COASTAL OCEAN MODELING

June 17-22, 2007
Colby-Sawyer College
New London, NH

Chair:
Francisco E. Werner

Vice Chair:
Richard P. Signell

Application Deadline: Applications for this meeting must be submitted by May 27, 2007.

Please apply early, as some conferences become oversubscribed (full) before this deadline. If the conference is oversubscribed, it will be stated here. You will still be able to submit your application. However, it will only be considered by the Conference Chair if there are cancellations, making more seats available.

Organizing Committee: John Allen, Julie Pullen, Mark Stacey and John Wilkin

SUNDAY
2:00 pm - 11:00 pm Arrival and Check-in
6:00 pm Dinner
7:30 pm - 7:40 pm Welcome / Introductory Comments by GRC Site Staff
7:40 pm - 9:30 pm INTEGRATION OF MODELING AND OBSERVING SYSTEMS

Discussion Leader: Huijie Xue (University of Maine, USA)

Nadia Pinardi (University of Bologna, Italy)
"Coastal ocean predictions: from marine meteorology to marine ecosystem management"
Predictability of Mesoscale Variability in the East Australian Current given Strong Constraint Data Assimilation

John Wilkin
Javier Zavala-Garay
and Hernan Arango

Institute of Marine and Coastal Sciences
Rutgers, The State University of New Jersey
New Brunswick, NJ, USA

jwilkin@rutgers.edu
http://marine.rutgers.edu
Mean steric height at 0 m and 150 m depth from hydrographic climatology.
East Australia Current ROMS* Model for IS4DVAR

**ROMS* Model Configuration**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Resolution</td>
<td>0.25 x 0.25 degrees</td>
</tr>
<tr>
<td>Grid</td>
<td>64 x 80 x 30</td>
</tr>
<tr>
<td>Δx, Δy</td>
<td>~ 25 km</td>
</tr>
<tr>
<td>Δt</td>
<td>1080 sec</td>
</tr>
<tr>
<td>Bathymetry</td>
<td>16 to 4895 m</td>
</tr>
<tr>
<td>Open boundaries</td>
<td>Global NCOM (2001 and 2002)</td>
</tr>
<tr>
<td>Forcing</td>
<td>Global NOGAPS, daily</td>
</tr>
<tr>
<td>De-correlation scale</td>
<td>100 km, 150 m</td>
</tr>
<tr>
<td>N outer, N inner loops</td>
<td>10, 3</td>
</tr>
</tbody>
</table>

* http://myroms.org

1/8° resolution version simulates complex EOF “eddy” and “wave” modes of satellite SST and SSH in EAC separation:

IS4DVAR*

- Given a first guess (the forward trajectory)...

*R Incremental Strong Constraint 4-Dimensional VARiational data assimilation
IS4DVAR

- Given a first guess (the forward trajectory)...
- and given the available data...
• Given a first guess (the forward trajectory)...
• and given the available data...
• what change (or increment) to the initial conditions (IC) produces a new forward trajectory that better fits the observations?
Basic IS4DVAR procedure:

1. Choose an $x(0) = x_b(0)$

2. Integrate NLROMS $t \in [0, \tau]$ and save $x(t)$
   
   (a) Choose a $\delta x(0)$

   (b) Integrate TLROMS $t \in [0, \tau]$ and compute $J$

   (c) Integrate ADROMS $t \in [\tau, 0]$ to yield $\frac{\partial J_0}{\partial \delta x(0)} = \lambda(0)$

   (d) Compute $\frac{\partial J}{\partial \delta x(0)} = B^{-1}\delta x(0) - \lambda(0)$

   (e) Use a descent algorithm to determine a “down gradient” correction to $\delta x(0)$ that will yield a smaller value of $J$

   (f) Back to (b) until converged

3. Compute new $x(0) = x(0) + \delta x(0)$ and back to (2) until converged

NLROMS = Non-linear forward model; TLROMS = Tangent linear; ADROMS = Adjoint
The best fit becomes the *analysis*

assimilation window
The final state becomes the IC for the forecast window.
The final state becomes the IC for the forecast window.

Forecast verification is with respect to data not yet assimilated.
4DVar Observations and Experiments

7-Day IS4DVAR Experiments
E1: SSH, SST
E2: SSH, SST, XBT

SSH 7-Day Averaged AVISO
SST Daily CSIRO HRPT

Days since 1 January 2001, 00:00
EAC IS4DVAR

Assimilating surface vs. sub-surface observations
EAC IS4DVAR

7-Day 4DVar Assimilation cycle
E1: SSH, SST Observations
E2: SSH, SST, XBT Observations

Observations

SSH

Temperature along XBT line

E1

E2

E1 – E2
Forecast SSH correlation and RMS error: Experiment E2

SSH Lag Pattern Correlation

SSH Lag Pattern RMS

Days since 1 January 2001 00:00
RMS error normalized by the expected variance in SSH

Forecast RMS error:
- typically < 0.5 out to 2 weeks forecast
- grows fastest at the open boundaries (errors in boundary data, or open boundary scheme)
Forecast uncertainty:
Ensemble predictions using Singular Vectors of the forecast

The eigenvectors of: \( R^T(t,0) W R(0,t) \)

...having the largest eigenvalues, are the fastest growing perturbations of the Tangent Linear model.

They correspond to the right Singular Vectors of \( R(0,t) \) (the ROMS TL propagator)

These describe perturbations to the initial conditions that lead to the greatest uncertainty in the forecast
Forecast uncertainty:
Ensemble predictions using Singular Vectors of the forecast

Perturb $\phi_0$ for ensemble of IC:
$r$ scales $\max|\delta\phi|$ to 3 cm

$$\delta\phi = r \sum_{i=1}^{10} a_i SV_i$$
$a_i$ are $N(0,1)$
Forecast uncertainty:
Ensemble predictions using Singular Vectors of the forecast

- The optimal perturbations when we include XBTs (experiment E2) are more realistic: they tend to be concentrated at the surface, where most of the instability takes place.
Example structures of the singular vectors for Experiments E1 and E2

Singular Vector 1

After assim. SSH+SST

E1

Perturbation after 10 days

E1

Vertical structure

E1

After assim. SSH+SST+XBT

E2

E2

Vertical structure

E2
Ensemble Prediction: E1

White contours: Ensemble set
Color: Ensemble mean
Black contour: Observed SSH

1-day forecast
8-day forecast
15-day forecast
Ensemble Prediction: E2

White contours: Ensemble set
Color: Ensemble mean
Black contour: Observed SSH

1-day forecast
8-day forecast
15-day forecast
Forecast uncertainty:
Ensemble predictions using Singular Vectors of the forecast

- The optimal perturbations when we include XBTs are more realistic: they tend to be concentrated at the surface, where most of the instability takes place.
- In an ensemble prediction system generated using SV perturbations, the spread for SVs of E2 is smaller and verifies better with observations than for SVs of E1.
- Subsurface XBT data significantly improves the forecast.
- We have a further source of subsurface information based on surface observations: synthetic-CTD
  - a statistically-based proxy deduced from historical EAC data
Synthetic XBT/CTD example:
Statistical projection of satellite SSH and SST using EOFs of subsurface $T(z)$, $S(z)$
E1: SSH, SST

E3*: SSH, SST, Syn-CTD

Syn-CTD 4-day CSIRO subsurface projection of satellite obs to T(z), S(z)
Comparison between ROMS temperature *analysis* (fit) and *withheld observations* (all available XBTs); the XBT data were not assimilated – they are used here only to evaluate the quality of the reanalysis.
Comparison between ROMS temperature *analysis (fit)* and *withheld observations* (all available XBTs); the XBT data were not assimilated – they are used here only to evaluate the quality of the reanalysis.
Comparison between ROMS subsurface temperature *predictions* and all *XBT observations* in 2001-2002.

- **Correlation**
- **RMS error (°C)**

E3: SSH+SST+
Syn-CTD

0 lag –
analysis skill
Comparison between ROMS subsurface temperature predictions and all XBT observations in 2001-2002

E3: SSH+SST+
Syn-CTD

0 lag –
analysis skill

1 week lag –
little loss of skill
Comparison between ROMS subsurface temperature \textit{predictions} and all \textit{XBT observations} in 2001-2002

- 0 lag – analysis skill
- 1 week lag – little loss of skill
- 2 week lag – forecast begins to deteriorate

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<tr>
<th></th>
<th>correlation</th>
<th>RMS error ($^{\circ}$C)</th>
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<td>0 lag – analysis skill</td>
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Comparison between ROMS subsurface temperature *predictions* and all *XBT observations* in 2001-2002

**correlation**

**RMS error (°C)**

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<td>3 week lag – forecast still better than …</td>
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Comparison between ROMS subsurface temperature *predictions* and all XBT *observations* in 2001-2002

0 lag – analysis skill

1 week lag – little loss of skill

2 week lag – forecast begins to deteriorate

3 week lag – forecast still better than …

no assimilation

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Conclusions

- Skillful ocean state predictions up to 2+ weeks
- Assimilation of SST and SSH only is not enough
- Assimilation of subsurface information:
  - improves estimate of the subsurface
  - makes forecasts more stable to uncertainty in IC
- Singular Vectors demonstrate ensemble predictions and uncertainty estimation
- Synthetic-CTD subsurface projection adds significant analysis and forecast skill
- The synthetic-CTD is a linear empirical relationship, suggesting a simple dynamical relationship could link surface to subsurface variability
  - this could be built in to the background error covariance
  - this idea is not new: Weaver et al 2006, A multivariate balance operator for variational ocean data assimilation, QJRMS
Future Work

- Include balance terms in the IS4DVAR
- Improve boundary forcing
  - better global forecast and/or boundary conditions
  - determine optimal boundary forcing via “weak constraint” data-assimilation (WS4DVAR)
- Use along-track SSH data instead of gridded multi-satellite analysis
- Explore sensitivity to length of assimilation window
- Computational effort: 1 week analysis + forecast takes 4 hours on 8-processors (Opteron 250, PGI, MPICH)
Thanks to:

- David Griffin (CSIRO) for the SST and Syn-CTD
- SIO VOS for XBT; AVISO for SSH
- John Evans (RU) 4DVAR observation file processing
\[ \frac{\partial S}{\partial t} = N(S), \]

\[ \frac{\partial s}{\partial t} = \left. \frac{\partial N(S)}{\partial S} \right|_{s_0} s = As, \quad (2) \]

Integral solutions of (2) can be written as \( s(t) = R(0, t)s(0) \), where \( R(0, t) \) is called the propa-
Notation

- **ROMS state vector** $\mathbf{x}(t) = [u \ v \ T \ S \ \zeta]^T$

- **NLROMS equation form**: 
  \[
  \frac{\partial \mathbf{x}(t)}{\partial t} = \mathbf{N}(\mathbf{x}(t)) + \mathbf{F}(t) \\
  \mathbf{x}(0) = \mathbf{x}_i \\
  \mathbf{x}(t)|_\Omega = \mathbf{x}_\Omega(t)
  \]

- **NLROMS propagator form**: 
  $\mathbf{x}(t_i) = \mathbf{M}(t_i, t_{i-1})(\mathbf{x}(t_{i-1}))$

- **Observation** $\mathbf{y}_i$ at time $t_i$ with observation error variance $\mathbf{O}$

- **Model equivalent at observation points** $\mathbf{H}_i \mathbf{x}(t_i) \equiv \mathbf{H}_i \mathbf{x}_i$

- **Unbiased background state** $\mathbf{x}_b$ with background error covariance $\mathbf{B}$
Strong constraint 4DVAR


• Seek $x(t)$ that minimizes

$$J(x) = \frac{1}{2} (x - x_b)^T B^{-1} (x - x_b) + \sum_{i=1}^{N} \frac{1}{2} (H_i x_i - y_i)^T O^{-1} (H_i x_i - y_i)$$

subject to equation (1) i.e., the model dynamics are imposed as a ‘strong’ constraint. $x(t)$ depends only on $x(0), x_{f\Omega}(t), F(t)$ “control variables”

• Cost function as function of control variables

$$J(x) = \frac{1}{2} (x(0) - x_b(0))^T B^{-1} (x(0) - x_b(0))$$

$$+ \sum_{i=1}^{N} \frac{1}{2} (H_i M(t_i, 0) x_i(0) - y_i)^T O^{-1} (H_i M(t_i, 0) x_i(0) - y_i)$$

• $J$ is not quadratic since $M$ is nonlinear.
S4DVAR procedure

Lagrange function

\[ L = J(x) + \sum_{i=1}^{N} \lambda_{i}^{T} \left( \frac{dx_{i}}{dt} - N(x_{i}) - F_{i} \right) \]

\[ F_{i} = F(i\Delta t) \quad x_{i} = x(i\Delta t) \]

Lagrange multiplier

\[ \lambda_{i} = \lambda(t_{i}) = \lambda(i\Delta t) \]

At extrema of \( L \), we require:

\[
\begin{align*}
\frac{\partial L}{\partial \lambda_{i}} &= 0 \Rightarrow \frac{dx_{i}}{dt} - N(x_{i}) - F_{i} = 0 & \text{NLROMS} \\
\frac{\partial L}{\partial x_{i}} &= 0 \Rightarrow -\frac{d\lambda_{i}}{dt} - \left( \frac{\partial N}{\partial x} \right)^{T} \lambda_{i} - \delta_{im} H^{T} O^{-1} (Hx_{m} - y_{m}) = 0 & \text{ADROMS} \\
\frac{\partial L}{\partial x(0)} &= 0 \Rightarrow B^{-1} (x(0) - x_{b}) - \lambda(0) = 0 & \text{coupling of NL & ADROMS} \\
\frac{\partial L}{\partial x(\tau)} &= 0 \Rightarrow \lambda(\tau) = 0 & \text{i.c. of ADROMS}
\end{align*}
\]

S4DVAR procedure:

1. Choose an \( x(0) = x_{b} \)
2. Integrate NLROMS \( t \in [0, \tau] \) and compute \( J \)
3. Integrate ADROMS \( t \in [\tau, 0] \) to get \( \lambda(0) \)
4. Compute \( \frac{\partial J}{\partial x(0)} = B^{-1} (x(0) - x_{b}) - \lambda(0) \)
5. Use a descent algorithm to determine a “down gradient” correction to \( x(0) \) that will yield a smaller value of \( J \)
6. Back to (2) until converged. But actually, it doesn’t converge well!
Adjoint model integration is forced by the model-data error.

$x_b = \text{model state at end of previous cycle, and } 1^{st} \text{ guess for the next forecast}$

In 4D-VAR assimilation the adjoint model computes the sensitivity of the initial conditions to mismatches between model and data.

A descent algorithm uses this sensitivity to iteratively update the initial conditions, $x_a$, to minimize $J_b + \Sigma(J_o)$.
Incremental Strong Constraint 4DVAR

Courtier et al, 1994, QJRMS, 120, 1367-1387
Weaver et al, 2003, MWR, 131, 1360-1378

- True solution \( x = x_b + \delta x \)

- NLROMS solution from Taylor series:

\[
x(t_i) = M(t_i, t_{i-1})x(t_{i-1}) = M(t_i, t_{i-1})(x_b(t_{i-1}) + \delta x(t_{i-1})) = M(t_i, t_{i-1})x_b(t_{i-1}) + \left( \frac{\partial M(t_i, t_{i-1})}{\partial x(t_{i-1})} \right)_{x_b(t_{i-1})} \delta x(t_{i-1}) + O(\delta x(t_{i-1})^2)
\]

- \( M(t_i, t_{i-1})x_b(t_{i-1}) + R(t_i, t_{i-1})\delta x(t_{i-1}) \quad R(t_i, t_{i-1}) \quad \text{---- TLROMS Propagator} \)

- Cost function is quadratic now

\[
J(x) \equiv \frac{1}{2} \delta x^T B^{-1} \delta x + \frac{1}{2} \sum_{i=1}^N (G_i \delta x - d_i)^T O^{-1} (G_i \delta x - d_i)
\]

\[
G_i = H_i R(0, t_i) \quad d_i = y_i - H_i M(t_i, 0)x_b(0) = y_i - H_i x_b(t_i)
\]
Basic IS4DVAR* procedure

*Incremental Strong Constraint 4-Dimensional Variational Assimilation

(1) Choose an \( x(0) = x_b(0) \)

(2) Integrate NLROMS \( t \in [0, \tau] \) and save \( x(t) \)
   
   (a) Choose a \( \delta x(0) \)
   
   (b) Integrate TLROMS \( t \in [0, \tau] \) and compute \( J \)
   
   (c) Integrate ADROMS \( t \in [\tau, 0] \) to yield \( \frac{\partial J}{\partial \delta x(0)} = \lambda(0) \)
   
   (d) Compute \( \frac{\partial J}{\partial \delta x(0)} = B^{-1} \delta x(0) - \lambda(0) \)
   
   (e) Use a descent algorithm to determine a “down gradient” correction to \( \delta x(0) \) that will yield a smaller value of \( J \)
   
   (f) Back to (b) until converged

(3) Compute new \( x(0) = x(0) + \delta x(0) \) and back to (2) until converged
Basic IS4DVAR* procedure

*Incremental Strong Constraint 4-Dimensional Variational Assimilation

1. Choose an \( \mathbf{x}(0) = \mathbf{x}_h(0) \)

2. Integrate NLROMS
   (a) Choose a \( \delta \mathbf{x}(0) \)
   (b) Integrate TLROMS
   (c) Integrate ADROMS
   (d) Compute \( \frac{\partial J}{\partial \delta \mathbf{x}(0)} \)
   (e) Use a descent algorithm to determine a "down gradient" correction to \( \delta \mathbf{x}(0) \)
   (f) Back to (b) until converged

3. Compute new \( \mathbf{x}(0) = \mathbf{x}(0) + \delta \mathbf{x}(0) \) and back to (2) until converged

The Devil is in the Details
Conjugate Gradient Descent
Long & Thacker, 1989, DAO, 13, 413-440

- Expand step (5) in S4DVAR procedure and step (e) in IS4DVAR procedure

- Two central component: (1) step size determination (2) pre-conditioning (modify the shape of $J$)

- New NLROMS initial condition: $\delta x_{n+1}(0) = \delta x_n(0) + \alpha d_n$  \[ \alpha \] ---- step-size (scalar)

- $d_n = -\left( \frac{\partial J}{\partial x(0)} \right)_n + \gamma_{n-1} d_{n-1}$  \[ \gamma_{n-1} = f\left( \frac{\partial J}{\partial x(0)} \right)_n, \frac{\partial J}{\partial x(0)} \right)_{n-1} \]  \[ d_n \] ---- descent direction

- Step-size determination:
  (a) Choose arbitrary step-size $\alpha_0$ and compute new $\delta x(0)$ and $\delta J_0$
  (b) For small correction, assume the system is linear, $\delta J_r$, yielded by any step-size $\alpha_r$, is $\delta J_r = f(\alpha_0, \alpha_r, \delta J_0)$
  (c) Optimal choice of step-size is the $\alpha_r$ who gives $\frac{\partial J_r}{\partial \alpha_r} = 0$

- Preconditioning:
  use Hessian for preconditioning: $E = \frac{\partial^2 J}{\partial x^2} = B^{-1} + H^T O^{-1} H$  \[ B \] is dominant because of sparse obs.

- Look for minimum $J$ in $v$ space
Background Error Covariance Matrix

Weaver & Courtier, 2001, QJRMS, 127, 1815-1846

- Split $B$ into two parts: $B = K_b B_u K_b^T$
  (1) unbalanced component $B_u$
  (2) balanced component $K_b$

- Unbalanced component $B_u = \Sigma C \Sigma$
  $\Sigma$ ---- diagonal matrix of background error standard deviation
  $C$ ---- symmetric matrix of background error correlation

- $B = B^{1/2} B^{T/2}$ for preconditioning, $B^{1/2} = K_b \Sigma C^{1/2}$

- Use diffusion operator to get $C^{1/2}$:
  assume Gaussian error statistics, error correlation $f(x) = \exp \left[ \frac{-(x - \mu)^2}{2\sigma^2} \right]$
  the solution of diffusion equation $\frac{\partial \eta}{\partial t} - \frac{\sigma}{2T} \frac{\partial^2 \eta}{\partial x^2} = 0$ over the interval $t = [0, T]$ with $\eta(0) = (x - \mu)^2$
  $\eta(x) = \frac{1}{\sqrt{2\pi\sigma}} \exp \left[ \frac{-(x - \mu)^2}{2\sigma^2} \right]

- $C = \Lambda L \Lambda$
  $L$ ---- the solution of diffusion operator
  $C^{1/2} = \Lambda L^{1/2} L^{1/2}$
  $\Lambda$ ---- matrix of normalization coefficients $\frac{1}{\sqrt{2\pi\sigma}}$