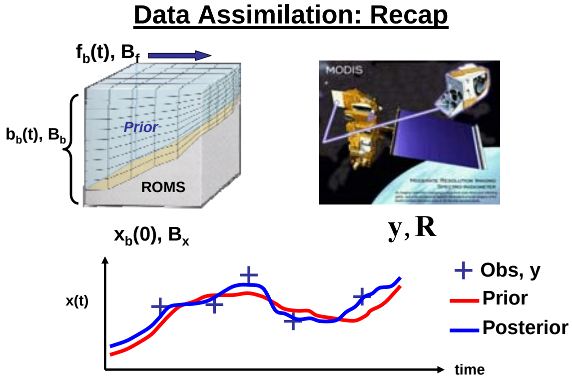
**Lecture 3:**
**Dual 4D-Var**

## 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



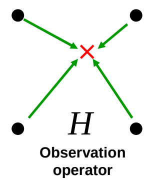

Model solutions depends on $x_b(0)$, $f_b(t)$, $b_b(t)$, $\eta(t)$

## Notation & Nomenclature: Recap

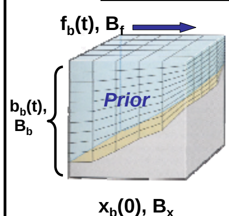
$$\mathbf{x} = \begin{bmatrix} \mathbf{T} \\ \mathbf{S} \\ \zeta \\ \mathbf{u} \\ \mathbf{v} \end{bmatrix} \quad \mathbf{z} = \begin{bmatrix} \mathbf{x}(0) \\ \mathbf{f}(t) \\ \mathbf{b}(t) \\ \boldsymbol{\eta}(t) \end{bmatrix} \quad \mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ \vdots \\ y_N \end{bmatrix} \quad \mathbf{d} = \left(\mathbf{y} - H(\mathbf{x}^{\mathrm{b}})\right)$$

State vector — Control vector — Observation vector

Prior — Innovation vector




## Incremental Formulation: Recap




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

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

(Courtier *et al.*, 1994)

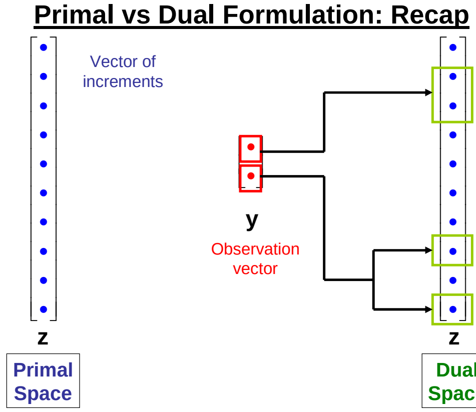
$$J = \frac{1}{2}\delta\mathbf{z}^T\mathbf{D}^{-1}\delta\mathbf{z} + \frac{1}{2}(\mathbf{G}\delta\mathbf{z} - \mathbf{d})^T\mathbf{R}^{-1}(\mathbf{G}\delta\mathbf{z} - \mathbf{d})$$

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

Prior (background) error covariance

Tangent Linear Model sampled at obs points — Obs Error Cov. — Innovation $\mathbf{d} = \mathbf{y} - \mathbf{H}\mathbf{x}_{\mathrm{b}}$

## 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):

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

Gain (primal):

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

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

## Two Spaces: Recap

**G** maps from model space to observation space

$\mathbf{G}^{\mathbf{T}}$ 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:**

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

## 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:**

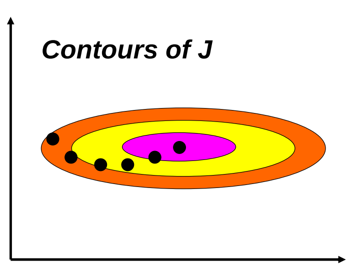
There is no physical significance attached to w

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

**then compute:**

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

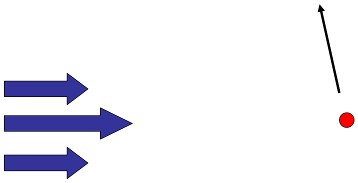
## Conjugate Gradient (CG) Methods



## Matrix-less Operations

There are no matrix multiplications!

$$GDG^T\delta$$



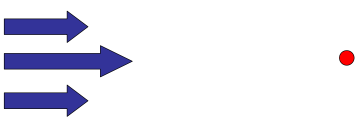
Zonal shear flow

## Matrix-less Operations

There are no matrix multiplications!

$$GDG^T\delta$$

Adjoint Model



Zonal shear flow

## Matrix-less Operations

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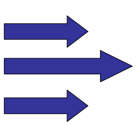
$$GDG^T\delta$$

Adjoint Model



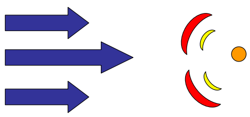
Zonal shear flow

## Matrix-less Operations

There are no matrix multiplications!

$$GDG^{T}\delta$$

↑ Adjoint Model

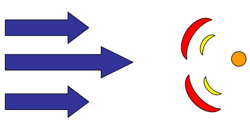



## Matrix-less Operations

There are no matrix multiplications!

$$GDG^{T}\delta$$

↑ Covariance

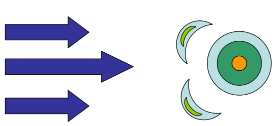



## Matrix-less Operations

There are no matrix multiplications!

$$GDG^{T}\delta$$

↑ Covariance

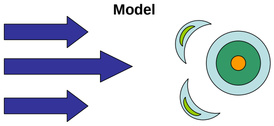


## Matrix-less Operations

There are no matrix multiplications!

$$GDG^T\delta$$

Tangent Linear Model



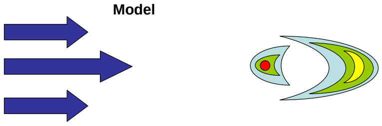
Zonal shear flow

## Matrix-less Operations

There are no matrix multiplications!

$$GDG^T\delta$$

Tangent Linear Model



Zonal shear flow

## Matrix-less Operations

There are no matrix multiplications!

$$GDG^T\delta$$

A covariance

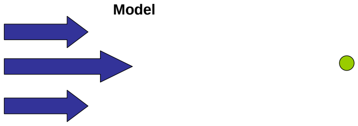
Zonal shear flow

## Matrix-less Operations

There are no matrix multiplications!

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

Tangent Linear Model

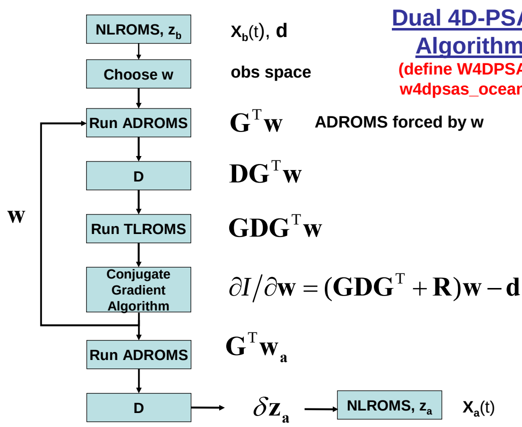


Zonal shear flow

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

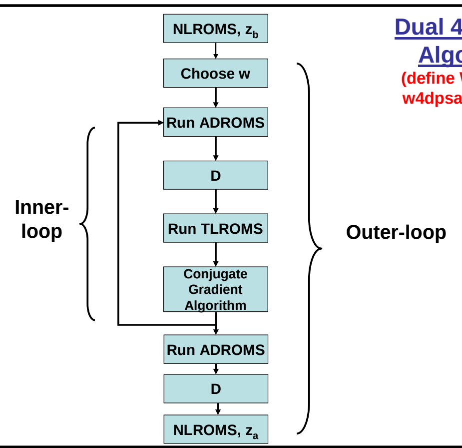
## Dual 4D-PSAS Algorithm

(define W4DPSAS, w4dpsas_ocean.h)



## Dual 4D-PSAS Algorithm

(define W4DPSAS, w4dpsas_ocean.h)

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

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## The Dual of State-Space

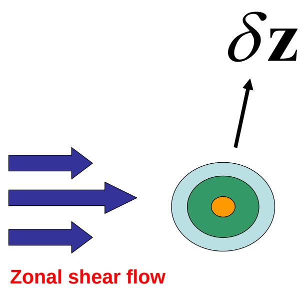
**ROMS state-vector increments:** $\delta\mathbf{x}(t) = \begin{bmatrix} \delta\mathbf{T}(t) \\ \delta\mathbf{S}(t) \\ \delta\zeta(t) \\ \delta\mathbf{u}(t) \\ \delta\mathbf{v}(t) \end{bmatrix}$

**The set of all continuous, linear functionals of $\delta$x(t) is called the *dual* of $\delta$x**

**For example, $y_m$=G$\delta$z belongs to the *dual* of $\delta$x**

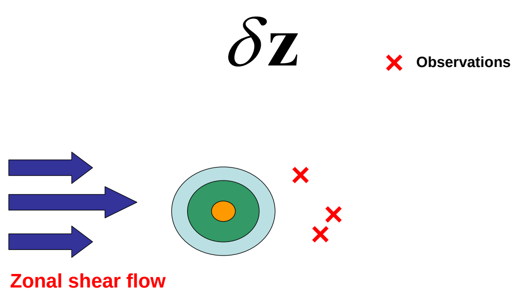
## The Dual of State-Space

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



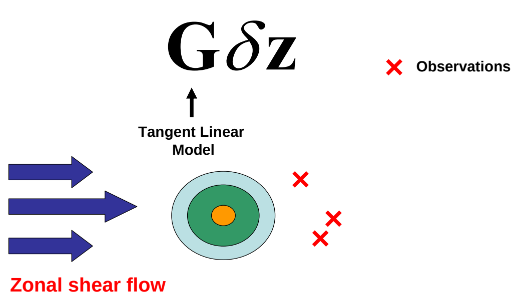

## The Dual of State-Space

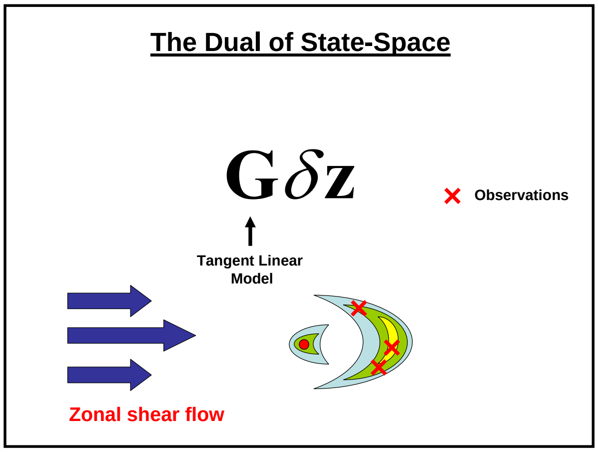
**Consider the assimilation window t=[0,T] for the zonal shear flow with 3 observations.**

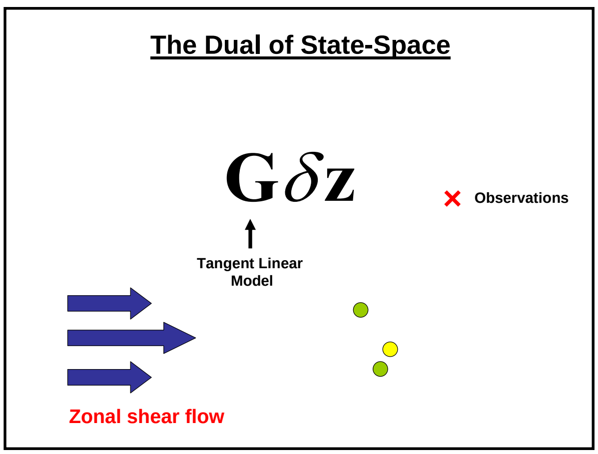


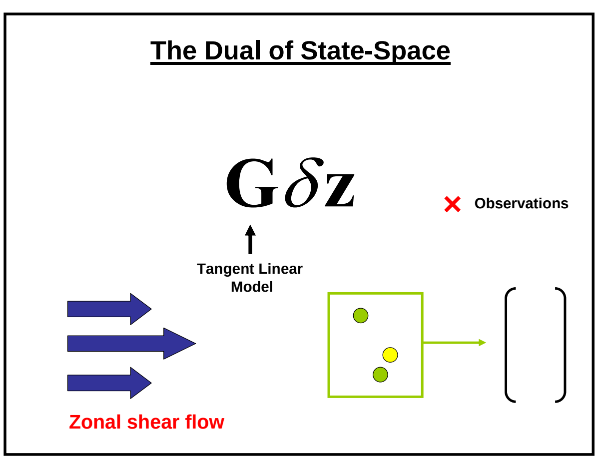

## The Dual of State-Space

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




The Dual of State-Space
Gδz
Observations
Tangent Linear Model
Zonal shear flow


The Dual of State-Space
Gδz
Observations
Tangent Linear Model
Zonal shear flow


The Dual of State-Space
Gδz
Observations
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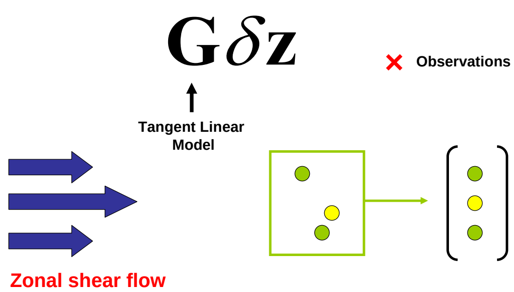
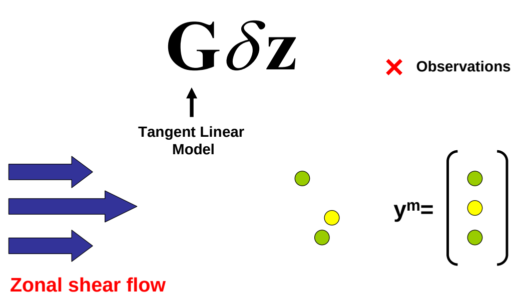
Zonal shear flow

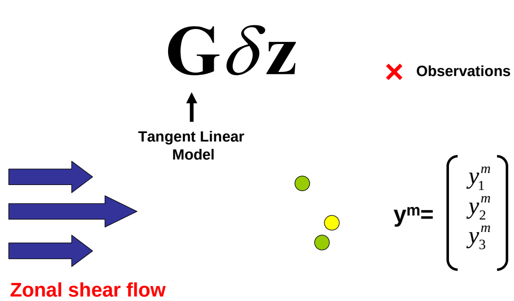
## The Dual of State-Space




## The Dual of State-Space




## The Dual of State-Space

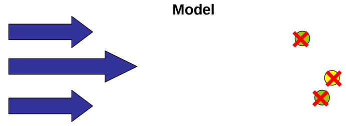


## The Dual of State-Space

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

Tangent Linear Model

× Observations



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

Innovation vector

Zonal shear flow

## The Dual of State-Space

The innovation vector belongs to the ***dual*** of $\delta\mathbf{x}(t)$.

**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:**

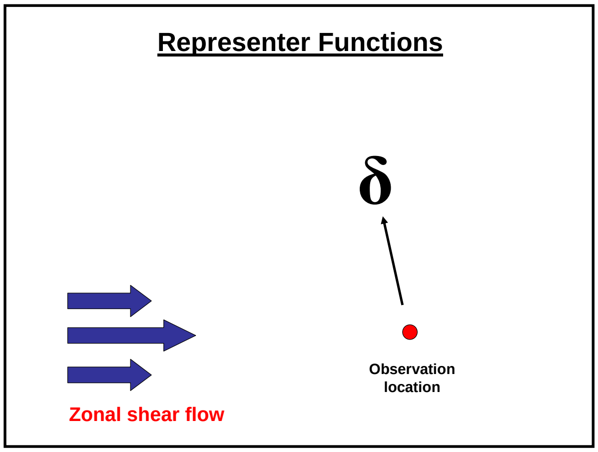
$$y_1^m - y_1^o = \boldsymbol{\rho}_1^{\mathrm{T}}\mathbf{u};\quad y_2^m - y_2^o = \boldsymbol{\rho}_2^{\mathrm{T}}\mathbf{u};\quad y_3^m - y_3^o = \boldsymbol{\rho}_3^{\mathrm{T}}\mathbf{u};$$

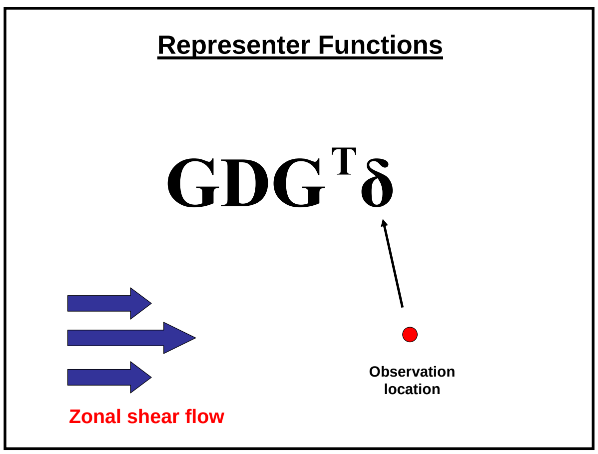
**where** $\rho_i$ **are referred to as "representer functions."**

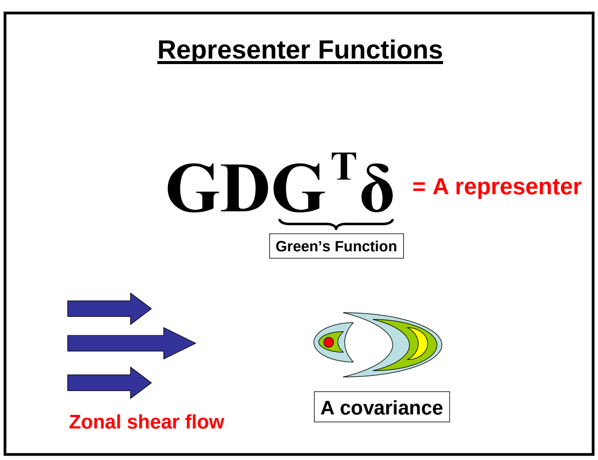
## The Dual of State-Space

**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
δ
Observation location
Zonal shear flow


Representer Functions
$GDG^T\delta$
Observation location
Zonal shear flow

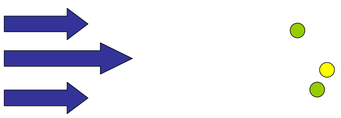

Representer Functions
$GDG^T\delta$
= A representer
Green's Function
A covariance
Zonal shear flow

## Representer Functions

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

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

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



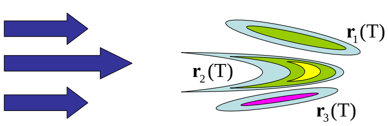
Zonal shear flow

## Representer Functions

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

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

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




Zonal shear flow

## 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:

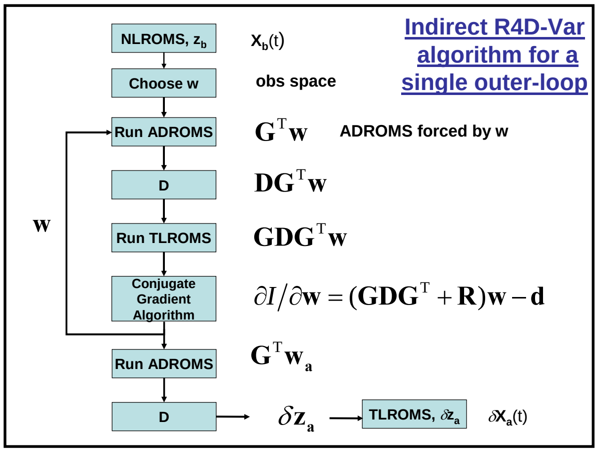
The elements of w are the weighting coefs for the $r_i(t)$

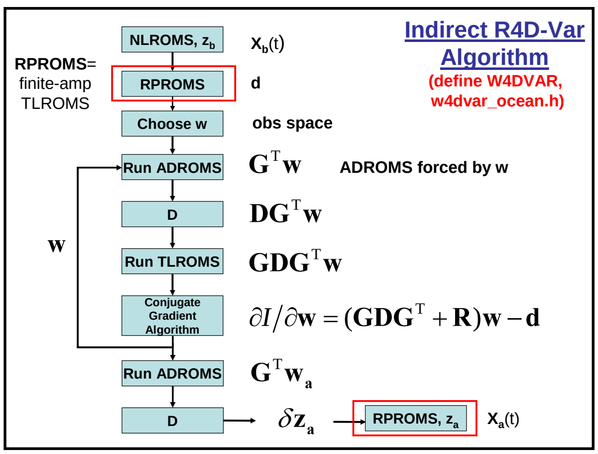
$$I(\mathbf{w})=\frac{1}{2}\mathbf{w}^T(\mathbf{GDG}^{\mathrm{T}}+\mathbf{R})\mathbf{w}-\mathbf{w}^T\mathbf{d}$$

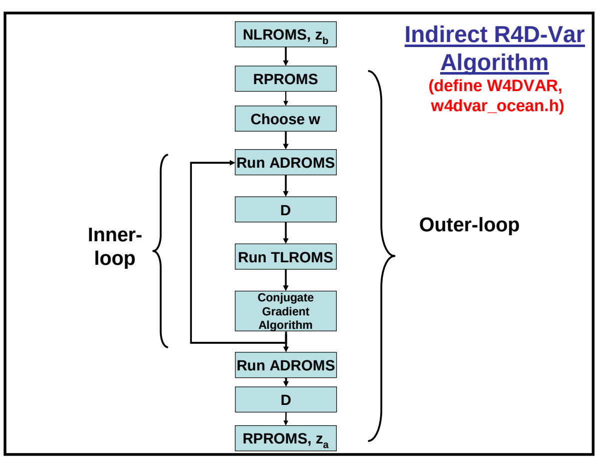
then compute:

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
NLROMS, $z_b$
$x_b(t)$
Choose w
obs space
Run ADROMS
$G^T w$
ADROMS forced by w
D
$DG^T w$
w
Run TLROMS
$GDG^T w$
Conjugate Gradient Algorithm
$\partial I/\partial w = (GDG^T + R)w - d$
Run ADROMS
$G^T w_a$
D
$\delta z_a$
TLROMS, $\delta z_a$
$\delta x_a(t)$


Indirect R4D-Var Algorithm
(define W4DVAR, w4dvar_ocean.h)
RPROMS= finite-amp TLROMS
NLROMS, $z_b$
$x_b(t)$
RPROMS
d
Choose w
obs space
Run ADROMS
$G^T w$
ADROMS forced by w
D
$DG^T w$
w
Run TLROMS
$GDG^T w$
Conjugate Gradient Algorithm
$\partial I/\partial w = (GDG^T + R)w - d$
Run ADROMS
$G^T w_a$
D
$\delta z_a$
RPROMS, $z_a$
$x_a(t)$


Indirect R4D-Var Algorithm
(define W4DVAR, w4dvar_ocean.h)
NLROMS, $z_b$
RPROMS
Choose w
Run ADROMS
D
Run TLROMS
Conjugate Gradient Algorithm
Run ADROMS
D
RPROMS, $z_a$
Inner-loop
Outer-loop

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

Correction for model error

## Weak Constraint 4D-Var

Tangent linear ROMS (TLROMS):

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

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

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:**

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

**Weak constraint:**

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

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

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

## Mechanics of Dual 4D-Var: Preconditioning

**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:**

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

**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:**

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

**Dual formulation of practical gain matrix:**

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

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

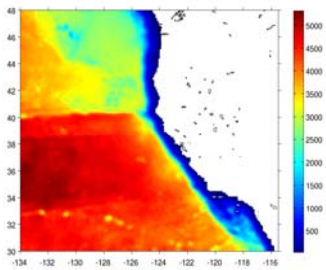
## An Example: ROMS CCS

COAMPS forcing $f_b(t), B_f$

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

$x_b(0), B_x$

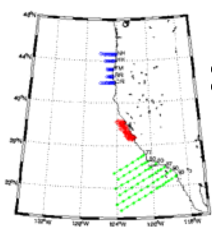
Previous assimilation cycle



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

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

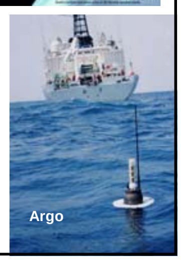
## Observations (y)



CalCOFI & GLOBEC



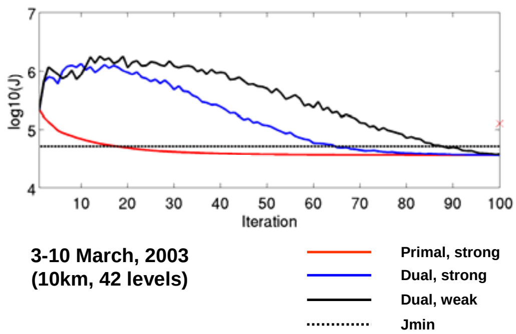
Ingleby and Huddleston (2007)




## 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, $\sigma$ from clim
  **f** $L_\tau$=300km, $L_Q$=100km, $\sigma$ from COAMPS
  **b** $L_h$=100 km, $L_v$=30m, $\sigma$ 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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