Lecture 2:
The Mechanics of 4D-Var

Outline

- The conjugate gradient algorithm
- Preconditioning
- Covariance modeling
- Background quality control

The Conjugate Gradient Algorithm (cgradient.h & congrad.F)

Recall the incremental cost function:

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

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

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

$$\underbrace{\left(\mathbf{D}^{-1}+\mathbf{G}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{G}\right)\delta\mathbf{z}-\mathbf{G}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{d}}=\mathbf{0}$$

i.e. solve $\mathbf{A}\delta\mathbf{z} = \mathbf{b}$

The Conjugate Gradient Algorithm

The ECMWF "congrad" of Fisher (1997) for inner-loop *k+1*:

$$\delta\hat{\mathbf{z}}_k = \delta\mathbf{z}_k + \tau_k \mathbf{h}_k$$ trial step

$$\hat{\mathbf{g}}_k = \partial J / \partial \delta\hat{\mathbf{z}}_k$$ TL & AD ROMS — gradient @ trial step

$$\alpha_k = -\tau_k \mathbf{h}_k^{\mathrm{T}} \mathbf{g}_k / \left(\mathbf{h}_k^{\mathrm{T}} (\hat{\mathbf{g}}_k - \mathbf{g}_k) \right)$$ optimum step

$$\delta\mathbf{z}_{k+1} = \delta\mathbf{z}_k + \alpha_k \mathbf{h}_k$$ new starting point

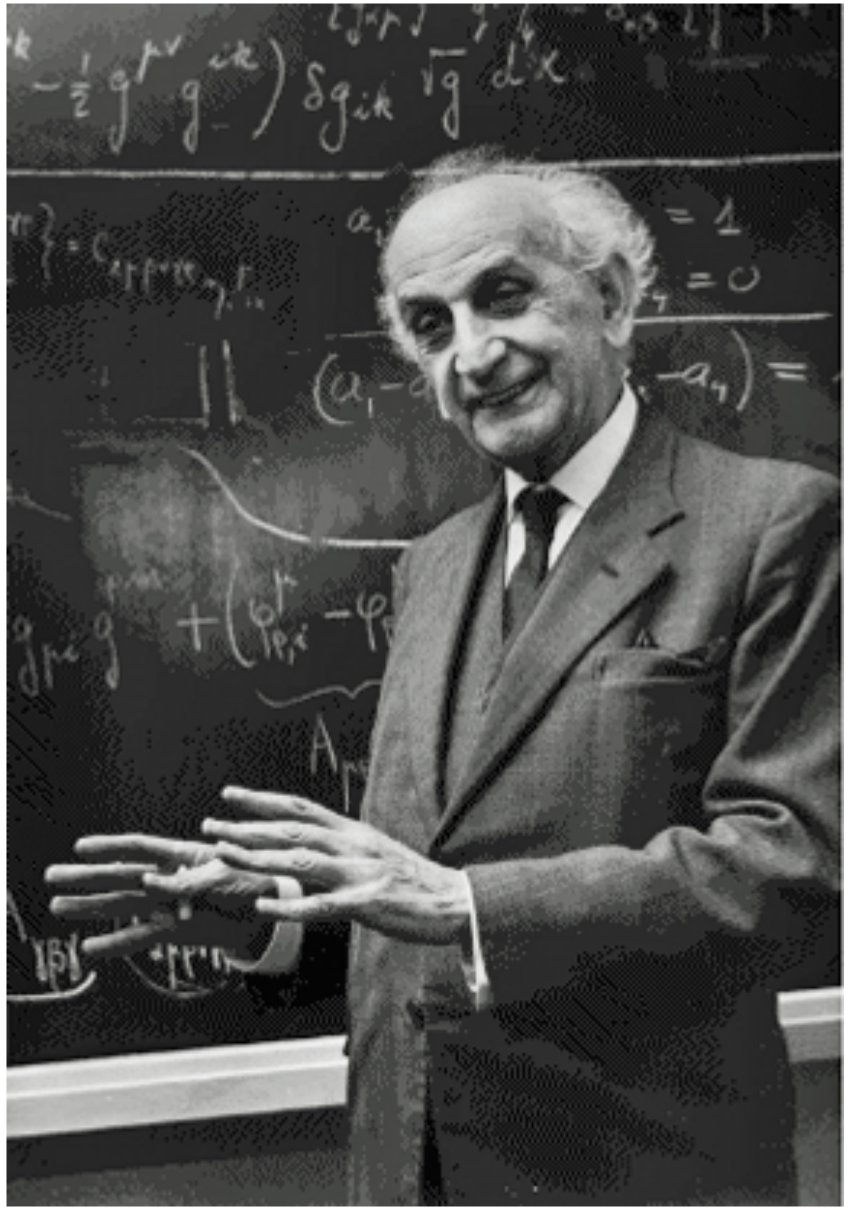
$$\mathbf{g}_{k+1} = \mathbf{g}_k + (\alpha_k / \tau_k)\left(\hat{\mathbf{g}}_k - \mathbf{g}_k\right)$$ gradient @new point

$$\beta_{k+1} = \mathbf{g}_{k+1}^{\mathrm{T}} \mathbf{g}_{k+1} / \mathbf{g}_k^{\mathrm{T}} \mathbf{g}_k$$

$$\mathbf{h}_{k+1} = -\mathbf{g}_{k+1} + \beta_{k+1} \mathbf{h}_k$$ new descent direction

The Lanczos Connection

Cornelius Lanczos (1893-1974)



The Lanczos Connection

The CG algorithm is equivalent to:

$$\mathbf{A}\mathbf{q}_{k+1} = \gamma_{k+1}\mathbf{q}_{k+2} + \delta_{k+1}\mathbf{q}_{k+1} + \gamma_k\mathbf{q}_k$$

"Lanczos recursion relation"

$$\mathbf{q}_k = \mathbf{g}_k \Big/ \|\mathbf{g}_k\|; \quad \delta_{\mathrm{k+1}} = (1/\alpha_{k+1} + \beta_{k+1}/\alpha_k); \quad \gamma_{\mathrm{k}} = -\beta_{k+1}^{1/2}/\alpha_k$$

$$\mathbf{V}_k = \left(\mathbf{q}_i\right)$$

$$\mathbf{A}\mathbf{V}_k = \mathbf{V}_k\mathbf{T}_k + \gamma_k\mathbf{q}_{k+1}\mathbf{e}_k^{\mathrm{T}}$$

Orthonormal Lanczos vectors

$$\mathbf{q}_i^{\mathrm{T}}\mathbf{q}_j = \delta_{ij}$$

$$\mathbf{V}_k^T\mathbf{V}_k = \mathbf{I}_k$$

$$\mathbf{T}_k = \begin{pmatrix} \delta_1 & \gamma_1 & & & & \\ \gamma_1 & \delta_2 & \gamma_2 & & & \\ & \ddots & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \gamma_{k-2} & \delta_{k-1} & \gamma_{k-1} \\ & & & & & \gamma_{k-1} & \delta_k \end{pmatrix}$$

The Lanczos Connection

Specifically:

$$\mathbf{A} \approx \mathbf{V}_k \mathbf{T}_k \mathbf{V}_k^T$$

$$\mathbf{A}^{-1} \approx \mathbf{V}_k \mathbf{T}_k^{-1} \mathbf{V}_k^T$$

The Lanczos Connection

Gain (primal form):

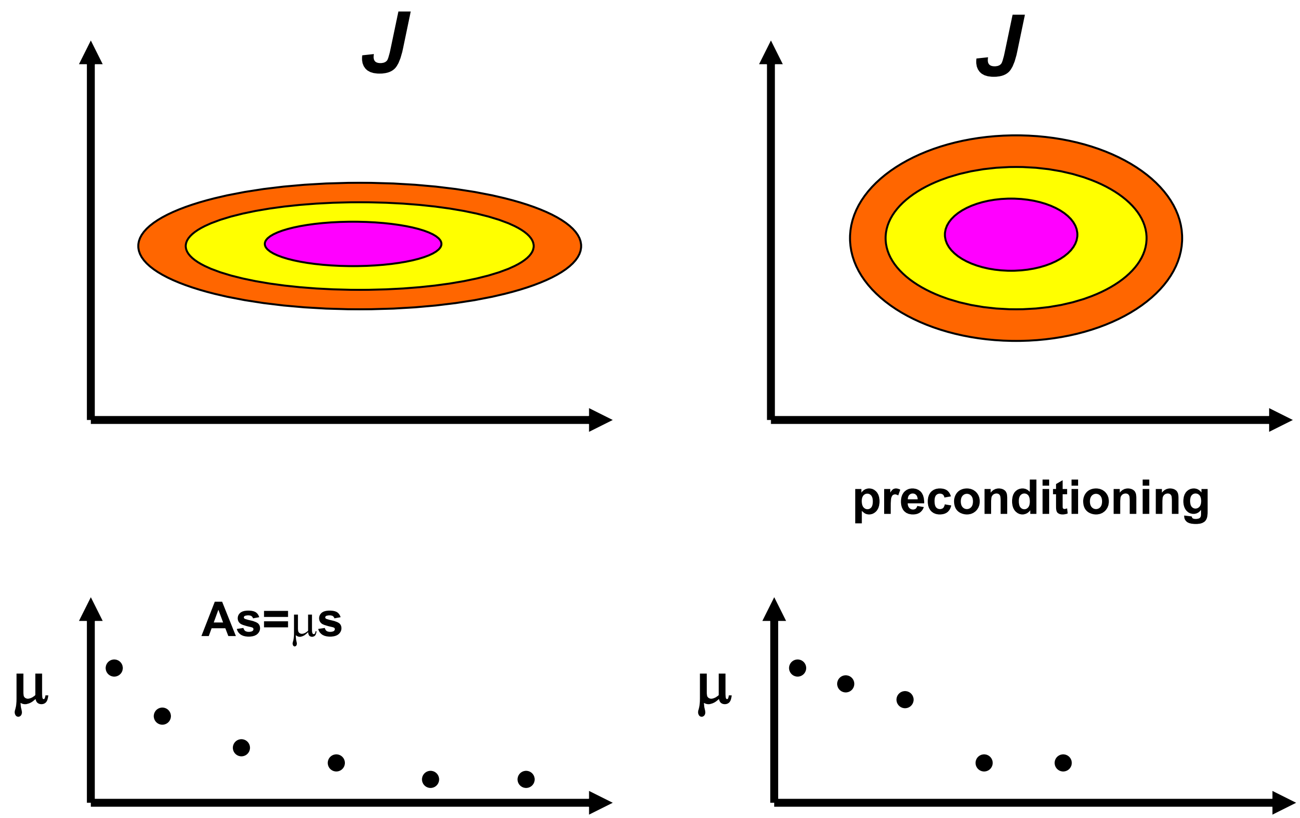
$$\mathbf{K} = (\mathbf{D}^{-1} + \mathbf{G}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{G})^{-1}\mathbf{G}^{\mathrm{T}}\mathbf{R}^{-1}$$

Practical gain matrix:

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

Useful for diagnostic applications (Lecture 5)
(The Lanczos vectors are in ADJname)

Preconditioning



Preconditioning seeks to cluster the eigenvalues of A via a transformation of variable

Preconditioning

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

$$\left(\mathbf{D}^{-1} + \mathbf{G}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{G}\right)\delta\mathbf{z} - \mathbf{G}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{d} = \mathbf{0}$$

i.e. solve $\mathbf{A}\delta\mathbf{z} = \mathbf{b}$

Minimize:

$$J = \frac{1}{2}\delta\mathbf{z}^{\mathrm{T}}\mathbf{A}\delta\mathbf{z} - \delta\mathbf{z}^{\mathrm{T}}\mathbf{b} + c$$

Introduce a new variable: $\mathbf{v} = \mathbf{A}^{1/2}\delta\mathbf{z}$

$$J = \frac{1}{2}\mathbf{v}^{\mathrm{T}}\mathbf{v} - \mathbf{v}^{\mathrm{T}}\mathbf{A}^{-\mathrm{T}/2}\mathbf{b} + c$$

At the minimum: $\partial J / \partial \mathbf{v} = \mathbf{v} - \mathbf{A}^{-\mathrm{T}/2}\mathbf{b} = \mathbf{0}$

Preconditioning

Recall the incremental cost function:

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

Introduce a new variable: $\mathbf{v} = \mathbf{D}^{-1/2}\delta\mathbf{z}$

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

$$= \frac{1}{2}\mathbf{v}^{\mathrm{T}}\left(\mathbf{I} + \mathbf{D}^{1/2}\mathbf{G}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{G}\mathbf{D}^{1/2}\right)\mathbf{v} - \mathbf{v}^{\mathrm{T}}\mathbf{D}^{1/2}\mathbf{G}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{d} + \frac{1}{2}\mathbf{d}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{d}$$

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

$$\left(\mathbf{I} + \mathbf{D}^{1/2}\mathbf{G}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{G}\mathbf{D}^{1/2}\right)\mathbf{v} - \mathbf{D}^{1/2}\mathbf{G}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{d} = \mathbf{0}$$

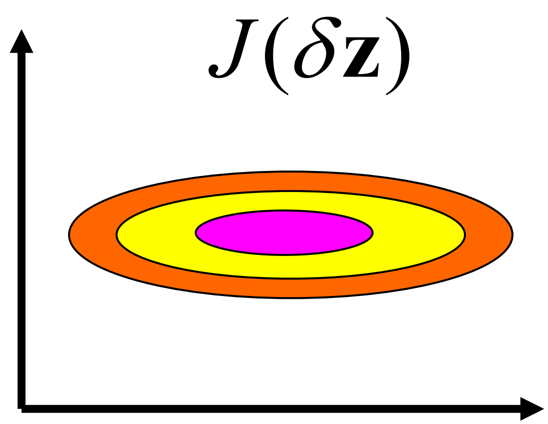
i.e. solve $\tilde{\mathbf{A}}\mathbf{v} = \tilde{\mathbf{b}}$ **then** $\delta\mathbf{z} = \mathbf{D}^{1/2}\mathbf{v}$

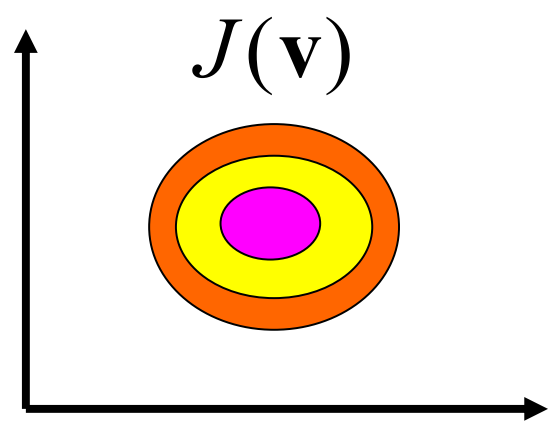
Preconditioning

Solve $\tilde{\mathbf{A}}\mathbf{v} = \tilde{\mathbf{b}}$

$$\tilde{\mathbf{A}} = \underbrace{\left(\mathbf{I} + \mathbf{D}^{1/2}\mathbf{G}^{T}\mathbf{R}^{-1}\mathbf{G}\mathbf{D}^{1/2}\right)}$$

Has eigenvalues clustered around 1





The Conjugate Gradient Algorithm

cgradient.h in v-space to minimize $J(\mathbf{v})$

$\hat{\mathbf{v}}_k = \mathbf{v}_k + \tau_k \mathbf{h}_k$	trial step
$\hat{\mathbf{g}}_k = \mathbf{D}^{\mathrm{T}/2}\, \partial J / \partial \delta \hat{\mathbf{z}}_k$	gradient @ trial step
$\alpha_k = -\tau_k \mathbf{h}_k^{\mathrm{T}} \mathbf{g}_k / \left(\mathbf{h}_k^{\mathrm{T}} (\hat{\mathbf{g}}_k - \mathbf{g}_{\mathbf{k}}) \right)$	optimum step
$\mathbf{v}_{k+1} = \mathbf{v}_k + \alpha_k \mathbf{h}_k$	new starting point
$\mathbf{g}_{k+1} = \mathbf{g}_k + (\alpha_k / \tau_k)\left(\hat{\mathbf{g}}_k - \mathbf{g}_k \right)$	gradient @new point
$\beta_{k+1} = \mathbf{g}_{k+1}^{\mathrm{T}} \mathbf{g}_{k+1} / \mathbf{g}_k^{\mathrm{T}} \mathbf{g}_k$	
$\mathbf{h}_{k+1} = -\mathbf{g}_{k+1} + \beta_{k+1} \mathbf{h}_k$	new descent direction
$\delta \mathbf{z}_{k+1} = \mathbf{D}^{1/2} \mathbf{v}_{k+1}$	project into state-space

The Lanczos Connection

Gain (primal form):

$$\mathbf{K} = \mathbf{D}^{1/2}(\mathbf{I} + \mathbf{D}^{\mathrm{T}/2}\mathbf{G}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{G}\mathbf{D}^{1/2})^{-1}\mathbf{D}^{\mathrm{T}/2}\mathbf{G}^{\mathrm{T}}\mathbf{R}^{-1}$$

Practical gain matrix:

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

Useful for diagnostic applications (Lecture 5)
(The Lanczos vectors are in ADJname)

Covariance Modeling

Recall the incremental cost function:

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

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

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

where $\mathbf{D} = \mathrm{diag}(\mathbf{B_x}, \mathbf{B_b}, \mathbf{B_f}, \mathbf{Q})$

Covariance Modeling

$\mathbf{B_x}$ = initial condition *prior* (or background) error covariance matrix

$\mathbf{B_f}$ = surface forcing *prior* error covariance matrix

$\mathbf{B_b}$ = open boundary condition *prior* error covariance matrix

Q = *prior* model error covariance matrix

Each covariance matrix is factorized according to:

$$\mathbf{B} = \mathbf{K_b} \boldsymbol{\Sigma} \mathbf{C} \boldsymbol{\Sigma}^{\mathrm{T}} \mathbf{K_b}^{\mathrm{T}}$$

C = univariate correlation matrix

Σ = diagonal matrix of error standard deviations

$\mathbf{K_b}$ = multivariate balance operator (for $\mathbf{B_x}$ and **Q** only)

Correlation Models

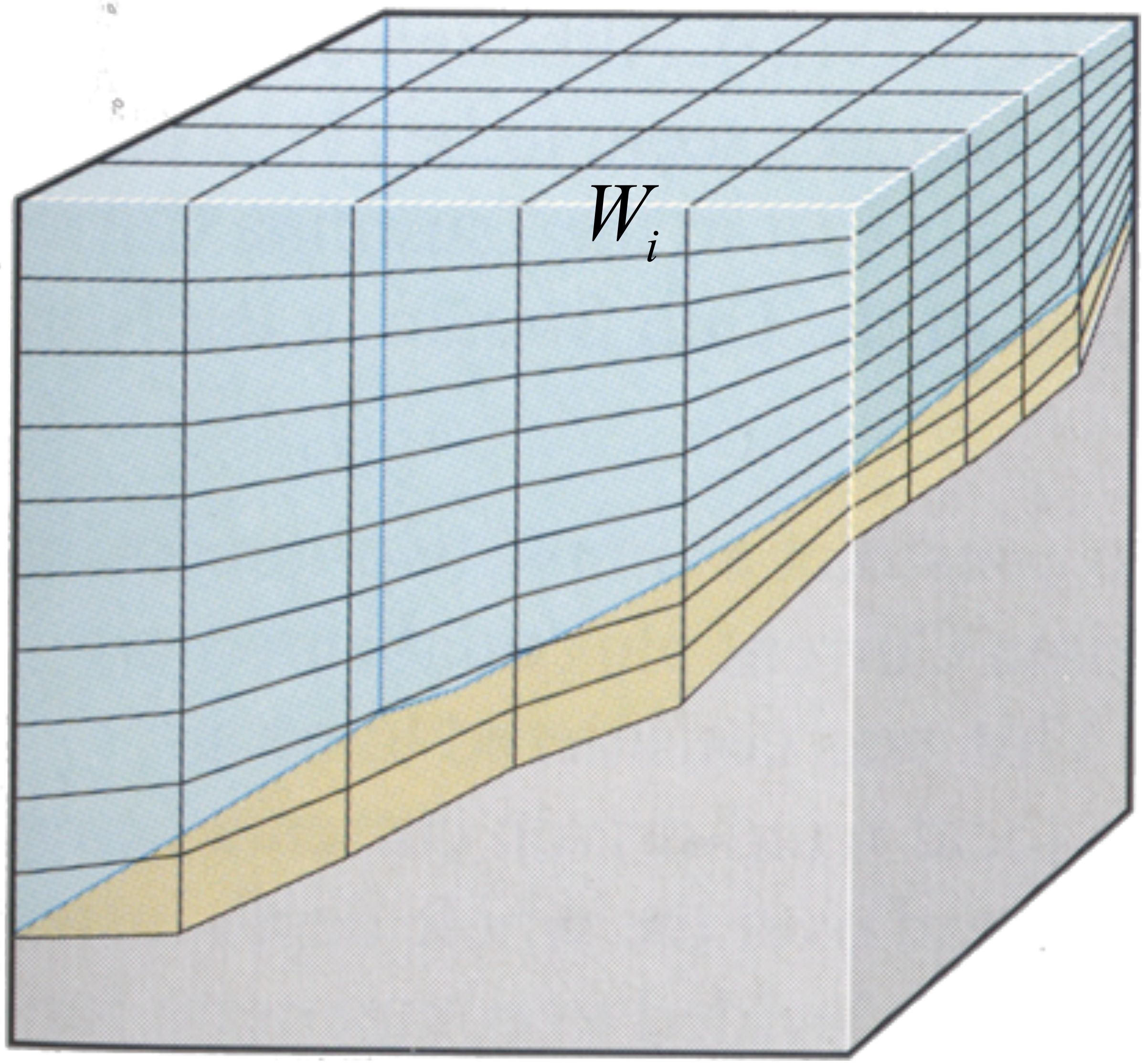
C is further factorized as:

$$\mathbf{C} = \mathbf{\Lambda} \mathbf{L}_{\mathbf{v}}^{1/2} \mathbf{L}_{\mathbf{h}}^{1/2} \mathbf{W}^{-1} \mathbf{L}_{\mathbf{h}}^{T/2} \mathbf{L}_{\mathbf{v}}^{T/2} \mathbf{\Lambda}^{T}$$

W = diagonal matrix of grid box volumes
$\mathbf{L_h}$ = horizontal correlation function model
$\mathbf{L_v}$ = vertical correlation function model
Λ = matrix of normalization coefficients

$\mathbf{L_h}$ and $\mathbf{L_v}$ are based on solutions of 2D and 1D pseudo diffusion equations respectively:

$$\partial\eta/\partial t - \kappa_h \nabla^2 \eta = 0 \qquad \partial\eta/\partial t - \kappa_v \, \partial^2\eta/\partial z^2 = 0$$



W_i

Correlation Models

C is further factorized as:

$$\mathbf{C} = \mathbf{\Lambda} \mathbf{L}_{\mathbf{v}}^{1/2} \mathbf{L}_{\mathbf{h}}^{1/2} \mathbf{W}^{-1} \mathbf{L}_{\mathbf{h}}^{T/2} \mathbf{L}_{\mathbf{v}}^{T/2} \mathbf{\Lambda}^{T}$$

W = diagonal matrix of grid box volumes
$\mathbf{L_h}$ = horizontal correlation function model
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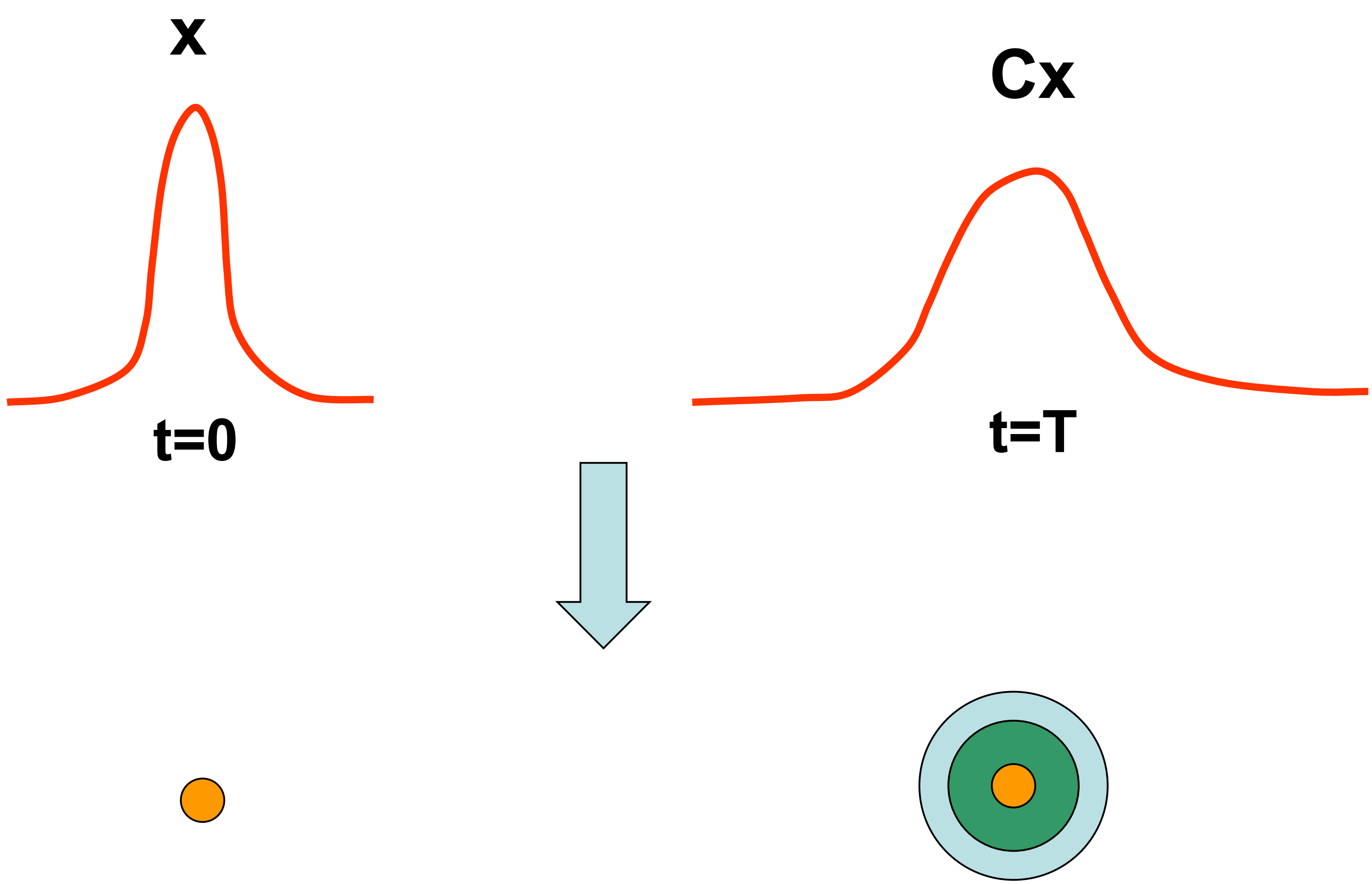
$\mathbf{L_h}$ and $\mathbf{L_v}$ are based on solutions of 2D and 1D pseudo diffusion equations respectively:

$$\partial\eta / \partial t - \kappa_h \nabla^2 \eta = 0 \qquad \partial\eta / \partial t - \kappa_v \, \partial^2 \eta / \partial z^2 = 0$$

Correlation Models



Correlation length, *L*: $$L^2 \approx 2\kappa T$$

Covariance Modeling

$$\mathbf{C} = \mathbf{\Lambda} \mathbf{L}_{\mathbf{v}}^{1/2} \mathbf{L}_{\mathbf{h}}^{1/2} \mathbf{W}^{-1} \mathbf{L}_{\mathbf{h}}^{T/2} \mathbf{L}_{\mathbf{v}}^{T/2} \mathbf{\Lambda}^{T}$$

Λ ensures that the range of **C** is ±1.

Suppose that **x** is divided into a balanced and unbalanced contribution: $\mathbf{x}=\mathbf{x_b}+\mathbf{x_u}$

Examples of balance relations: geostrophy, hydrostatic

$$\left(\mathbf{B_x}\right)_{\mathbf{u}} = \mathbf{\Sigma C \Sigma}^{T}$$

$$\mathbf{B_x} = \mathbf{K_b}\left(\mathbf{B_x}\right)_{\mathbf{u}} \mathbf{K_b}^{T}$$

The Balance Operator

(define BALANCE_OPERATOR)

Following Weaver et al (2005):

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

Total state vector increments

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

Unbalanced state vector increments (except for δT)

$$\left(\mathbf{B}_x\right)_u = \left\langle \delta\hat{\mathbf{x}}\delta\hat{\mathbf{x}}^T \right\rangle$$

$$\delta\mathbf{x} = \mathbf{K}_b\delta\hat{\mathbf{x}}$$

$$\mathbf{B}_x = \left\langle \delta\mathbf{x}\delta\mathbf{x}^T \right\rangle$$

$$= \mathbf{K}_b \left\langle \delta\hat{\mathbf{x}}\delta\hat{\mathbf{x}}^T \right\rangle \mathbf{K}_b^T$$

$$= \mathbf{K}_b \left(\mathbf{B}_u\right)_x \mathbf{K}_b^T$$

The Balance Operator

$$\delta \mathbf{S} = \boxed{\mathbf{K}_{ST}} \delta \mathbf{T} + \delta \mathbf{S}_{\mathbf{u}}$$

T-S relation

$$\delta \varsigma = \boxed{\mathbf{K}_{\varsigma\rho}} \delta \rho + \delta \varsigma_{\mathbf{u}}$$

Level of no motion or elliptic eqn

$$\delta \mathbf{u} = \boxed{\mathbf{K}_{up}} \delta \mathbf{p} + \delta \mathbf{u}_{\mathbf{u}}$$

Geostrophic balance

$$\delta \mathbf{v} = \boxed{\mathbf{K}_{vp}} \delta \mathbf{p} + \delta \mathbf{v}_{\mathbf{u}}$$

Geostrophic balance

$$\delta \rho = \boxed{\mathbf{K}_{\rho T}} \delta \mathbf{T} + \boxed{\mathbf{K}_{\rho S}} \delta \mathbf{S}$$

Linear equation of state

$$\delta \mathbf{p} = \boxed{\mathbf{K}_{p\rho}} \delta \rho + \boxed{\mathbf{K}_{p\varsigma}} \delta \varsigma$$

Hydrostatic balance

The Balance Operator

$$\delta \mathbf{x} = \mathbf{K_b} \delta \hat{\mathbf{x}}$$

$$\mathbf{K_b} = \begin{pmatrix} \mathbf{I} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{K}_{ST} & \mathbf{I} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{K}_{\varsigma T} & \mathbf{K}_{\varsigma S} & \mathbf{I} & \mathbf{0} & \mathbf{0} \\ \mathbf{K}_{uT} & \mathbf{K}_{uS} & \mathbf{K}_{u\varsigma} & \mathbf{I} & \mathbf{0} \\ \mathbf{K}_{vT} & \mathbf{K}_{vS} & \mathbf{K}_{v\varsigma} & \mathbf{0} & \mathbf{I} \end{pmatrix}$$

The Balance Operator

$\mathbf{K}_{ST}$ from *prior* (background) *T-S* relationship

$$\delta S_b = \gamma \left.\frac{\partial S}{\partial z}\right|_S \left.\frac{\partial z}{\partial T}\right|_T \delta T$$

$$\gamma = \left.\begin{matrix} 0 \\ 1 \end{matrix}\right\} \text{depending on mixed layer}$$

The Balance Operator

$$\mathbf{K_b} = \begin{pmatrix} \mathbf{I} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{K}_{ST} & \mathbf{I} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \boxed{\mathbf{K}_{\varsigma T}} & \boxed{\mathbf{K}_{\varsigma S}} & \mathbf{I} & \mathbf{0} & \mathbf{0} \\ \mathbf{K}_{uT} & \mathbf{K}_{uS} & \mathbf{K}_{u\varsigma} & \mathbf{I} & \mathbf{0} \\ \mathbf{K}_{vT} & \mathbf{K}_{vS} & \mathbf{K}_{v\varsigma} & \mathbf{0} & \mathbf{I} \end{pmatrix}$$

The Balance Operator

$$\left.\begin{aligned}\mathbf{K}_{\varsigma T} &= \mathbf{K}_{\varsigma\rho}\left(\mathbf{K}_{\rho T} + \mathbf{K}_{\rho S}\mathbf{K}_{ST}\right)\\ \mathbf{K}_{\varsigma S} &= \mathbf{K}_{\varsigma\rho}\mathbf{K}_{\rho S}\end{aligned}\right\}\delta\rho = \rho_0\left(-\alpha\delta T + \beta\delta S\right)$$

Either:

(i) $\delta\varsigma_b = -\int_{z_r}^{0} \delta\rho / \rho_0 dz$ (level of no motion z_r)

(ii) $\nabla(h\nabla\,\delta\varsigma_b) = -\nabla\int_{-h}^{0}\int_{z}^{0}\delta\rho / \rho_0 dz' dz + \ldots$

(define ZETA_ELLIPTIC)

The Balance Operator

$$\mathbf{K_b} = \begin{pmatrix} \mathbf{I} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{K}_{ST} & \mathbf{I} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{K}_{\varsigma T} & \mathbf{K}_{\varsigma S} & \mathbf{I} & \mathbf{0} & \mathbf{0} \\ \boxed{\mathbf{K}_{uT}} & \boxed{\mathbf{K}_{uS}} & \boxed{\mathbf{K}_{u\varsigma}} & \mathbf{I} & \mathbf{0} \\ \mathbf{K}_{vT} & \mathbf{K}_{vS} & \mathbf{K}_{v\varsigma} & \mathbf{0} & \mathbf{I} \end{pmatrix}$$

The Balance Operator

$$\mathbf{K}_{uT} = \mathbf{K}_{up}\left(\mathbf{K}_{p\rho} + \mathbf{K}_{p\varsigma}\mathbf{K}_{\varsigma\rho}\right)\left(\mathbf{K}_{\rho T} + \mathbf{K}_{\rho S}\mathbf{K}_{ST}\right)$$

$$\mathbf{K}_{uS} = \mathbf{K}_{up}\left(\mathbf{K}_{p\rho} + \mathbf{K}_{p\varsigma}\mathbf{K}_{\varsigma\rho}\right)\mathbf{K}_{\rho S}$$

$$\mathbf{K}_{u\varsigma} = \mathbf{K}_{up}\mathbf{K}_{p\varsigma}$$

$\mathbf{K}_{p\rho}$ hydrostatic balance

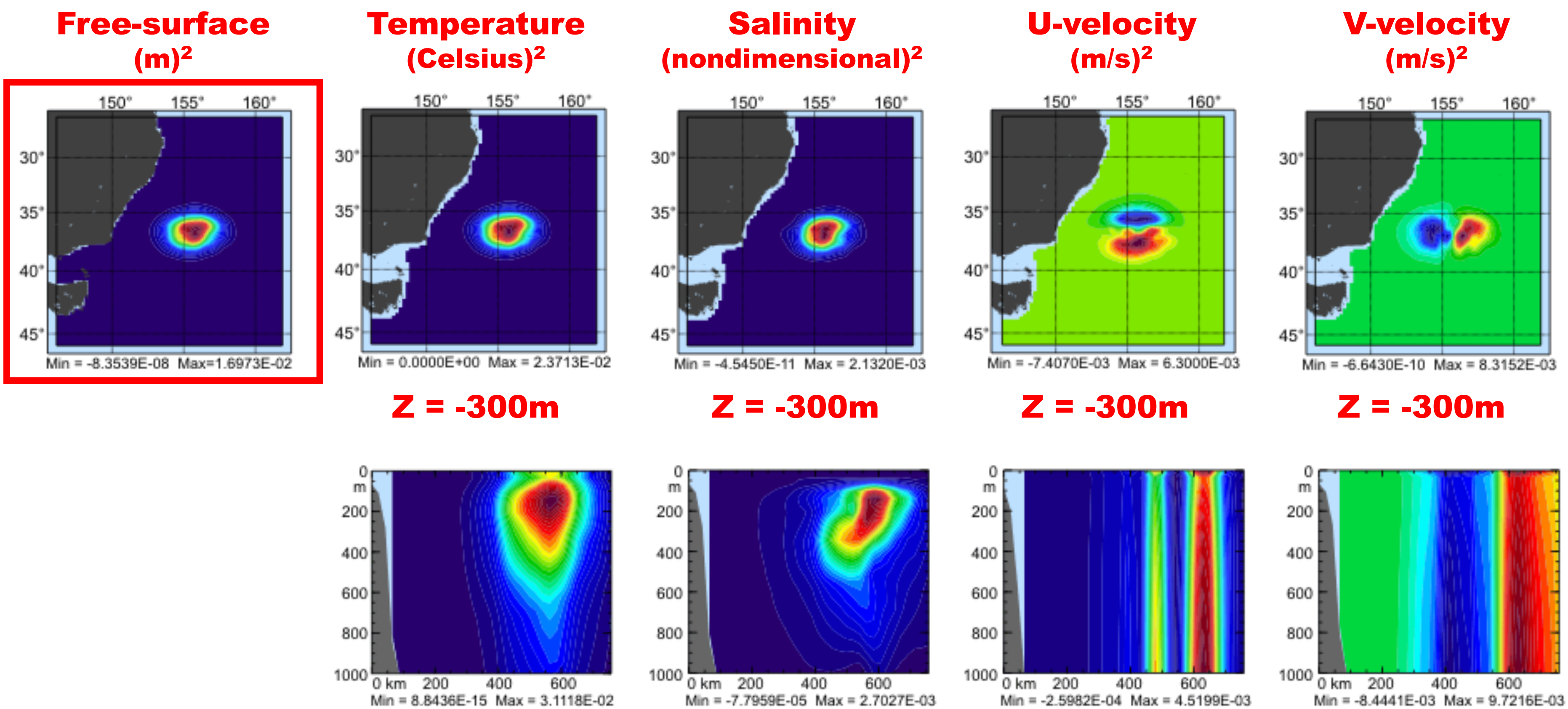
$\mathbf{K}_{up}$ geostrophic balance

$\mathbf{K}_{p\varsigma}$ free-surface contribution to *p*

The Balance Operator

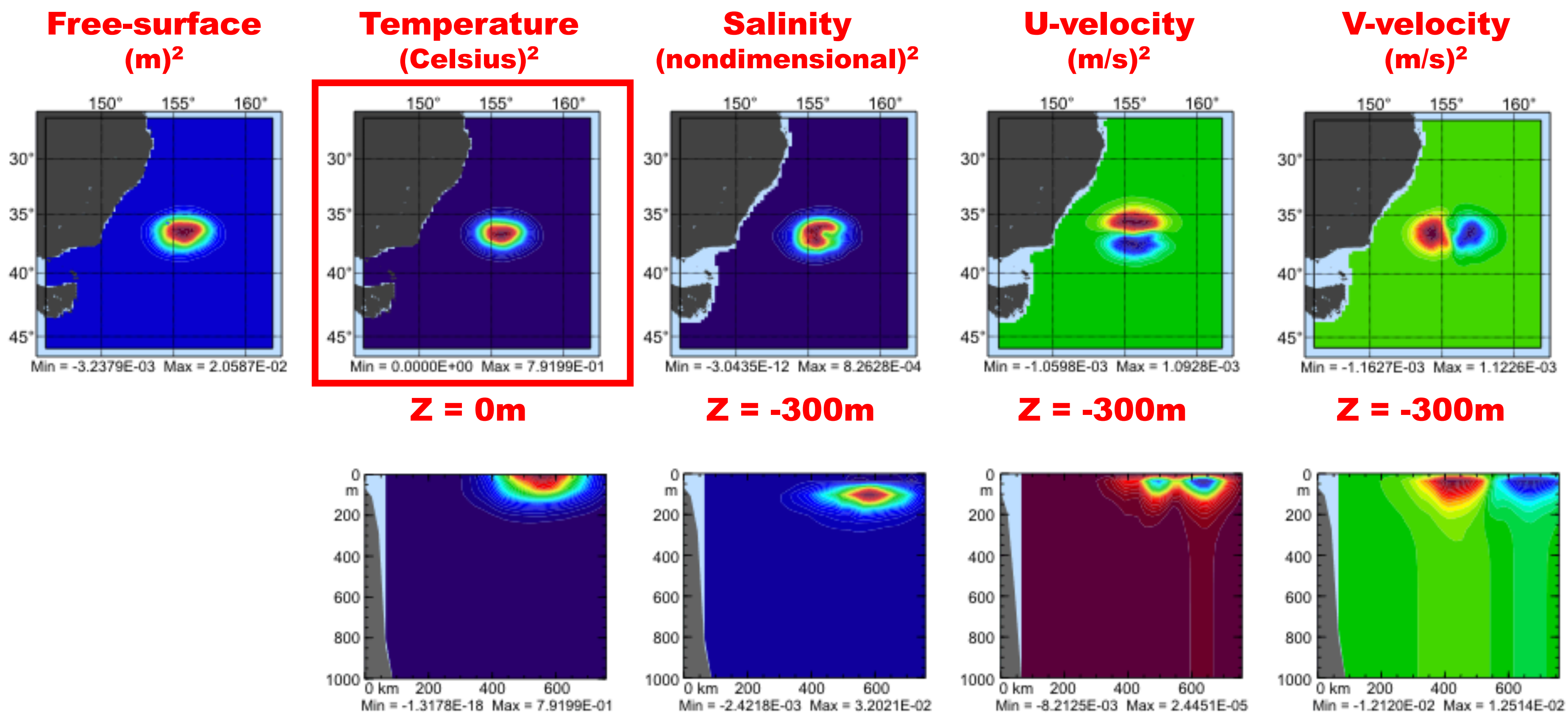
$$\mathbf{B}_{\mathbf{x}} = \mathbf{K}_{\mathbf{b}} \left(\mathbf{B}_{\mathbf{x}}\right)_{\mathbf{u}} \mathbf{K}_{\mathbf{b}}^{\mathrm{T}} = \begin{pmatrix} \mathbf{B}_{TT} & \mathbf{B}_{ST}^{T} & \mathbf{B}_{\varsigma T}^{T} & \mathbf{B}_{uT}^{T} & \mathbf{B}_{vT}^{T} \\ \mathbf{B}_{ST} & \mathbf{B}_{SS} & \mathbf{B}_{\varsigma S}^{T} & \mathbf{B}_{uS}^{T} & \mathbf{B}_{vS}^{T} \\ \mathbf{B}_{\varsigma T} & \mathbf{B}_{\varsigma S} & \mathbf{B}_{\varsigma\varsigma} & \mathbf{B}_{u\varsigma}^{T} & \mathbf{B}_{v\varsigma}^{T} \\ \mathbf{B}_{uT} & \mathbf{B}_{uS} & \mathbf{B}_{u\varsigma} & \mathbf{B}_{uu} & \mathbf{B}_{vu}^{T} \\ \mathbf{B}_{vT} & \mathbf{B}_{vS} & \mathbf{B}_{v\varsigma} & \mathbf{B}_{vu} & \mathbf{B}_{vv} \end{pmatrix}$$

IS4DVAR Balanced Operator Covariances: EAC



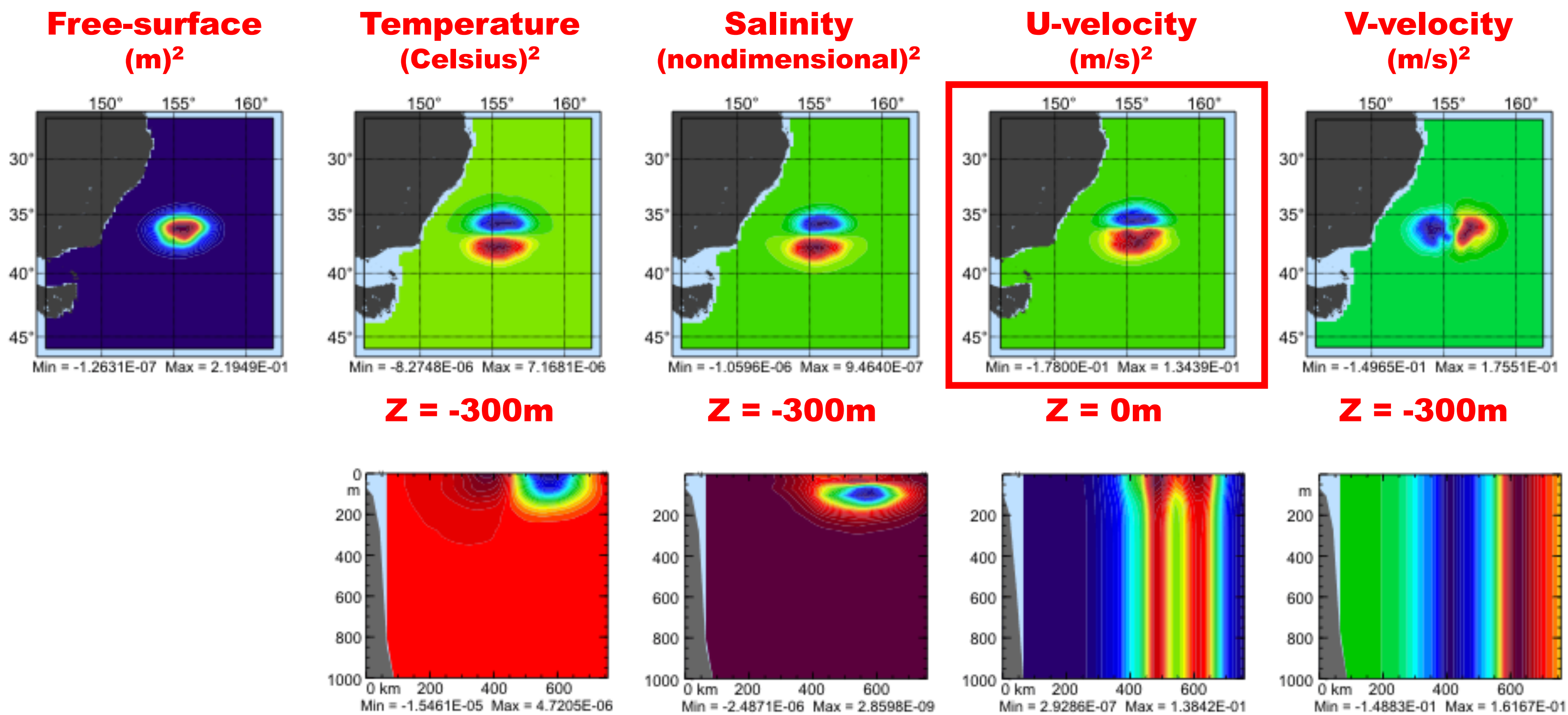
The cross-covariances are computed from a single sea surface height observation using multivariate physical balance relationships.

IS4DVAR Balanced Operator Covariances: EAC



The cross-covariances are computed from a single temperature observation at the surface using multivariate physical balance relationships.

IS4DVAR Balanced Operator Covariances: EAC



The cross-covariances are computed from a single U-velocity observation at the surface using multivariate physical balance relationships.

Initial condition *prior:*

$$\mathbf{B_x} = \mathbf{K_b \Sigma_x C_x \Sigma_x^T K_b^T}$$

Surface forcing *prior:*

$$\mathbf{B_f} = \mathbf{\Sigma_f C_f \Sigma_f^T}$$

No balance

Open boundary condition *prior:*

$$\mathbf{B_b} = \mathbf{\Sigma_b C_b \Sigma_b^T}$$

No balance

Model error *prior:*

$$\mathbf{Q} = \mathbf{K_b \Sigma_q C_q \Sigma_q^T K_b^T}$$

Preconditioning Again

General form of the *prior* error covariance matrix:

$$\mathbf{D} = \mathbf{K_b} \mathbf{\Sigma} \mathbf{C} \mathbf{\Sigma}^{\mathrm{T}} \mathbf{K_b^{\mathrm{T}}}$$

Introduce a new variable:

$$\mathbf{v} = \mathbf{U}^{-1} \delta \mathbf{z}$$

where

$$\mathbf{D} = \mathbf{U} \mathbf{U}^{\mathrm{T}}$$

$$\mathbf{U} = \mathbf{K_b} \mathbf{\Sigma} \mathbf{C}^{1/2}$$

The Conjugate Gradient Algorithm

cgradient.h in v-space to minimize $J(\mathbf{v})$

$$\hat{\mathbf{v}}_k = \mathbf{v}_k + \tau_k \mathbf{h}_k$$ trial step

$$\hat{\mathbf{g}}_k = \mathbf{C}^{\mathrm{T}/2}\boldsymbol{\Sigma}^{\mathrm{T}}\mathbf{K}_{\mathbf{b}}^{\mathrm{T}}\,\partial J/\partial\delta\hat{\mathbf{z}}_k$$ gradient @ trial step

$$\alpha_k = -\tau_k \mathbf{h}_k^{\mathrm{T}}\mathbf{g}_k \Big/ \left(\mathbf{h}_k^{\mathrm{T}}(\hat{\mathbf{g}}_k - \mathbf{g}_{\mathbf{k}})\right)$$ optimum step

$$\mathbf{v}_{k+1} = \mathbf{v}_k + \alpha_k \mathbf{h}_k$$ new starting point

$$\mathbf{g}_{k+1} = \mathbf{g}_k + (\alpha_k/\tau_k)\left(\hat{\mathbf{g}}_k - \mathbf{g}_k\right)$$ gradient @new point

$$\beta_{k+1} = \mathbf{g}_{k+1}^{\mathrm{T}}\mathbf{g}_{k+1} / \mathbf{g}_k^{\mathrm{T}}\mathbf{g}_k$$

$$\mathbf{h}_{k+1} = -\mathbf{g}_{k+1} + \beta_{k+1}\mathbf{h}_k$$ new descent direction

$$\delta\mathbf{z}_{k+1} = \mathbf{K}_{\mathbf{b}}\boldsymbol{\Sigma}\mathbf{C}^{1/2}\mathbf{v}_{k+1}$$ project into state-space

The Lanczos Connection

Gain (primal form):

$$\mathbf{K} = \mathbf{K_b}\boldsymbol{\Sigma}\mathbf{C}^{1/2}(\mathbf{I}+\mathbf{D}^{\mathrm{T}/2}\mathbf{G}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{G}\mathbf{D}^{1/2})^{-\mathbf{1}}\mathbf{C}^{\mathrm{T}/2}\boldsymbol{\Sigma}^{\mathrm{T}}\mathbf{K}_{\mathbf{b}}^{\mathrm{T}}\mathbf{G}^{\mathrm{T}}\mathbf{R}^{-1}$$

Practical gain matrix:

$$\tilde{\mathbf{K}}_k = \mathbf{K_b}\boldsymbol{\Sigma}\mathbf{C}^{1/2}\mathbf{V}_k\mathbf{T}_k^{-1}\mathbf{V}_k^{\mathrm{T}}\mathbf{C}^{\mathrm{T}/2}\boldsymbol{\Sigma}^{\mathrm{T}}\mathbf{K}_{\mathbf{b}}^{\mathrm{T}}\mathbf{G}^{\mathrm{T}}\mathbf{R}^{-1}$$

Useful for diagnostic applications (Lecture 5)
(The Lanczos vectors are in ADJname)

Background Quality Control
(define BGQC)

- **Some observations will be outliers for a variety of reasons (e.g. bad obs, bad model, or both, non-Gaussian behavior, etc)**
- **It is important to exclude these data from the data assimilation system since they can adversely affect the analysis.**
- **Observations are screened in ROMS according to the background error and observation error variances.**
- **The approach used in ROMS parallels that used in the ECMWF NWP system.**
- **An observation is rejected if the normalized innovation exceeds a specified multiple of the standard expected error.**
- **Specifically:**

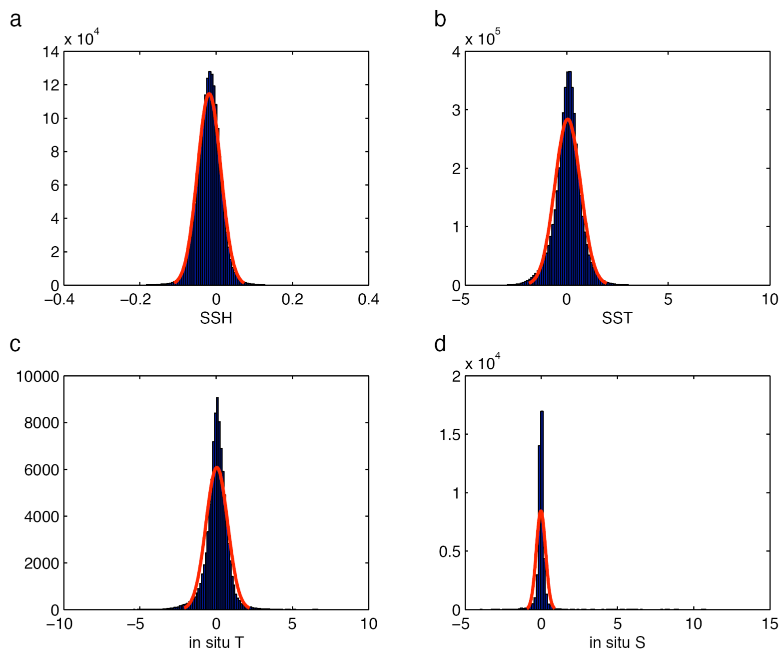
$$\left(y_i - H_i\left(\mathbf{x}_b\right)\right)^2 > \alpha^2\left(1+\sigma_o^2/\sigma_b^2\right)$$

- α **is a user-specified parameter.**

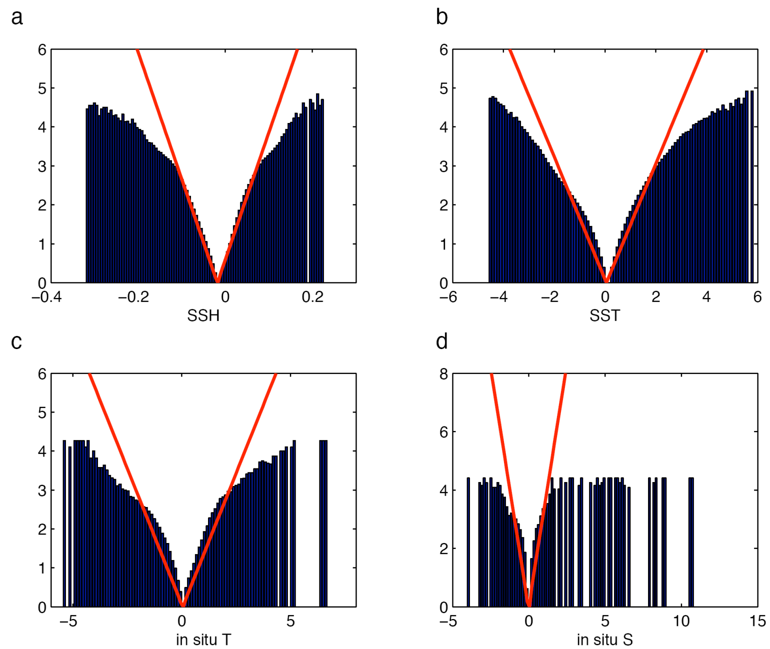
(see Andersson and Järvinen (1999, *QJRMS*, 125, 697-722).

Background Quality Control

(define BGQC)



Frequency distribution, *f*, (i.e. pdf) of 4D-Var innovations.



Distribution of $\hat{f} = \sqrt{-2\ln(f/\max(f))}$. The red lines show $y = \pm\left|x/(\sigma_b^2 + \sigma_o^2)^{1/2}\right|$. Choose α based on red line.

Issues & Things to do

- Relax horizontal homogeneity and isotropy of L_x and L_y correlation lengths.
- Elliptic solver for free-surface balance:
  - cannot handle islands at the moment
  - add additional boundary condition option
- Cannot assimilate obs right at the open boundary.
- Div and curl of $\delta\tau$ are not constrained.
- No restart option for 4D-Var.
- Variational bias correction.
- Variational QC.

Summary

- Lanczos formulation of CG: cgradient.h
- Lanczos vectors saved in ADJname
- Covariance models using diffusion operators:

  define VCONVOLUTION

  define IMPLICIT_VCONV, etc

  $\mathbf{\Sigma}$ - tl_variability.F

  $\mathbf{\Sigma}^{T}$ - ad_variability.F

  $\mathbf{C}^{1/2}$- tl_convolution.F

  $\mathbf{C}^{T/2}$- ad_convolution.F
- Multivariate balance operator:

  define BALANCE_OPERATOR

  $\mathbf{K_b}$ - tl_balance.F

  $\mathbf{K_b^T}$- ad_balance.F

- Background QC: define BGQC

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