

Ensemble Assimilation of Ocean Data into the GEOS-5 Coupled GCM

Christian Keppenne^{1,2,*}, Guillaume Vernieres^{1,2}, Michele Rienecker¹, Robin Kovach^{1,2}, Jossy Jacob^{1,2} and Atanas Trayanov^{1,2}

> ¹NASA GMAO ²SAIC

Outline:

- NASA GMAO coupled model
- Coupled ensemble assimilation with GMAO ODAS-2
 - Atmospheric analysis "replay" procedure
 - Augmented ocean ensemble Kalman filter
 - Adaptive observation errors
 - Adaptive background-error covariance localization and inflation/deflation
 - Hybrid particle filter
 - Online bias correction
- System validation
 - Assimilation of sea level height
 - Online bias correction
 - Multivariate projection method
 - Assimilation of in situ T and/or S
- Outlook

*contact: christian.keppenne@nasa.gov

June 15, 2010

Atmospheric Observing System

GEOS-5 ADAS 14 May 2008 OOUTC 1,557,926 observations - 90% from satellites



Ocean Observing System

ODAS-2 data

- Topex/Jason SSH anomalies
- Argo in situ T and S profiles
- In situ T from TAO, XBT, Pirata and Rama
- Reynolds SST
- Levitus surface salinity while waiting for Aquarius 15N



The density and vertical coverage of in situ data has increased tremendously but the ocean is still poorly observed vs. the atmosphere. Hence, assimilating surface measurements from remote sensing is a must.

In situ data: 1 month (Jan. 2010)



Jason altimeter track: 1 day - ~2500 obs./day





ODAS-1

- Ocean-only runs
- · OGCM: Poseidon 4
- Analysis algorithms
 - EnKF
 - MvOI (EnKF analysis with steady-state fixed ensemble)
 - UOI (functional univariate background covariances)



ODAS-2

- · GEOS-5 Coupled Model:
 - OGCM: MOM-4 (0.5°X 0.167-0.5°X 40L) or any other ESMF-ready model
 - AGCM: GEOS-5 AGCM (1.25°X 1°X 72L)
- Analysis algorithms
 - Atmosphere: "replay" of GMAO atmospheric analysis
 - · Ocean: "Augmented" hybrid EnKF/lagged EnKF/particle filter approach
- ODAS implemented as ESMF gridded-component -> model independent







Augmented EnKF

The data assimilation problem

$$\frac{d\mathbf{x}}{dt} = \mathbf{M}(\mathbf{x}, \mathbf{f}) + \mathbf{q}$$

$$y = H(x_t) + r$$

$$E((\boldsymbol{x}-\boldsymbol{x}_{t})(\boldsymbol{x}-\boldsymbol{x}_{t})^{T}) = \boldsymbol{P} \qquad E(\boldsymbol{q}\boldsymbol{q}^{T}) = \boldsymbol{Q}$$

$$E(\boldsymbol{r}\boldsymbol{r}^{T}) = \boldsymbol{R}$$

- x : model state vector
- \boldsymbol{X}_t : unknown true state
- y: measurements

Objective: Find the best possible estimate of
$$x_t$$
 given x, y and their error distributions

The Kalman Filter (Kalman 1960)

$$\frac{d\boldsymbol{P}}{dt} = \frac{d}{dt} \left[E\left(\left(\boldsymbol{x} - \boldsymbol{x}_{t} \right) \left(\boldsymbol{x} - \boldsymbol{x}_{t} \right)^{T} \right) \right] = \frac{d\boldsymbol{M}}{d\boldsymbol{x}} \boldsymbol{P} \left[\frac{d\boldsymbol{M}}{d\boldsymbol{x}} \right]^{T} + \boldsymbol{Q}$$
$$\boldsymbol{x}^{a} = \boldsymbol{x}^{f} + \boldsymbol{P} \boldsymbol{H}^{T} \left(\boldsymbol{H} \boldsymbol{P} \boldsymbol{H}^{T} + \boldsymbol{R} \right)^{-1} \left(\boldsymbol{y} - \boldsymbol{H} \left(\boldsymbol{x}^{f} \right) \right)$$

The ensemble Kalman Filter

Evensen (1994, 1996)

Replace background-covariance evolution with ensemble integration

$$\frac{d\mathbf{x}_i}{dt} = \mathbf{M}(\mathbf{x}_i, \mathbf{f}) + \mathbf{q}_i \qquad E((\mathbf{x} - \mathbf{x}_t)(\mathbf{x} - \mathbf{x}_t)^T) = \mathbf{P}$$
$$\mathbf{P} \approx \frac{1}{n-1} \sum_i (\mathbf{x}_i - \overline{\mathbf{x}})(\mathbf{x}_i - \overline{\mathbf{x}})^T$$

given $z_i = H(x_i - \overline{x}), \quad i = 1, \dots n, \qquad Z = \frac{1}{\sqrt{n-1}} [z_i], \quad X = \frac{1}{\sqrt{n-1}} [x_i - \overline{x}],$

the update for ensemble member x_i is computed as (from right to left -> only matrix-vector products):

$$\boldsymbol{x}_{i}^{\mathrm{a}} = \boldsymbol{x}_{i}^{\mathrm{f}} + \boldsymbol{X}\boldsymbol{Z}^{\mathrm{T}}(\boldsymbol{Z}\boldsymbol{Z}^{\mathrm{T}} + \boldsymbol{R})^{-1}(\boldsymbol{y} - \boldsymbol{H}\boldsymbol{x}_{i} + \boldsymbol{\varepsilon}_{i})$$

$$P \longrightarrow C_{p} \circ P$$

$$R \longrightarrow C_{r} \circ R$$

$$X Z^{T} (Z Z^{T} + R)^{-1} \longrightarrow C_{p} \circ X Z^{T} (C_{p} \circ Z Z^{T} + C_{r} \circ R)^{-1}$$

 $\circ \equiv$ Hadamard (Schur) product

ODAS-2 Augmented EnKF

3 Sources of background-error covariance information

$$\boldsymbol{P}^{f} = \boldsymbol{P}_{dyn}^{f} + \boldsymbol{P}_{stat}^{f} + \boldsymbol{P}_{func}^{f}$$

 P_{dvn} : State-dependent error-covariance basis vectors from ensemble integration

- Current state of each ensemble member minus low pass filter
- Past states of each ensemble member minus a low pass filter



P_{stat}: Static ensemble of time-independent "error EOFs"

Error EOFs calculated from a time series of differences between a coupled model run constrained by replaying the GMAO atmospheric analysis and unconstrained short-term forecasts



P_{func}: Pseudo-Gaussian univariate covariance term

ODAS-1 Error-Covariance Localization

- Static, not flow adaptive 3D localization along (x, y, z) space dimensions
- Also apply Gaussian filter to deviations from ensemble mean $x_i \overline{x}$, $i = 1 \cdots n$

Marginal Kalman gain: T obs @(On,156E,150m) on 12/31/01 horizontal section through <T',T'> covariances





ODAS-2 flow-adaptive and observation-adaptive analysis

- Flow adaptive error-covariance localization following neutral density [(x, y, z, ρ) dimensions]
- Adaptive optimization of error-covariance localization scales (x, y, z) used with each observation
- Adaptive estimation of representation error associated with each observation
- Adaptive background-error covariance inflation/deflation
- Adaptive rescaling of analysis increments
- Particle pre-filter



ODAS-2 adaptive error covariance localization: successive stages

Traditional approach (as in ODAS-1)
 C(δx, δy, δz, δt) is an approximately Gaussian compactly supported correlation function

$$\boldsymbol{P}_c = \boldsymbol{P} \circ \boldsymbol{C}$$

- 2. Tried hierarchical ensemble filter (Anderson 2007)
 - Observations must be processed serially ($\alpha_{kl} P_{kl}$ is not a covariance)

$$\alpha = \frac{1}{m - 1} \left(\frac{(\sum_{i=1}^{m} \beta_i)^2}{\sum_{i=1}^{m} \beta_i^2} - 1 \right)$$

- 3. Bishop's (2007) flow adaptive moderation of spurious covariances
 - Some long-range spurious features are amplified.
 - Assimilation performance (OMFA statistics) worse than case 1

$$c_{ij}^{m} = \left(\frac{\boldsymbol{P}_{ij}}{\sqrt{\boldsymbol{P}_{ii}\boldsymbol{P}_{jj}}}\right)^{m}$$

$$G = diag(C^{m}), \qquad C^{mq} = G^{-1/2}(C^{m})^{q}G^{-1/2}$$

- 4. Back to approach 1 with localization in (x, y, z, t, neutral density) space
 - Respects flow-dependent gradients such as thermocline and fronts
 - Adaptive optimization of localization scales involved in processing each observation
 - Assimilation performance better than case 1

ODAS-2 flow-dependent error-covariance localization along neutral density surfaces

Covariance localization is the most numerically intensive part of the ensemble assimilation system

$$P \to C_{p} \circ P, \qquad R \to C_{r} \circ R, \qquad C = [c_{ij}],$$

$$c_{ij} = c_{0} (2 \frac{|x_{i} - x_{j}|}{l_{i}^{x} + l_{j}^{x}}) c_{0} (2 \frac{|y_{i} - y_{j}|}{l_{i}^{y} + l_{j}^{y}}) c_{0} (2 \frac{|z_{i} - z_{j}|}{l_{i}^{z} + l_{j}^{z}}) c_{0} (2 \frac{|p_{i} - p_{j}|}{l_{i}^{p} + l_{j}^{p}}) c_{0} (\frac{|t_{i} - t_{j}|}{l_{i}^{t} + l_{j}^{t}})$$

 C_0 is a compactly supported analytical covariance function (Gaspari and Cohn 1985)

ODAS-1: $I_x(y)$ and $I_y(y)$ proportional to Rossby radius of deformation ODAS-2: $I_x(x,y,z,t)$, $I_y(x,y,z,t)$, $I_z(x,y,z,t) \& I_p(x,y,z,t)$ optimized iteratively for each datum





Jan 2007

ODAS-2 flow-dependent error covariances

Marginal Kalman gain: unit T innovation at 95m



Marginal Kalman gain: unit SSH innovation along equator



ODAS-2 adaptive error-covariance localization

For each observation y_0 , process neighboring observations as though they were perfect (R=0) and optimize the localization by iteratively solving for the I_x , I_y & I_z that minimize

$$y_0 - \boldsymbol{H}_0 \boldsymbol{C} \circ \boldsymbol{P} \boldsymbol{H}_n^T \left(\boldsymbol{H}_n \boldsymbol{C} \circ \boldsymbol{P} \boldsymbol{H}_n^T \right)^{-1} \left(\boldsymbol{y}_n - \boldsymbol{H}_n \boldsymbol{x} \right)$$

- y_0 : an observation
- y_n : set of neighboring observations of same variable excluding y_0
- H_{y} : maps the state vector to y_{n}
- H_0 : maps the state vector to y_0

Relative zonal localization



Example:

optimized I_x and I_y localization scales for Reynolds SST data on Jan. 1 2007 expressed as a fraction of the default Rossyby-radius dependent localization



ODAS-2 adaptive representation-error estimation



For each individual observation, after optimization of the covariance localization parameters I_x , I_y & I_z , the representation error is estimated as

$$\sigma_0 = \left| y_0 - \boldsymbol{H}_0 \boldsymbol{C} \circ \boldsymbol{P} \boldsymbol{H}_n^T \left(\boldsymbol{H}_n \boldsymbol{C} \circ \boldsymbol{P} \boldsymbol{H}_n^T \right)^{-1} \left(\boldsymbol{y}_n - \boldsymbol{H}_n \boldsymbol{x} \right) \right|$$

Estimated representation error for Reynolds SST data Jan. 1 2007



Difference in SST increment : adaptive (errors + localization + covariance inflation) – standard assimilation (adaptive inflation only)

ODAS-2 adaptive localization and representation-error estimation



Optimal horizontal scales: ~60% of Rossby-radius dependent scales @250m, larger @1000m
Optimal vertical localization scales: minimum in thermocline. Default (250m) is too short near 1000m
Representation error estimate (σ_{obs}): maximum in thermocline, very small below 1000m

ODAS-2 adaptive error-covariance inflation

Following Desroziers et al. we have:

$$E\left[\left(\boldsymbol{y} - \boldsymbol{H}\boldsymbol{x}^{\mathrm{f}}\right)\left(\boldsymbol{y} - \boldsymbol{H}\boldsymbol{x}^{\mathrm{f}}\right)^{\mathrm{T}}\right] = Tr\left(\boldsymbol{H}\boldsymbol{P}^{\mathrm{f}}\boldsymbol{H}^{\mathrm{T}} + \boldsymbol{R}\right)$$
$$E\left[\left(\boldsymbol{y} - \boldsymbol{H}\boldsymbol{x}^{\mathrm{f}}\right)\left(\boldsymbol{H}\left(\boldsymbol{x}^{\mathrm{a}} - \boldsymbol{x}^{\mathrm{f}}\right)\right)^{\mathrm{T}}\right] = Tr\left(\boldsymbol{H}\boldsymbol{P}\boldsymbol{H}^{\mathrm{T}}\right)$$

Iterate until global convergence is satisfied:

Not prohibitively expensive because does not require calculation of $C_{\circ}HPH^{T}$

$$\alpha = \frac{\boldsymbol{P} \rightarrow \alpha \boldsymbol{P}}{\sum \left[\left(\boldsymbol{y}_i - \boldsymbol{H}_i \boldsymbol{x}^{\mathrm{f}} \right) \boldsymbol{H}_i \left(\boldsymbol{x}^{\mathrm{a}} - \boldsymbol{x}^{\mathrm{f}} \right) \right]}{Tr \left(\boldsymbol{H} \boldsymbol{P}^{\mathrm{f}} \boldsymbol{H}^{\mathrm{T}} + \boldsymbol{R} \right)} \boldsymbol{P}$$

 $H_i(x)$: observation operator (e.g., interpolation) for observation i (scalar)

Assimilation increment rescaling

Parallel algorithm involves each CPU minimizing RMS analysis error variance for a subset of all the observations (all the observations that influence state variables pertaining to that CPU). The increment, Δ , is then optimized globally by rescaling it ($\Delta \rightarrow \gamma \Delta$) such as to globally minimize

$$f(\boldsymbol{\gamma}) = \sum_{i} (y_{i} - \boldsymbol{H}_{i} \boldsymbol{x}^{a})^{2} = \sum_{i} (y_{i} - \boldsymbol{H}_{i} (\boldsymbol{x}^{f} + \boldsymbol{\gamma} \Delta))^{2}$$

$$\frac{d}{d\gamma}f(\gamma) = 0 \longrightarrow \gamma = \frac{\sum((y_i - H_i \mathbf{x}^f)H_i \Delta)}{\sum(H_i \Delta)^2}$$

| | | | | | | | | | | | | | / | | | |
|--|--|--|--|--|--|--|---|--|---|--|--|---|---|---|--|--|
| | | | | | | | | | | | | | | | | |
| | | | | | | | Γ | | Γ | | | 7 | | Γ | | |
| | | | | | | | | | | | | | | | | |
| | | | | | | | | | | | | | | | | |
| | | | | | | | | | | | | | | | | |
| | | | | | | | | | Γ | | | | | | | |

ODAS-2 particle pre-filter

Motivation: ensemble mean is not necessarily a realizable state. Hence we want to improve upon this state by shifting the ensemble mean to the ensemble member that is closest to the observations (a realizable state).

- Find ensemble member x_p that is closest to the data in terms of RMS OMF Displace the whole ensemble by an increment $\Delta_p = x_p x_m$ where x_m is the ensemble mean Thereafter, apply the ensemble Kalman filter analysis



ODAS-2 particle pre-filter example: assimilate in situ ARGO T data. Validate against ARGO S data

- · CGCM
- Data
 - Daily assimilation of ARGO T profiles 04/01/06 05/31/06 (active data set)
 - ARGO S profiles used for validation (passive data set)
- Initial condition
- 03/01/06 coupled model restart from single coupled model run with atm. Anal. Replay
- Ensemble initialization (03/01/06 04/01/06)
 - initial perturbation from linear combinations of model signal EOFs
 - daily perturbations with 1% of initial perturbation amplitude
- Assimilation (04/01/06-05/31/06)
 - · CE-16: 16-member control ensemble no assimilation
 - EnKF-16x11: 16 streams (model integrations) and 10 past instances in each stream (lag = 1 day)
 - HPEnKF-16x11: reordering particle pre-filter HPF-16 used prior to each EnKF-16x11 analysis

ODAS-2 particle pre-filter example: assimilate in situ ARGO T data. Validate against ARGO S data



Online bias correction and assimilation of SSH anomalies

- Challenge 1: model bias changes as the data are assimilated
- Challenge 2: must derive T(z), S(z) u(z) and v(z) from scalar η measurements

a) Standard assimilation



b) Assimilation with online bias estimation (OBE)



Side by side estimation of

- bias
- unbiased error component

$$\eta = \int_{z} f(\rho(z)) dz$$

 $P = P^{f} + P^{b}$ after Dee and Dasilva (1998) $b^{a} = b^{f} - P^{b}H^{T}(H(P^{b} + P^{f})H^{T} + R)^{-1}(y - H(x^{f} - b^{f}))$ $x^{a} = x^{f} + P^{f}H^{T}(HP^{f}H^{T} + R)^{-1}(y - H(x^{f} - b^{a}))$ $b^{f}_{k+1} = b^{a}_{k}$ y - H(x): total innovationy - H(x - b): unbiased innovation

$$\begin{array}{l} \boldsymbol{P}^{b} \rightarrow \boldsymbol{C}^{b} \circ \boldsymbol{P}^{b} \\ \boldsymbol{P}^{f} \rightarrow \boldsymbol{C}^{f} \circ \boldsymbol{P}^{f} \end{array}$$

SSH bias estimate snapshot 04/01/2006





Online bias correction and assimilation of SSH anomalies

Note: ensemble initialization during first two months of EnKF run



RMS T OMFA statistics at TAO mooring locations (April-July 2007)

T improvement over control: control RMS T OMF - ODAS RMS T OMF

Validation of surface data assimilation using passive (not assimilated) sub-surface Argo data



Assimilation of SST + SSS alone does not improve the subsurface T much (vs. control)
SLA assimilation with online bias correction improves upon control, but not in Nino-4 area (0-300m)
Assimilating SST + SSS + SLA mostly corrects the 0-300m Nino-4 area deficiencies

S improvement over control: control RMS S OMF - ODAS RMS S OMF

Validation of surface data assimilation using passive (not assimilated) sub-surface Argo data



RMS S OMF diff. 0-300m









RMS S OMF diff. 300-2000m





- SLA assimilation alone very effective is improving S over the control
- Best results for S seen when assimilating SST + SSS + SLA



- analyz



T and S forecast and analysis compared to some un-assimilated in situ profiles near the altimeter track at the time of the first assimilation

Summary

- Ocean data assimilation into GMAO CGCM with "replay" of the GMAO atmospheric analysis
- Combining static and dynamic ensembles (including lagged ensemble) gives best performance
- Multivariate background covariances effective in improving unobserved model variables
- SLA assimilation improves subsurface T & S, but best results with SST + SSS + SLA assim.
- Ensemble data assimilation system ready for production runs
- Started 1950-present retrospective analysis

Outlook

- Moving towards fully coupled data assimilation system through data assimilation into the skin layer (building upon NCEP GSI work)
- Ready for new data types, starting with Aquarius

GMAO ODAS webpage: http://gmao.gsfc.nasa.gov/research/oceanassim