

Constructing a background error covariance model for variational ocean data assimilation

...with an emphasis on the tropics



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Acknowledgments:

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Outline

- The variational assimilation problem.
- Some remarks about **B**.
- General approach to modelling **B** for the ocean:
 - modelling correlation functions
 - parametrising variances
 - including balance and conservation constraints
- Examples from 3D-Var and 4D-Var with the OPA OGCM.

The variational assimilation problem

Minimize $J = J_b + J_o$

Background term

$$J_b = \frac{1}{2} (\mathbf{x} - \mathbf{x}^b)^T \mathbf{B}^{-1} (\mathbf{x} - \mathbf{x}^b)$$

Observation term

$$J_o = \frac{1}{2} (G(\mathbf{x}) - \mathbf{y}^o)^T \mathbf{R}^{-1} (G(\mathbf{x}) - \mathbf{y}^o)$$

The incremental approximation

Minimize $J = J_b + J_o$

Background term

$$J_b = \frac{1}{2} \delta \mathbf{x}^T \mathbf{B}^{-1} \delta \mathbf{x}$$

where $\delta \mathbf{x} = \mathbf{x} - \mathbf{x}^b$

Observation term (quadratic)

$$J_o = \frac{1}{2} (\mathbf{G} \delta \mathbf{x} - \mathbf{d})^T \mathbf{R}^{-1} (\mathbf{G} \delta \mathbf{x} - \mathbf{d})$$

where $\mathbf{d} = \mathbf{y}^o - G(\mathbf{x}^b)$

Preconditioning with \mathbf{B}

Background term

$$J_b = \frac{1}{2} \delta \mathbf{x}^T \mathbf{B}^{-1} \delta \mathbf{x}$$

Preconditioned background term

Define $\mathbf{v} = \mathbf{U}^{-I} \delta \mathbf{x}$

where $\mathbf{B}^{-1} = \left(\mathbf{U}^{-I}\right)^T \left(\mathbf{U}^{-I}\right)$ and $\mathbf{B} = \mathbf{U} \mathbf{U}^T$

then $J_b = \frac{1}{2} \mathbf{v}^T \mathbf{v}$

Preconditioning with \mathbf{B}

- \mathbf{v} is the control vector for the minimization problem.
- On the first **inner** iteration we take $\delta\mathbf{x} = 0$ so $\mathbf{v} = 0$.
- Consequently, on each inner iteration, we only need to specify the **inverse of the change of variable**:

$$\delta\mathbf{x} = \mathbf{U} \mathbf{v}$$

and its **adjoint** for computing the gradient of J_o

$$\mathbf{v}^* = \mathbf{U}^T \delta\mathbf{x}^*$$

Some general remarks about **B**

- **B** largely determines how observational increments are smoothed in space and transferred between different model variables.

Linear solution:
$$\delta \mathbf{x}^a = \mathbf{B} \mathbf{G}^T \underbrace{(\mathbf{G} \mathbf{B} \mathbf{G}^T + \mathbf{R})^{-1}}_{\hat{\mathbf{x}}} \mathbf{d}$$

- **B** is important in both 3D-Var and 4D-Var.
- **B** is also important for ensemble methods for generating realistic initial perturbations (using the square root factor **U**).

Some general remarks about **B**

- **Difficulty diagnosing statistics:** there is not enough (and never will be) enough information to determine all the elements of **B** (typically $> O(10^{11})$).
- **Computational difficulty:** **B** is too large to store as a full matrix.
- **B** must be approximated using a **model**.
- In 3D-Var/4D-Var, **B** must be implemented as an **operator** :

$$\hat{\mathbf{x}} \xrightarrow{\mathbf{B}} \mathbf{x}$$

unless the analysis space is sufficiently small (e.g., coefficients of a few ensemble members or EOFs).

Some general remarks about **B**

- Constructing an effective **B** model involves substantial development and tuning!

Some specific remarks about **B** for the ocean

- The background state variables in an OGCM:
 - temperature (T), salinity (S), sea-surface height (SSH), horizontal velocity (u, v).
 - (e.g., Weaver et al. 2003 - MWR; Vialard et al. 2003 - MWR)

but may also include the surface forcing fields:

 - wind stress ($taux, tauy$), heat flux (Q), evaporation-precipitation ($E-P$).
 - (e.g., Bonekamp et al. 2001 – JGR)
- Ocean observations are relatively sparse so it is difficult to estimate background error statistics from innovations. Considerable spatial and temporal averaging is required (e.g., Martin et al. 2002).

Some specific remarks about **B** for the ocean

- With few observations the role of **B** is critical for exploiting the available data-sets effectively (e.g., surface altimeter data).
- Added complexity due to the presence of **continental boundaries** (natural inhomogeneity, boundary conditions, scales, spectra, balance).
- Rich variety of scales: **mesoscale** (Gulf Stream, Kuroshio regions) $\sim O(10\text{km})$ and **synoptic** scale (tropics) $\sim O(100\text{km})$. (*e.g., see Martin et al. 2002*)

A general approach for modelling **B**

- By definition,

$$\mathbf{B} = \begin{pmatrix} E[T' T'^T] & E[T' S'^T] & E[T' \eta'^T] & E[T' u'^T] & E[T' v'^T] \\ E[S' T'^T] & E[S' S'^T] & E[S' \eta'^T] & E[S' u'^T] & E[S' v'^T] \\ E[\eta' T'^T] & E[\eta' S'^T] & E[\eta' \eta'^T] & E[\eta' u'^T] & E[\eta' v'^T] \\ E[u' T'^T] & E[u' S'^T] & E[u' \eta'^T] & E[u' u'^T] & E[u' v'^T] \\ E[v' T'^T] & E[v' S'^T] & E[v' \eta'^T] & E[v' u'^T] & E[v' v'^T] \end{pmatrix}$$

where T' , S' etc. denote the difference between the background and “true” values of the state variables (assumed unbiased).

A general approach for modelling **B**

(cf. Derber & Bouttier 1999 - Tellus)

- Suppose (to be justified shortly)

“balanced” variables

“unbalanced” variables

$$\begin{aligned} T' &= T'_B \\ S' &= S'_B + S'_U = \underbrace{K_{ST} T'}_{S'_B} + S'_U \\ \eta' &= \eta'_B + \eta'_U = \underbrace{K_{\eta T} T' + K_{\eta S} S'}_{\eta'_B} + \eta'_U \\ u' &= u'_B + u'_U = \underbrace{K_{uT} T' + K_{uS} S' + K_{u\eta} \eta'}_{u'_B} + u'_U \\ v' &= v'_B + v'_U = \underbrace{K_{vT} T' + K_{vS} S' + K_{v\eta} \eta'}_{v'_B} + v'_U \end{aligned}$$

A general approach for modelling \mathbf{B}

- Substitute the expressions for T', S', η', u', v' into the general expression for \mathbf{B} and assume that $T'_B, S'_U, \eta'_U, u'_U, v'_U$ are mutually uncorrelated.
- Then we can write $\mathbf{B} = \mathbf{K} \mathbf{B}_U \mathbf{K}^T$ where

$$\mathbf{K} = \begin{pmatrix} I & 0 & 0 & 0 & 0 \\ K_{ST} & I & 0 & 0 & 0 \\ K_{\eta T} & K_{\eta S} & I & 0 & 0 \\ K_{uT} & K_{uS} & K_{u\eta} & I & 0 \\ K_{vT} & K_{vS} & K_{v\eta} & 0 & I \end{pmatrix}, \quad \mathbf{B}_U = \begin{pmatrix} B_{TT} & 0 & 0 & 0 & 0 \\ 0 & B_{S_US_U} & 0 & 0 & 0 \\ 0 & 0 & B_{\eta_U \eta_U} & 0 & 0 \\ 0 & 0 & 0 & B_{u_U u_U} & 0 \\ 0 & 0 & 0 & 0 & B_{v_U v_U} \end{pmatrix}$$

where $B_{TT} \equiv E[T' T'^T] = E[T'_B T'^T_B]$, $B_{S_US_U} \equiv E[S'_U S'^T_U]$, etc.

A strong constraint approach for modelling \mathbf{B}

- Consider the special case where $S'_U = \eta'_U = u'_U = v'_U = 0$

$$\mathbf{B} = \underbrace{\begin{pmatrix} I \\ K_{ST} \\ K_{\eta T} \\ K_{uT} \\ K_{vT} \end{pmatrix}}_{\mathbf{K}} B_{TT} \underbrace{\left(I \quad K_{ST}^T \quad K_{\eta T}^T \quad K_{uT}^T \quad K_{vT}^T \right)}_{\mathbf{K}^T}$$

- Here \mathbf{K} is a “strong constraint” (*Lorenc 2002*).
- We only need a univariate statistical model for

$$B_{TT} = \Sigma_T C_{TT} \Sigma_T$$

- All other covariances are determined implicitly from B_{TT} using \mathbf{K} and \mathbf{K}^T .

A strong constraint approach for modelling **B**

- **B** has a **nullspace** associated with the “unbalanced” components S'_U , η'_U , u'_U and v'_U .
- The **reduced** control variable is

$$v_T = \Sigma_T^{-1} C_{TT}^{-1/2} \mathbf{K}^{-I} \delta \mathbf{x}$$
$$\left(\begin{array}{c} \\ \\ \\ \end{array} \right) = \left(\begin{array}{c} \\ \\ \\ \end{array} \right) \left(\begin{array}{c} \\ \\ \\ \end{array} \right) \left(\begin{array}{c} \\ \\ \\ \end{array} \right)$$

A strong constraint approach for modelling **B**

- Recall that for the preconditioned variational problem, we need to specify only the inverse of the change of variable:

$$\delta \mathbf{x} = \mathbf{K} \Sigma_T \mathbf{C}_{TT}^{1/2} \mathbf{v}_T$$

and its adjoint for computing the gradient of J_0 of :

$$\mathbf{v}_T^* = (\mathbf{C}_{TT}^{1/2})^T \Sigma_T \mathbf{K}^T \delta \mathbf{x}^*$$

A strong constraint approach for modelling **B**

- Recall that for the preconditioned variational problem, we need to specify only the inverse of the change of variable:

$$\delta \mathbf{x} = \mathbf{K} \Sigma_T \mathbf{C}_{TT}^{1/2} \mathbf{v}_T$$

and its adjoint for computing the gradient of J_o :

$$\mathbf{v}_T^* = \left(\mathbf{C}_{TT}^{1/2} \right)^T \Sigma_T \mathbf{K}^T \delta \mathbf{x}^*$$

Univariate correlation modelling using a diffusion equation

(Derber & Rosati 1989 - JPO; Egbert et al. 1994 - JGR; Weaver & Courtier 2001 - QJRMS)

1D case:

■ Consider $\frac{\partial \eta}{\partial t} - \kappa \frac{\partial^2 \eta}{\partial z^2} = 0$ with constant $\kappa > 0$.

on $-\infty < z < \infty$ with $\eta(z, t) \rightarrow 0$ as $z \rightarrow \pm\infty$

■ Integrate from $t = 0$ and $t = T$ with $\eta(z, 0)$ as IC:

$$\eta(z, T) = \frac{1}{\sqrt{4\pi\kappa T}} \int_{z'} e^{-(z-z')^2 / 4\kappa T} \eta(z', 0) dz'$$

Solution:
$$\eta(z, T) = \frac{1}{\sqrt{4\pi\kappa T}} \int_{z'} e^{-(z-z')^2/4\kappa T} \eta(z', 0) dz'$$

■ This integral solution defines, after normalization, a correlation operator \mathcal{C} :

$$\eta(z, 0) \xrightarrow{\mathcal{C}} \sqrt{4\pi\kappa T} \eta(z, T)$$

■ The kernel of \mathcal{C} is a Gaussian correlation function

$$f(z; \kappa T) = e^{-z^2/2L^2}$$

where $L = \sqrt{2\kappa T}$ is the length scale.

■ Basic idea: To compute the action of \mathcal{C} on a discrete grid we can iterate a diffusion operator.

This is much cheaper than solving an integral equation directly.

Theoretical generalization: a family of isotropic correlation functions on the sphere

(Wahba 1985; Weaver & Courtier 2001-QJRMS)

- Consider the differential operator

$$\eta(\lambda, \phi) = \left(1 - \sum_{p=1}^P \alpha_p (-\nabla^2)^p \right)^{-M} \hat{\eta}(\lambda, \phi)$$

with constant $\alpha_p > 0$ and integers $M > 0$, $P > 0$.

- Consider solutions of the form

$$\eta(\lambda, \phi) = \sum_{n=0}^{\infty} \sum_{m=-n}^n \eta_n^m Y_n^m(\lambda, \phi)$$

where $Y_n^m(\lambda, \phi)$ are the spherical harmonics, with

$$\nabla^2 Y_n^m = \left(-n(n+1) / a^2 \right) Y_n^m$$

Theoretical generalization: a family of isotropic correlation functions on the sphere

- The integral representation of the differential operator is

$$\eta(\lambda, \phi) = \frac{1}{4\pi a^2} \int_{\Sigma} f(\theta) \hat{\eta}(\lambda, \phi) d\Sigma \quad (\text{A})$$

where $f(\theta) = \sum_{n=0}^{\infty} f_n P_n^0(\cos\theta)$

and $f_n(\alpha_p, P, M) = \sqrt{2n+1} \left(1 + \frac{1}{M} \sum_{p=1}^P \alpha_p (n(n+1)/a^2)^p \right)^{-M}$

- The $f_n > 0$ so (A) is a valid (positive definite) covariance operator (e.g., see Gaspari and Cohn 1999 - QJRMS).

Theoretical generalization: a family of isotropic correlation functions on the sphere

- The length scale L of the correlation functions can be defined by (*Daley 1991*):

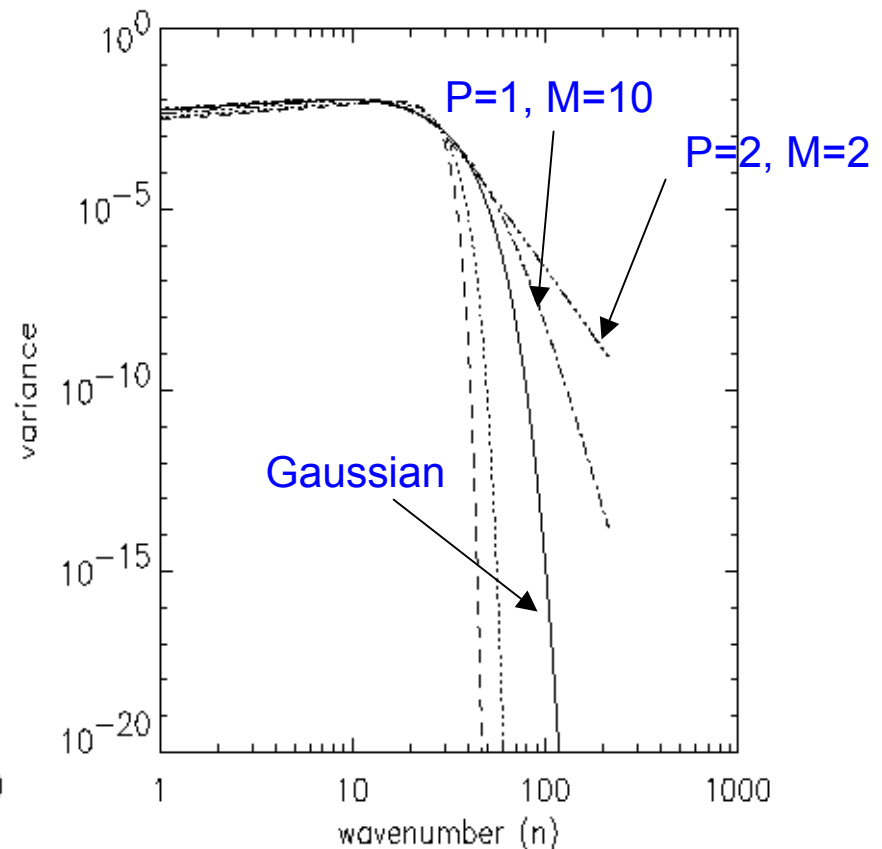
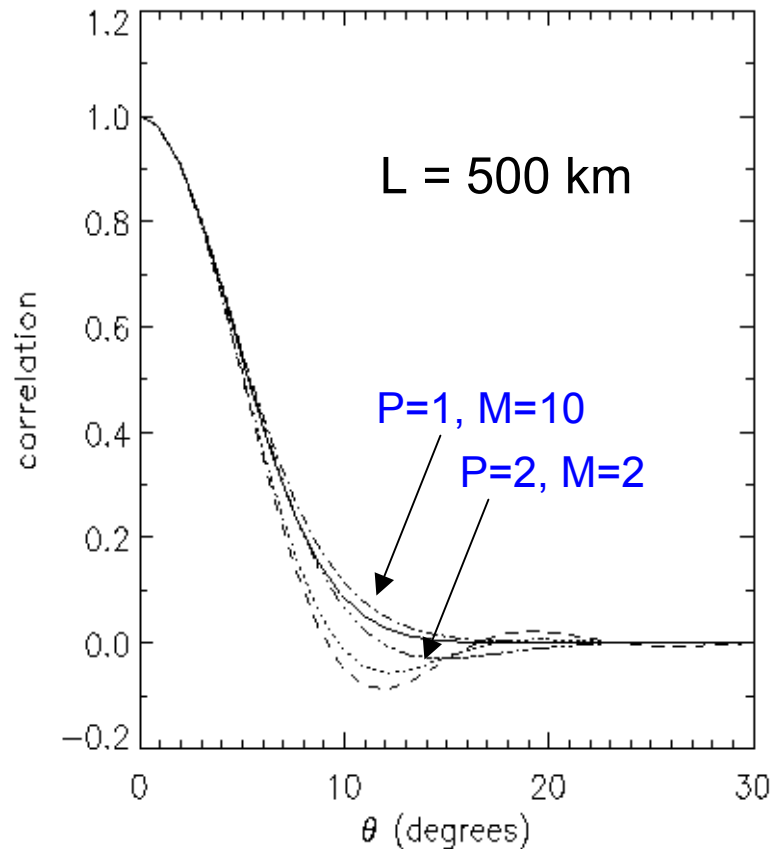
$$L^2 = - \frac{f}{\nabla^2 f} \Big|_{\theta=0}$$

Examples

$$f(\theta) = \sum_{n=0}^{\infty} f_n P_n^0(\cos \theta) \quad f_n = \sqrt{2n+1} \left(1 + \frac{1}{M} \sum_{p=1}^P \alpha_p \left(n(n+1)/a^2 \right)^p \right)^{-M}$$

shape $f(\theta)$

spectrum f_n



Theoretical generalization: a family of isotropic correlation functions on the sphere

- We can identify the previous differential operator as the solution of a **generalized diffusion equation (GDE)**

$$\frac{\partial \eta}{\partial t} + \sum_{p=1}^P \kappa_p (-\nabla^2)^p \eta = 0$$

using **implicit time discretization**

$$\eta(\lambda, \phi, T) = \left(1 - \sum_{p=1}^P \kappa_p \Delta t (-\nabla^2)^p \right)^{-M} \eta(\lambda, \phi, 0) \quad (\text{A})$$

where $\kappa_p \Delta t \leftrightarrow \alpha_p$; $\eta(\lambda, \phi, 0) \leftrightarrow \hat{\eta}(\lambda, \phi)$
 $T \leftrightarrow M \Delta t$; $\eta(\lambda, \phi, T) \leftrightarrow \eta(\lambda, \phi)$

- We can use direct or iterative algorithms for solving (A) in grid-point space.

Some remarks on numerical implementation

- The full correlation operator is formulated in **grid-point space** as a sequence of operators

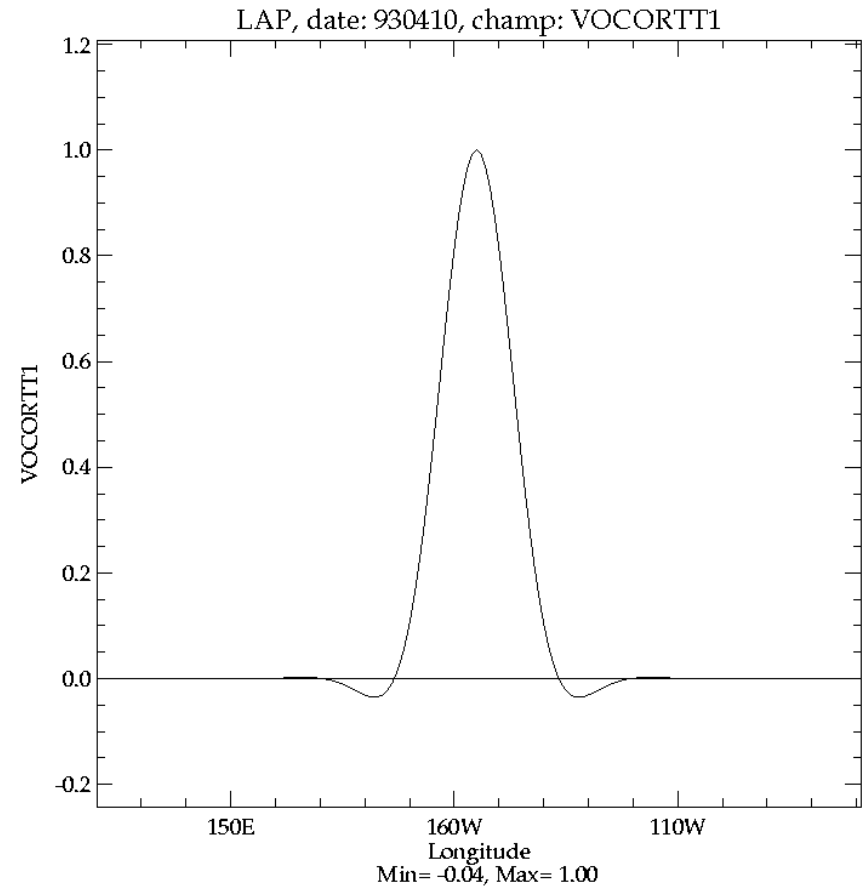
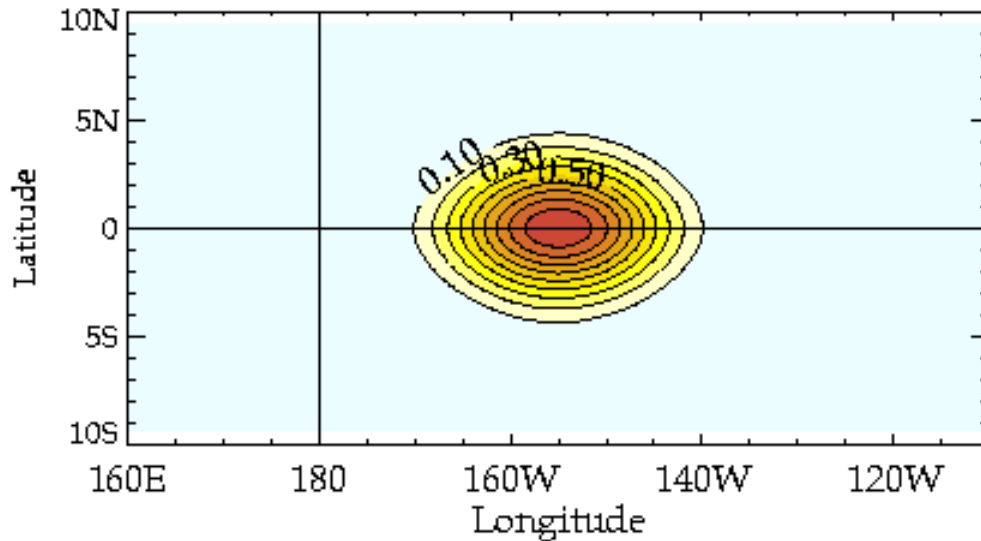
$$\begin{aligned}\mathbf{C} &= \mathbf{\Lambda} \mathbf{L}^{1/2} \mathbf{W}^{-1} \mathbf{L}^{T/2} \mathbf{\Lambda} \\ &= \underbrace{\left(\mathbf{\Lambda} \mathbf{L}^{1/2} \mathbf{W}^{-1/2} \right)}_{\mathbf{C}^{1/2}} \underbrace{\left(\mathbf{W}^{-1/2} \mathbf{L}^{T/2} \mathbf{\Lambda} \right)}_{\mathbf{C}^{T/2}}\end{aligned}$$

- \mathbf{L} is the diffusion operator and is formulated in 3D as a product $\mathbf{L} = \mathbf{L}_h \mathbf{L}_v$ of a 2D (horizontal) and 1D (vertical) operator.
- \mathbf{W} is a diagonal matrix of volume elements, and appears in \mathbf{C} because of the self-adjointness of \mathbf{L} .
- The factor $\mathbf{L}^{1/2}$ means $M/2$ iterations of the diffusion operator.

GDE-generated correlation functions

Example: T-T correlations at the equator

P=2, M=4



Some remarks on numerical implementation

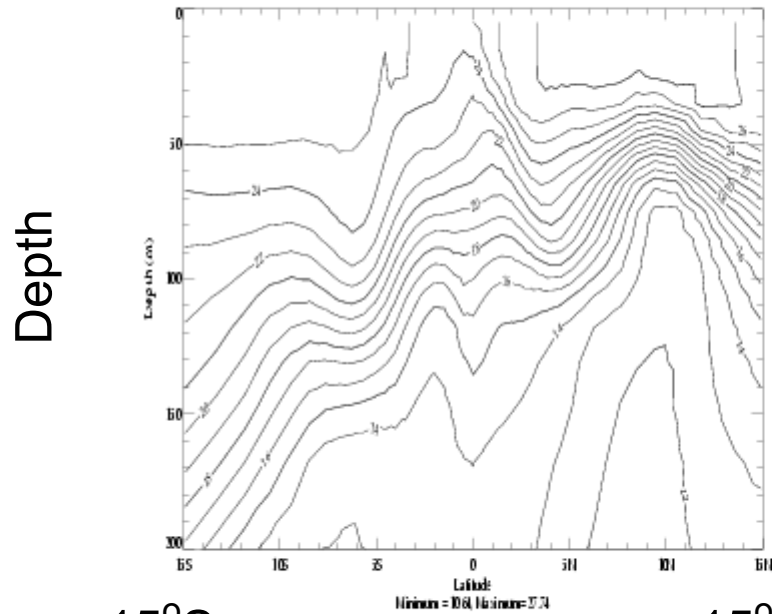
- We can let $\nabla^2 \rightarrow \nabla \cdot R \nabla$ where R is a diffusion tensor that can be used to stretch and/or rotate the coordinates in the correlation model to account for anisotropic or flow-dependent structures.
- BCs are imposed directly within the discrete expression for ∇^2 using a land-ocean mask.
- Λ contains normalization factors to ensure the variances of \mathbf{C} are equal to one.
- The diffusion and recursive filter (*Lorenc 1991 – QJRMS; Purser et al. 2003 - MWR; Derber lecture*) approaches to correlation modelling have many similarities.

GDE-generated correlation functions

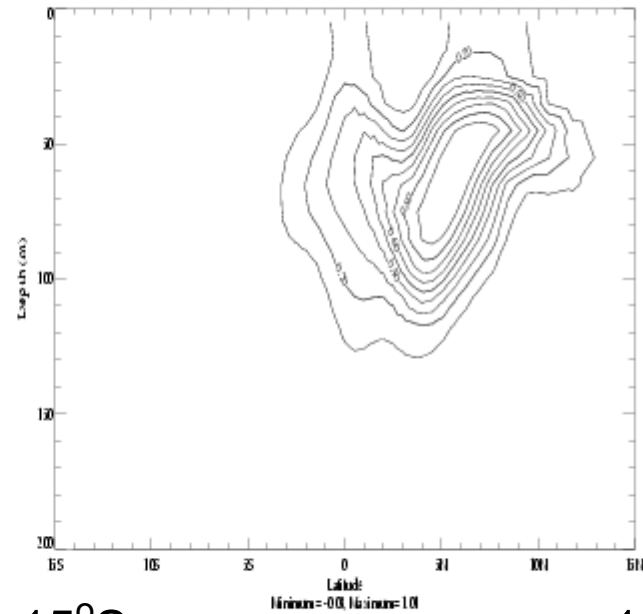
Example: flow-dependent correlations

(Weaver & Courtier 2001-QJRM; cf. Riishojgaard 1998-Tellus;
Daley & Barker 2001-MWR)

Background isothermals



T-T correlations



15°S

15°N

15°N

Some remarks on numerical implementation

- We can let $\nabla^2 \rightarrow \nabla \cdot R \nabla$ where R is a diffusion tensor that can be used to stretch and/or rotate the coordinates in the correlation model to account for anisotropic or flow-dependent structures.
- BCs are imposed directly within the discrete expression for ∇^2 using a land-ocean mask.
- Λ contains normalization factors to ensure the variances of \mathbf{C} are equal to one.
- The diffusion and recursive filter (*Lorenc 1991 – QJRMS; Purser et al. 2002 – MWR; Derber lecture*) approaches to correlation modelling have many similarities.

The normalization matrix Λ

- The elements of Λ are the inverse of the square root of the diagonal elements of the cov. filter

$$\mathbf{L}^{1/2} \mathbf{W}^{-1} \mathbf{L}^{T/2}$$

- With constant “diffusion” coefficient and in the absence of boundaries

$$\Lambda = \lambda \mathbf{I}$$

- With spatially varying “diffusion” coefficients or in the presence of boundaries

$$\Lambda = \text{diag} (\lambda_i), \quad i = 1, \dots, N$$

Computing the normalization factors

- Define the square root of the covariance filter

$$\hat{\mathbf{v}} = \mathbf{L}^{1/2} \mathbf{W}^{-1/2} \mathbf{v}$$

- Algorithm 1 : Exact

– Let $\mathbf{v} = (0, \dots, 0, \underset{\substack{\uparrow \\ i\text{-th grid point}}}{1}, 0, \dots, 0)$

– Then $\lambda_i^{-2} = \hat{\mathbf{v}}^T \hat{\mathbf{v}}$

– One application of the square root filter is needed for each grid point $i \implies$ Expensive!

Computing the normalization factors

- Define the square root of the covariance filter

$$\hat{\mathbf{v}} = \mathbf{L}^{1/2} \mathbf{W}^{-1/2} \mathbf{v}$$

- Algorithm 2 : Randomization

(Fisher & Courtier 1995; Andersson lecture)

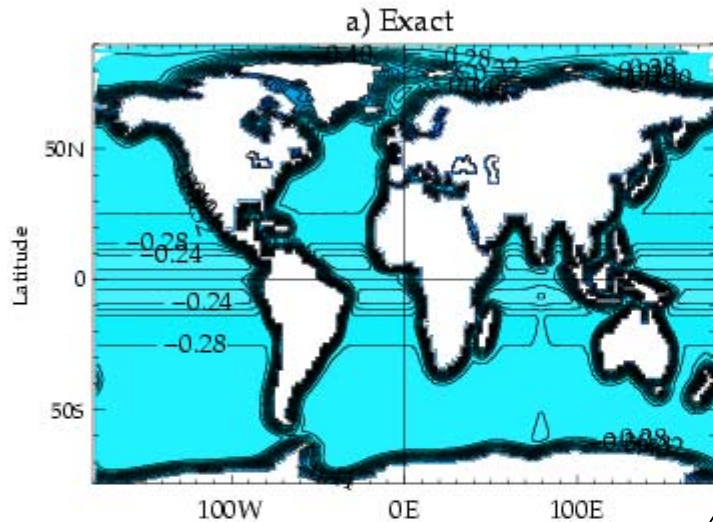
– Choose \mathbf{v} such that $E[\mathbf{v}] = \mathbf{0}$ and $E[\mathbf{v} \mathbf{v}^T] = \mathbf{I}$

– Then $\lambda_i^{-2} \approx \text{diag}_i \left(\frac{1}{Q-1} \sum_{q=1}^Q \hat{\mathbf{v}}_q \hat{\mathbf{v}}_q^T \right)$

– The estimate of λ_i improves as Q gets large.

– Estimate of the randomization error = $1/\sqrt{2Q}$

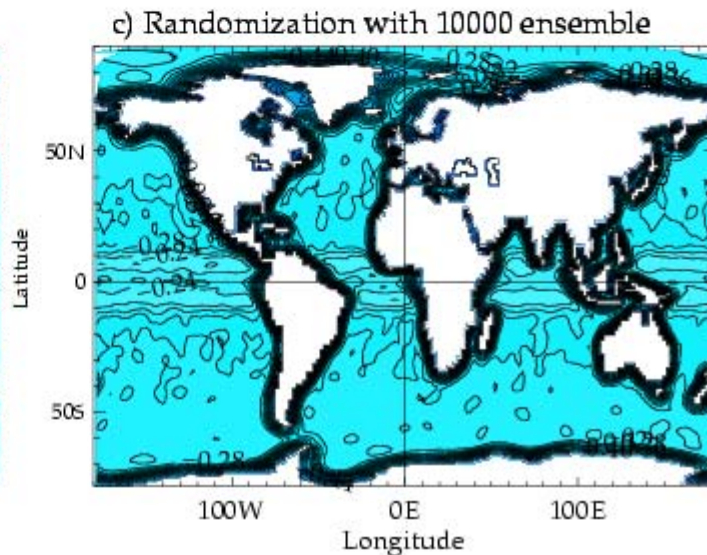
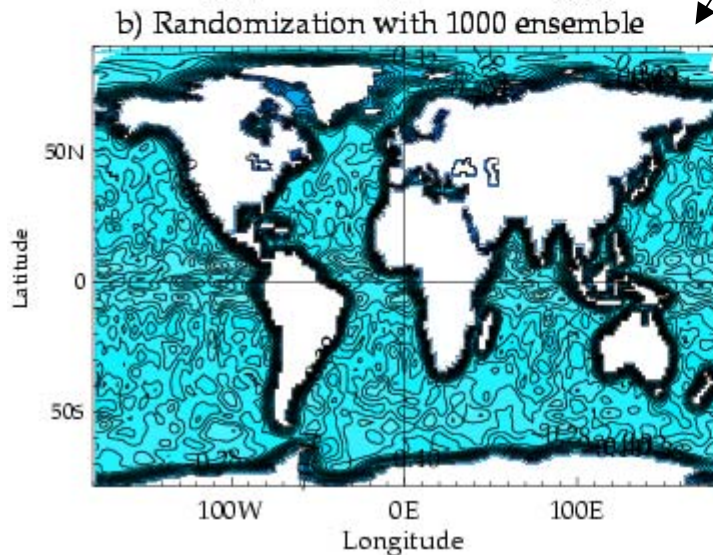
Computing the normalization factors



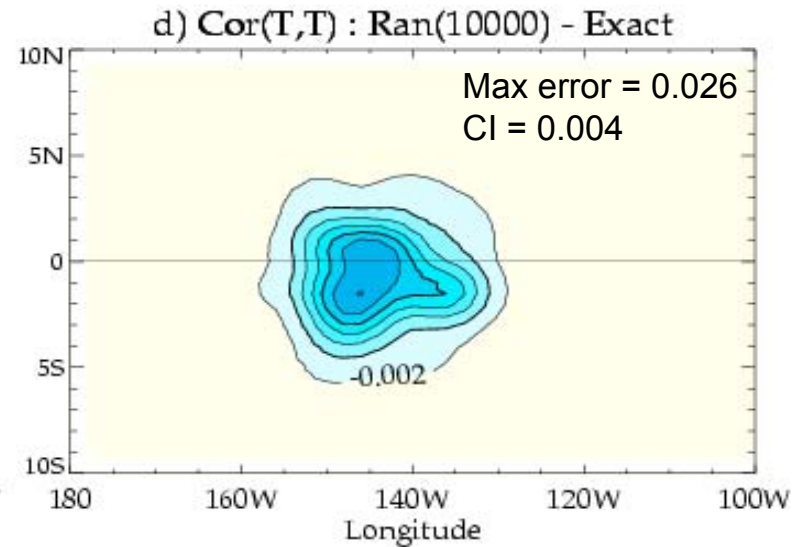
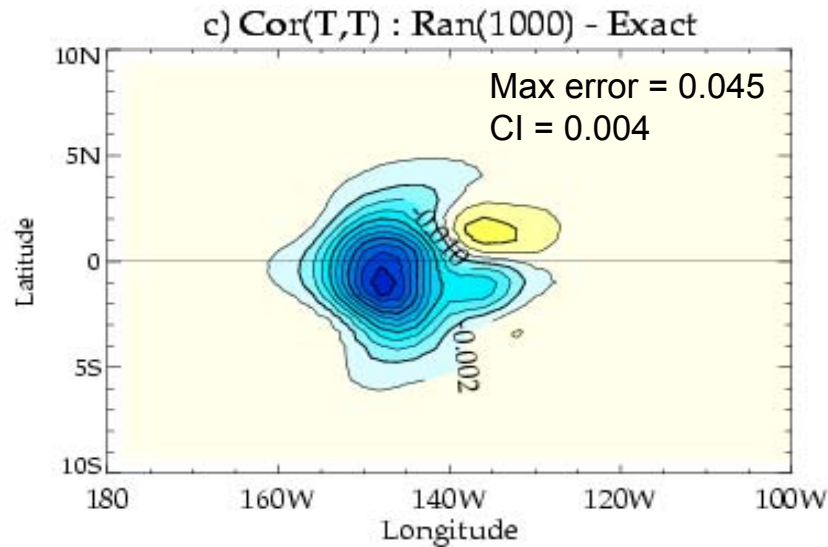
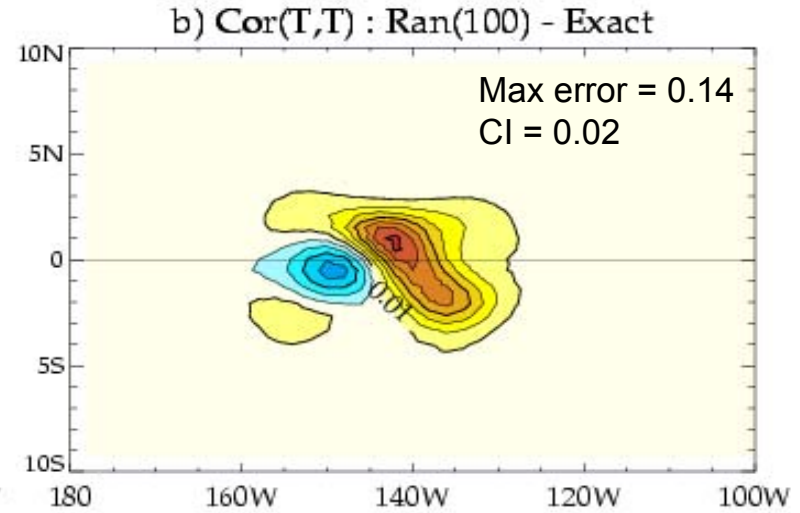
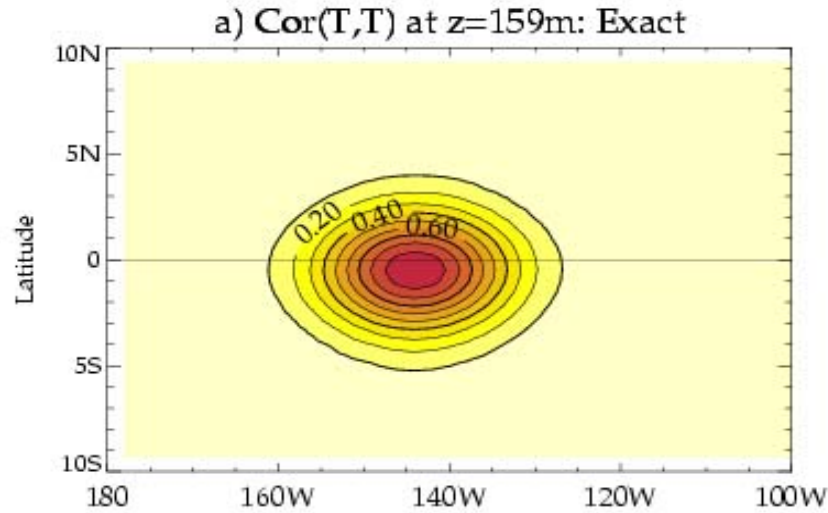
CPU ~ 51 hrs for one level!

CPU ~ 1hr for all grid pts
Std error ~ 2.2%

CPU ~ 10 hrs for all grid pts
Std error ~ 0.7%



Impact of randomization on the correlations



A strong constraint approach for modelling **B**

- Recall that for the preconditioned variational problem we need to specify only the inverse of the change of variable

$$\delta \mathbf{x} = \mathbf{K} \left(\Sigma_T \right) C_{TT}^{1/2} \mathbf{v}_T$$

and its adjoint for computing the gradient of J_o :

$$\mathbf{v}_T^* = \left(C_{TT}^{1/2} \right)^T \left(\Sigma_T \right) \mathbf{K}^T \delta \mathbf{x}^*$$

A flow-dependent parametrisation for Σ_T

(Behringer et al. 1998 - MWR ; Alves et al. 2003 - QJRMS)

- Assume that the elements σ_T^b of Σ_T are a function of the background vertical temperature gradient $\partial T^b / \partial z$.

Physical justification:

- Errors in the temperature (T) state are expected to be largest in regions of strong variability; e.g., in the thermocline where $\partial T^b / \partial z$ is large.
- Assuming that the background T profile (T^b) and “true” T profile (T^t) differ because of a vertical displacement error δz then (cf. Cooper and Haines 1996 – JGR)

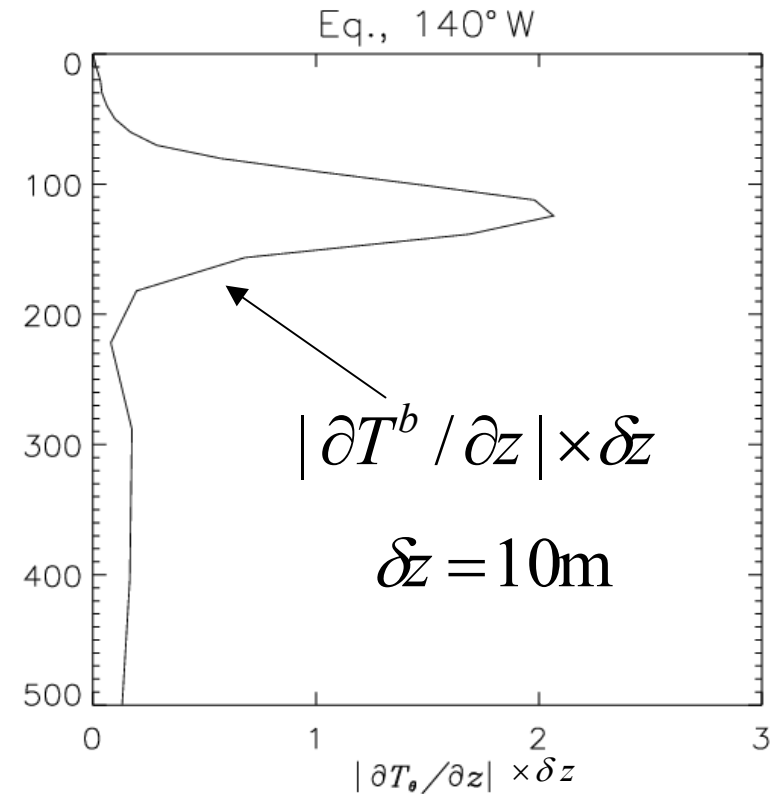
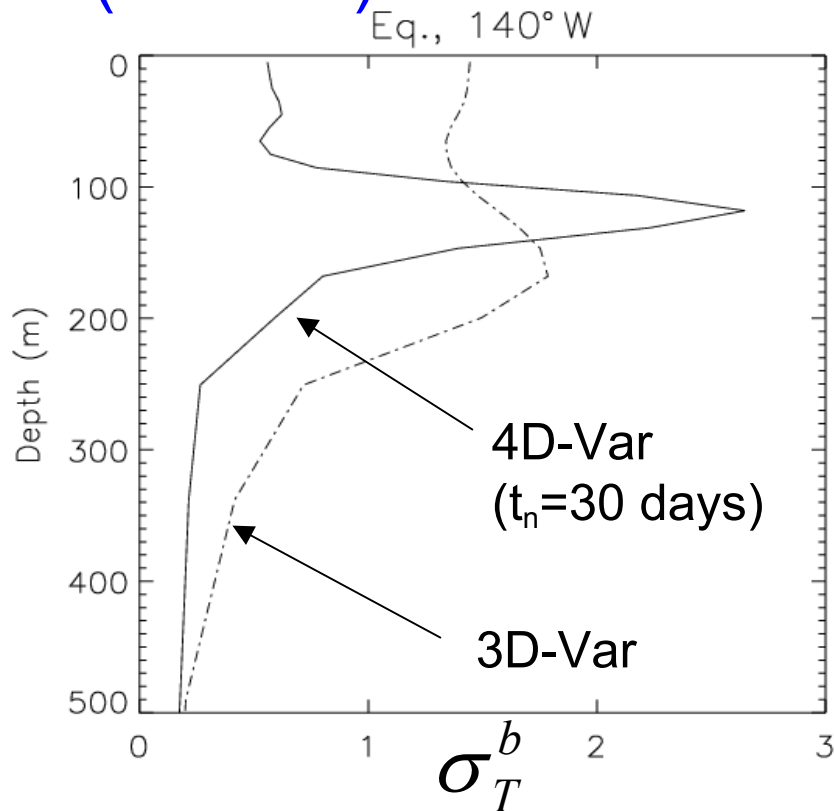
$$T^t(z) = T^b(z + \delta z) \approx T^b(z) + \underbrace{\left(\partial T^b / \partial z\right) \times \delta z}_{\varepsilon^b}$$

Diagnosing σ_T^b in 4D-Var

(Weaver et al. 2003 – MWR)

In 3D-Var: $\mathbf{P}^b(t_n) = \mathbf{B}$

In 4D-Var: $\mathbf{P}^b(t_n) = \mathbf{M}(t_n, t_0) \mathbf{B} \mathbf{M}(t_n, t_0)^T$
(cf. EKF)



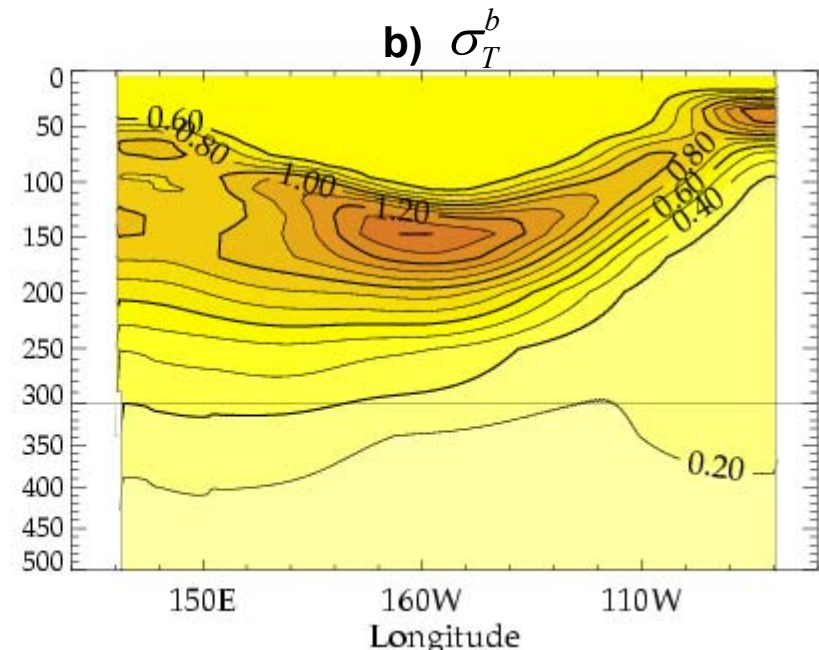
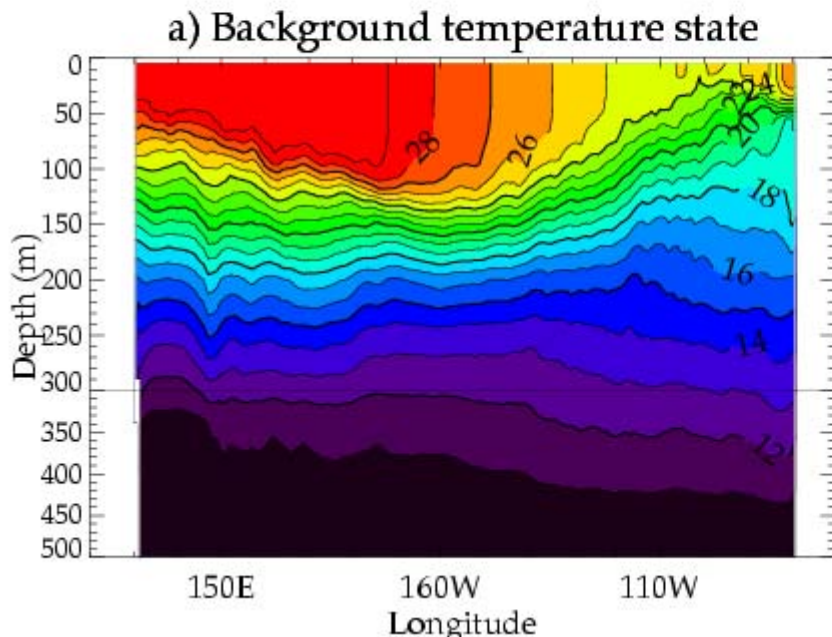
A flow-dependent parametrisation for σ_T^b

Example:

$$\sigma_T^b(\lambda, \phi, z) = \begin{cases} \sigma_{\min}^b & \text{in the mixed layer} \\ \min\left(\left(\partial T^b / \partial z\right) \times \delta z, \sigma_{\max}^b\right) & \text{below the mixed layer} \end{cases}$$

with $\sigma_{\min}^b = 0.5^\circ\text{C}$, $\sigma_{\max}^b = 1.5^\circ\text{C}$ and $\delta z = 10\text{m}$

$\sigma_T^b(\lambda, \phi, z)$ is smoothed in each level using the correlation filter



A strong constraint approach for modelling **B**

- Recall that for the preconditioned variational problem, we need to specify only the inverse of the change of variable:

$$\delta \mathbf{x} = \mathbf{K} \Sigma_T C_{TT}^{1/2} \mathbf{v}_T$$

and its adjoint for computing the gradient of J_o :

$$\mathbf{v}_T^* = (C_{TT}^{1/2})^T \Sigma_T \mathbf{K}^T \delta \mathbf{x}^*$$

A general approach for modelling **B**

(cf. Derber & Bouttier 1999 - Tellus)

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A flow-dependent model for K_{ST}

(Ricci et al. 2003)

- Use a local **T-S relation** from the background state
(Troccoli and Haines 1999 - JAOT; Troccoli et al. 2002 - JPO)

$$S^b = S(T^b)$$

- Water mass T-S properties are largely preserved in regions where **isentropic** processes dominate (e.g., in the tropical thermocline).
- For small perturbations T' about T^b

$$S(T) = S(T^b + T') \cong S(T^b) + \underbrace{\left(\frac{\partial S}{\partial T} \right) \Big|_{\substack{S=S^b \\ T=T^b}}}_{S'} \times T'$$

A flow-dependent model for K_{ST} cont.

- Assume that local perturbations to the T-S relation arise through **vertical displacements** of the background isopycnals :

$$\left. \frac{\partial S}{\partial T} \right|_{S=S^b, T=T^b} = \frac{\left. \frac{\partial S}{\partial z} \right|_{S=S^b}}{\left. \frac{\partial T}{\partial z} \right|_{T=T^b}}$$

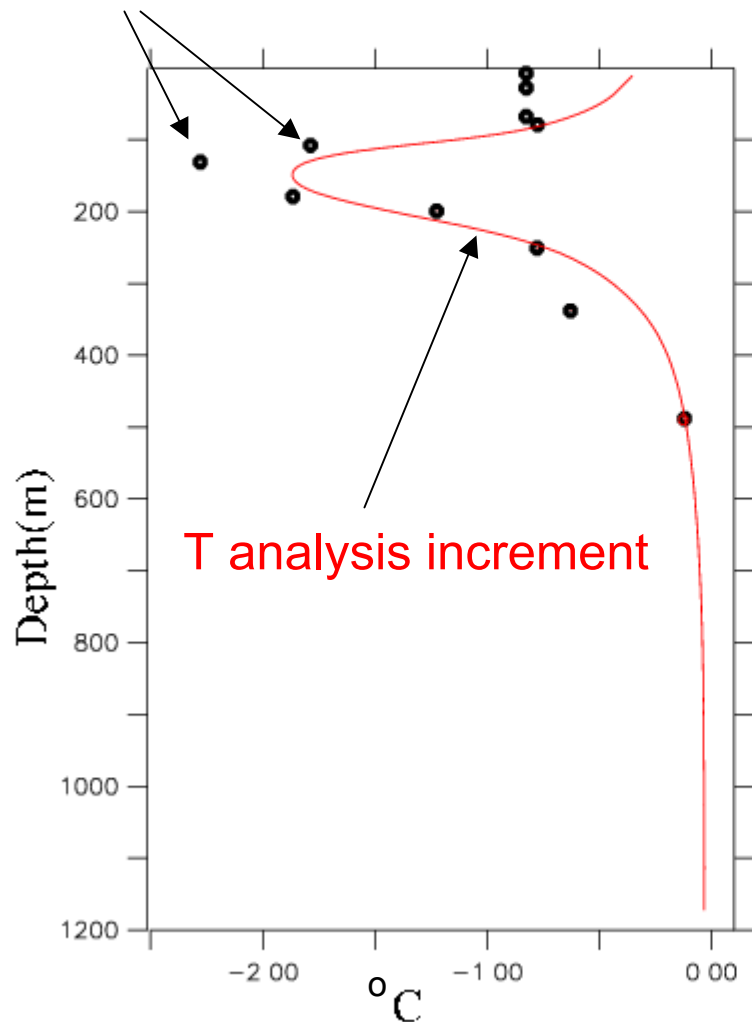
- We avoid applying a T-S constraint in regions where **nonisentropic** processes are important (e.g., in the mixed layer) :

$$S' = w(\mathbf{x}^b) \times \left. \frac{\partial S}{\partial T} \right|_{S=S^b, T=T^b} \times T'$$

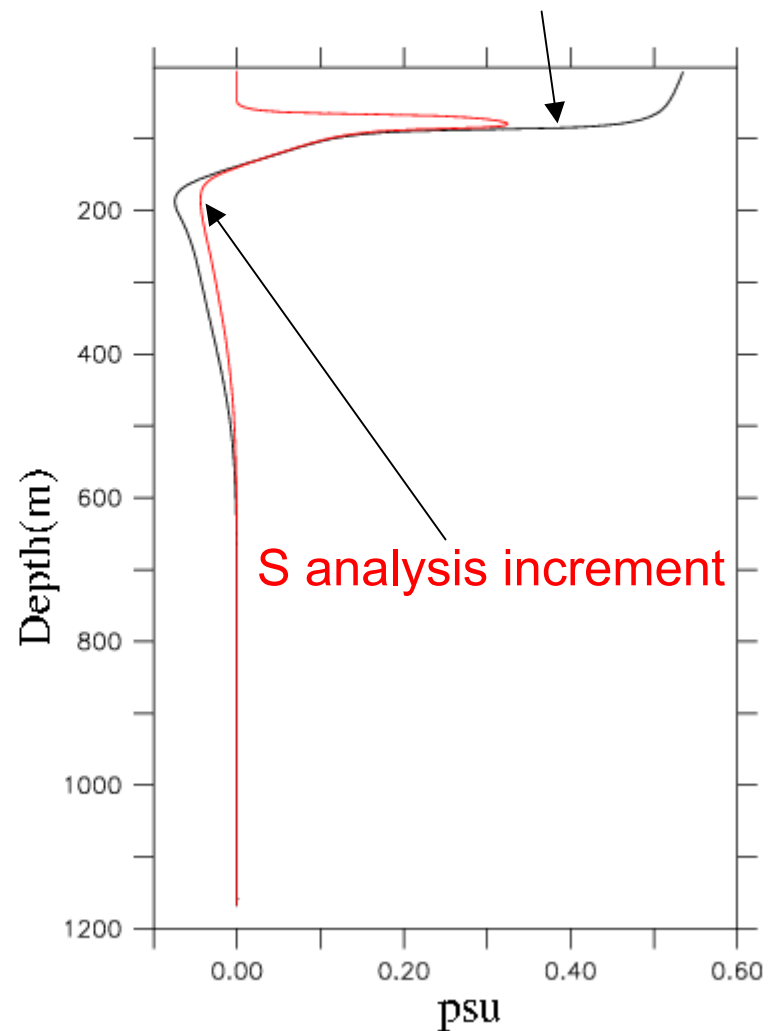
where $w(\mathbf{x}^b) = 0$ or 1 depending on conditions in \mathbf{x}^b .

Impact of the multivariate T-S constraint in 3D-Var: a twin experiment.

T "innovation"



S "true" increment



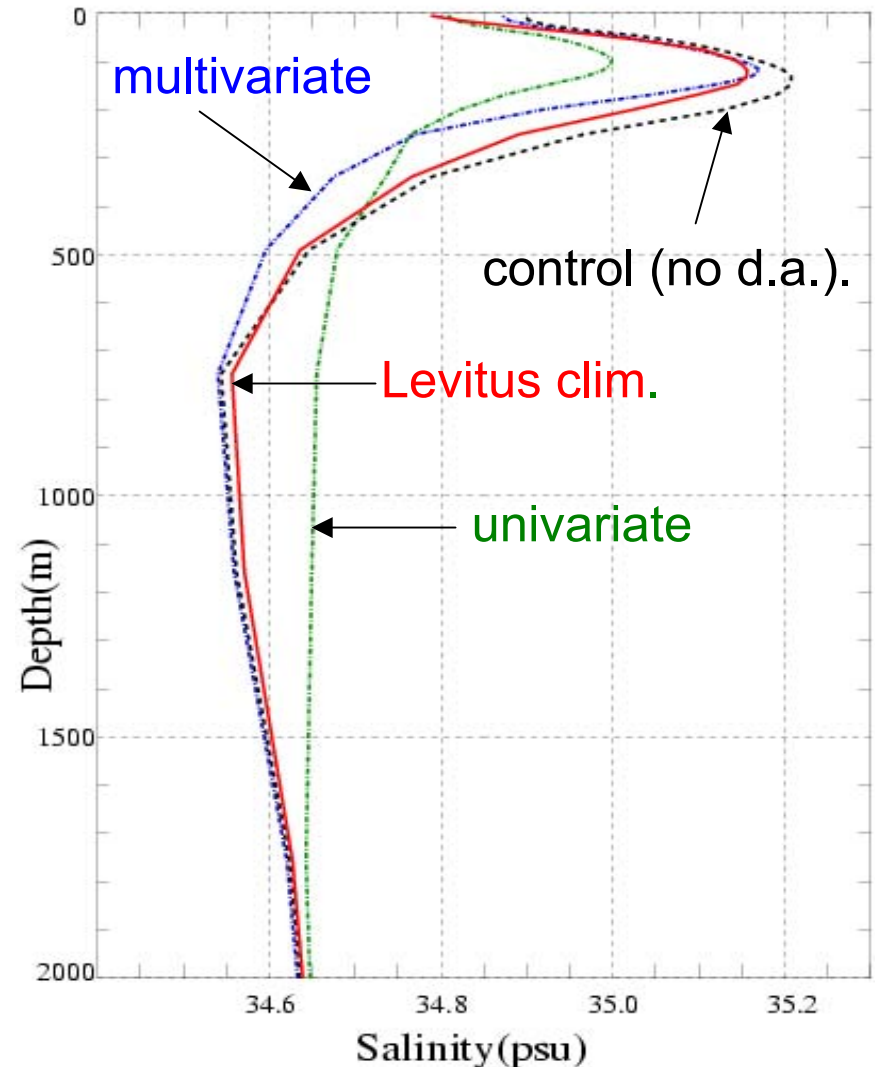
Impact of the multivariate T-S constraint on the salinity mean state in 3D-Var

- Univariate (T) case:

- Spurious circulation develops.
- Artificial decrease / increase of the salinity in the upper / deeper ocean.
- Destruction of the salinity maximum.

- Multivariate (T-S) case:

- Realistic dynamical balances restored.
- Better conservation of water masses.
- Salinity maximum restored.



Multivariate T-S constraint

Effect on water masses in 3D-Var

Control (no d.a.)

Levitus

Univariate **B**

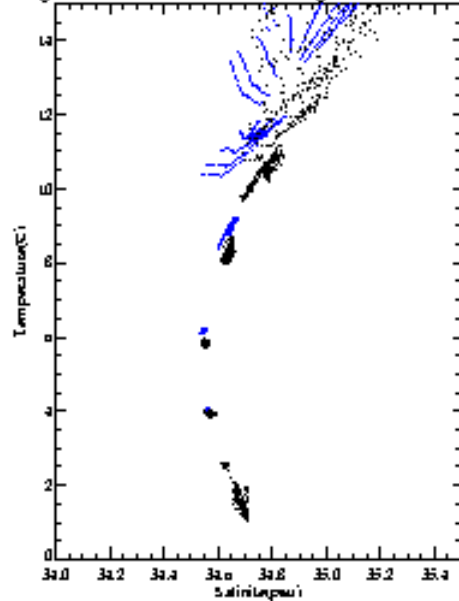
Levitus

Multivariate **B**

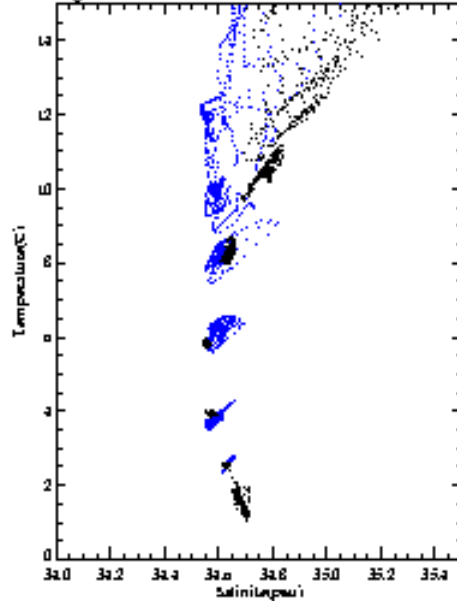
Levitus

Temperature

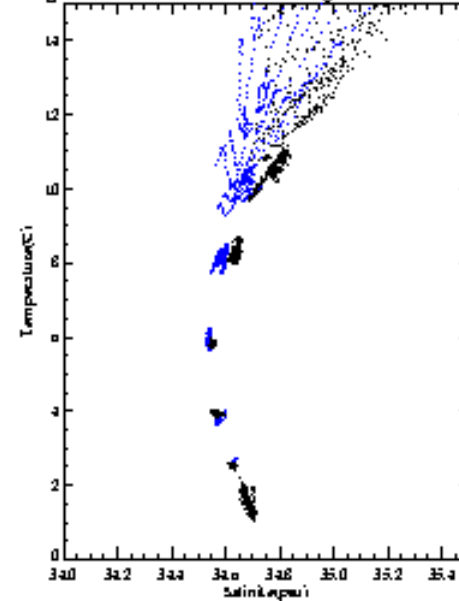
Diagrammes IS-Nino4-Climatologie Levitus 89-VE1 96



Diagrammes IS-Nino4-Clim. Levitus 89-SR2 96



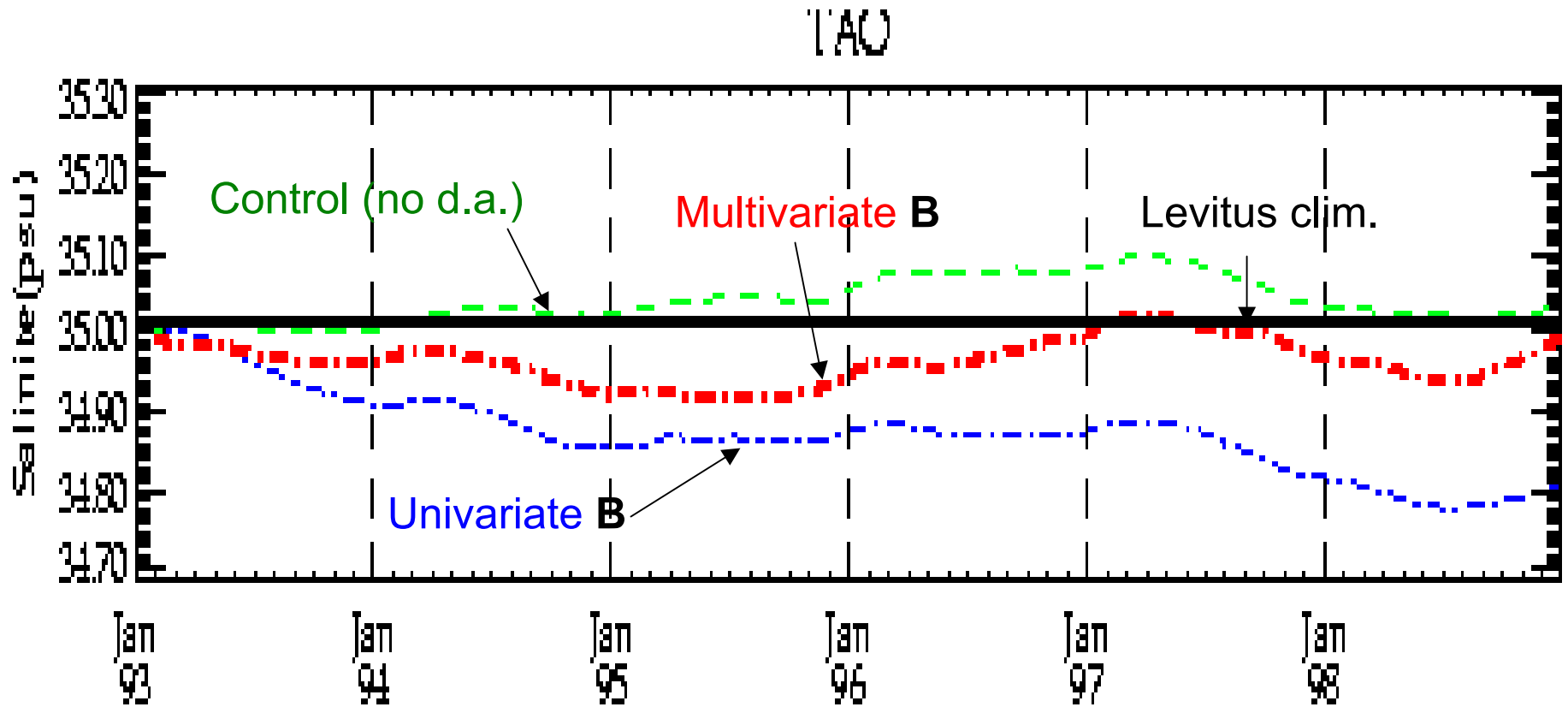
Diagrammes IS-Nino4-Climatologie Levitus 89-SR1 96



Salinity

Multivariate T-S constraint

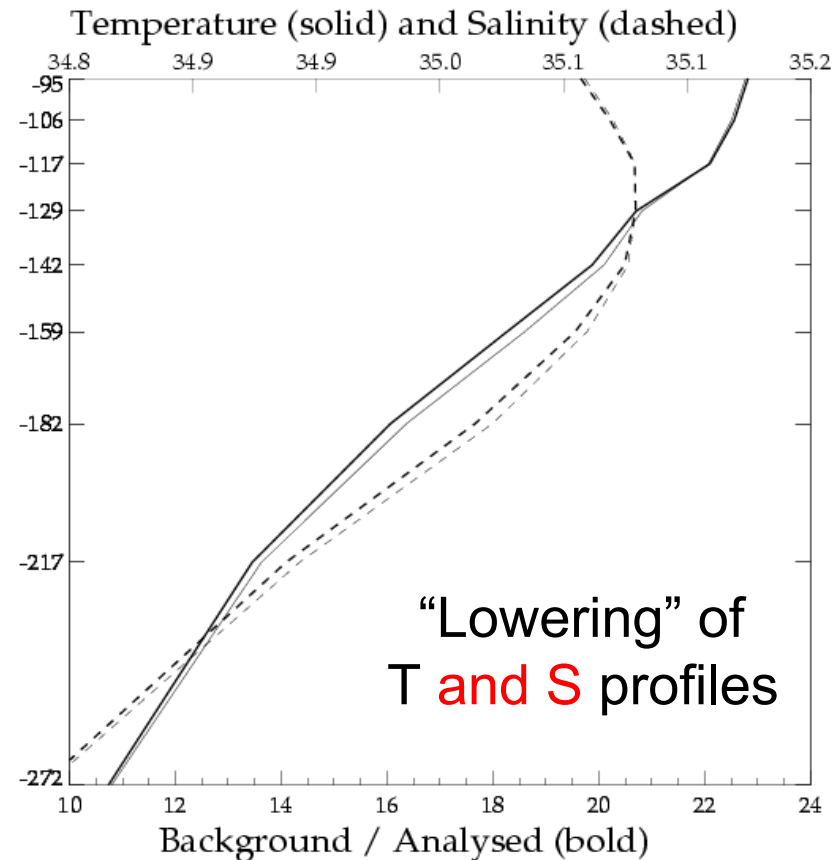
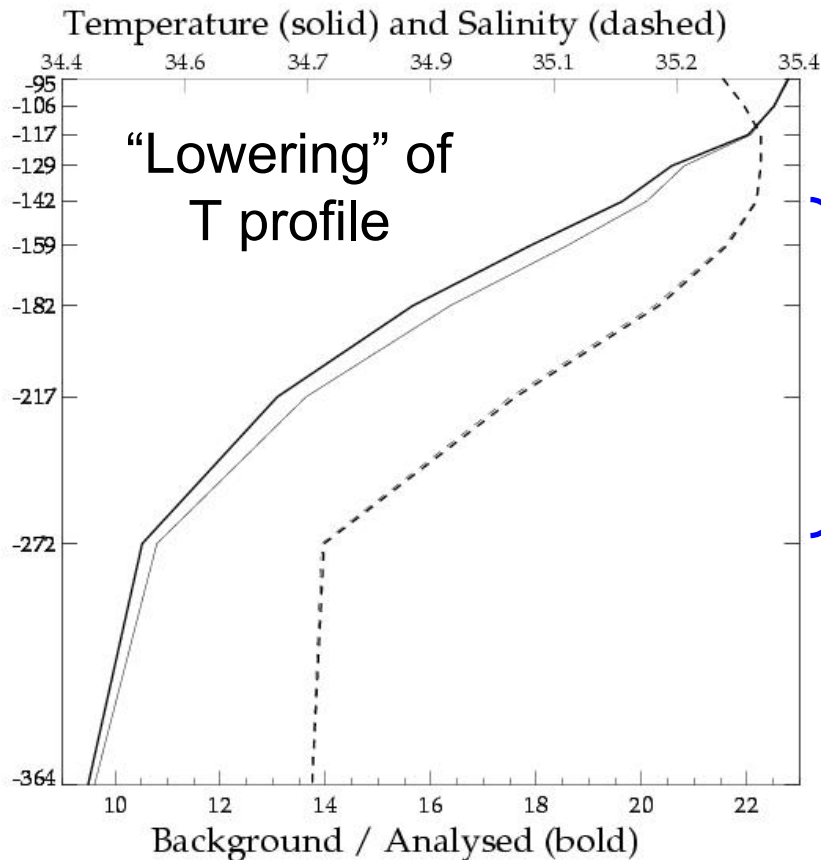
Effect on salinity drift in 3D-Var



Impact of the multivariate T-S constraint in 4D-Var: a single SSH obs experiment

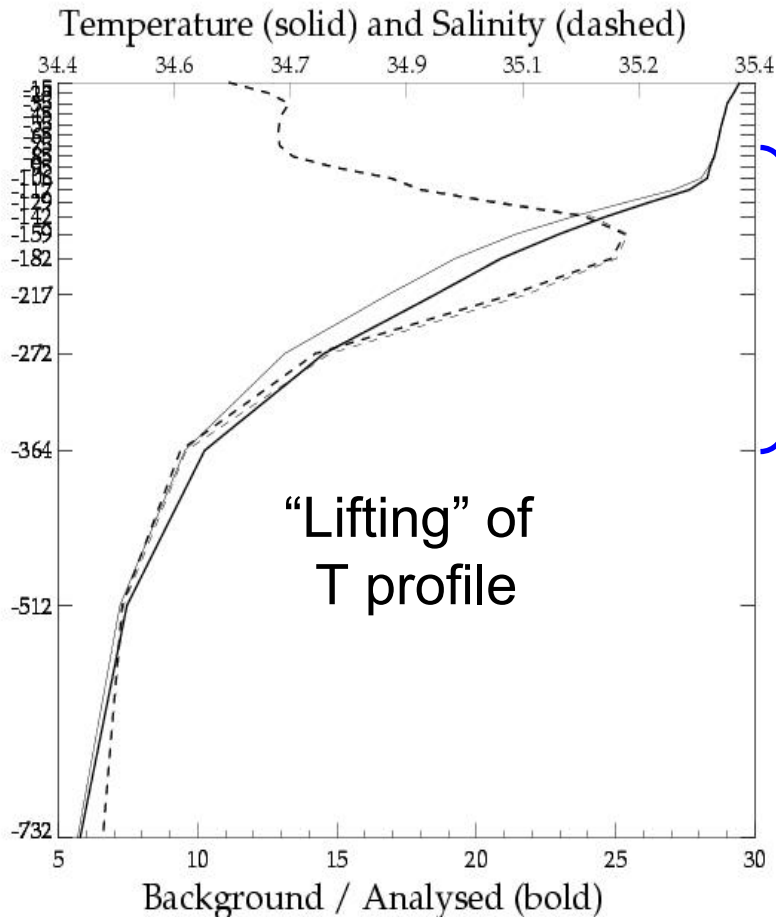
Univariate **B**

Multivariate **B**

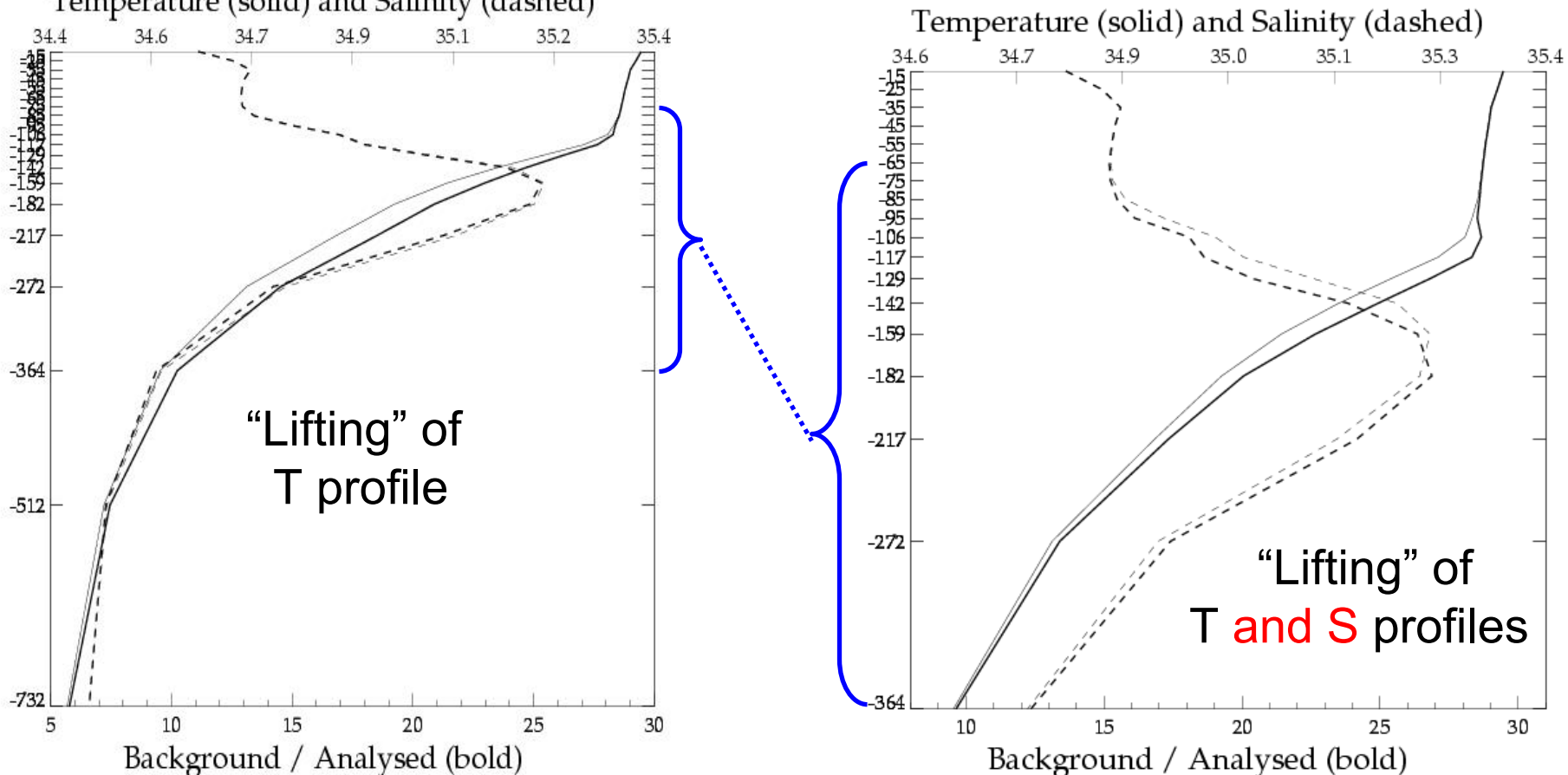


Impact of the multivariate T-S constraint in 4D-Var: a single SSH obs experiment

Univariate **B**



Multivariate **B**



A general approach for modelling **B**

(cf. Derber & Bouttier 1999 - Tellus)

- Suppose (to be justified shortly)

“balanced” variables

“unbalanced” variables

$$\begin{aligned} T' &= T'_B \\ S' &= S'_B + S'_U = \underbrace{K_{ST} T'}_{S'_B} + S'_U \\ \eta' &= \eta'_B + \eta'_U = \underbrace{K_{\eta T} T' + K_{\eta S} S'}_{\eta'_B} + \eta'_U \\ u' &= u'_B + u'_U = \underbrace{K_{uT} T' + K_{uS} S' + K_{u\eta} \eta'}_{u'_B} + u'_U \\ v' &= v'_B + v'_U = \underbrace{K_{vT} T' + K_{vS} S' + K_{v\eta} \eta'}_{v'_B} + v'_U \end{aligned}$$

A flow-dependent model for $K_{\eta T}$ and $K_{\eta S}$

- Linearized equation of state :

$$\rho' / \rho_0 = -\alpha T' + \beta S'$$

where $\alpha = \partial\rho / \partial T|_{T=T^b}$ and $\beta = \partial\rho / \partial S|_{S=S^b}$.

- Dynamic height of the surface relative to $z = z_{ref}$:

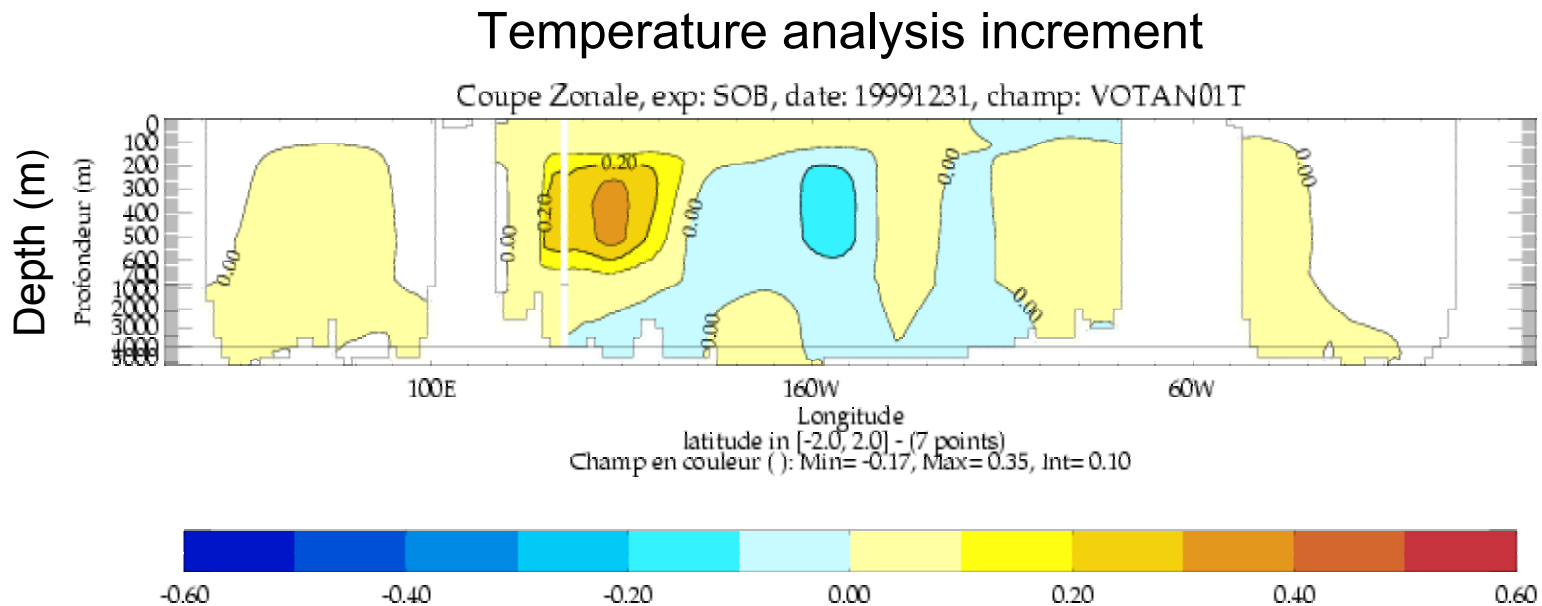
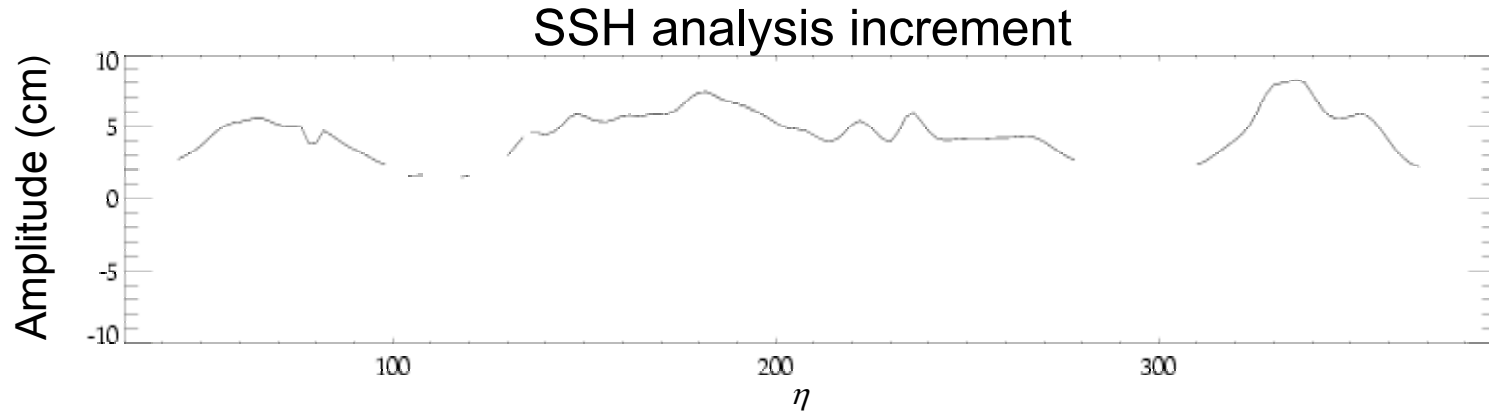
$$\eta' = - \int_{z_{ref}}^0 (\rho' / \rho_0) dz$$

where ρ_0 is a reference density.

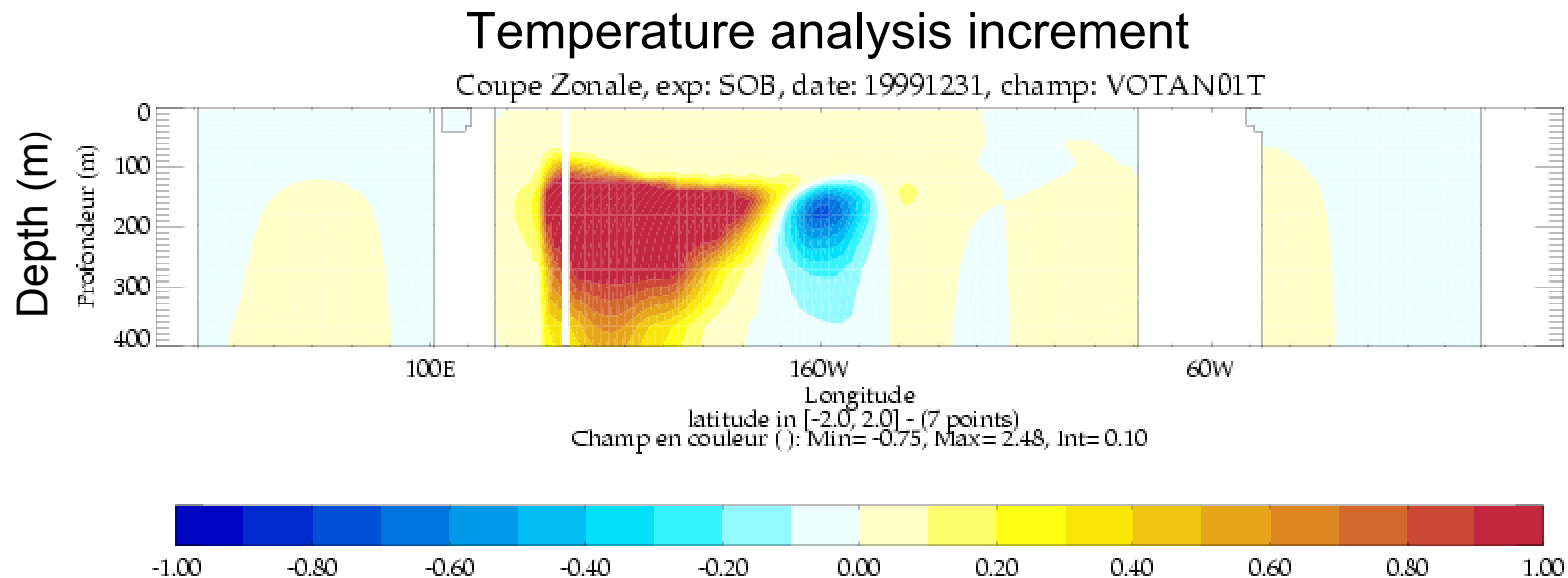
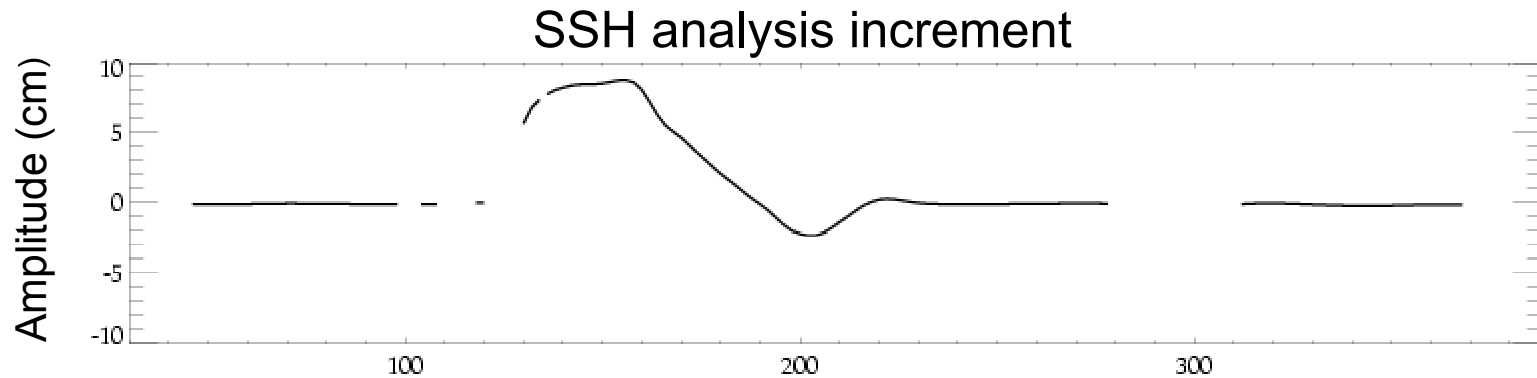
Impact of a single SSH obs in 4D-Var

Ex: SSH innovation = 10 cm at (0°, 160°W) at t = 30 days.

a) univariate **B** ; b) constant σ_T^b in the upper 600m.



Ex: As previous example but with: **a)** a multivariate \mathbf{B} ; **b)** an extra constraint in \mathbf{B} to enforce $\overline{\eta'} = 0$; and **c)** vertical T -gradient dependent σ_T^b



A model for $K_{u(T,S,\eta)}$, $K_{v(T,S,\eta)}$

- Hydrostatic approximation :

$$p' = \int_z^0 \rho' g dz + \rho_0 g \eta'$$

- Combine hydrostatic and dynamic height relations :

$$p' = \int_{z_{ref}}^z \rho' g dz$$

- Geostrophic (f-plane) approximation :

$$f u' = - (1 / \rho_0) (\partial p' / \partial y)$$

$$f v' = (1 / \rho_0) (\partial p' / \partial x)$$

A model for $K_{u(T,S,\eta)}$, $K_{v(T,S,\eta)}$ near the equator

(cf. Burgers et al. 2002 - JPO ; Balmaseda lecture)

■ Geostrophic f-plane approximation :

$$f u'_f = - (1 / \rho_0) (\partial p' / \partial y)$$

$$f v'_f = (1 / \rho_0) (\partial p' / \partial x)$$

■ Geostrophic β -plane ($f = \beta y$) approximation :

$$\beta u'_\beta = - (1 / \rho_0) (\partial^2 p' / \partial y^2)$$

$$\beta v'_\beta = (1 / \rho_0) (\partial^2 p' / \partial x \partial y)$$

A model for $K_{u(T,S,\eta)}$, $K_{v(T,S,\eta)}$ near the equator

- Combining the **f-plane** and **β -plane** solutions
(*Lagerloef et al. 1999 – JGR*) :

$$u' = W_{\beta} u'_{\beta} + (1 - W_{\beta}) u'_f$$

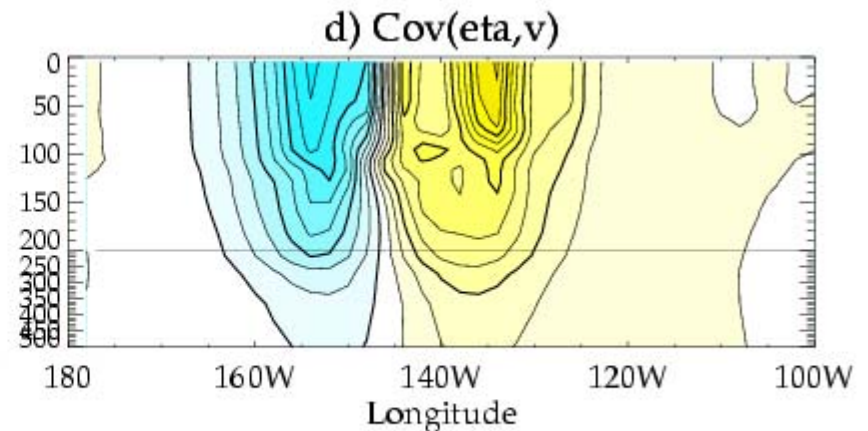
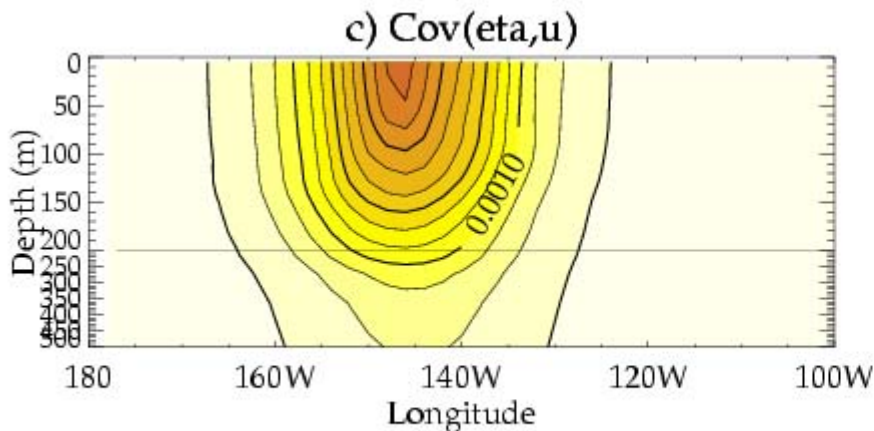
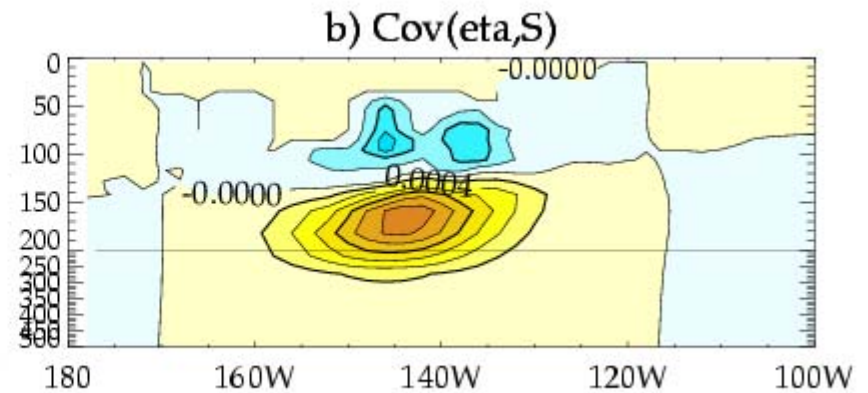
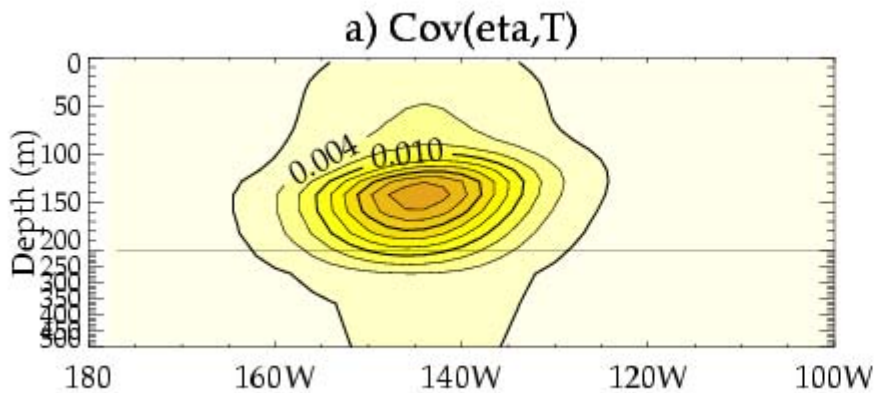
$$v' = W_{\beta} v'_{\beta} + (1 - W_{\beta}) v'_f$$

where $W_{\beta} = \exp(-y^2 / 2L_{\beta}^2)$.

- L_{β} is a length scale $\sim O(\text{eq. Rossby radius}) \sim 1^{\circ} - 2^{\circ}$.
- More elaborate linear models (e.g., which include surface forcing, friction) could be used.
(e.g., *Lagerloef et al. 1999-JGR; Bonjean & Lagerloef 2002-JPO*)

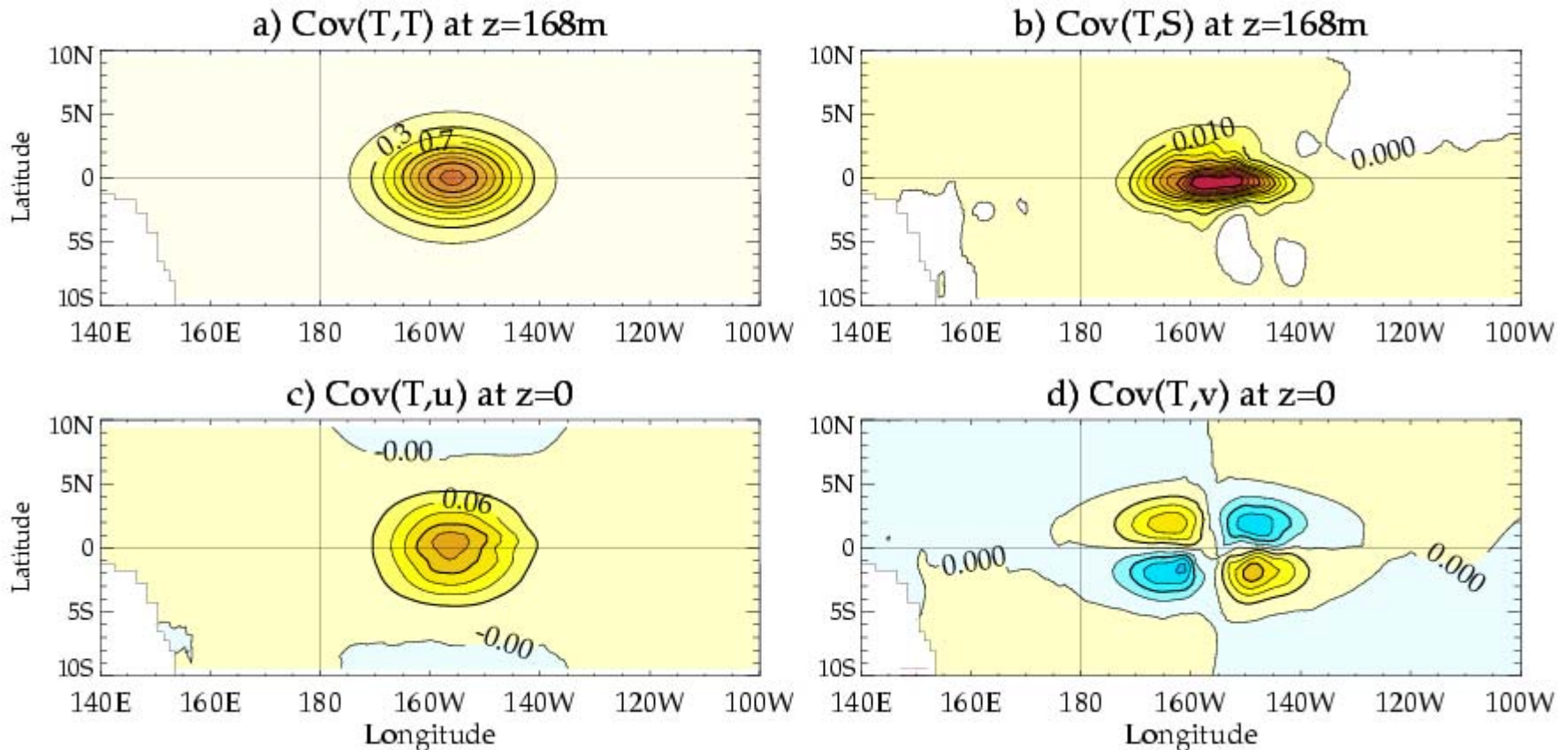
Multivariate covariance structures

Example: covariance relative to a SSH (η) point at $(0^\circ, 144^\circ\text{W})$



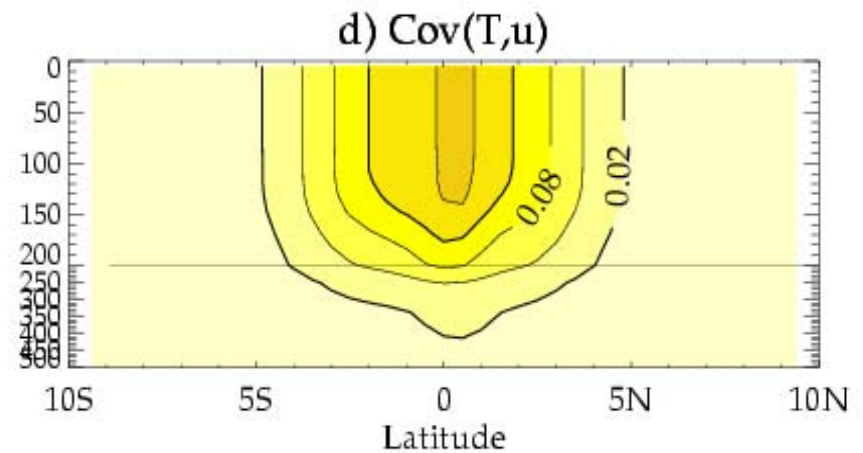
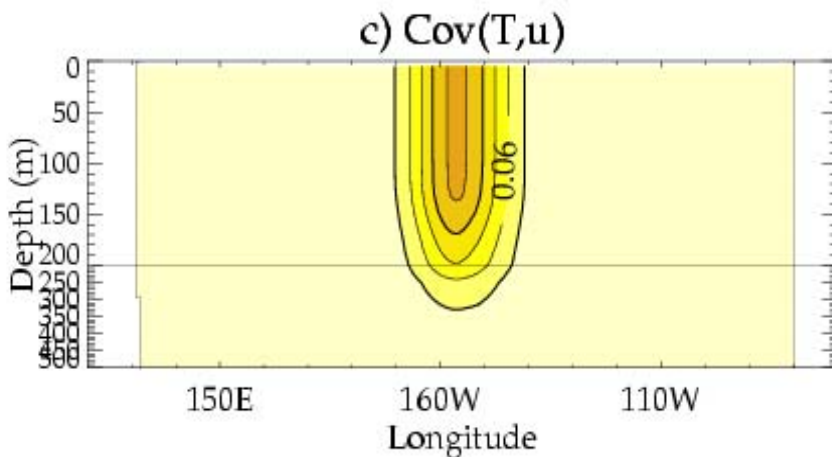
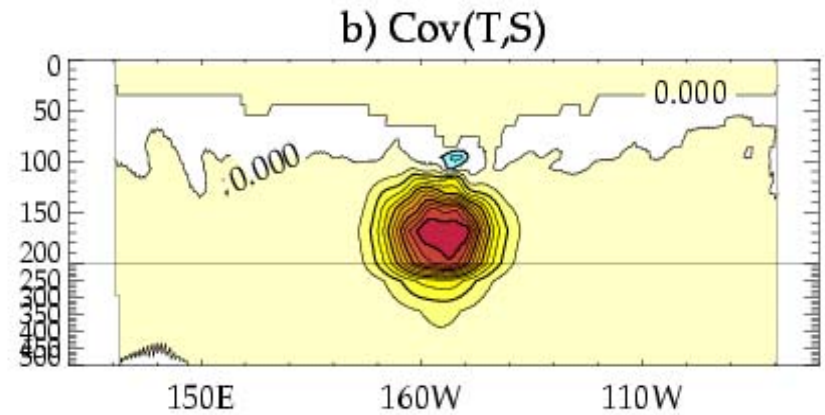
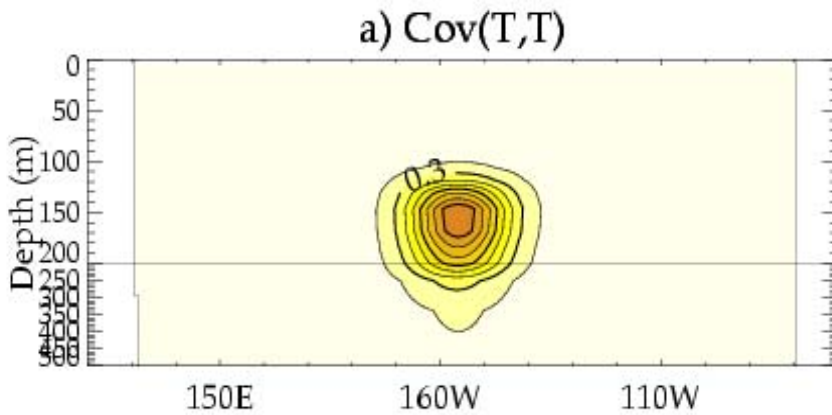
Multivariate covariance structures

Example: covariance relative to a T point at $(0^\circ, 156^\circ\text{W}, 168\text{m})$



Multivariate covariance structures

Example: covariance relative to a T point at (0°, 156°W, 168m)

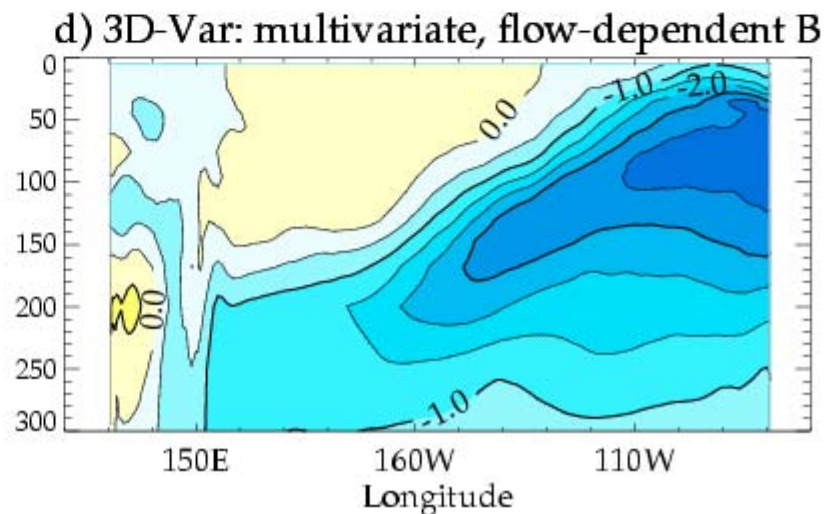
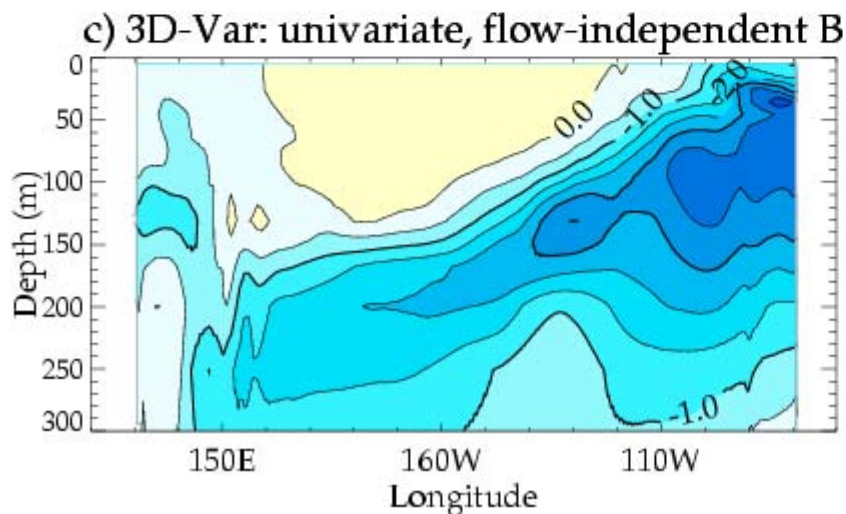
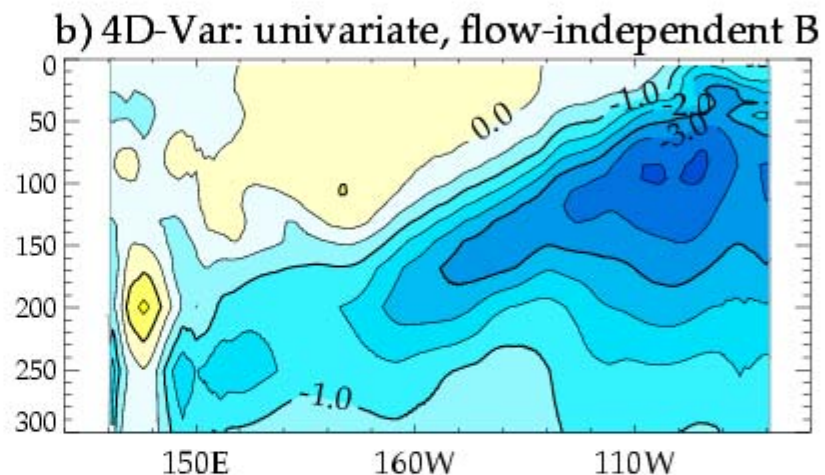
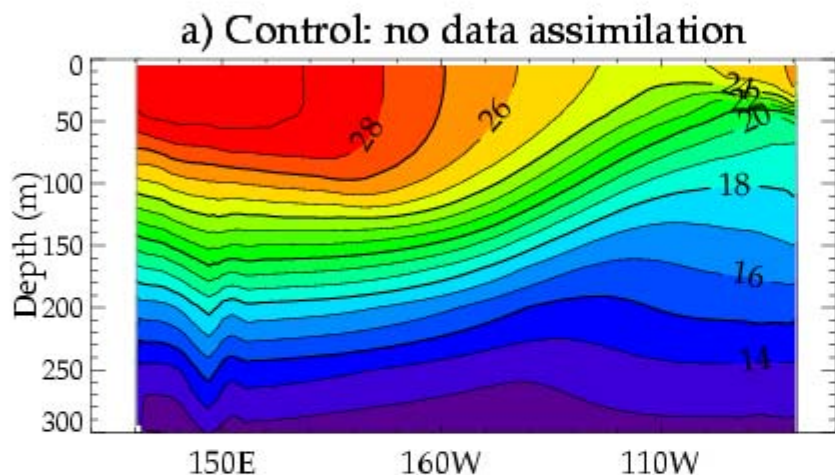


Impact on the temperature mean state

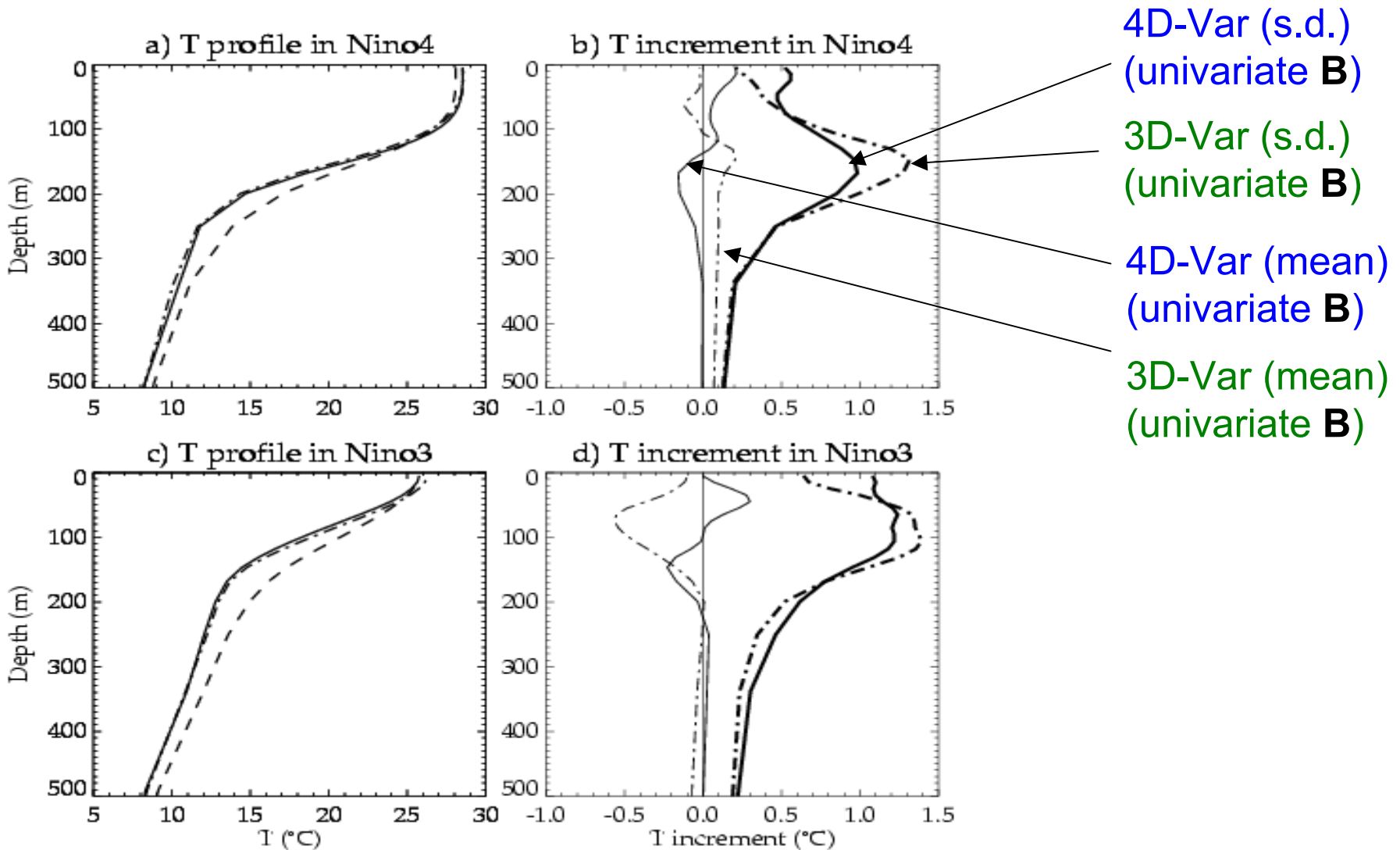
(*cf. Vialard et al. 2003 - MWR*)

Assimilation data-set = *in situ* temperatures from the GTSPP

1993-96 climatology: b) – d) are the difference from the control



Mean and standard deviation of the analysis increments

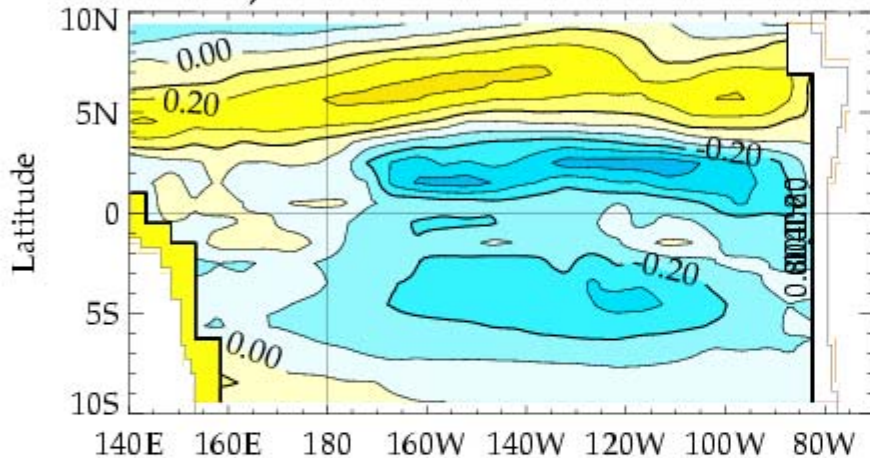


Impact on the mean zonal velocity

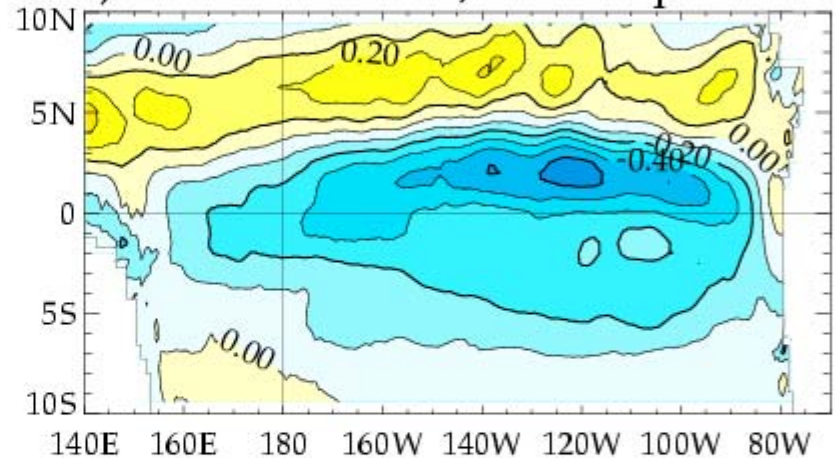
(cf. Vialard et al. 2003 - MWR)

1993-96 climatology

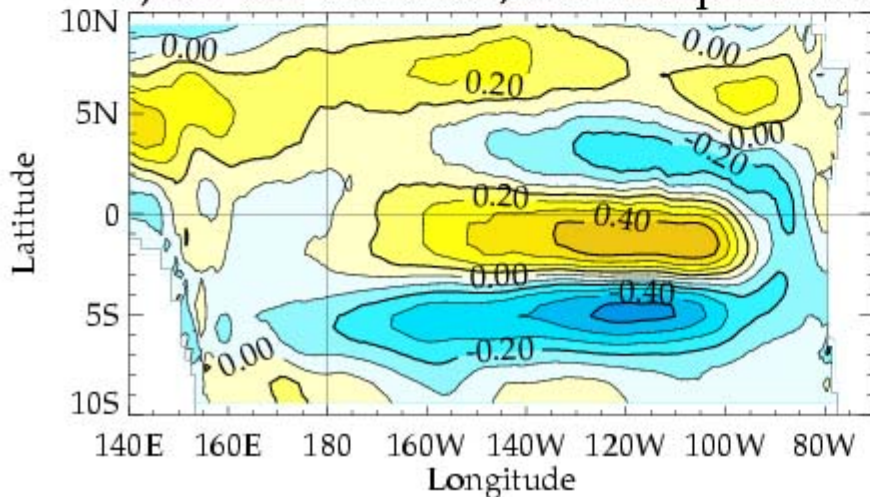
a) Reverdin et al. 1987-92 clim.



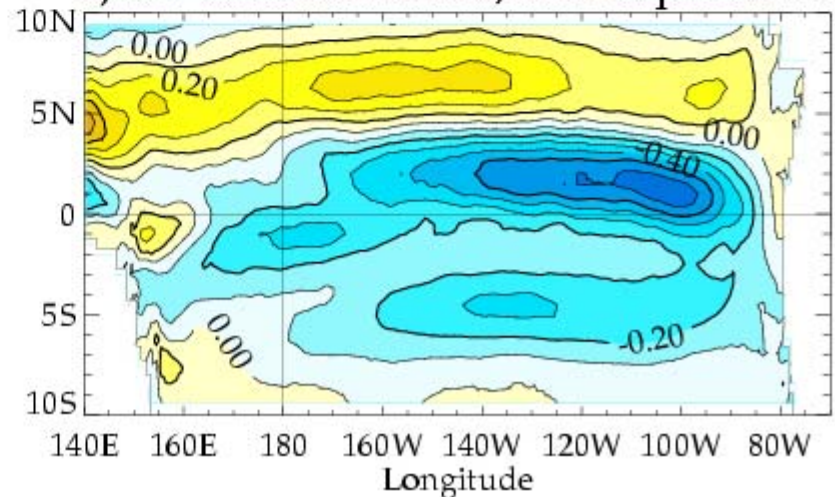
b) 4D-Var: univariate, flow-independent B



c) 3D-Var: univariate, flow-independent B



d) 3D-Var: multivariate, flow-dependent B

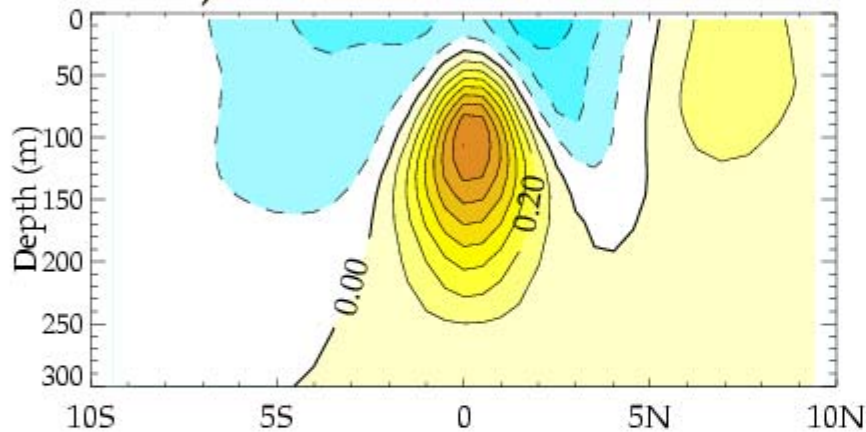


Impact on the mean zonal velocity

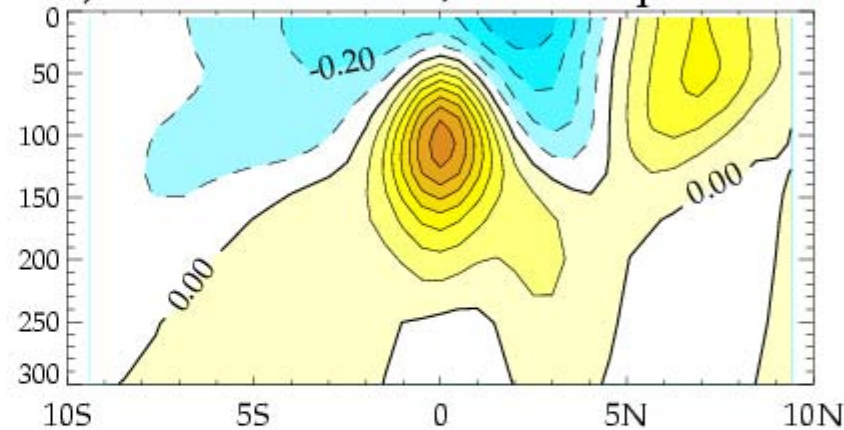
(cf. Vialard et al. 2003 - MWR)

1993-96 climatology

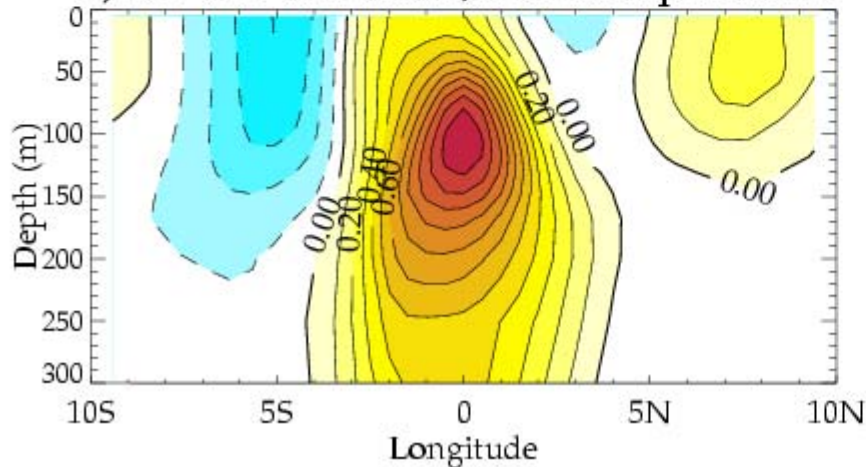
a) Control: no data assimilation



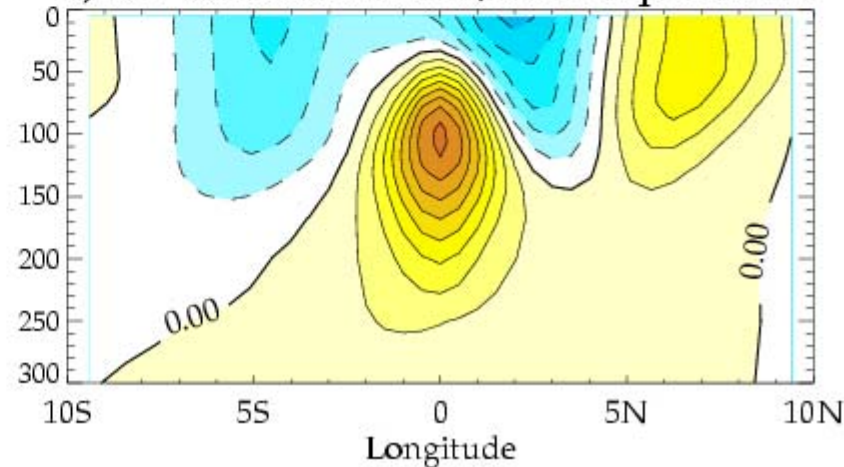
b) 4D-Var: univariate, flow-independent B



c) 3D-Var: univariate, flow-independent B



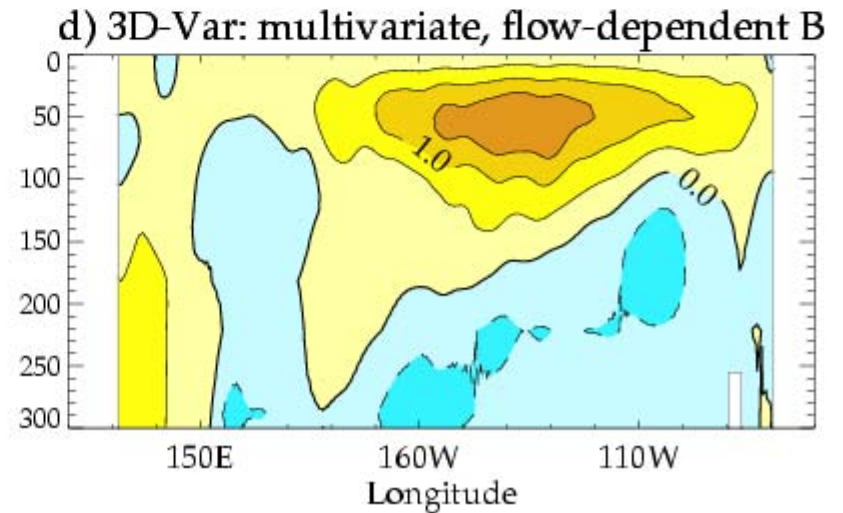
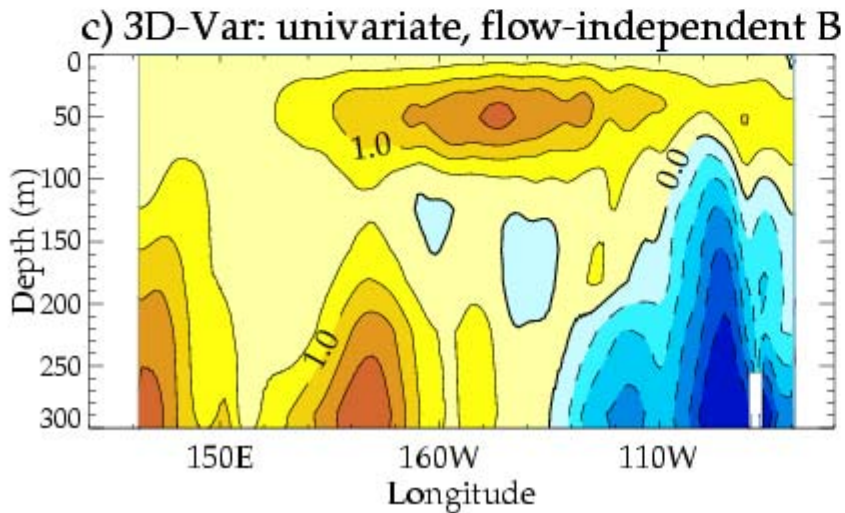
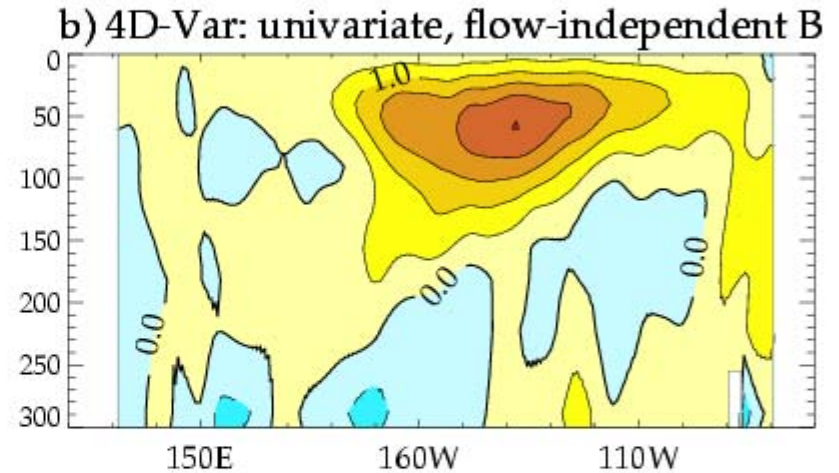
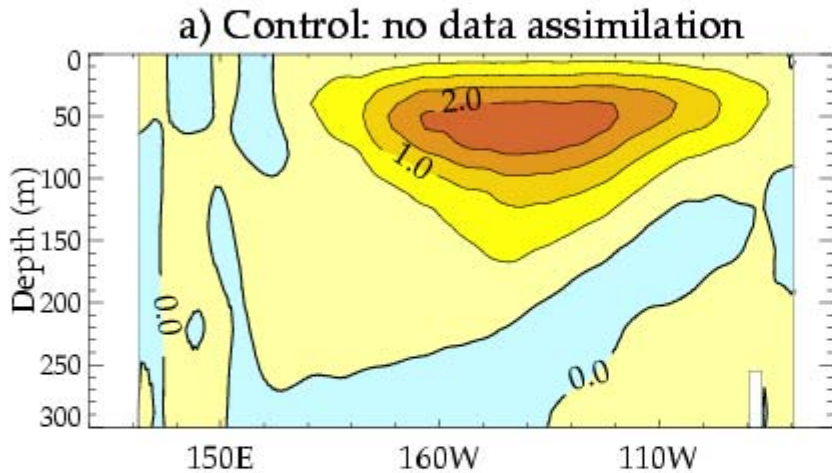
d) 3D-Var: multivariate, flow-dependent B



Impact on the mean vertical velocity

(cf. Vialard et al. 2003 - MWR)

1993-96 climatology



Concluding remarks...

- Univariate data assimilation schemes tend to disrupt the dynamical balances along the equator and produce spurious circulations (*Bell et al. 2003 - QJRMSS; Burgers et al. 2002 - JPO; Vialard et al. 2003 – MWR; Balmaseda lecture*).
- Improving the background error covariance models to include multivariate constraints and flow-dependent features is one way of restoring realistic balances in the model and significantly improving the analyses (*cf. Burgers et al. 2002 - JPO; Troccoli et al. 2002 – MWR; Balmaseda lecture*).
- General methodologies for modelling **B** developed in NWP are applicable to the ocean problem as well. (Ocean assimilators can exploit the wealth of experience in NWP).
- However, the details differ: need for specific algorithms for dealing with boundaries; different balance or conservation relationships, different scales,...

Research issues...

- * Develop techniques for the ocean for diagnosing the statistics of background error (ensemble methods, innovation-based methods). (*cf. Fisher lecture*)
- Develop **weak constraint** versions of the balance operators (* is a prerequisite).
- How do the improved covariance models benefit 4D-Var? More comparisons between 3D-Var and 4D-Var are needed.