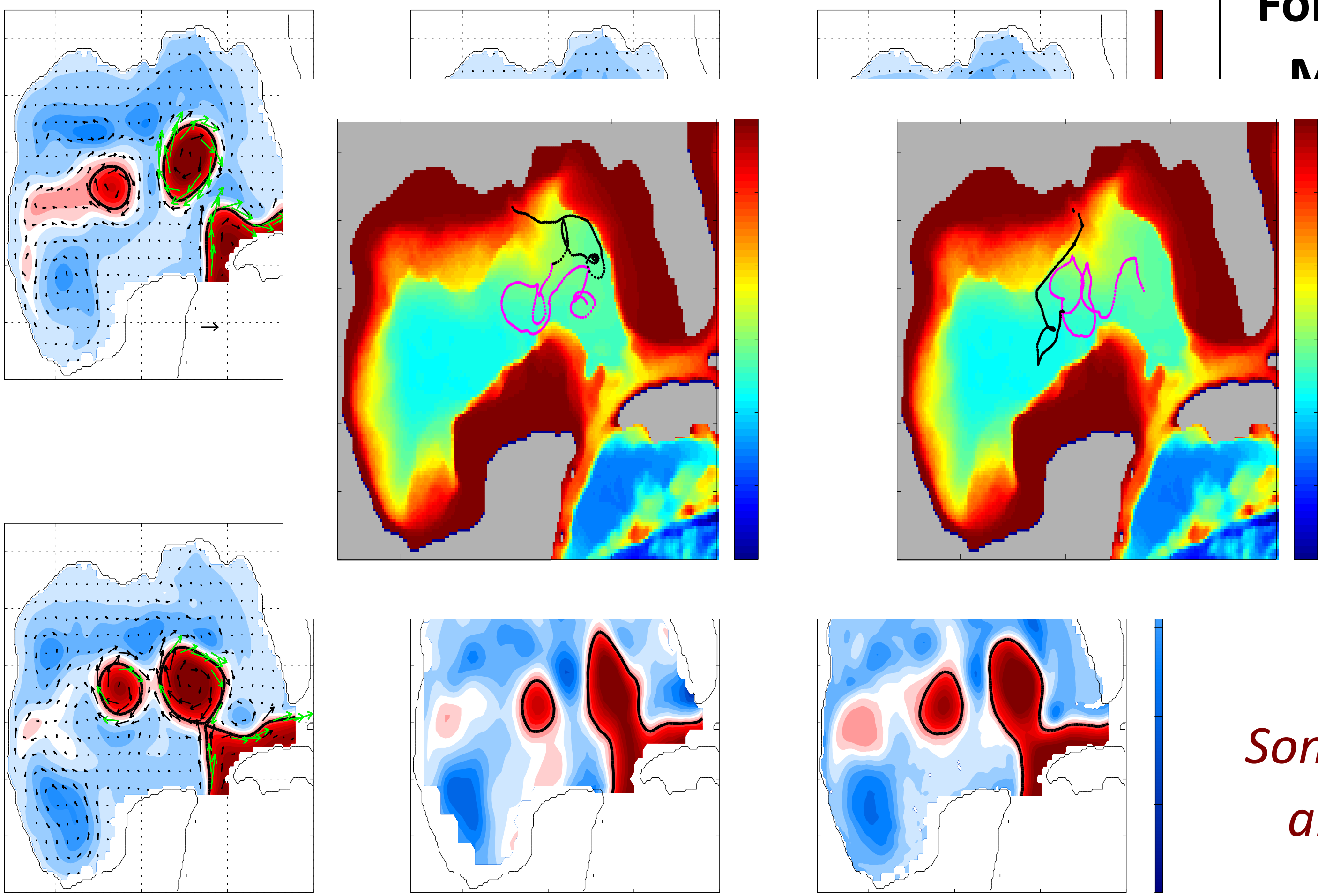
Assimilation of Gliders Data in 4DVAR

Forecast - 4 weeks

March 15, 2012



SSH

SSH + 1 Glider

SSH + 2 Gliders

Some "calibrations" are still needed!

AEnKF

- Another way to interpret it is to split the Kalman Gain into two parts:

$$\mathbf{K} = \mathbf{P}\mathbf{H}^T \left(\mathbf{H}\mathbf{P}\mathbf{H}^T + \mathbf{R}^e\right)^{-1}$$

$$\mathbf{K}^r = \mathbf{B}\mathbf{H}^T \left(\mathbf{H}\mathbf{P}\mathbf{H}^T + \mathbf{H}\mathbf{B}\mathbf{H}^T + \mathbf{R}\right)^{-1}$$

  We use $\mathbf{K}$ *to update the ensemble as in the regular EnKF, and we use* $\mathbf{K}^r$ *to estimate a new member.*

- We could use $\mathbf{K}^r$ for each member, as in LIH methods, so that same increments are added to all members. This would however increase correlations between members and does not improve "diversity".

Numerical Ocean Model – MITgcm

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$$\frac{\partial u}{\partial t} + \vec{u} \cdot \nabla u = -\frac{1}{\rho_0}\frac{\partial P}{\partial x} + \frac{1}{\rho_0}\frac{\partial \tau^x}{\partial z} - \frac{\partial \kappa \partial u}{\partial z^2} - \nu \frac{\partial^2 u}{\partial x^2}$$

$$\frac{\partial v}{\partial t} + \vec{u} \cdot \nabla v = -\frac{1}{\rho_0}\frac{\partial P}{\partial y} + \frac{1}{\rho_0}\frac{\partial \tau^y}{\partial z} - \frac{\partial \kappa \partial u}{\partial z^2} - \nu \frac{\partial^2 v}{\partial x^2}$$

Momentum Eq.

$$\nabla \cdot \vec{u} = 0$$

Continuity Eq.
(incompressible)

$$\frac{\partial T}{\partial t} + \vec{u} \cdot \nabla T + \frac{\partial k \partial T}{\partial^2 z} + \nu \frac{\partial^2 T}{\partial x^2} + \nu \frac{\partial^2 T}{\partial y^2} = 0$$

$$\frac{\partial S}{\partial t} + \vec{u} \cdot \nabla S + \frac{\partial k \partial S}{\partial^2 z} + \nu \frac{\partial^2 S}{\partial x^2} + \nu \frac{\partial^2 S}{\partial y^2} = 0$$

Tracer Eq. for T & S

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

SSH Eq.

$$\frac{\partial P}{\partial z} = -\rho g$$

Pressure Eq.
(Hydrostatic)

$$\rho = \rho_0(1 + \alpha(T - T_0) + \beta(S - S_0))$$

State Eq. for density