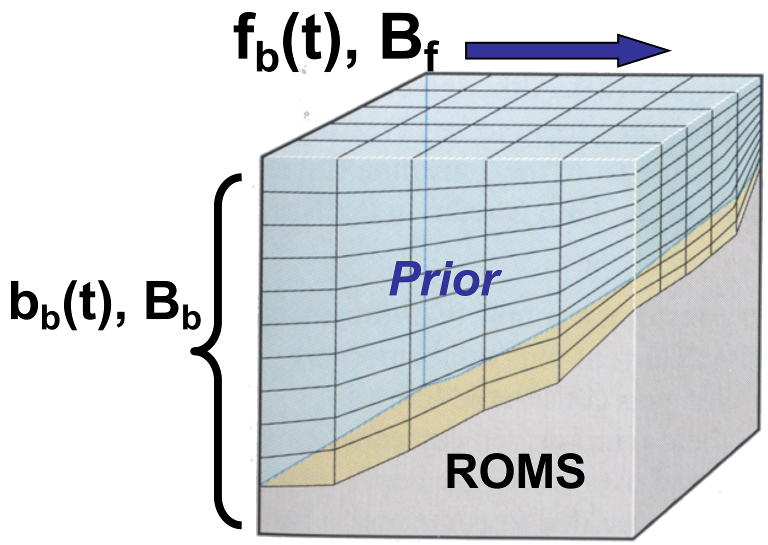
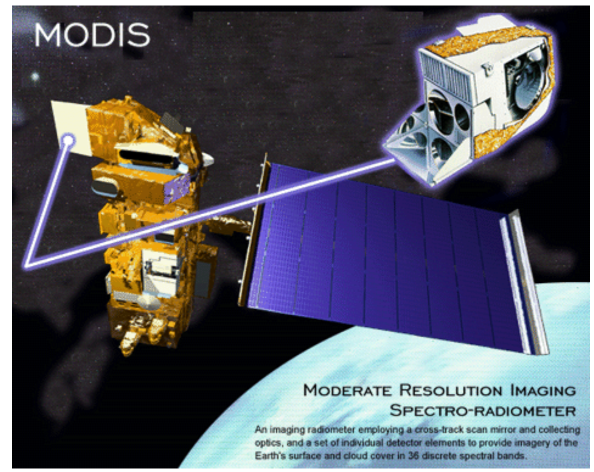
Lecture 1:
4D-Var: Some Basics

Outline

- ROMS 4D-Var overview
- 4D-Var concepts
- Primal formulation of 4D-Var
- Incremental approach used in ROMS
- The ROMS I4D-Var algorithm

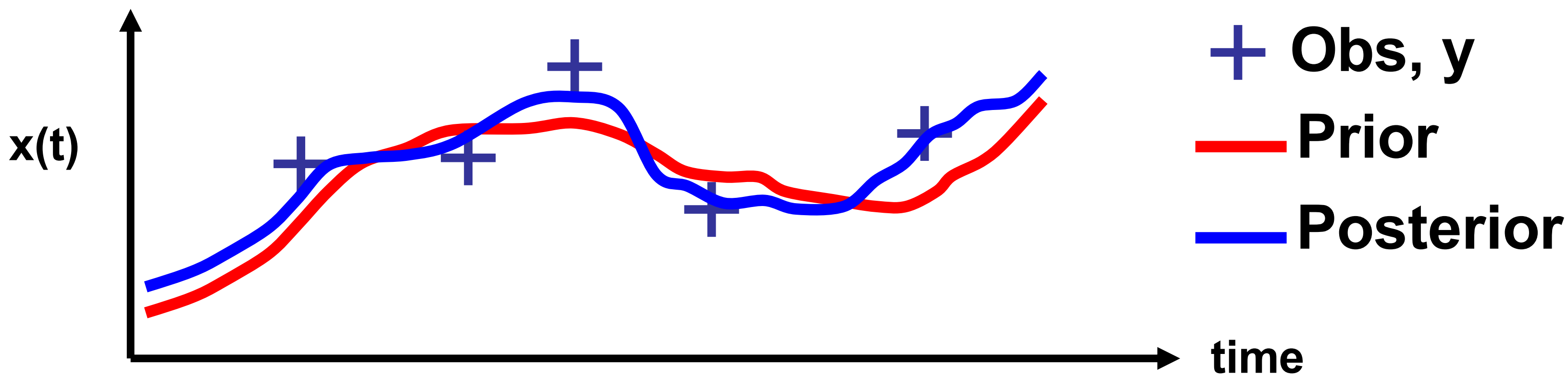
Data Assimilation





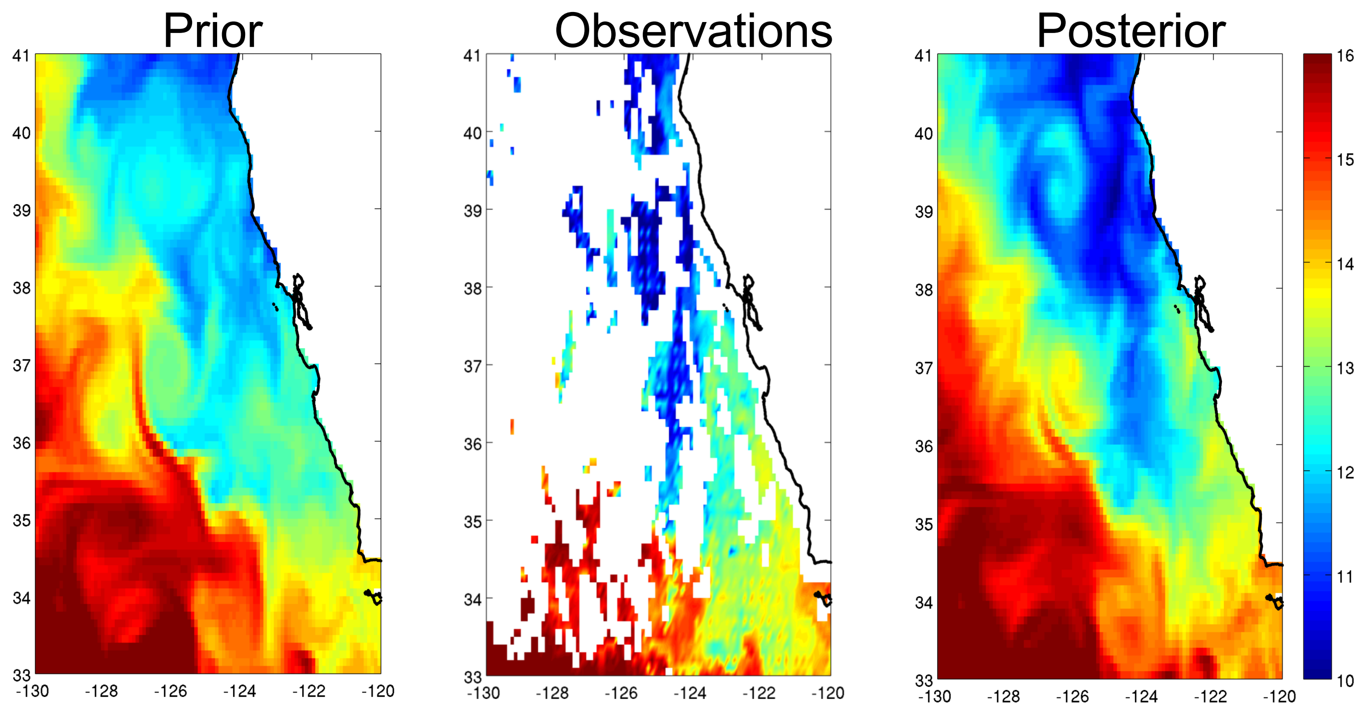
$x_b(0)$, B_x

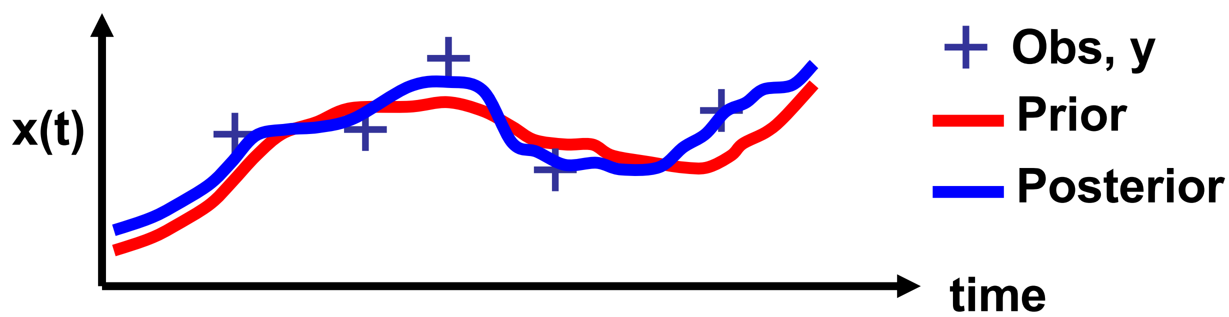
y, R



Model solutions depends on $x_b(0)$, $f_b(t)$, $b_b(t)$, $\eta(t)$

California SST Analysis, Jan. 2010





The problem can be approached in several ways:
(i) as a weighted, constrained least-squares problem
(ii) as an optimal control problem
(iii) as a Bayesian estimation problem

Essentially all equivalent

Notation & Nomenclature

$$\mathbf{x} = \begin{bmatrix} \mathbf{T} \\ \mathbf{S} \\ \boldsymbol{\zeta} \\ \mathbf{u} \\ \mathbf{v} \end{bmatrix}$$

State vector

$$\mathbf{z} = \begin{bmatrix} \mathbf{x}(0) \\ \mathbf{f}(t) \\ \mathbf{b}(t) \\ \boldsymbol{\eta}(t) \end{bmatrix}$$

Control vector

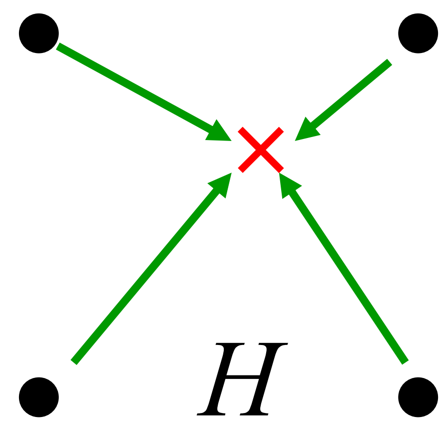
$$\mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ \vdots \\ y_N \end{bmatrix}$$

Observation vector

Prior

$$\mathbf{d} = \left(\mathbf{y} - H(\mathbf{z}_\mathbf{b})\right)$$

Innovation vector



Observation operator

Thomas Bayes
(1702-1761)

Bayes Theorem

(Shamelessly plagiarized from Wikle and Berliner, 2007)

Conditional probability:

$$p(\mathbf{z}\,|\,\mathbf{y}) = p(\mathbf{y}\,|\,\mathbf{z})\, p(\mathbf{z}) / p(\mathbf{y})$$

Posterior distribution | **Data distribution** | **Prior** | **Marginal**

p(**y**) – a normalizing constant

$$= c \, \exp\left(-1/2\left(\mathbf{y} - H(\mathbf{z})\right)^{\mathrm{T}} \mathbf{R}^{-1}\left(\mathbf{y} - H(\mathbf{z})\right)\right)$$

$$\ldots 1/2 \left(\ldots \right)^{\mathrm{T}} \ldots^{-1} \left(\ldots \right)\Big)$$

p(**z**|**y**) – the posterior update of our *prior* knowledge about **z** as summarized by p(**z**) given **y**

p(**y**|**z**) – quantifies distribution of measurement error (probability of obs **y** given unobservables **z**)

Maximum likelihood esti... ...um of

$$J_{NL}(\mathbf{z}) = \frac{1}{2}(\mathbf{z} - \ldots (\mathbf{x}))^{\mathrm{T}} \mathbf{R}^{-1}(\mathbf{y} - H(\mathbf{x}))$$

p(**z**) – quantifies our *prior* understanding of the unobservables **z**

which maxim...

Bayes Theorem

Conditional probability:

(Wikle and Berliner, 2007)

$$p(\mathbf{z}\,|\,\mathbf{y}) = p(\mathbf{y}\,|\,\mathbf{z})\,p(\mathbf{z})/p(\mathbf{y})$$

Posterior distribution | Data distribution | Prior | Marginal

$$= c\ \exp\left(-1/2\left(\mathbf{y}-H(\mathbf{z})\right)^{\mathrm{T}}\mathbf{R}^{-1}\left(\mathbf{y}-H(\mathbf{z})\right)\right)$$

("likelihood")

$$\times\ \exp\left(-1/2\left(\mathbf{z}-\mathbf{z}_{\mathbf{b}}\right)^{\mathrm{T}}\mathbf{D}^{-1}\left(\mathbf{z}-\mathbf{z}_{\mathbf{b}}\right)\right)$$

Maximum likelihood estimate: identify the minimum of

$$J_{NL}(\mathbf{z}) = \frac{1}{2}(\mathbf{z}-\mathbf{z}_{\mathbf{b}})^{\mathrm{T}}\mathbf{D}^{-1}(\mathbf{z}-\mathbf{z}_{\mathbf{b}}) + \frac{1}{2}(\mathbf{y}-H(\mathbf{x}))^{\mathrm{T}}\mathbf{R}^{-1}(\mathbf{y}-H(\mathbf{x}))$$

which maximizes $p(\mathbf{z}|\mathbf{y})$.

Variational Data Assimilation

Conditional Probability: $P(\mathbf{z}\,|\,\mathbf{y}) \propto \exp\left(-J_{NL}\right)$

$$J_{NL}(\mathbf{z}) = \frac{1}{2}(\mathbf{z}-\mathbf{z}_{\mathbf{b}})^{\mathrm{T}}\mathbf{D}^{-1}(\mathbf{z}-\mathbf{z}_{\mathbf{b}}) + \frac{1}{2}(\mathbf{y}-H(\mathbf{z}))^{\mathrm{T}}\mathbf{R}^{-1}(\mathbf{y}-H(\mathbf{z}))$$

Observation error covariance

$$\mathbf{D} = \underbrace{\mathrm{diag}(\mathbf{B}_{\mathbf{x}}, \mathbf{B}_{\mathbf{b}}, \mathbf{B}_{\mathbf{f}}, \mathbf{Q})}$$

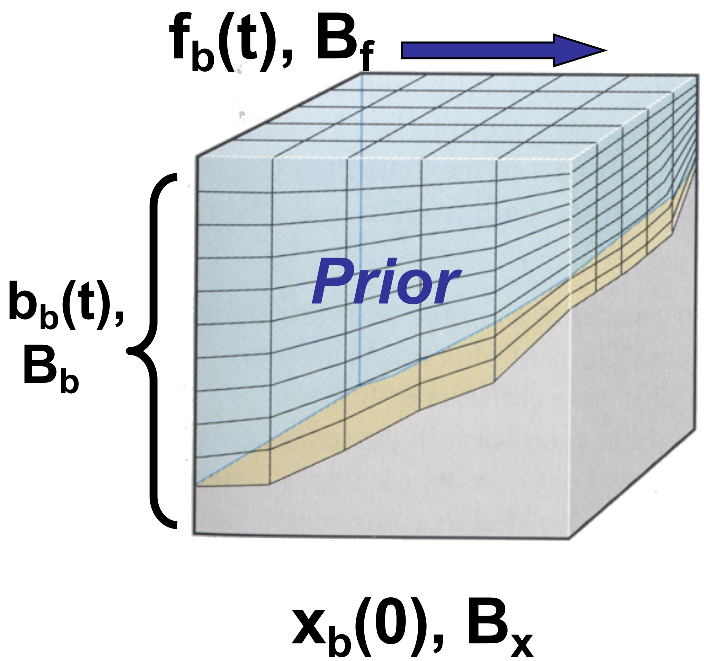
Background error covariance

J_{NL} is called the "cost" or "penalty" function.

Problem: Find z=z_a that minimizes *J (i.e. maximizes P)* using principles of variational calculus.
z_a is *also* the "maximum likelihood" or "minimum variance" estimate.

Incremental Formulation

(Courtier *et al.*, 1994)



$$\delta\mathbf{z} = (\delta\mathbf{x}^T(0), \delta\mathbf{b}(t), \delta\mathbf{f}(t), \boldsymbol{\eta}(t))^T$$

initial condition increment — boundary condition increment — forcing increment — corrections for model error

$$J = \frac{1}{2}\delta\mathbf{z}^T\mathbf{D}^{-1}\delta\mathbf{z} + \frac{1}{2}\left(\mathbf{G}\delta\mathbf{z} - \mathbf{d}\right)^T\mathbf{R}^{-1}\left(\mathbf{G}\delta\mathbf{z} - \mathbf{d}\right)$$

$$\mathbf{D} = \mathrm{diag}(\mathbf{B}_x, \mathbf{B}_b, \mathbf{B}_f, \mathbf{Q})$$

Prior (background) error covariance

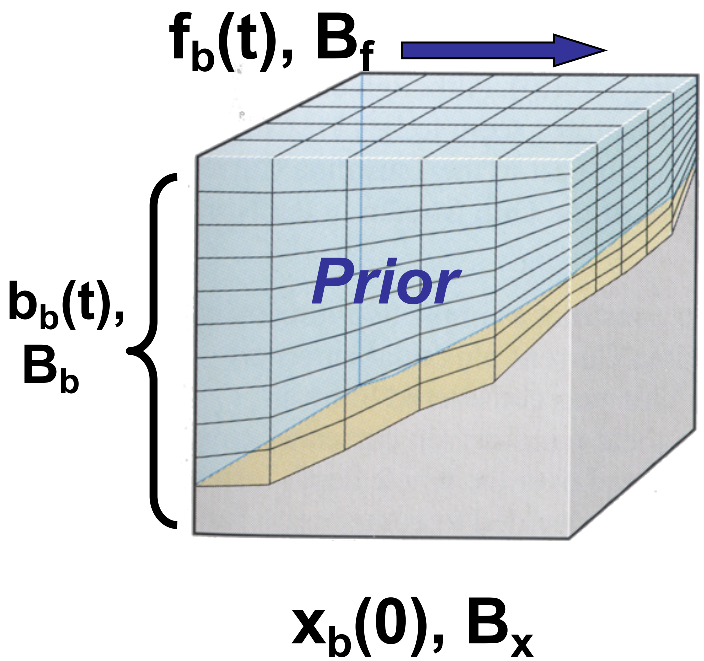
Tangent Linear Model sampled at obs points

Obs Error Cov.

Innovation

$$\mathbf{d} = \mathbf{y} - H(\mathbf{z}_b)$$

Incremental Formulation



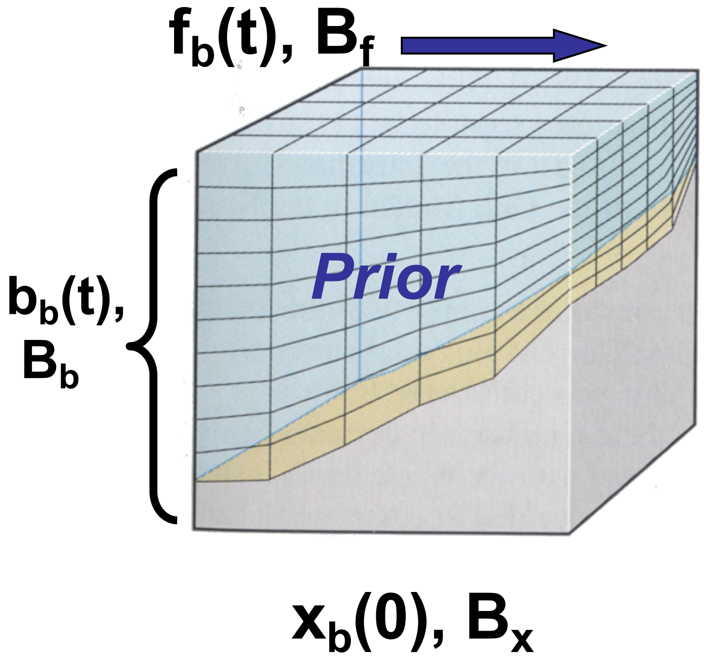
$$\delta \mathbf{z} = (\delta \mathbf{x}^T(0), \delta \mathbf{b}(t), \delta \mathbf{f}(t), \boldsymbol{\eta}(t))^T$$

- $\delta \mathbf{x}^T(0)$: initial condition increment
- $\delta \mathbf{b}(t)$: boundary condition increment
- $\delta \mathbf{f}(t)$: forcing increment
- $\boldsymbol{\eta}(t)$: corrections for model error

$$J = \frac{1}{2}\delta \mathbf{z}^T \mathbf{D}^{-1} \delta \mathbf{z} + \frac{1}{2}\left(\mathbf{G}\delta \mathbf{z} - \mathbf{d}\right)^T \mathbf{R}^{-1}\left(\mathbf{G}\delta \mathbf{z} - \mathbf{d}\right)$$

The minimum of *J* is identified iteratively by searching for $\partial J/\partial \delta \mathbf{z} = 0$

Incremental Formulation



$$\delta \mathbf{z} = (\delta \mathbf{x}^T(0), \delta \mathbf{b}(t), \delta \mathbf{f}(t), \boldsymbol{\eta}(t))^T$$

initial condition increment; boundary condition increment; forcing increment; corrections for model error

$$\mathbf{z} = \mathbf{z_b} + \delta \mathbf{z}$$

Assumptions:

(i) $\delta \mathbf{z} \ll \mathbf{z}_b$

(ii) $\mathbf{x}(t) = \mathbf{x}_b(t) + \delta \mathbf{x}(t)$

(iii) $\delta \mathbf{x}(t) \simeq \mathbf{M}\delta \mathbf{z}$

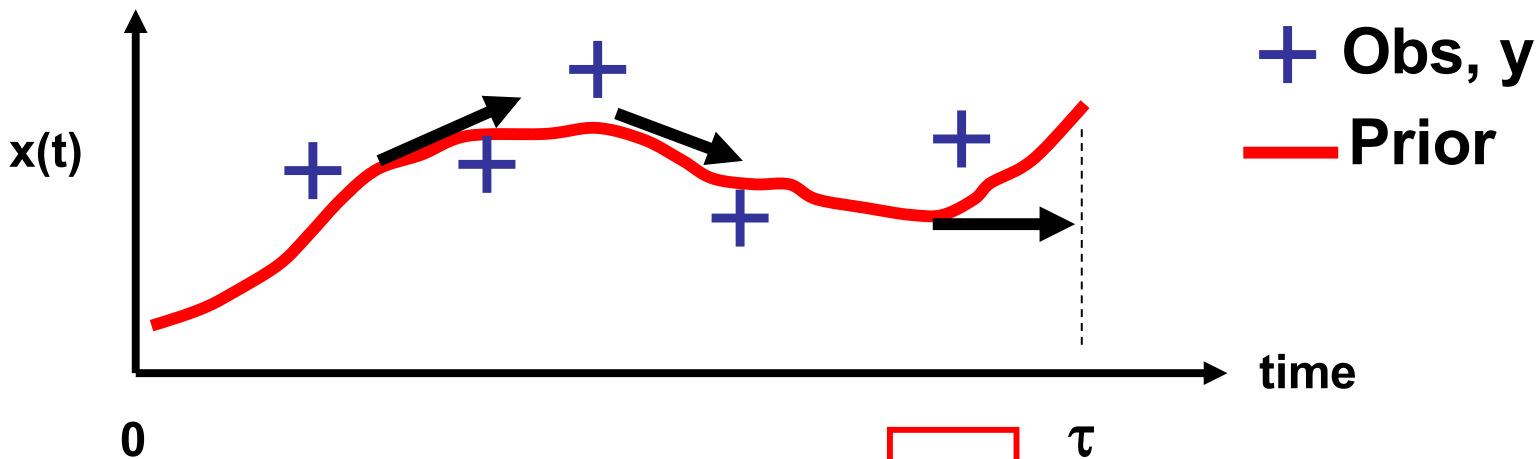
(iv) $\mathbf{H} * \delta \mathbf{x}(t) \simeq \mathbf{H} * \mathbf{M}\delta \mathbf{z} = \mathbf{G}\delta \mathbf{z}$

$\mathbf{M}$ = Tangent Linear Model

$\mathbf{H}$ = Tangent Linear H

The Tangent Linear Model

(TLROMS)



Prior is solution of model: $\mathbf{x}_b(t_i) = M(\mathbf{x}_b(t_{i-1}), \mathbf{f}_b(t_i), \mathbf{b}_b(t_i))$

Nonlinear model

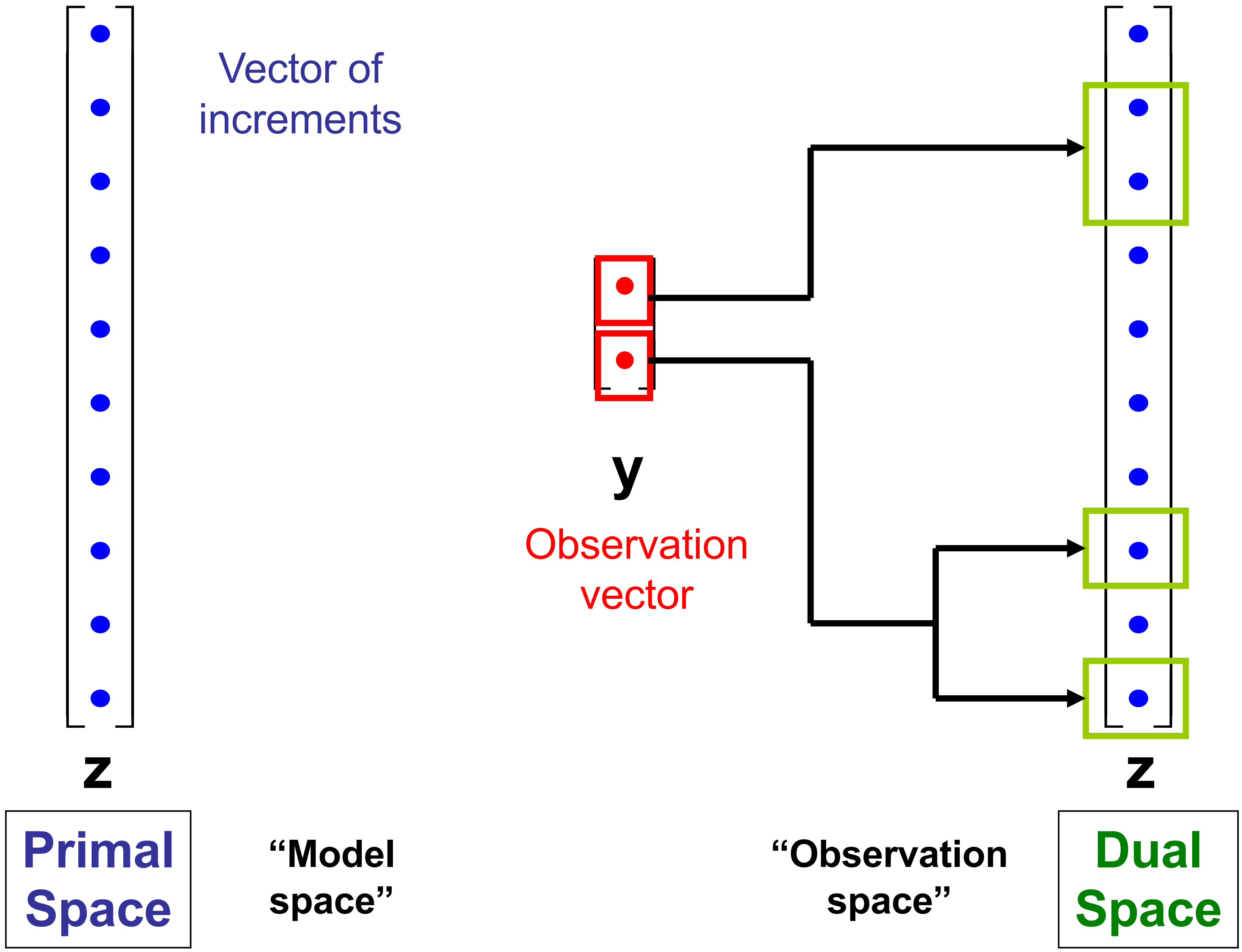
Increment: $\delta\mathbf{x}(t) \ll \mathbf{x}_b(t); \quad \delta\mathbf{f}(t) \ll \mathbf{f}_b(t);$ etc

$$\mathbf{x}(t_i) = \mathrm{M}(\mathbf{x}_b(t_{i-1}) + \delta\mathbf{x}(t_{i-1}), \cdots)$$

$$\simeq \mathrm{M}(\mathbf{x}_b(t_{i-1}), \cdots) + \mathbf{M}_{\mathbf{x}_b}\delta\mathbf{z}$$

Tangent linear model

Primal vs Dual Formulation



The Solution

Analysis: $$\mathbf{z_a} = \mathbf{z_b} + \mathbf{Kd}$$

Gain matrix (dual form):

$$\mathbf{K} = \mathbf{DG}^{\mathrm{T}}(\mathbf{GDG}^{\mathrm{T}} + \mathbf{R})^{-1}$$

Gain matrix (primal form):

$$\mathbf{K} = (\mathbf{D}^{-1} + \mathbf{G}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{G})^{-1}\mathbf{G}^{\mathrm{T}}\mathbf{R}^{-1}$$

Two Spaces

Gain (dual):

$$\mathbf{K} = \mathbf{D}\mathbf{G}^{\mathrm{T}} \underbrace{(\mathbf{G}\mathbf{D}\mathbf{G}^{\mathrm{T}} + \mathbf{R})}_{N_{\mathrm{obs}} \times N_{\mathrm{obs}}}^{-1}$$

Gain (primal):

$$\mathbf{K} = \underbrace{(\mathbf{D}^{-1} + \mathbf{G}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{G})}_{N_{\mathrm{model}} \times N_{\mathrm{model}}}^{-1} \mathbf{G}^{\mathrm{T}}\mathbf{R}^{-1}$$

$$N_{\mathrm{obs}} \ll N_{\mathrm{model}}$$

Two Spaces

G maps from model space
to observation space

$\mathbf{G}^T$ maps from observation space
to model space

Comments:

- ROMS supports both the primal and dual formulations of 4D-Var
- We are going to encourage you to use the dual formulation because it is more efficient and has more utility
- However, it is useful to start with a discussion of the primal form since much of the 4D-Var literature focusses on the primal form.

Iterative Solution of Primal Formulation

(define IS4DVAR, is4dvar_ocean.h)

Recall the incremental cost function:

$$J = \underbrace{\frac{1}{2}\delta\mathbf{z}^T\mathbf{D}^{-1}\delta\mathbf{z}}_{J_b} + \underbrace{\frac{1}{2}\left(\mathbf{G}\delta\mathbf{z}-\mathbf{d}\right)^{\mathrm{T}}\mathbf{R}^{-1}\left(\mathbf{G}\delta\mathbf{z}-\mathbf{d}\right)}_{J_o}$$

At the minimum of *J* we have $\partial J/\partial\delta\mathbf{z} = \mathbf{0}$

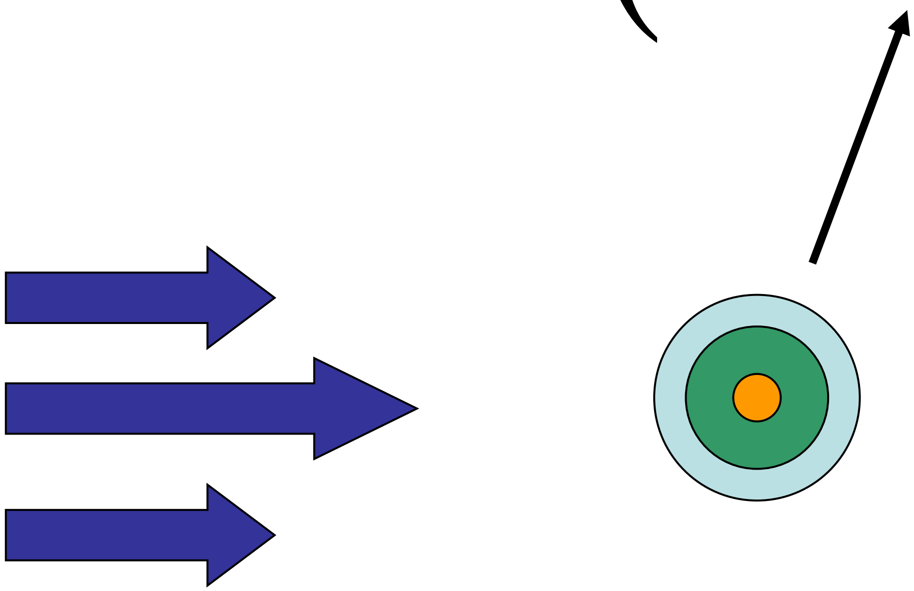
$$\partial J/\partial\delta\mathbf{z} = \mathbf{D}^{-1}\delta\mathbf{z} + \mathbf{G}^{\mathrm{T}}\mathbf{R}^{-1}\left(\mathbf{G}\delta\mathbf{z}-\mathbf{d}\right)$$

Given *J* and $\partial J/\partial\delta\mathbf{z}$, we can identify the $\delta\mathbf{z}$ that minimizes *J*

Matrix-less Operations

There are no matrix multiplications!

$$\mathbf{G}^{T}\mathbf{R}^{-1}\left(\mathbf{G}\delta\mathbf{z}-\mathbf{d}\right)$$



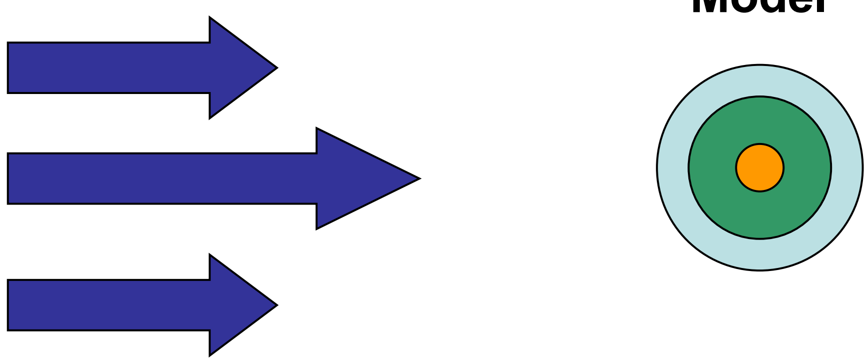
Zonal shear flow

Matrix-less Operations

There are no matrix multiplications!

$$\mathbf{G}^{T}\mathbf{R}^{-1}\left(\mathbf{G}\delta\mathbf{z}-\mathbf{d}\right)$$

↑ Tangent Linear Model



Zonal shear flow

Matrix-less Operations

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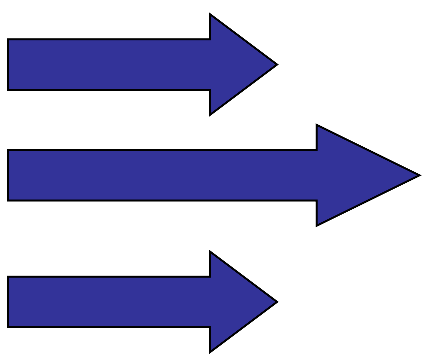
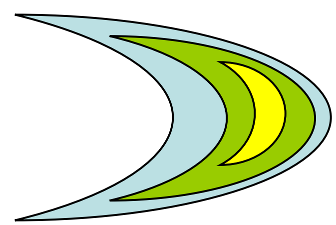
$$\mathbf{G}^{T}\mathbf{R}^{-1}\left(\mathbf{G}\delta\mathbf{z}-\mathbf{d}\right)$$

↑

Tangent Linear Model





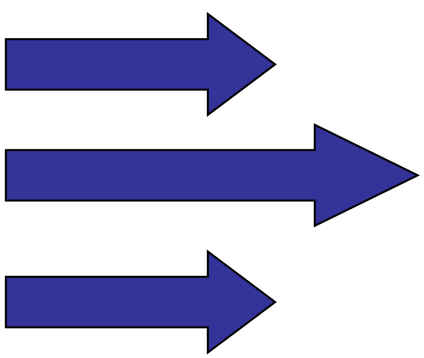
Zonal shear flow

Matrix-less Operations

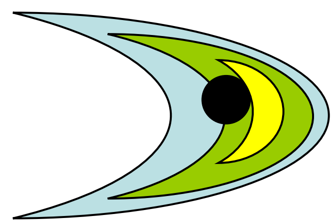
There are no matrix multiplications!

$$\mathbf{G}^{T}\mathbf{R}^{-1}\underbrace{\left(\mathbf{G}\delta\mathbf{z}-\mathbf{d}\right)}$$

Consider a single Observation



Zonal shear flow



Matrix-less Operations

There are no matrix multiplications!

$$\mathbf{G}^{T}\mathbf{R}^{-1}\underbrace{\left(\mathbf{G}\delta\mathbf{z}-\mathbf{d}\right)}_{\text{Consider a single Observation}}$$

Zonal shear flow

Matrix-less Operations

There are no matrix multiplications!

$$\mathbf{G}^{T}\mathbf{R}^{-1}\left(\mathbf{G}\delta\mathbf{z}-\mathbf{d}\right)$$

Inverse Obs Error Covariance

Zonal shear flow

Matrix-less Operations

There are no matrix multiplications!

$$\mathbf{G}^{T}\mathbf{R}^{-1}\left(\mathbf{G}\delta\mathbf{z}-\mathbf{d}\right)$$

↑

Inverse Obs Error Covariance

Zonal shear flow

Matrix-less Operations

There are no matrix multiplications!

$$\mathbf{G}^{T}\mathbf{R}^{-1}\left(\mathbf{G}\delta\mathbf{z}-\mathbf{d}\right)$$

↑

Adjoint Model

Zonal shear flow

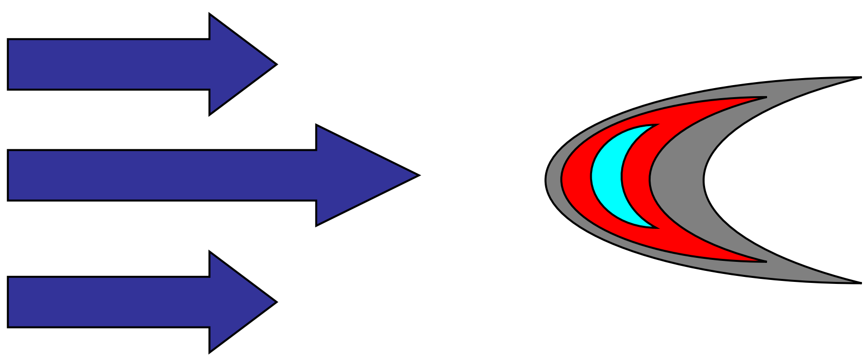
Matrix-less Operations

There are no matrix multiplications!

$$\mathbf{G}^{T}\mathbf{R}^{-1}\left(\mathbf{G}\delta\mathbf{z}-\mathbf{d}\right)$$

↑

Adjoint Model

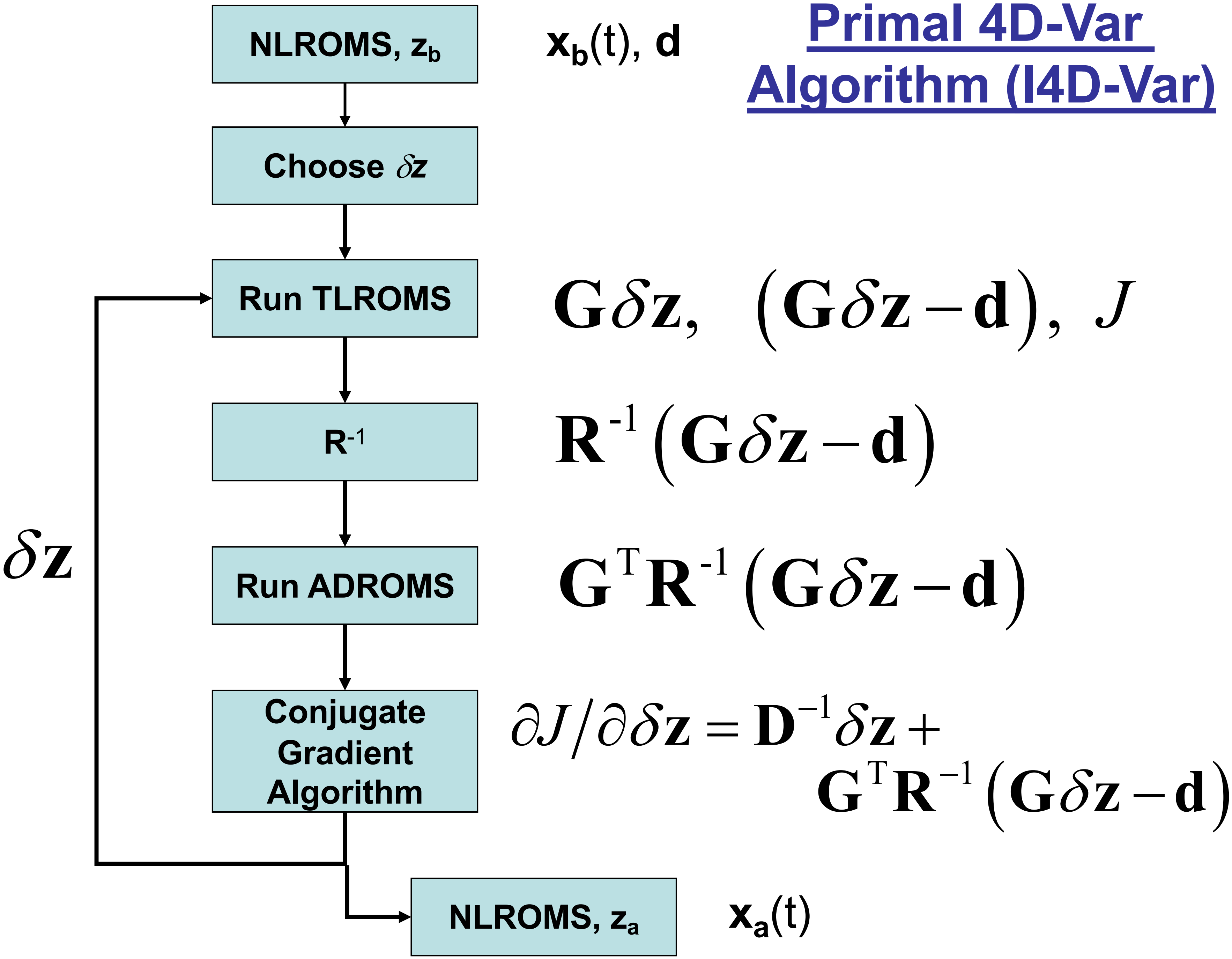


Zonal shear flow

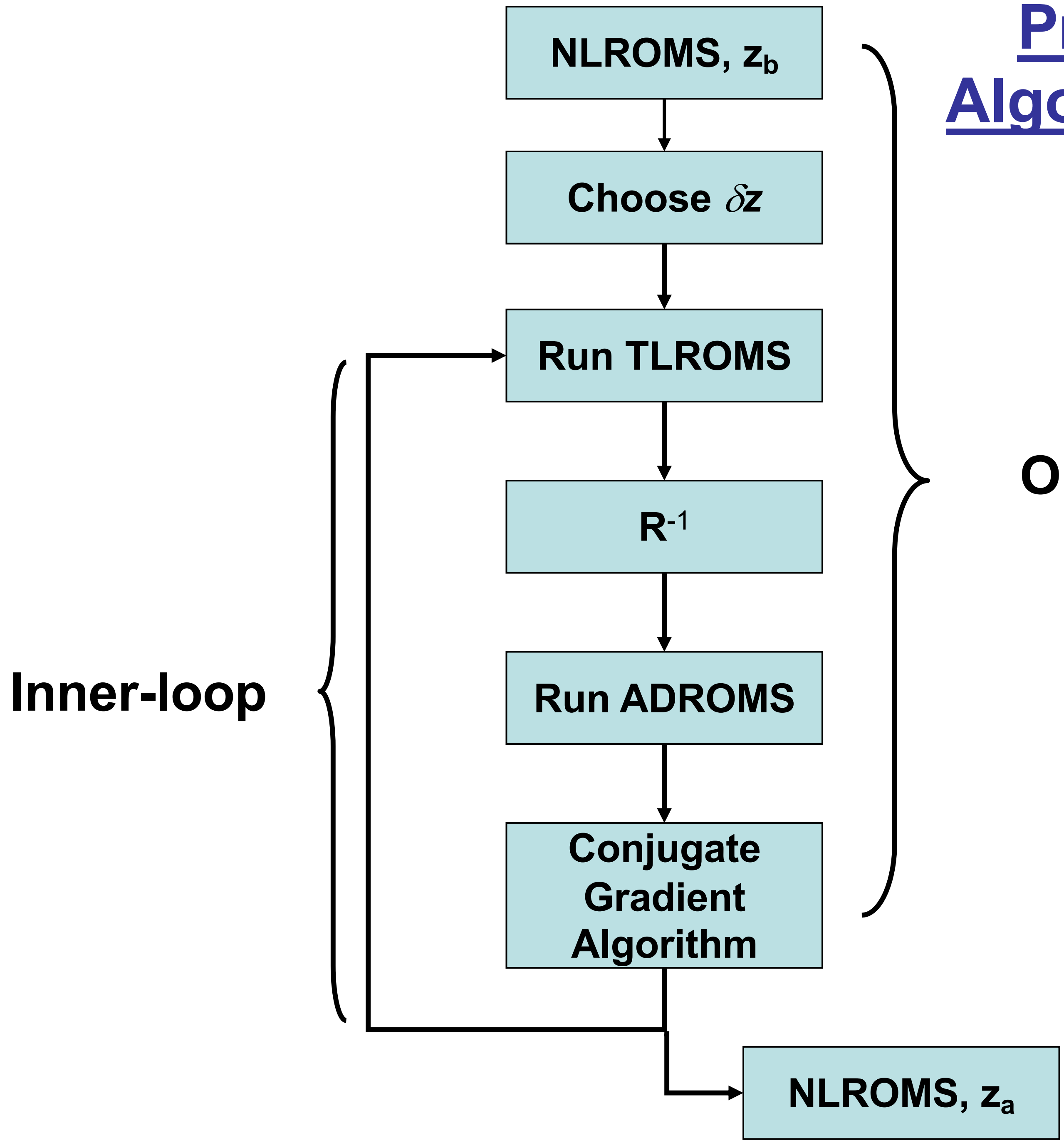
Green's Function

$$\partial J_o / \partial \delta \mathbf{z}$$

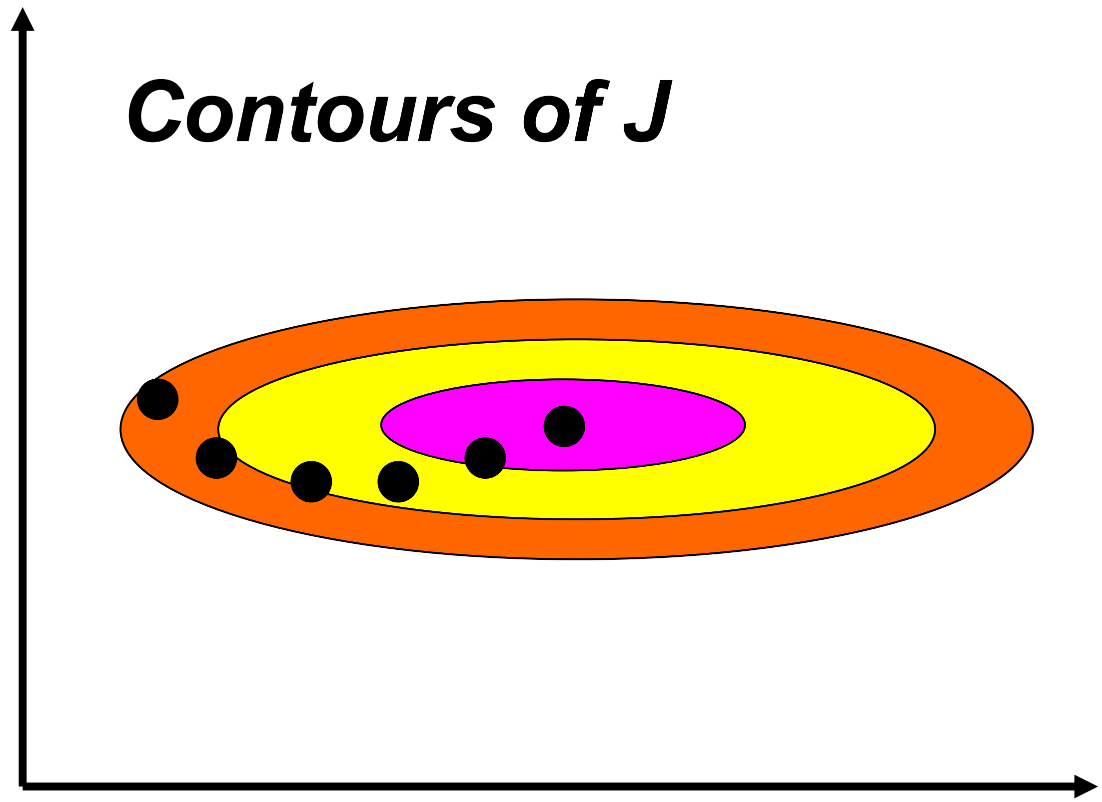
Primal 4D-Var Algorithm (I4D-Var)



Primal 4D-Var Algorithm (I4D-Var)



Conjugate Gradient (CG) Methods



An Example: ROMS CCS

COAMPS forcing

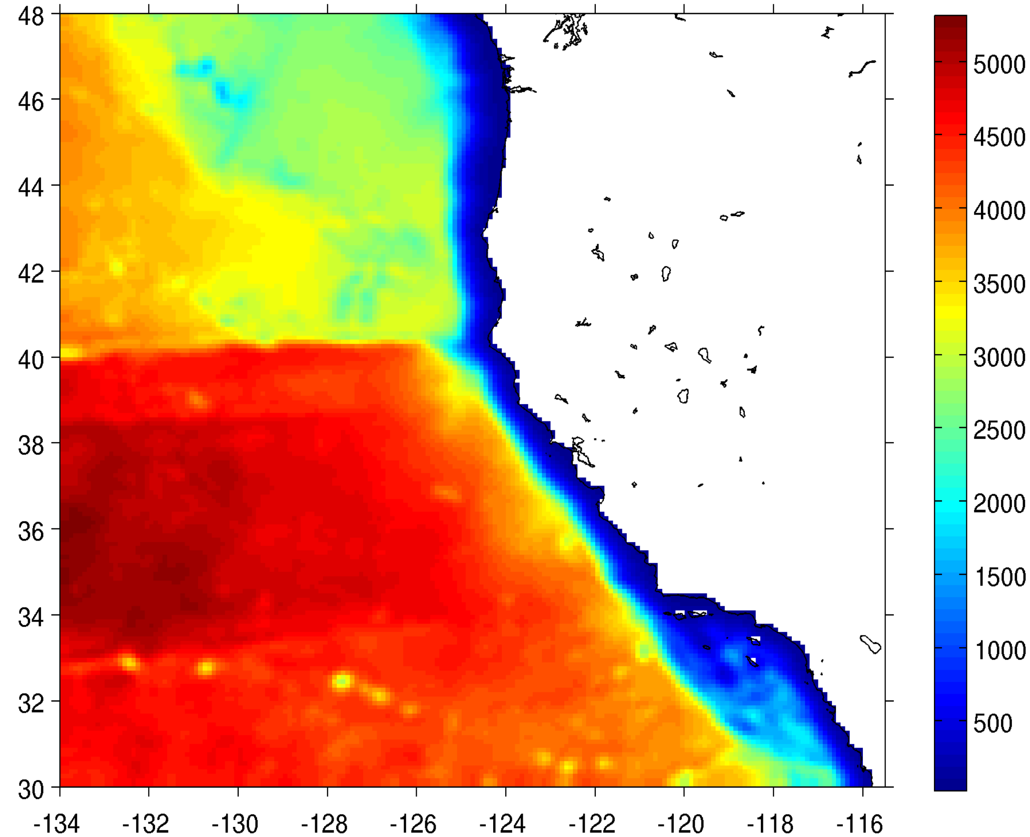
$f_b(t), B_f$

ECCO open boundary conditions

$b_b(t), B_b$

$x_b(0), B_x$

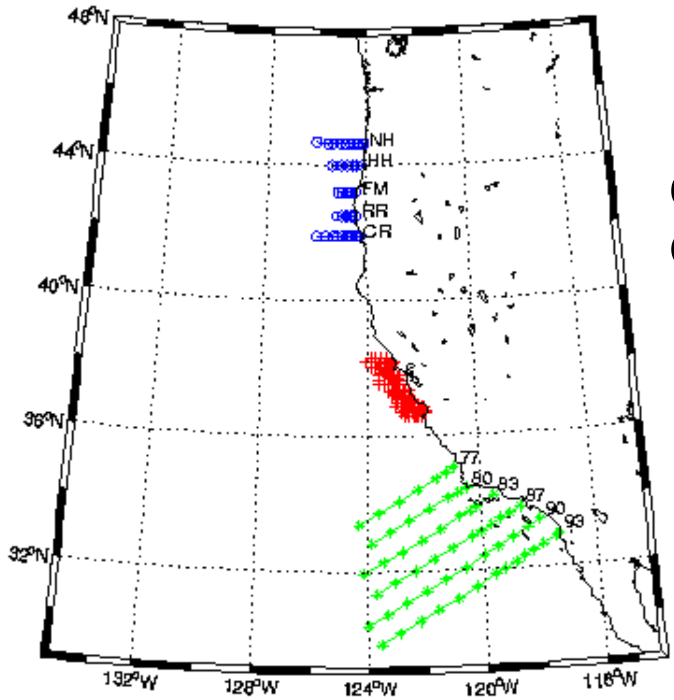
Previous assimilation cycle



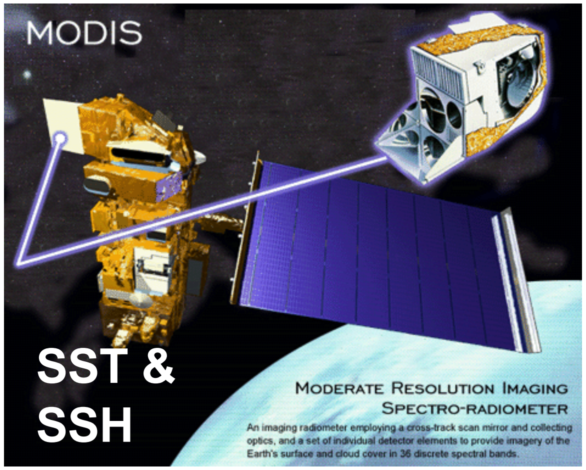
30km, 10 km & 3 km grids, 30- 42 levels

Veneziani et al (2009)
Broquet et al (2009)
Moore et al (2010)

Observations (y)



CalCOFI & GLOBEC



Ingleby and Huddleston (2007)

4D-Var Configuration

- Case studies for a representative case 3-7 March, 2003.
- 1 outer-loop, 25 inner-loops
- 4 day assimilation window
- *Prior* **D***:* **x** L_h=50 km, L_v=30m, σ from clim

  f L_τ=300km, L_Q=100km, σ from COAMPS

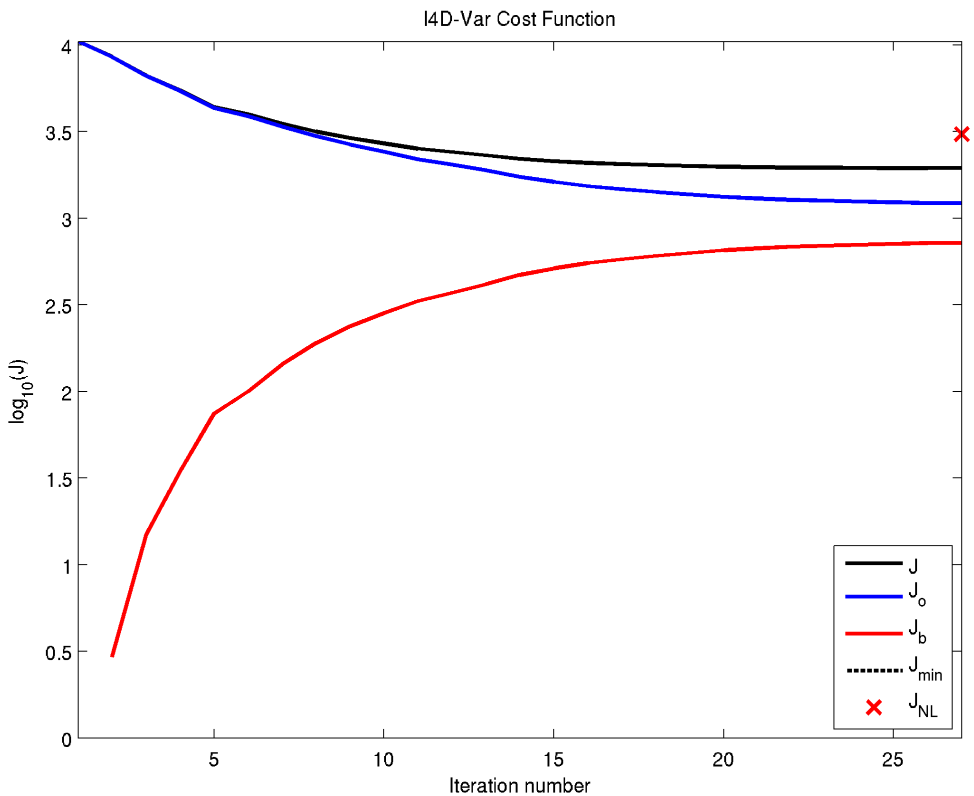
  b L_h=100 km, L_v=30m, σ from clim
- Super observations formed
- Obs error **R** (diagonal):

  SSH 2 cm

  SST 0.4 C

  hydrographic 0.1 C, 0.01psu

I4DVAR Cost Function



Summary

- Strong constraint incremental 4D-Var, primal formulation:

  define IS4DVAR

  Drivers/is4dvar_ocean.h
- Matrix-less iterations to identify cost function minimum using TLROMS and ADROMS

References

- Broquet, G., C.A. Edwards, A.M. Moore, B.S. Powell, M. Veneziani and J.D. Doyle, 2009: Application of 4D-variational data assimilation to the California Current System. *Dyn. Atmos. Oceans*, **48**, 69-91.
- Courtier, P., J.-N. Thépaut and A. Hollingsworth, 1994: A strategy for operational implemenation of 4D-Var using an incremental approach. *Q. J. R. Meteorol. Soc*., **120**, 1367-1388.
- Ingleby, B. and M. Huddleston, 2007: Quality control of ocean temperature and salinity profiles - historical and real-time data. *J. Mar. Systems*, **65**, 158-175.
- Moore, A.M., H.G. Arango, G. Broquet, B.S. Powell, J. Zavala-Garay and A.T. Weaver, 2011: The Regional Ocean Modeling System (ROMS) 4-dimensional data assimilation systems. I: System overview and formulation. *Prog. Oceanogr.*, **91**, 34-49.
- Veneziani, M., C.A. Edwards, J.D. Doyle and D. Foley, 2009: A central California coastal ocean modeling study: 1. Forward model and the influence of realistic versus climatological forcing. *J. Geophys. Res*., **114**, C04015, doi:10.1029/2008JC004774.
- Wikle, C.K. and L.M. Berliner, 2007: A Bayesian tutorial for data assimilation. *Physica D*, **230**, 1-16.