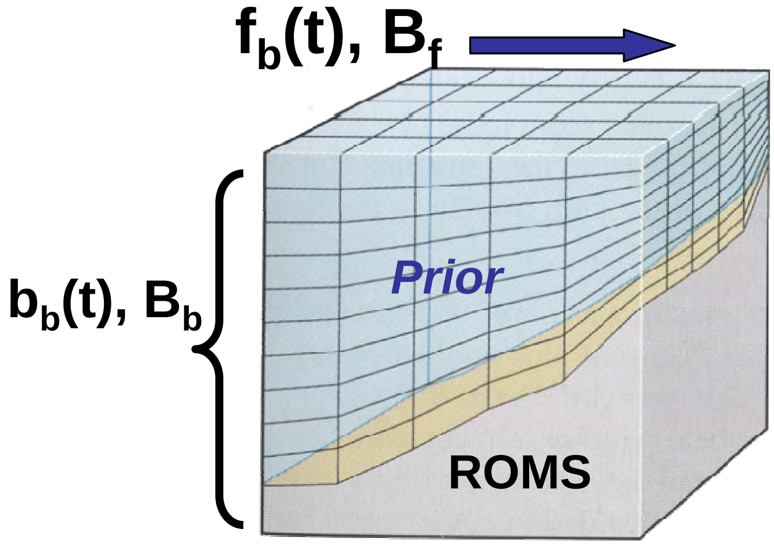
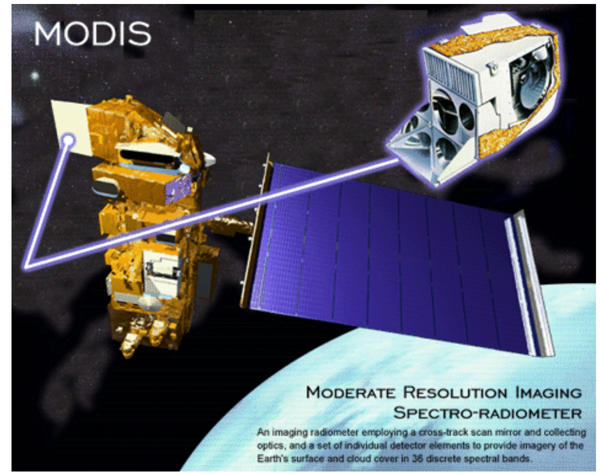
Lecture 3:
Dual 4D-Var

Outline

- 4D-Var recap
- Dual 4D-Var (4D-PSAS & R4D-Var)
- The ROMS 4D-PSAS & R4D-Var algorithms
- Weak constraint 4D-Var

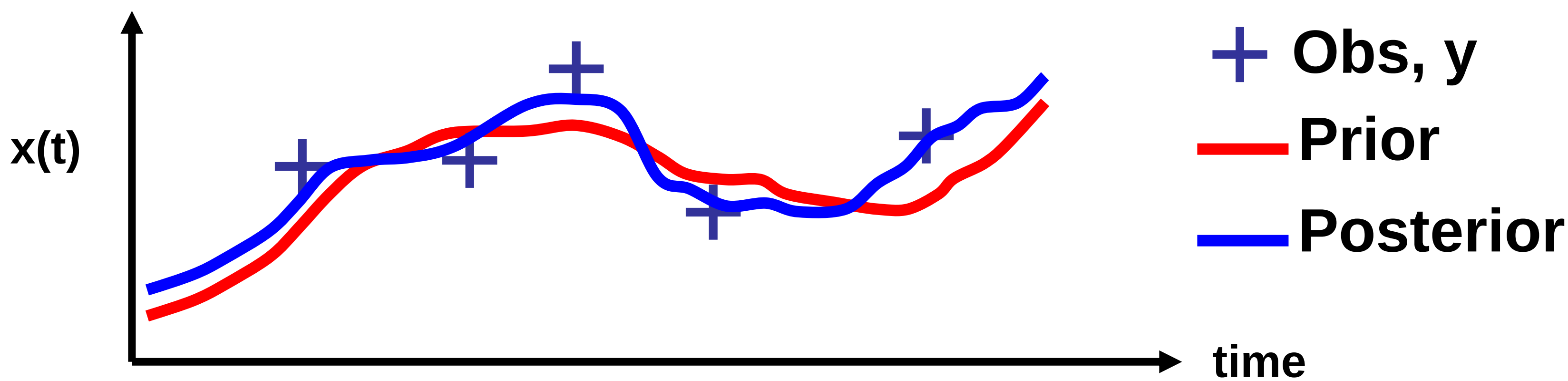
Data Assimilation: Recap





$x_b(0)$, B_x

y, R



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

Notation & Nomenclature: Recap

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

State vector

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

Control vector

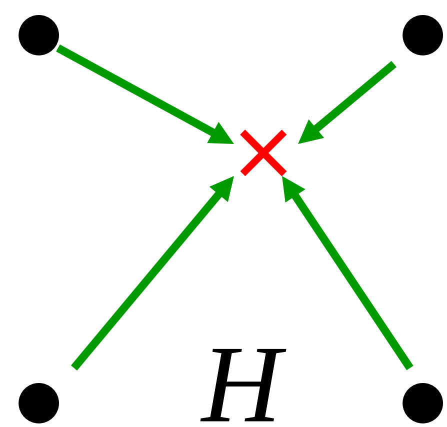
$$\mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ \vdots \\ y_N \end{bmatrix}$$

Observation vector

Prior

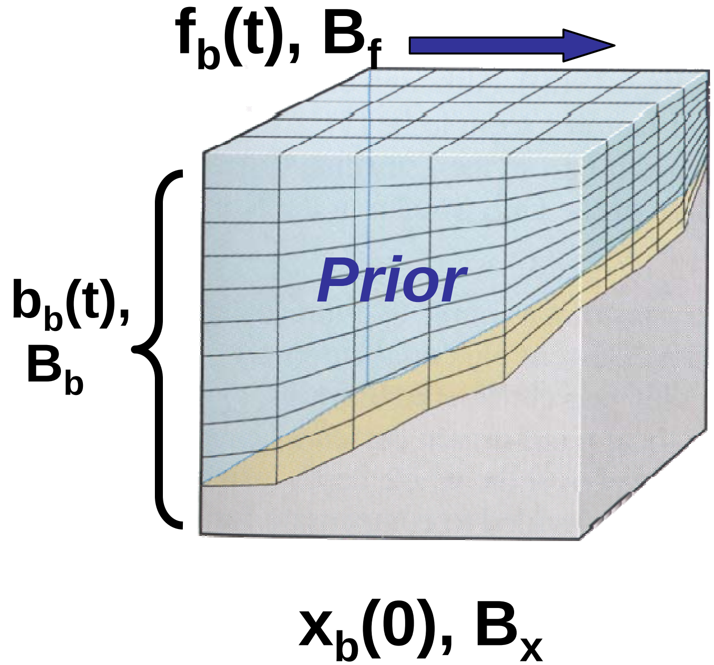
$$\mathbf{d} = \left(\mathbf{y} - H\left(\mathbf{x}^{\mathrm{b}}\right)\right)$$

Innovation vector



Observation operator

Incremental Formulation: Recap



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

initial condition increment

boundary condition increment

forcing increment

corrections for model error

(Courtier *et al*., 1994)

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

$$\mathbf{D} = \underbrace{\mathrm{diag}(\mathbf{B}_{\mathbf{x}}, \mathbf{B}_{\mathbf{b}}, \mathbf{B}_{\mathbf{f}}, \mathbf{Q})}_{\text{Prior (background) error covariance}}$$

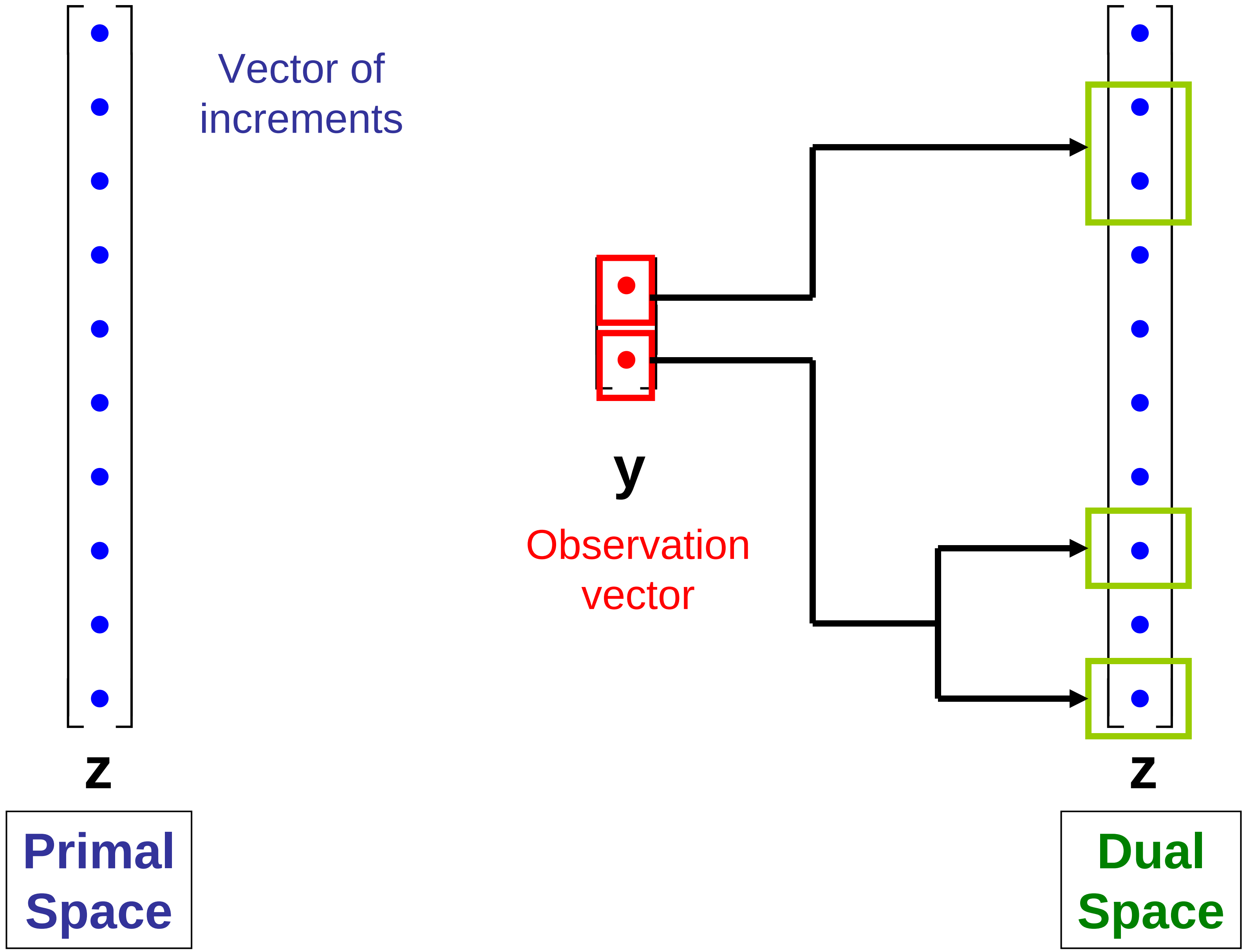
Tangent Linear Model sampled at obs points

Obs Error Cov.

Innovation

$$\mathbf{d} = \mathbf{y} - \mathbf{H}\mathbf{x}_{\mathbf{b}}$$

Primal vs Dual Formulation: Recap



The Solution: Recap

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

Gain (dual form):

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

Gain (primal form):

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

Two Spaces: Recap

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):

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

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

Two Spaces: Recap

G maps from model space
to observation space

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

Primal Formulation: Recap

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

Goal of 4D-Var is to identify:

$$\delta\mathbf{z} = \mathbf{Kd} = (\mathbf{D}^{-1} + \mathbf{G}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{G})^{-1}\mathbf{G}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{d}$$

Solve the equivalent linear system:

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

by minimizing:

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

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

Dual Formulation

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

Goal of 4D-Var is to identify:

$$\delta\mathbf{z} = \mathbf{Kd} = \mathbf{DG}^{\mathrm{T}}(\mathbf{GDG}^{\mathrm{T}} + \mathbf{R})^{-1}\mathbf{d}$$

Solve the equivalent linear system:

$$(\mathbf{GDG}^{\mathrm{T}} + \mathbf{R})\mathbf{w} = \mathbf{d}; \qquad \delta\mathbf{z} = \mathbf{DG}^{\mathrm{T}}\mathbf{w}$$

by minimizing:

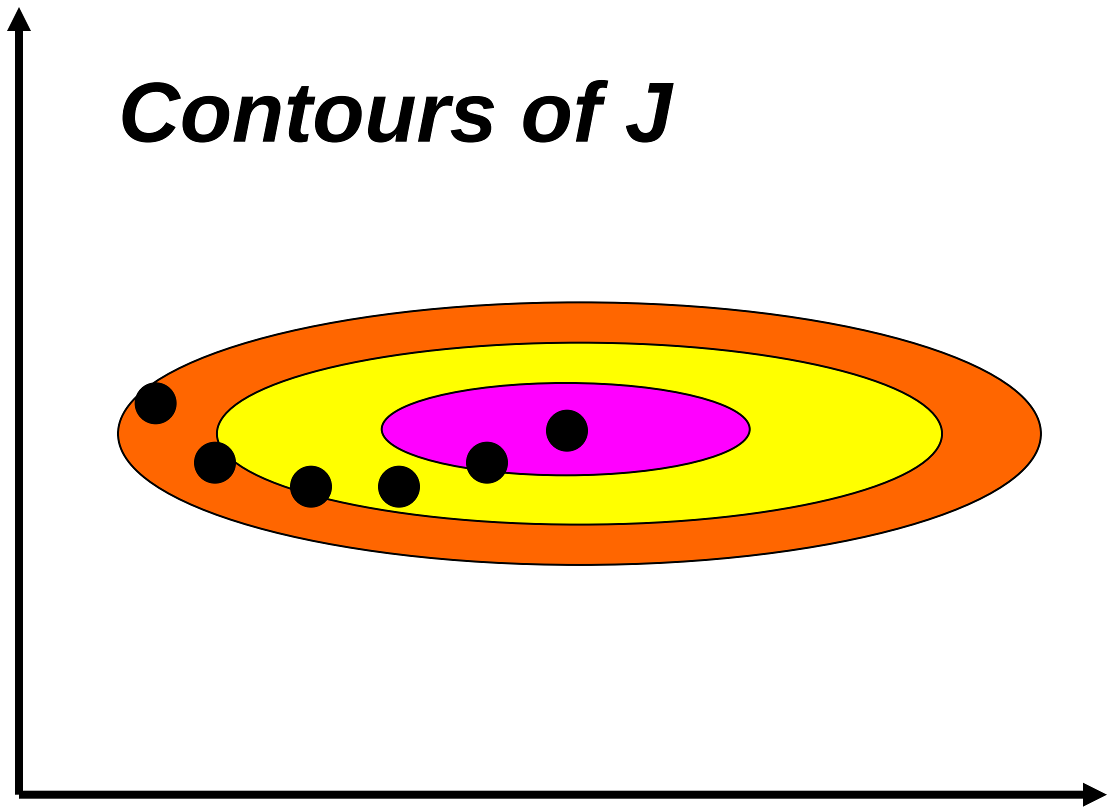
There is no physical significance attached to w

$$I(\mathbf{w}) = \frac{1}{2}\mathbf{w}^{T}(\mathbf{GDG}^{\mathrm{T}} + \mathbf{R})\mathbf{w} - \mathbf{w}^{T}\mathbf{d}$$

then compute:

$$\delta\mathbf{z} = \mathbf{DG}^{\mathrm{T}}\mathbf{w}$$

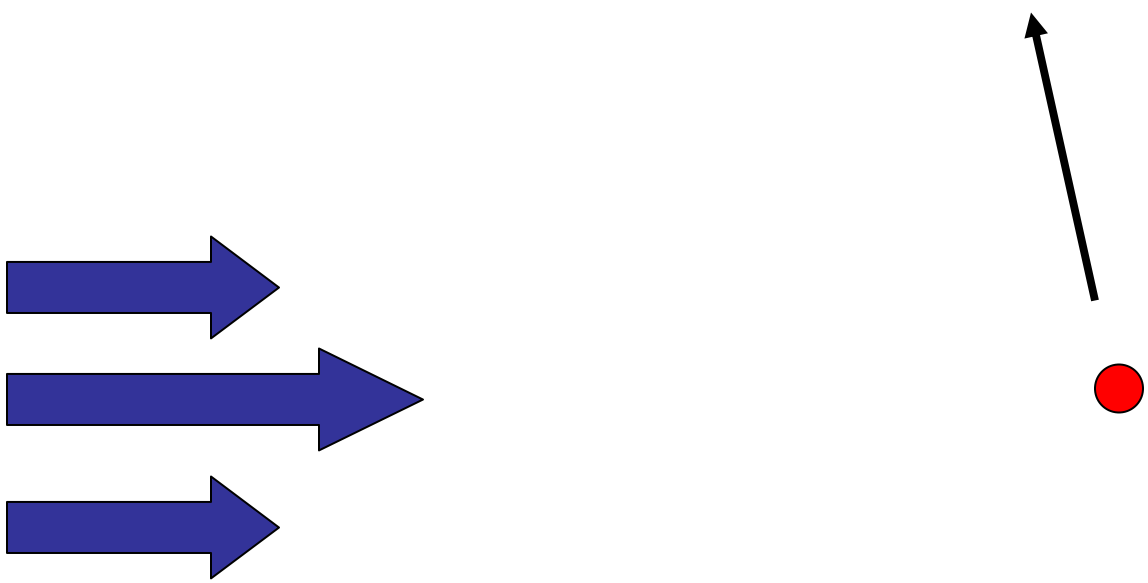
Conjugate Gradient (CG) Methods



Matrix-less Operations

There are no matrix multiplications!

$$\mathbf{G D G^{T} \delta}$$



Zonal shear flow

Matrix-less Operations

There are no matrix multiplications!

$$\mathbf{G D G}^{T} \delta$$

Adjoint Model

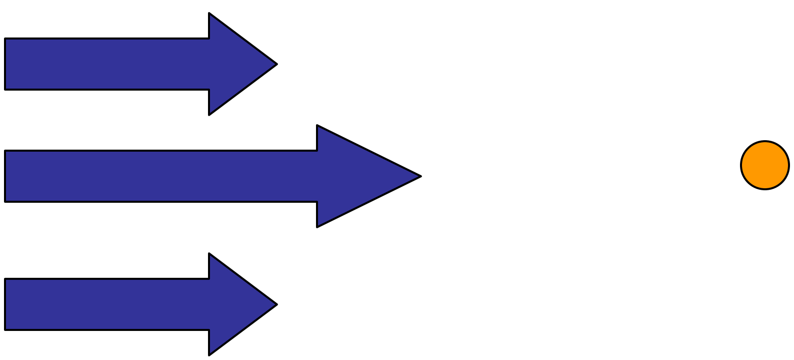
Zonal shear flow

Matrix-less Operations

There are no matrix multiplications!

$$\mathbf{G D G^{T} \delta}$$

Adjoint Model



Zonal shear flow

Matrix-less Operations

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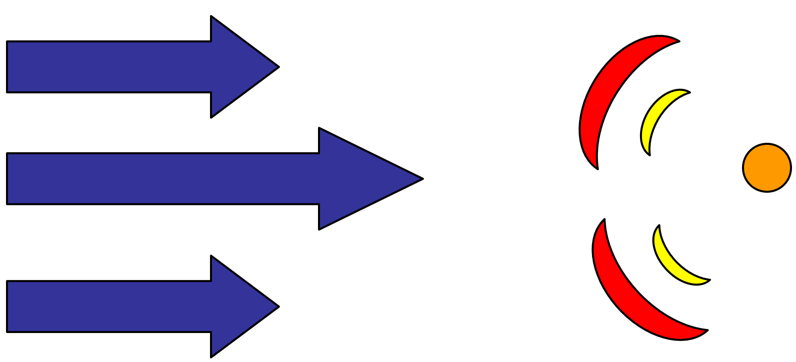
Adjoint Model



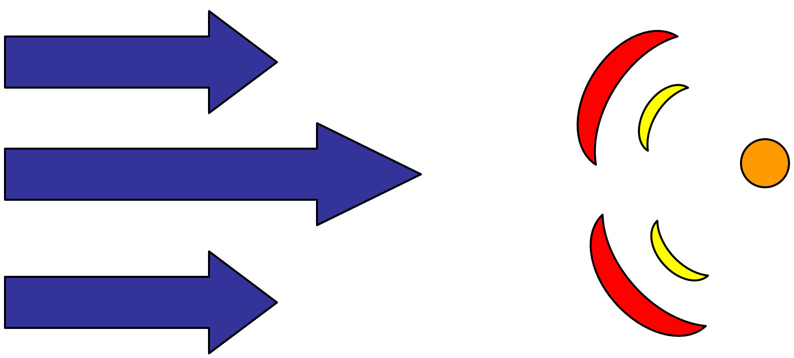
Zonal shear flow

Matrix-less Operations

There are no matrix multiplications!

$$\mathbf{G D G}^{T} \boldsymbol{\delta}$$

Covariance

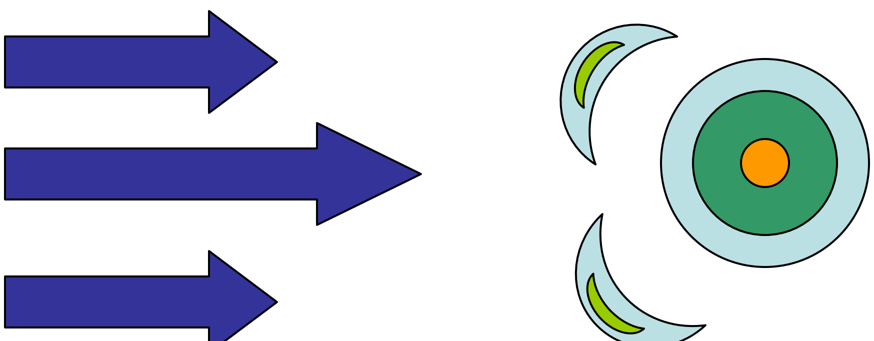


Zonal shear flow

Matrix-less Operations

There are no matrix multiplications!

$$\mathbf{G}\underbrace{\mathbf{D}}_{\text{Covariance}}\mathbf{G}^{T}\boldsymbol{\delta}$$



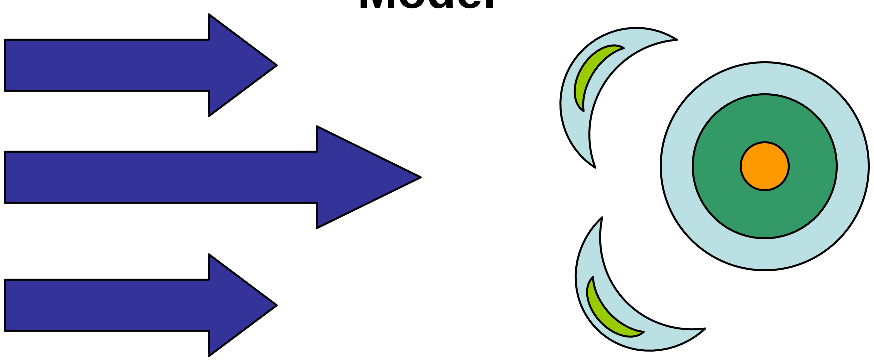
Zonal shear flow

Matrix-less Operations

There are no matrix multiplications!

$$\mathbf{GDG}^{T}\boldsymbol{\delta}$$

Tangent Linear Model



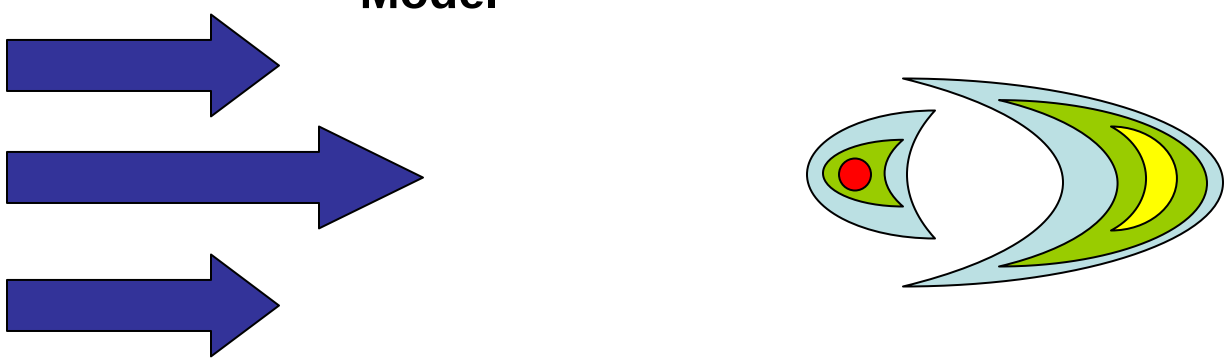
Zonal shear flow

Matrix-less Operations

There are no matrix multiplications!

$$\mathbf{GDG}^{\mathrm{T}}\boldsymbol{\delta}$$

Tangent Linear Model

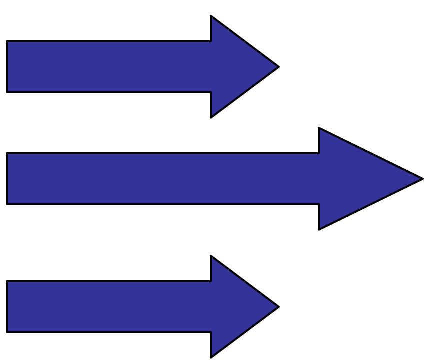


Zonal shear flow

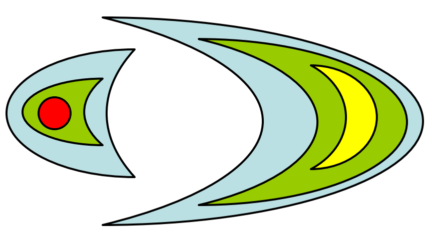
Matrix-less Operations

There are no matrix multiplications!

$$\mathbf{GDG}^{T}\boldsymbol{\delta}$$



Zonal shear flow



A covariance

Matrix-less Operations

There are no matrix multiplications!

$$\mathbf{GDG}^{\mathrm{T}}\boldsymbol{\delta}$$

Tangent Linear Model

Zonal shear flow

Physical-space Statistical Analysis System (PSAS) – Da Silva *et al.* (1995)

Dual 4D-PSAS Algorithm

(define W4DPSAS, w4dpsas_ocean.h)

NLROMS, z_b — $x_b(t)$, **d**

Choose w — obs space

Run ADROMS — $\mathbf{G}^T\mathbf{w}$ — ADROMS forced by w

D — $\mathbf{D}\mathbf{G}^T\mathbf{w}$

w

Run TLROMS — $\mathbf{G}\mathbf{D}\mathbf{G}^T\mathbf{w}$

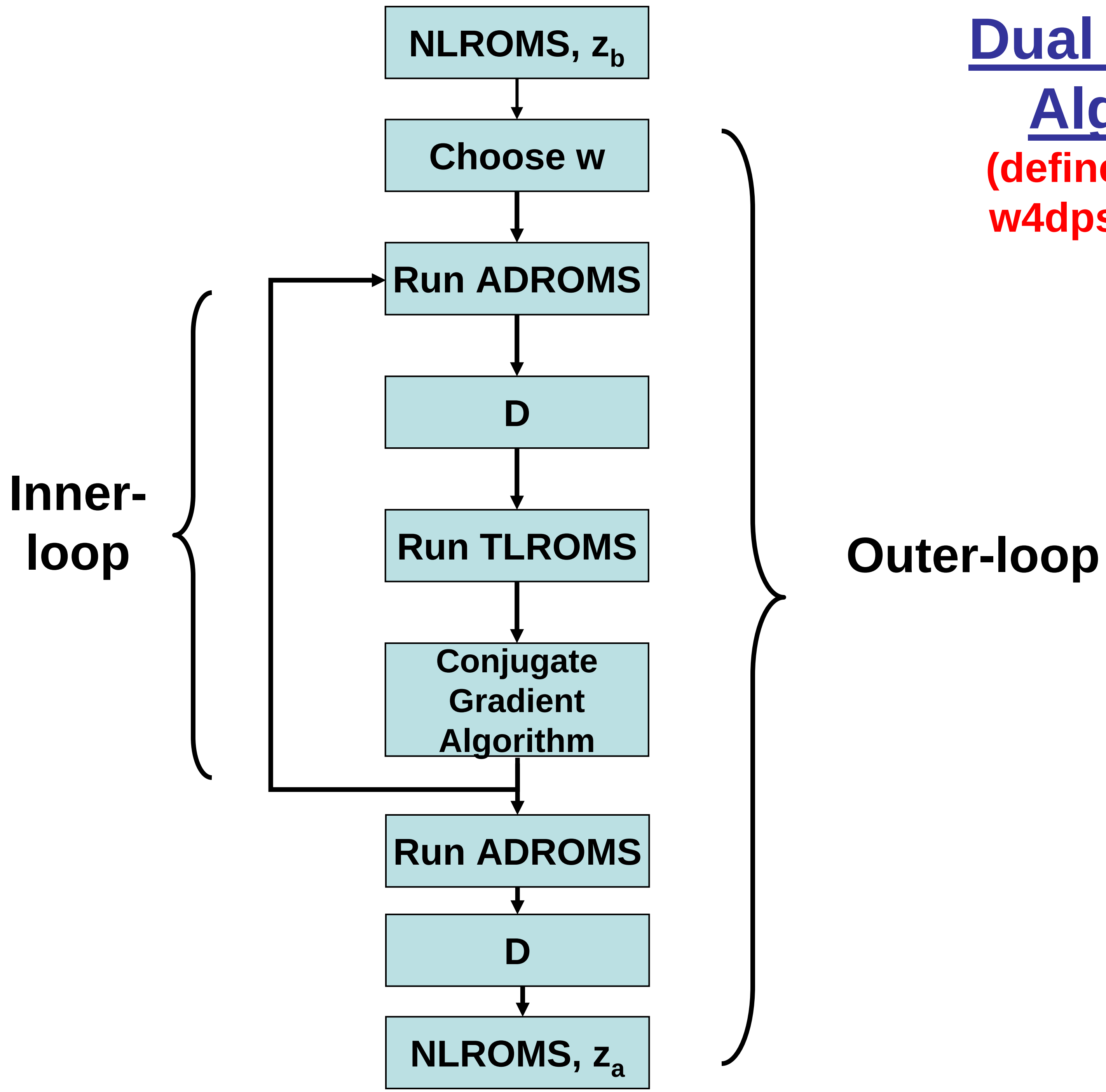
Conjugate Gradient Algorithm — $\partial I/\partial \mathbf{w} = (\mathbf{G}\mathbf{D}\mathbf{G}^T + \mathbf{R})\mathbf{w} - \mathbf{d}$

Run ADROMS — $\mathbf{G}^T\mathbf{w}_\mathbf{a}$

D → $\delta \mathbf{z}_\mathbf{a}$ → NLROMS, z_a — $x_a(t)$

Dual 4D-PSAS Algorithm

(define W4DPSAS, w4dpsas_ocean.h)



The method of representers (R4D-Var)
Bennett (2002)

The Dual of State-Space

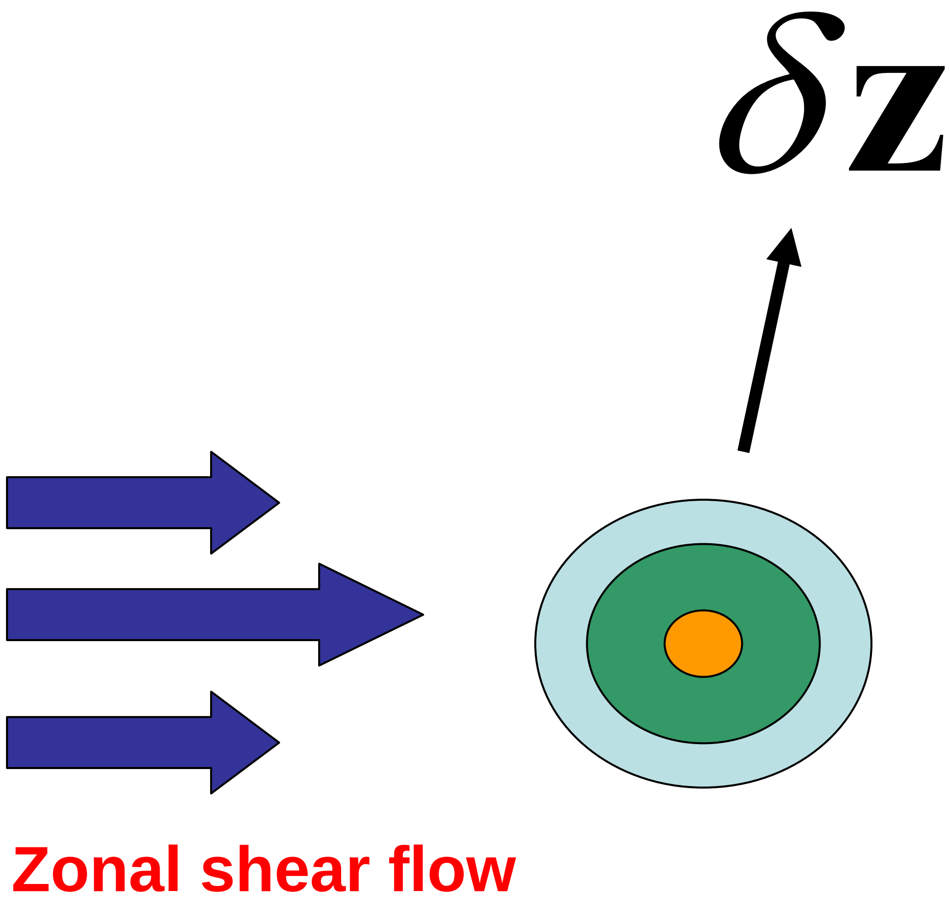
ROMS state-vector increments: $$\delta\mathbf{x}(t) = \begin{bmatrix} \delta\mathbf{T}(t) \\ \delta\mathbf{S}(t) \\ \delta\boldsymbol{\zeta}(t) \\ \delta\mathbf{u}(t) \\ \delta\mathbf{v}(t) \end{bmatrix}$$

The set of all continuous, linear functionals of δx(t) is called the *dual* of δx

For example, y_m=Gδz belongs to the *dual* of δx

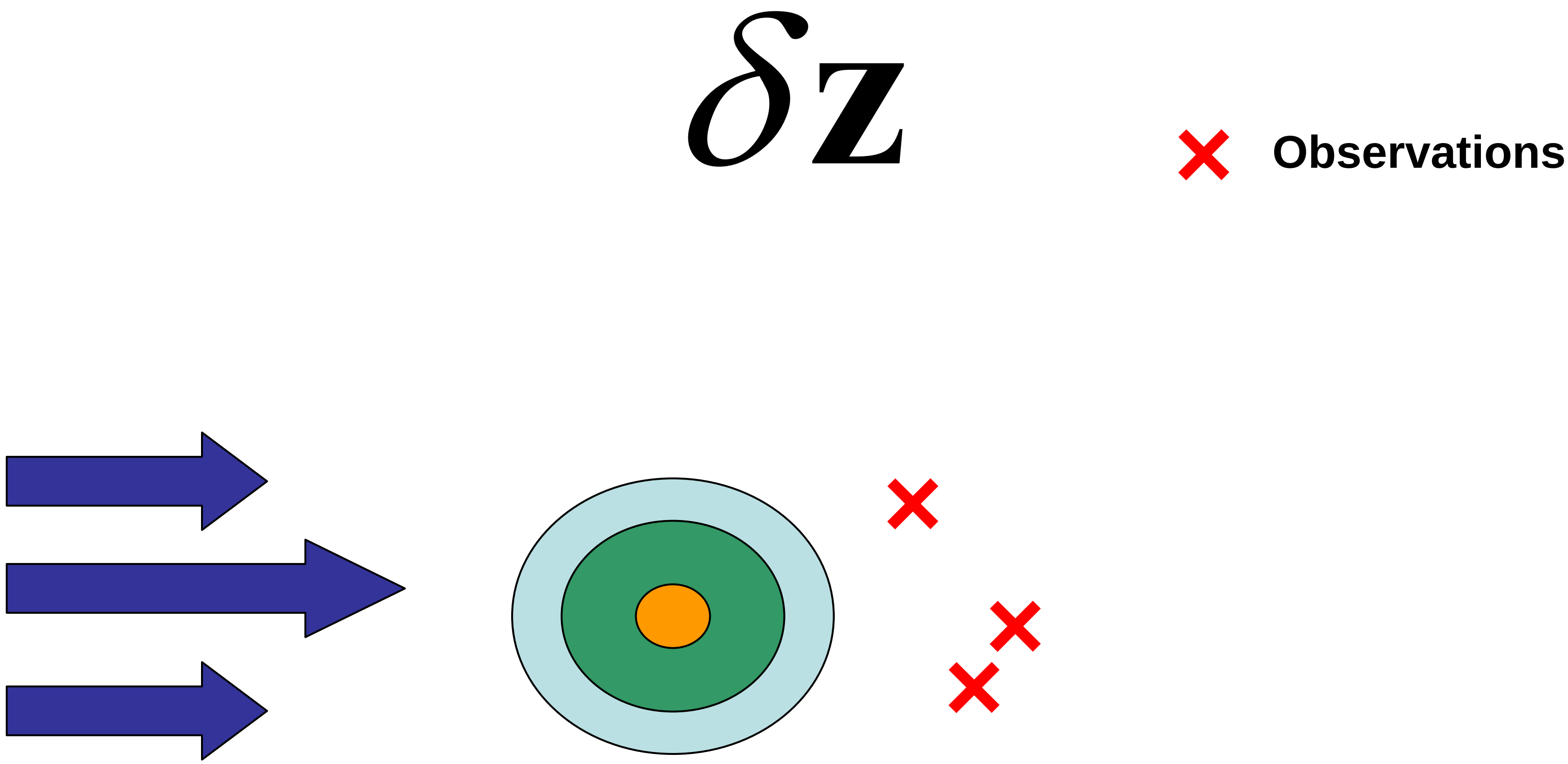
The Dual of State-Space

Consider the assimilation window t=[0,T] for the zonal shear flow…



The Dual of State-Space

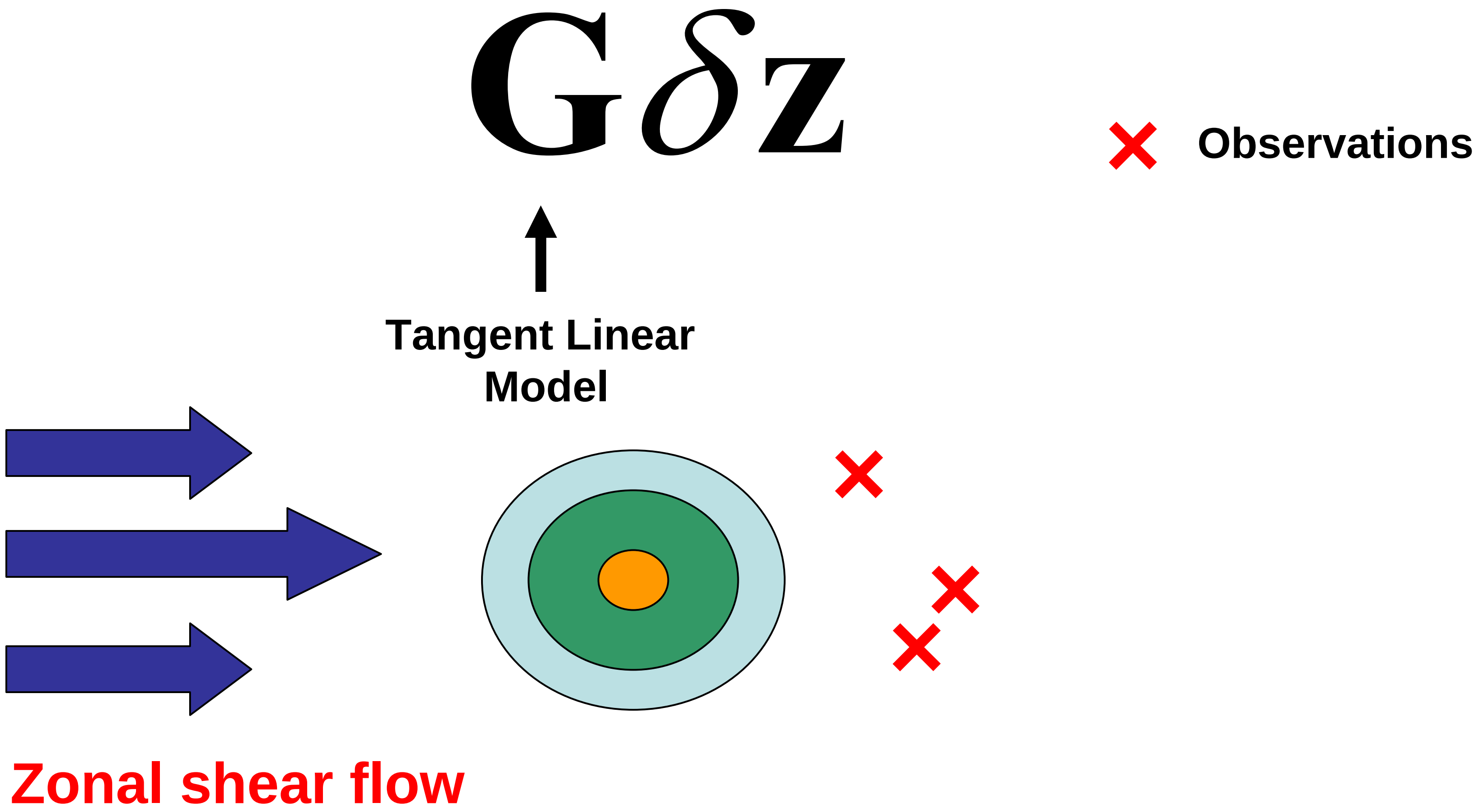
Consider the assimilation window t=[0,T] for the zonal shear flow with 3 observations.



Zonal shear flow

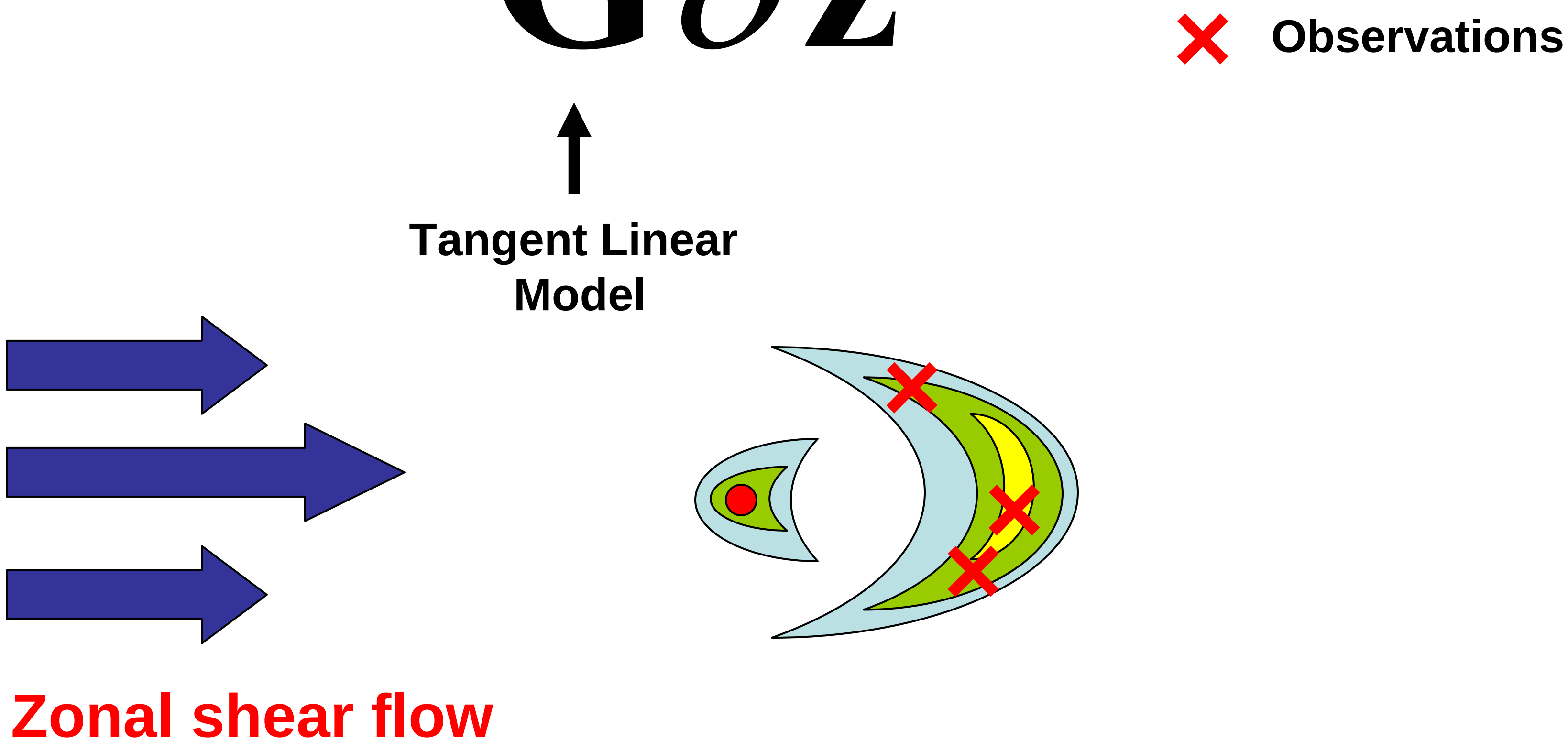
The Dual of State-Space

Consider the assimilation window t=[0,T] for the zonal shear flow with 3 observations.



The Dual of State-Space

$$\mathbf{G}\delta\mathbf{z}$$

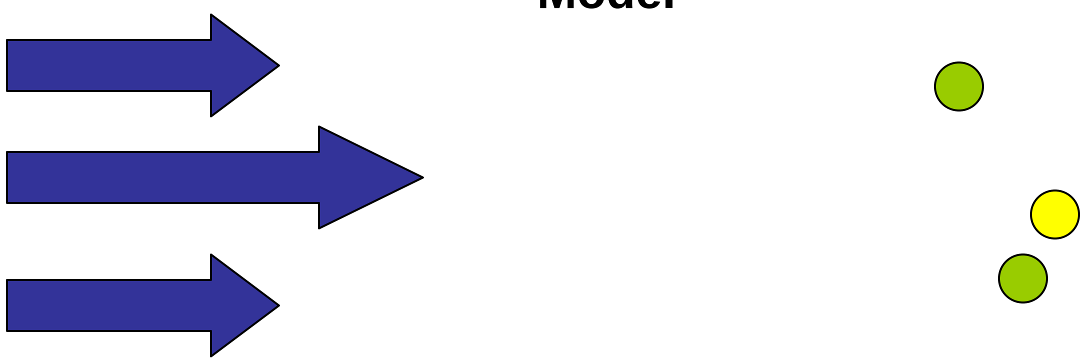


The Dual of State-Space

$$\mathbf{G}\delta\mathbf{z}$$

Tangent Linear Model

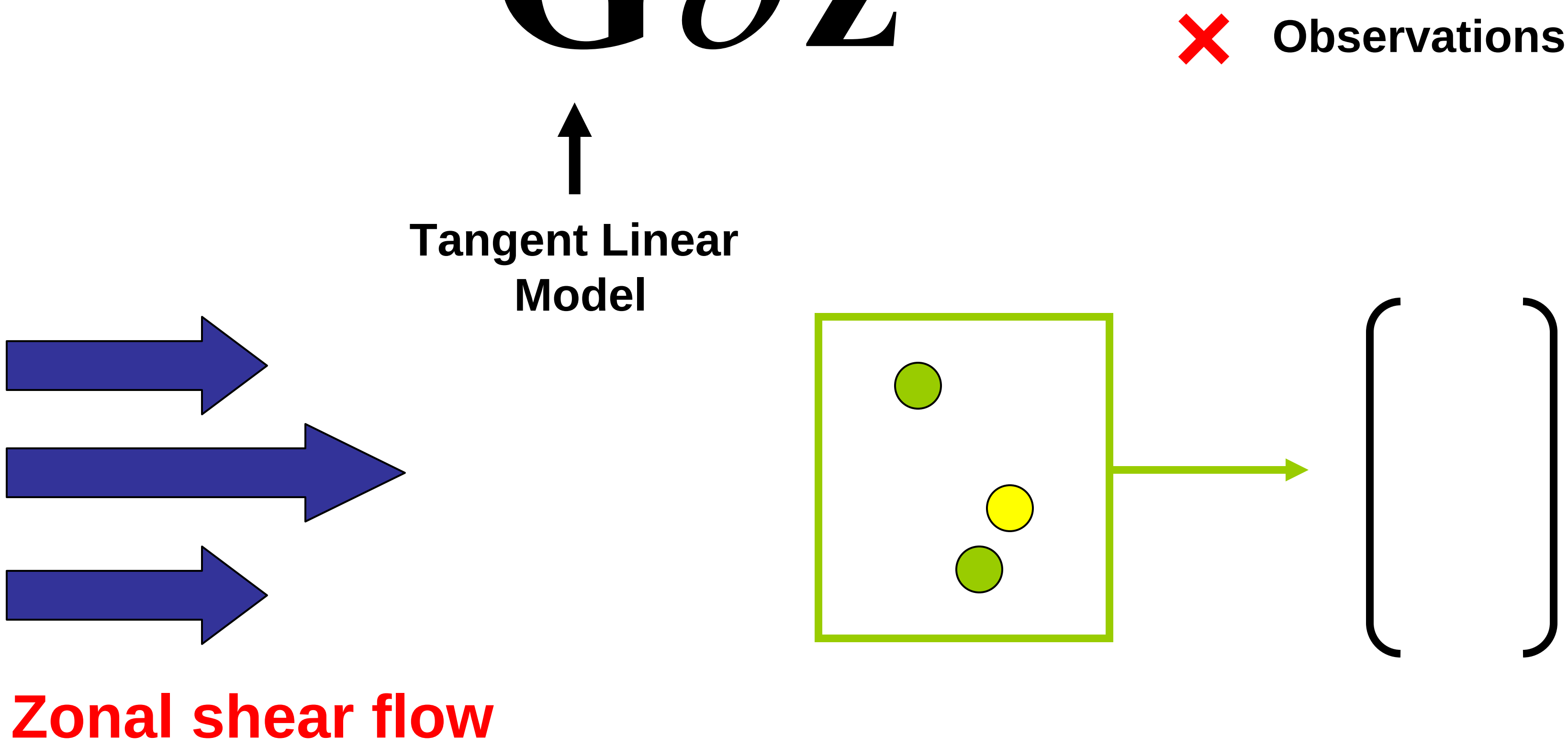
Observations



Zonal shear flow

<u>The Dual of State-Space</u>

$$\mathbf{G}\delta\mathbf{z}$$

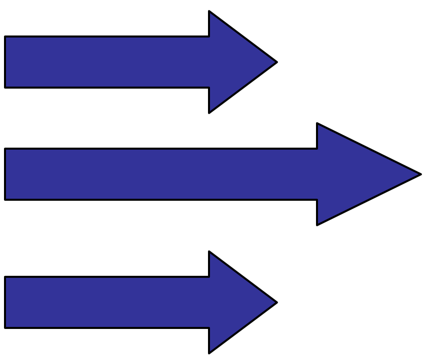


The Dual of State-Space

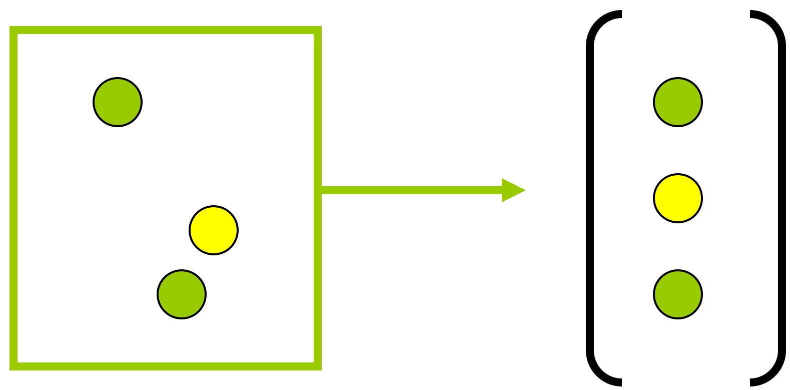
$$\mathbf{G}\delta\mathbf{z}$$

Tangent Linear Model

Observations



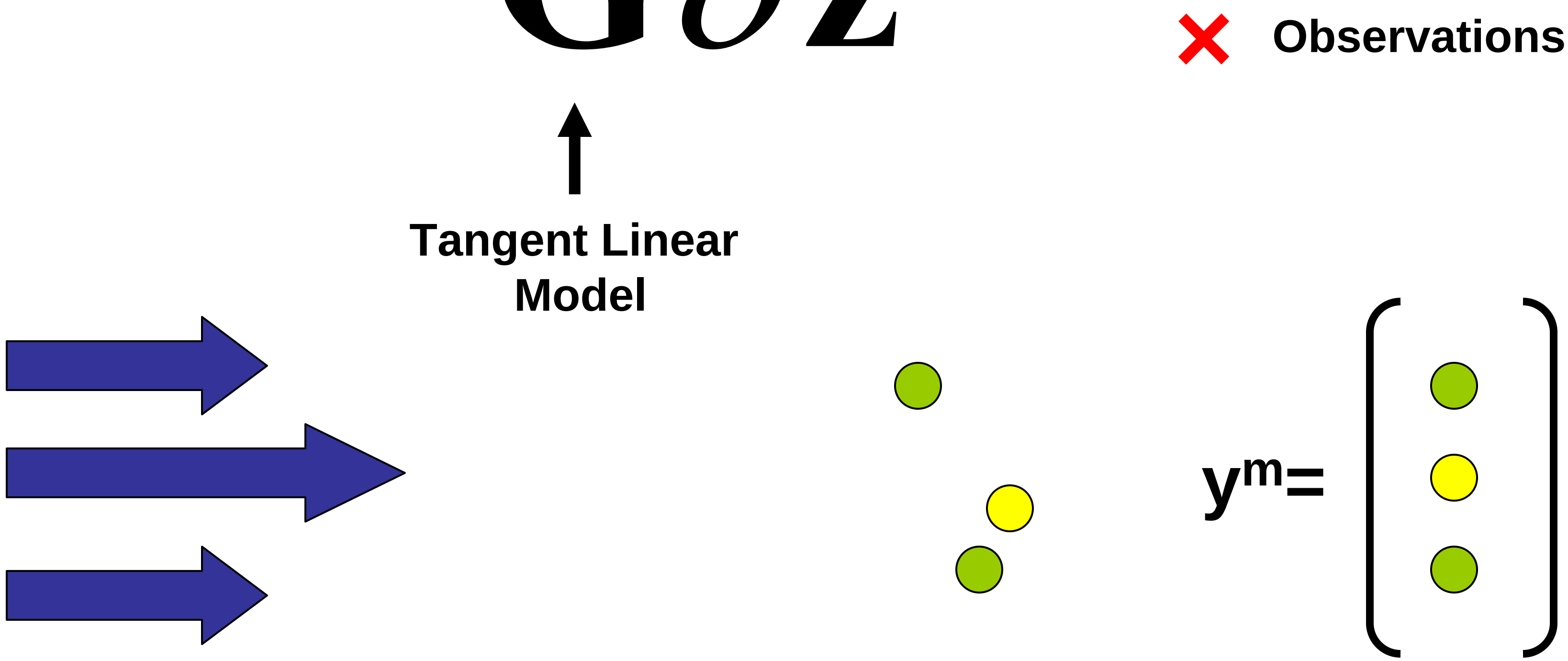
Zonal shear flow



The Dual of State-Space

$$\mathbf{G}\delta\mathbf{z}$$

Tangent Linear Model



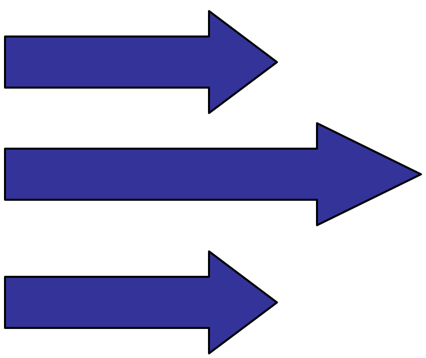
Zonal shear flow

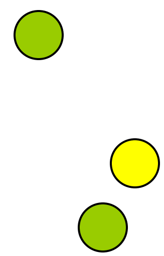
The Dual of State-Space

$$\mathbf{G}\delta\mathbf{z}$$

✕ **Observations**

Tangent Linear Model





$$\mathbf{y^m} = \begin{pmatrix} y_1^m \\ y_2^m \\ y_3^m \end{pmatrix}$$

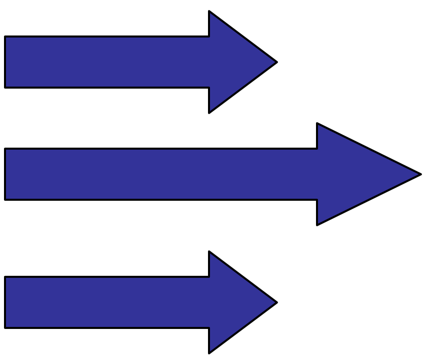
Zonal shear flow

The Dual of State-Space

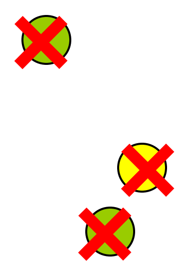
$$\mathbf{G}\delta\mathbf{z}$$

Tangent Linear Model

Observations



Zonal shear flow



$$\mathbf{d} = \begin{bmatrix} y_1^m - y_1^o \\ y_2^m - y_2^o \\ y_3^m - y_3^o \end{bmatrix}$$

Innovation vector

The Dual of State-Space

The innovation vector belongs to the *dual* of δ**x**(t).

Let $\mathbf{u} = \begin{bmatrix} \delta\mathbf{x}(0) \\ \delta\mathbf{x}(t_1) \\ \delta\mathbf{x}(t_2) \\ \vdots \\ \delta\mathbf{x}(\mathrm{T}) \end{bmatrix}$ **for** *t*=[0,T]

According to Riesz representation theorem:

$$y_1^m - y_1^o = \boldsymbol{\rho}_1^{\mathrm{T}}\mathbf{u}; \;\; y_2^m - y_2^o = \boldsymbol{\rho}_2^{\mathrm{T}}\mathbf{u}; \;\; y_3^m - y_3^o = \boldsymbol{\rho}_3^{\mathrm{T}}\mathbf{u};$$

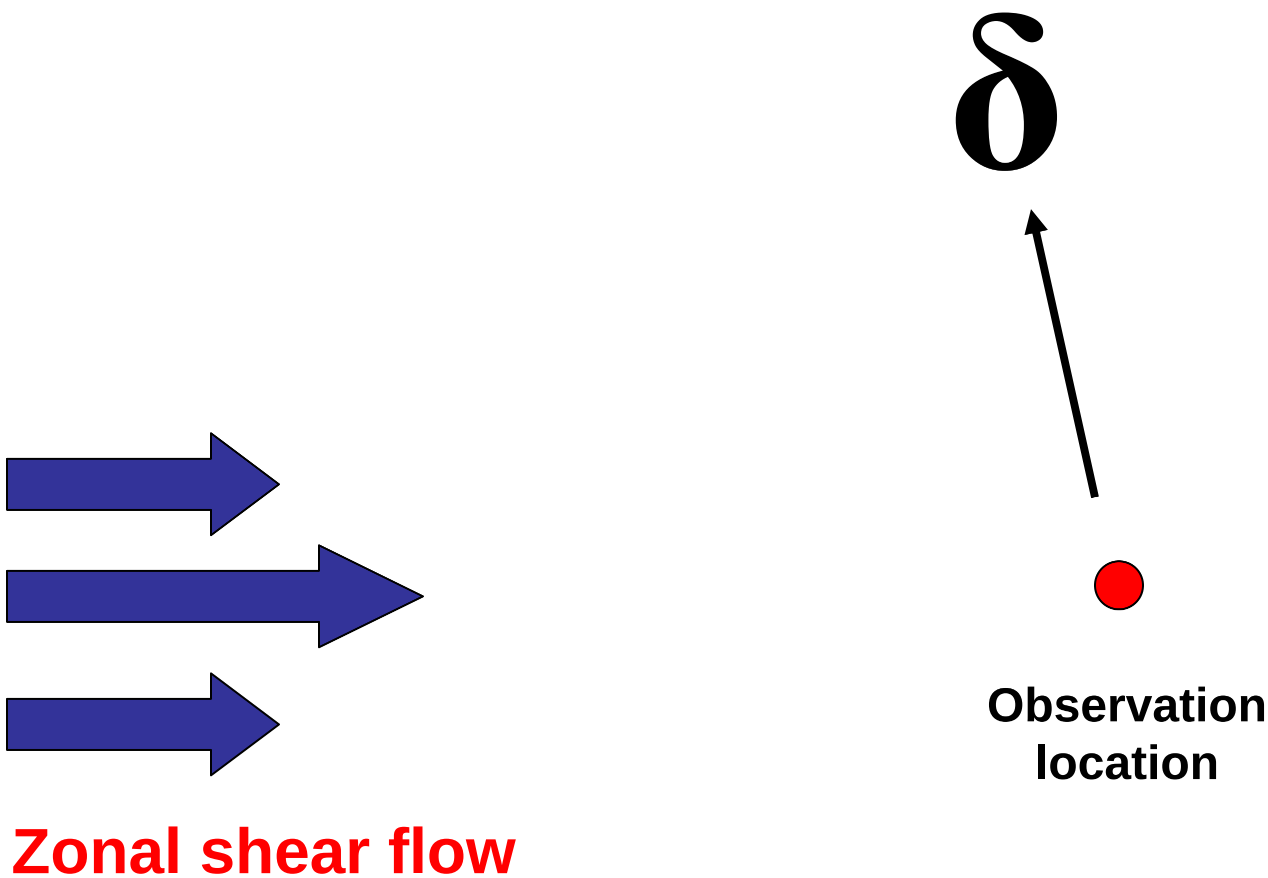
where ρ_i **are referred to as "representer functions."**

The Dual of State-Space

Let $$\boldsymbol{\rho}_i = \begin{bmatrix} \mathbf{r}_i(0) \\ \mathbf{r}_i(t_1) \\ \mathbf{r}_i(t_2) \\ \vdots \\ \mathbf{r}_i(\mathrm{T}) \end{bmatrix}$$ **for** *t*=[0,T]

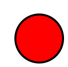
and $$\mathcal{R}(\mathrm{t}) = \left(\mathbf{r}_i(\mathrm{t})\right)$$

Representer Functions

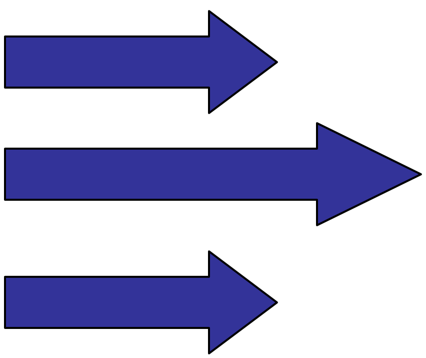


Representer Functions

$$\mathbf{GDG}^{T}\boldsymbol{\delta}$$



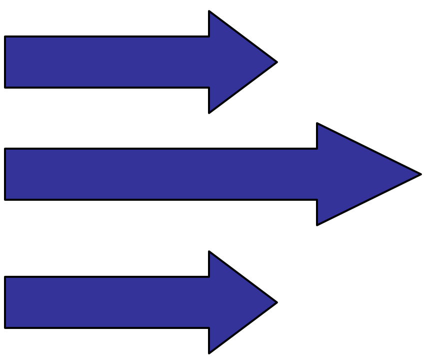
Observation location



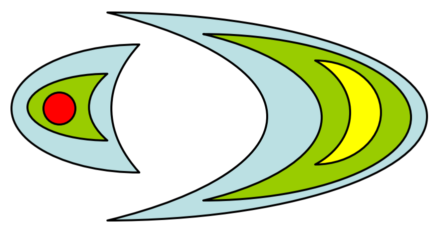
Zonal shear flow

Representer Functions

$$\mathbf{GD}\underbrace{\mathbf{G}^{T}\boldsymbol{\delta}}_{\text{Green's Function}} \quad \text{= A representer}$$



Zonal shear flow



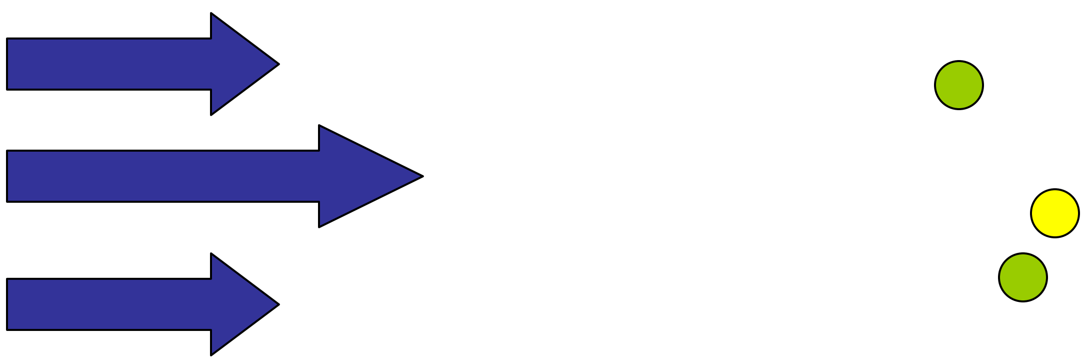
A covariance

Representer Functions

The analysis increments can be written as the weighted sum of the representers

$$\mathbf{x_a}(\mathrm{t}) = \mathbf{x_b}(\mathrm{t}) + \sum_{i=1}^{3} w_i \mathbf{r}_i(\mathrm{t}) = \mathbf{x_b}(\mathrm{t}) + \mathcal{R}(\mathrm{t})\mathbf{w}$$

$$\mathcal{R}(\mathrm{t}) = \left(\mathbf{r}_i(\mathrm{t})\right)$$



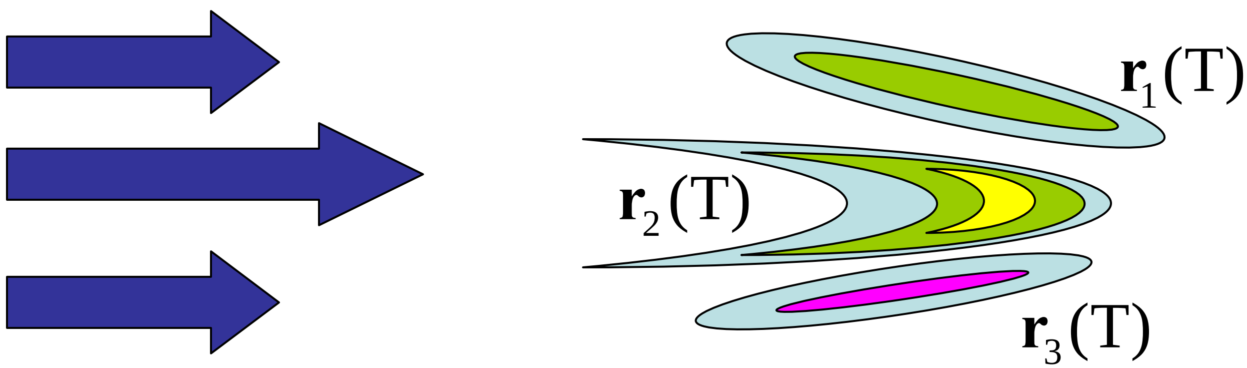
Zonal shear flow

Representer Functions

The analysis increments can be written as the weighted sum of the representers

$$\mathbf{x}_\mathbf{a}(\mathrm{t}) = \mathbf{x}_\mathbf{b}(\mathrm{t}) + \sum_{i=1}^{3} w_i \mathbf{r}_i(\mathrm{t}) = \mathbf{x}_\mathbf{b}(\mathrm{t}) + \mathcal{R}(\mathrm{t})\mathbf{w}$$

$$\mathcal{R}(\mathrm{t}) = \left(\mathbf{r}_i(\mathrm{t})\right)$$



Zonal shear flow

Indirect Representer Algorithm

(Egbert *et al*, 1994)

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

Goal of 4D-Var is to identify:

$$\delta\mathbf{z} = \mathbf{Kd} = \mathbf{DG}^{\mathrm{T}}(\mathbf{GDG}^{\mathrm{T}} + \mathbf{R})^{-1}\mathbf{d}$$

Solve the equivalent linear system:

$$(\mathbf{GDG}^{\mathrm{T}} + \mathbf{R})\mathbf{w} = \mathbf{d}; \quad \boxed{\delta\mathbf{z} = \mathbf{DG}^{\mathrm{T}}\mathbf{w} \equiv \mathcal{R}(0)\mathbf{w}}$$

by minimizing:

The elements of w are the weighting coefs for the $r_i(t)$

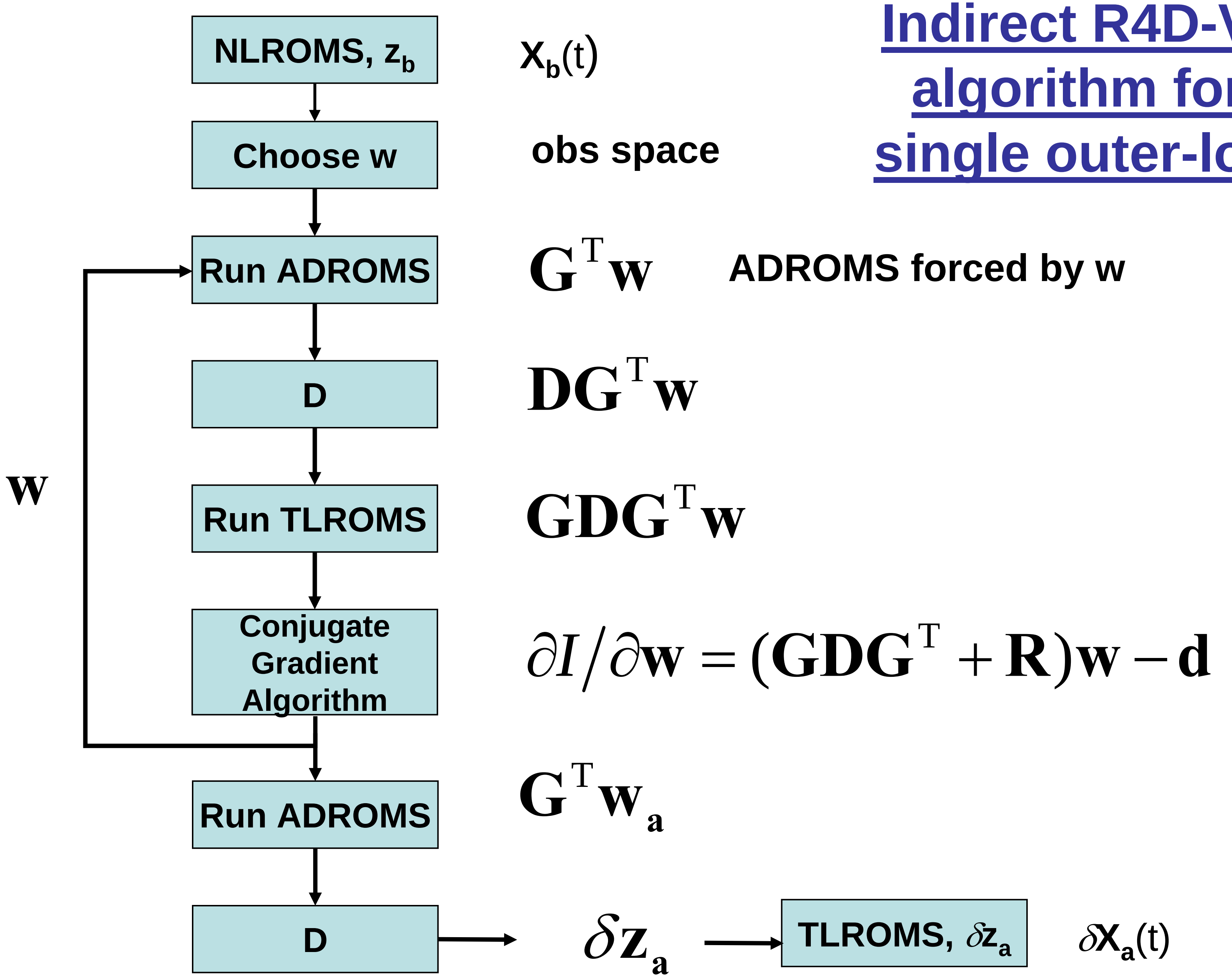
$$I(\mathbf{w}) = \frac{1}{2}\mathbf{w}^T(\mathbf{GDG}^{\mathrm{T}} + \mathbf{R})\mathbf{w} - \mathbf{w}^T\mathbf{d}$$

then compute:

TLROMS

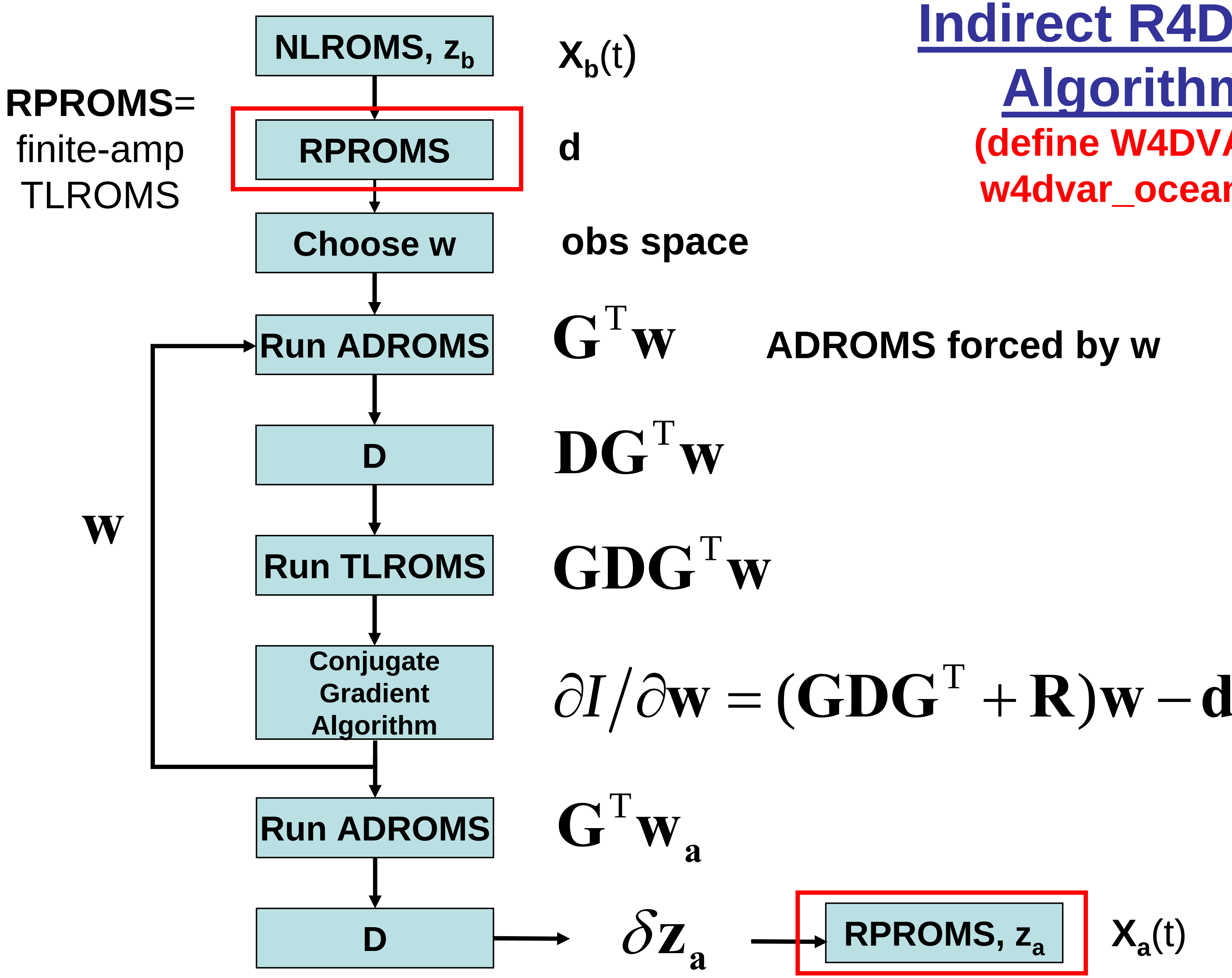
$$\boxed{\delta\mathbf{z} = \mathbf{DG}^{\mathrm{T}}\mathbf{w} \equiv \mathcal{R}(0)\mathbf{w}; \quad \delta\mathbf{x}(\mathrm{t}) = \mathcal{M}\delta\mathbf{z} = \mathcal{R}(\mathrm{t})\mathbf{w}}$$

Indirect R4D-Var algorithm for a single outer-loop



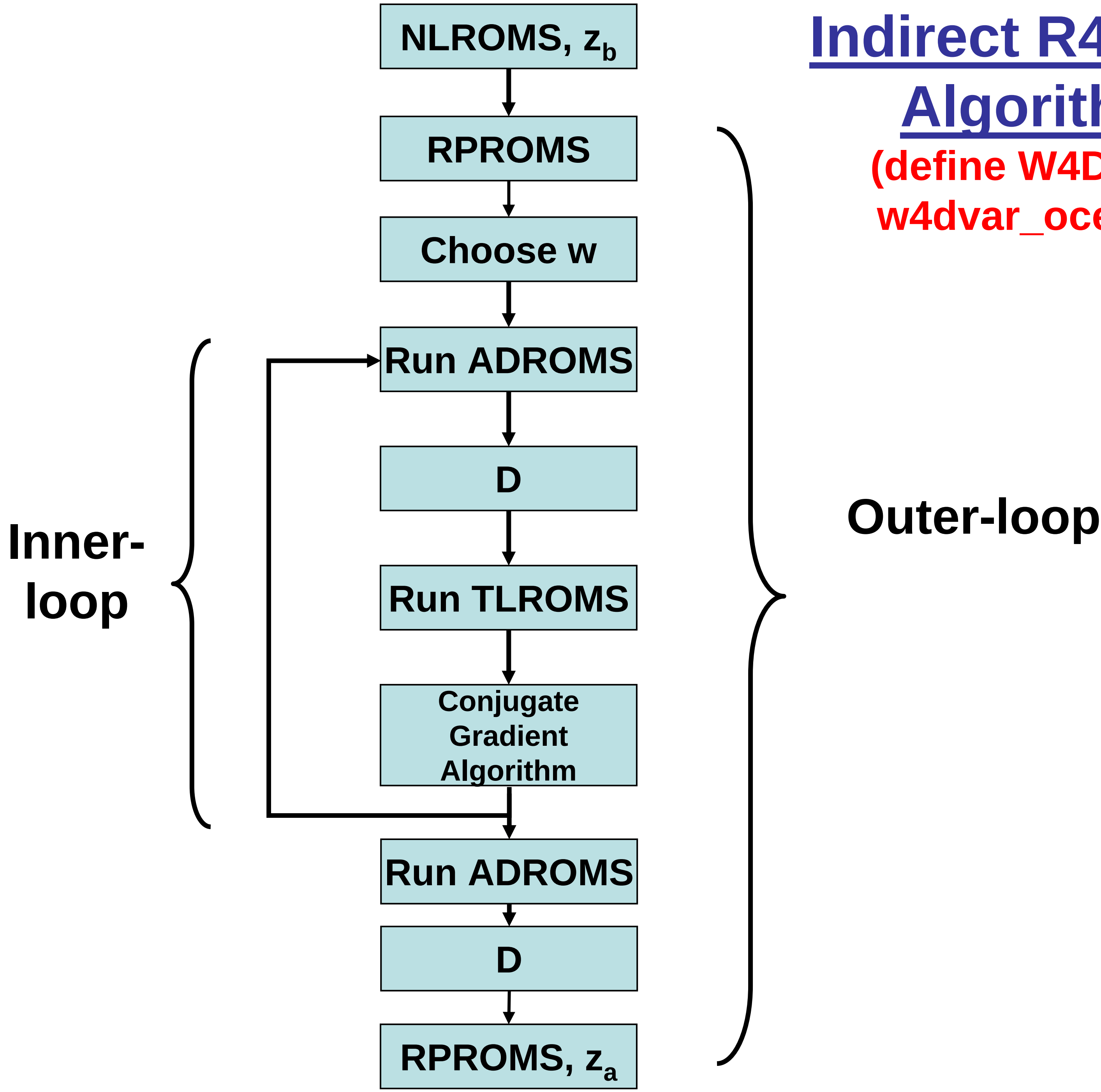
Indirect R4D-Var Algorithm

(define W4DVAR, w4dvar_ocean.h)



Indirect R4D-Var Algorithm

(define W4DVAR, w4dvar_ocean.h)



Weak Constraint 4D-Var

Nonlinear ROMS (NLROMS):

$$\mathbf{x}(t_i) = M(t_i, t_{i-1})(\mathbf{x}(t_{i-1}), \mathbf{f}(t_i), \mathbf{b}(t_i))$$

Nonlinear ROMS (NLROMS) with model error:

$$\mathbf{x}(t_i) = M(t_i, t_{i-1})(\mathbf{x}(t_{i-1}), \mathbf{f}(t_i), \mathbf{b}(t_i), \boldsymbol{\varepsilon}(t_i))$$

Model error *prior*: 0

Model error *prior* covariance: $\mathbf{Q}$

(no explicit time correlation in Q, but there is some in practice)

4D-Var control vector:

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

Correction for model error

Weak Constraint 4D-Var

Tangent linear ROMS (TLROMS):

$$\delta \mathbf{x}(t_i) = \mathbf{M}(t_i, t_{i-1})\delta \mathbf{u}(t_{i-1})$$

$$\delta \mathbf{u}(t_i) = \begin{bmatrix} \delta \mathbf{x}(t_i) \\ \delta \mathbf{f}(t_i) \\ \delta \mathbf{b}(t_i) \\ \boxed{\delta \boldsymbol{\eta}(t_i)} \end{bmatrix}$$

4D forcing for TLROMS

Strong constraint: $\delta \boldsymbol{\eta}(t_i) = \mathbf{0}$

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):

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

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

Two Spaces

Strong constraint:

$$N_{\mathrm{model}} = N_x + N_{times}\left(N_f + N_b\right)$$

Weak constraint:

$$N_{\mathrm{model}} = N_x + N_{times}\left(N_f + N_b + \boxed{N_x}\right)$$

Weak constraint is only practical in dual formulation of 4D-Var since N_{obs} **is unaffected:**

$$\mathbf{K} = \mathbf{DG}^{\mathrm{T}}\underbrace{\left(\mathbf{GDG}^{\mathrm{T}} + \mathbf{R}\right)}_{N_{\mathrm{obs}} \times N_{\mathrm{obs}}}{}^{-1}$$

Mechanics of Dual 4D-Var: Preconditioning

Analysis: $\mathbf{z}_{\mathbf{a}} = \mathbf{z}_{\mathbf{b}} + \mathbf{Kd}$

Goal of 4D-Var is to identify:

$$\delta\mathbf{z} = \mathbf{Kd} = \mathbf{DG}^{\mathrm{T}}(\mathbf{GDG}^{\mathrm{T}} + \mathbf{R})^{-1}\mathbf{d}$$

Solve the equivalent linear system:

$$(\mathbf{GDG}^{\mathrm{T}} + \mathbf{R})\mathbf{w} = \mathbf{d}; \qquad \delta\mathbf{z} = \mathbf{DG}^{\mathrm{T}}\mathbf{w}$$

by minimizing:

$$I(\mathbf{w}) = \frac{1}{2}\mathbf{w}^{T}(\mathbf{GDG}^{\mathrm{T}} + \mathbf{R})\mathbf{w} - \mathbf{w}^{T}\mathbf{d}$$

Preconditioning via the change of variable

$$\mathbf{v} = \mathbf{R}^{-1/2}\mathbf{w}$$

Mechanics of Dual 4D-Var: Lanczos vectors

Lanczos formulation of conjugate gradient algorithm in observation space is used (congrad.F).

Dual formulation of gain matrix:

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

Dual formulation of practical gain matrix:

$$\tilde{\mathbf{K}}_k = \mathbf{D}\mathbf{G}^{\mathrm{T}}\mathbf{R}^{-1/2}\mathbf{V}_k\mathbf{T}_k^{-1}\mathbf{V}_k^{\mathrm{T}}\mathbf{R}^{-1/2}$$

Many practical diagnostic applications using this formulation (Lectures 4 & 5).

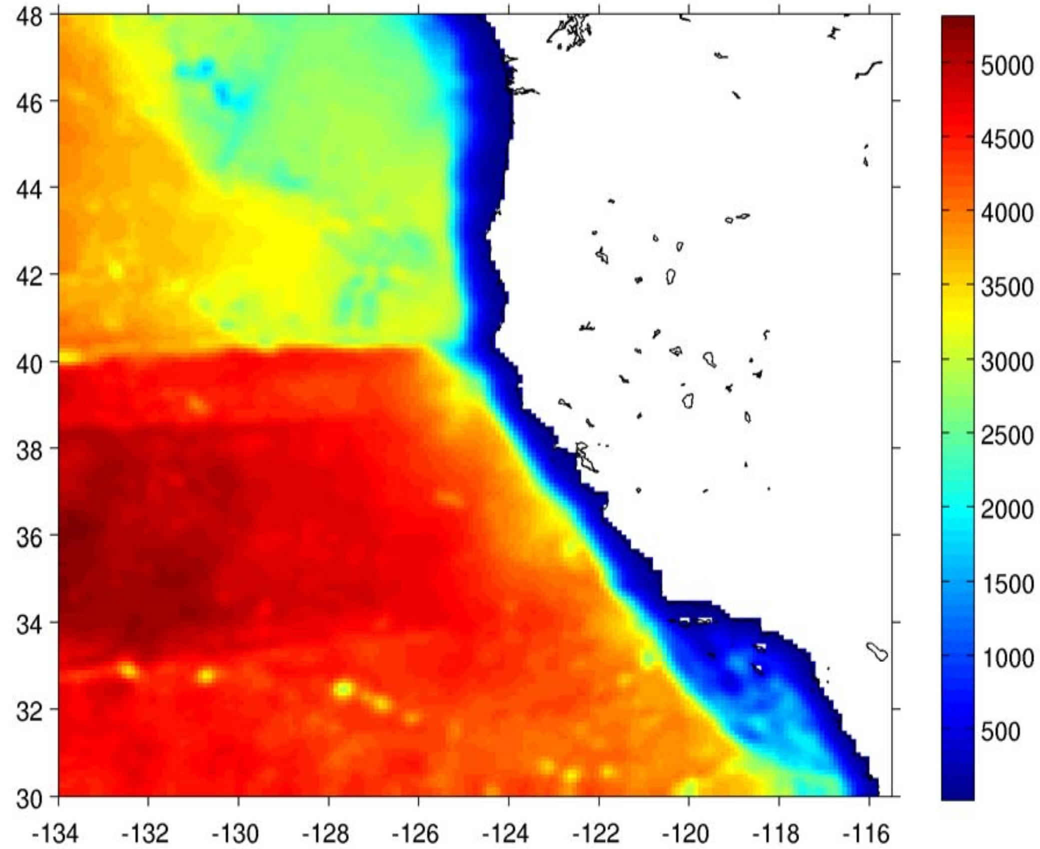
An Example: ROMS CCS

COAMPS forcing $f_b(t), B_f$

ECCO open boundary conditions $b_b(t), B_b$

$x_b(0), B_x$

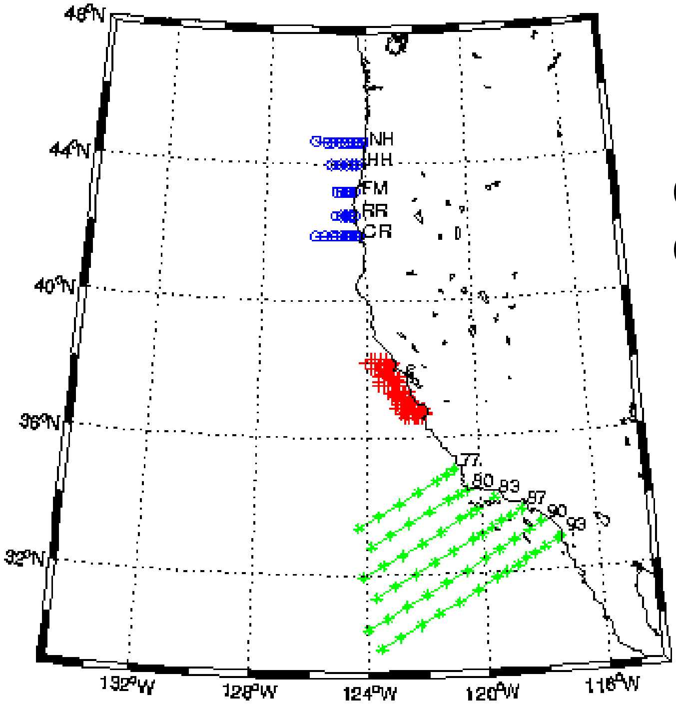
Previous assimilation cycle



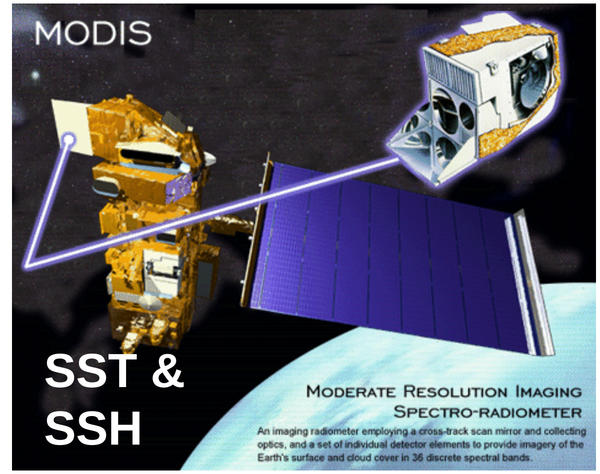
30km, 10 km & 3 km grids, 30- 42 levels

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

Observations (y)



CalCOFI & GLOBEC

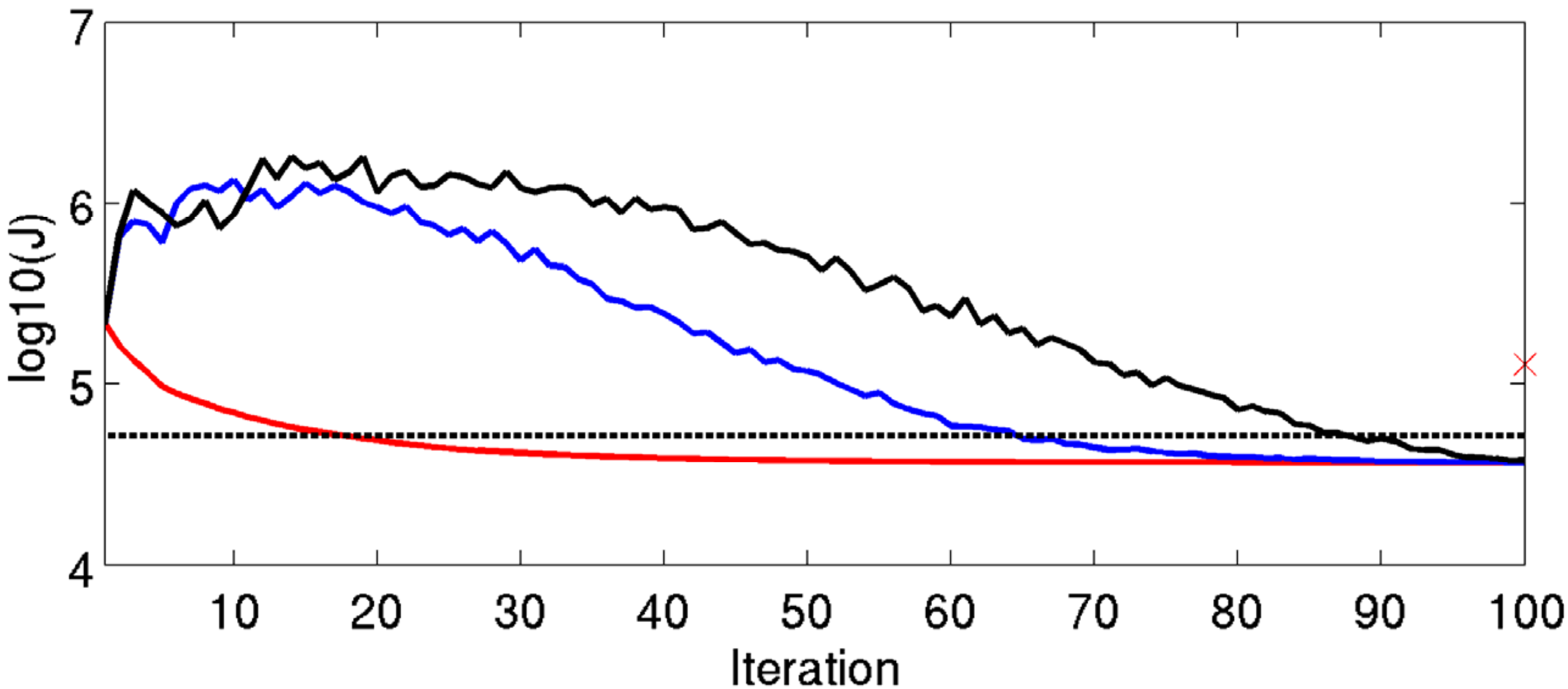


Ingleby and Huddleston (2007)

4D-Var Configuration

- Case studies for a representative case 3-10 March, 2003.
- 1 outer-loop, 100 inner-loops
- 7 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

4D-Var Performance



3-10 March, 2003
(10km, 42 levels)

Issues, Things to do, & Coming Soon

- Slow convergence of dual 4D-Var compared to primal formulation:
  - **w** has no physical significance, so $\delta \mathbf{z} = \mathbf{D}\mathbf{G}^{\mathrm{T}}\mathbf{w}$ need not be physically realizable
  - minimum residual method may be the answer (El Akkraoui and Gauthier, 2010)

Summary

- Strong and weak constraint 4D-Var, dual formulation:

  define W4DPSAS

  Drivers/w4dpsas_ocean.h

  define W4DVAR

  Drivers/w4dvar_ocean.h

- Matrix-less iterations to identify cost function minimum using TLROMS and ADROMS

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