Is it worth replacing 3DFgat by 4DVAR in CERA's ocean component?

Can we improve coupled consistency through data assimilation?

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Convergence of (approximate) Gauss-Newton

The original 4DVar problem:

$$J(\mathbf{x}) = \frac{1}{2}\left(\mathbf{x}-\mathbf{x}^b\right)^T \mathbf{B}^{-1}\left(\mathbf{x}-\mathbf{x}^b\right) + \frac{1}{2}\left(\mathcal{H}(\mathcal{M}(\mathbf{x}))-\mathbf{y}^o\right)^T \mathbf{R}^{-1}\left(\mathcal{H}(\mathcal{M}(\mathbf{x}))-\mathbf{y}^o\right)$$

It can be put in a more compact form, let $F : \mathbb{R}^n \longrightarrow \mathbb{R}^{n+p}$ such that

$$F(\mathbf{x}) = \begin{pmatrix} \mathbf{B}^{-1/2}\left(\mathbf{x}-\mathbf{x}^b\right) \\ \mathbf{R}^{-1/2}\left(\mathcal{H}(\mathcal{M}(\mathbf{x}))-\mathbf{y}^o\right) \end{pmatrix}$$

Original cost function can then be rewritten

$$J(\mathbf{x}) = \frac{1}{2}\|F(\mathbf{x})\|_2^2$$

Denoting $\mathbf{F}_\mathbf{x} = \begin{pmatrix} \mathbf{B}^{-1/2} \\ \mathbf{R}^{-1/2}\mathbf{H}_\mathbf{x}\mathbf{M}_\mathbf{x} \end{pmatrix}$ the jacobian (tangent linear) of F differentiated around $\mathbf{x}$, gradient and Hessian of J read

$$\nabla_\mathbf{x} J = \mathbf{F}_\mathbf{x}^T F(\mathbf{x}) \quad \in \quad \mathbb{R}^n$$
$$\nabla_\mathbf{x}^2 J = \mathbf{F}_\mathbf{x}^T \mathbf{F}_\mathbf{x} + Q(\mathbf{x}) \quad \in \quad \mathbb{R}^{n\times n}$$

where $Q(\mathbf{x})$ denotes the second order terms

Convergence of (approximate) Gauss-Newton

At each iterations

- Newton solves: $\nabla^2_{\mathbf{x}^{(k)}} J \delta \mathbf{x}^{(k+1)} = -\nabla_{\mathbf{x}^{(k)}} J$
- Gauss-Newton solves: $\mathbf{F}^T_{\mathbf{x}^{(k)}} \mathbf{F}_{\mathbf{x}^{(k)}} \delta \mathbf{x}^{(k+1)} = -\nabla_{\mathbf{x}^{(k)}} J$

Convergence of (approximate) Gauss-Newton

At each iterations

- Newton solves: $\left(\mathbf{F}_{\mathbf{x}^{(k)}}^T \mathbf{F}_{\mathbf{x}^{(k)}} + Q(\mathbf{x}^{(k)})\right) \delta\mathbf{x}^{(k+1)} = -\mathbf{F}_{\mathbf{x}^{(k)}}^T F(\mathbf{x}^{(k)})$
- Gauss-Newton solves: $\mathbf{F}_{\mathbf{x}^{(k)}}^T \mathbf{F}_{\mathbf{x}^{(k)}} \delta\mathbf{x}^{(k+1)} = -\mathbf{F}_{\mathbf{x}^{(k)}}^T F(\mathbf{x}^{(k)})$

Convergence of (approximate) Gauss-Newton

At each iterations

- Newton solves: $\delta \mathbf{x}^{(k+1)} = -\left(\mathbf{F}^T_{\mathbf{x}^{(k)}}\mathbf{F}_{\mathbf{x}^{(k)}} + Q(\mathbf{x}^{(k)})\right)^{-1}\mathbf{F}^T_{\mathbf{x}^{(k)}}F(\mathbf{x}^{(k)})$
- Gauss-Newton solves: $\delta \mathbf{x}^{(k+1)} = -\left(\mathbf{F}^T_{\mathbf{x}^{(k)}}\mathbf{F}_{\mathbf{x}^{(k)}}\right)^{-1}\mathbf{F}^T_{\mathbf{x}^{(k)}}F(\mathbf{x}^{(k)}) = \mathbf{F}^+_{\mathbf{x}^{(k)}}F(\mathbf{x}^{(k)})$

Convergence of (approximate) Gauss-Newton

At each iterations

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Under several conditions, Gauss Newton will converge toward a minimum of the original problem if $\exists\eta^{(k)} < 1$:

$$\left\|\left(\mathbf{F}_{\mathbf{x}^{(k)}}^T \mathbf{F}_{\mathbf{x}^{(k)}}\right)^{-1} Q(\mathbf{x}^{(k)})\right\|_2 \leq \eta^{(k)}$$

Convergence of (approximate) Gauss-Newton

At each iterations

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Convergence of (approximate) Gauss-Newton

At each iterations

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In practice further approximations are made (lower resolution, simplified physics, CERA, 3DFgat, ...), the approximate Gauss-Newton iteration then solves

$$\widetilde{\mathbf{F}}_{\mathbf{x}^{(k)}}^T\widetilde{\mathbf{F}}_{\mathbf{x}^{(k)}}\delta\mathbf{x}^{(k+1)} = -\widetilde{\mathbf{F}}_{\mathbf{x}^{(k)}}^T F(\mathbf{x}^{(k)})$$

One can show that for such an approximation of the cost function, this sufficient condition becomes

$$\left\| \mathbf{I} - \left(\widetilde{\mathbf{F}}^T_{\mathbf{x}^{(k)}} \widetilde{\mathbf{F}}_{\mathbf{x}^{(k)}} \right)^{-1} \left(\widetilde{\mathbf{F}}^T_{\mathbf{x}^{(k)}} \mathbf{F}_{\mathbf{x}^{(k)}} + \tilde{Q}(\mathbf{x}^{(k)}) \right) \right\|_2 \leq \eta^{(k)}$$

But the minimum is not the same as the original problem

$$\|\tilde{\mathbf{x}}^* - \mathbf{x}^*\|_2 \leq \frac{1}{1-\nu} \left\| \left(\widetilde{\mathbf{F}}^+_{\tilde{\mathbf{x}}^*} - \mathbf{F}^+_{\tilde{\mathbf{x}}^*} \right) F(\tilde{\mathbf{x}}^*) \right\|_2 = \frac{1}{1-\nu} \left\| \mathbf{F}^+_{\tilde{\mathbf{x}}^*} F(\tilde{\mathbf{x}}^*) \right\|_2$$

($\mathbf{F}^+ = \left(\mathbf{F}^T \mathbf{F}\right)^{-1} \mathbf{F}^T$)

In the linear case the above sufficient condition becomes necessary.

One can show that for such an approximation of the cost function, this sufficient condition becomes

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($\mathbf{F}^+ = \left(\mathbf{F}^T \mathbf{F}\right)^{-1} \mathbf{F}^T$)

In the linear case the above sufficient condition becomes necessary.

As a summary all what matters is:

how good $\widetilde{\mathbf{F}}_\mathbf{x} = \begin{pmatrix} \mathbf{B}^{-1/2} \\ \mathbf{R}^{-1/2}\mathbf{H}_\mathbf{x}\widetilde{\mathbf{M}}_\mathbf{x} \end{pmatrix}$ is an approximation of $\mathbf{F}_\mathbf{x} = \begin{pmatrix} \mathbf{B}^{-1/2} \\ \mathbf{R}^{-1/2}\mathbf{H}_\mathbf{x}\mathbf{M}_\mathbf{x} \end{pmatrix}$.

Back to the first question

Is it worth replacing 3DFgat by 4DVAR in CERA20C's ocean component?

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the answer is no ...

Back to the first question

Is it worth replacing 3DFgat by 4DVAR in CERA20C's ocean component?

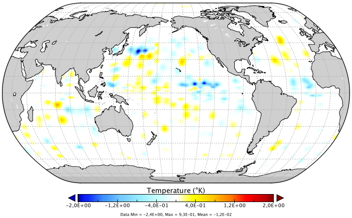
the answer is no ...

It just does not change a bit ...

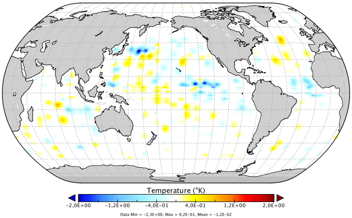
incremental 4Dvar vs incremental 3Dvar

ORCA 1, One day assimilation window, T and S assimilation

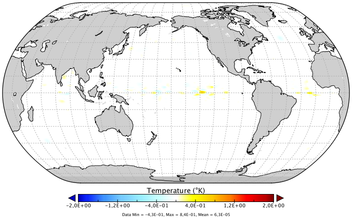
4Dvar (1 day) T300 increment



3Dvar (1 day) T300 increment

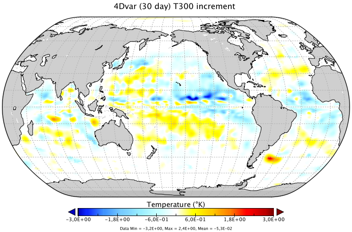


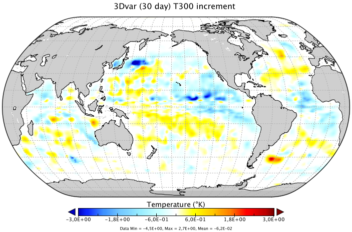
4Dvar - 3Dvar (1 day) difference T300 increment

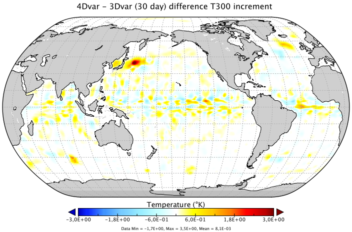


incremental 4Dvar vs incremental 3Dvar

ORCA 1, 30 day assimilation window, T and S assimilation







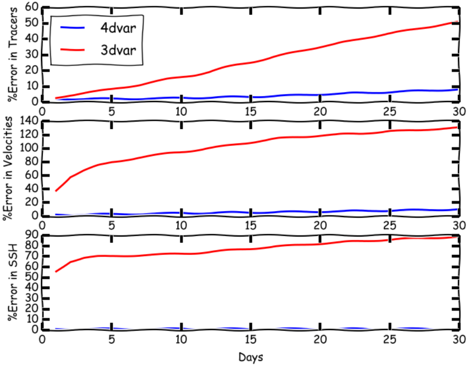
Considering the standard inner loop's incremental formulation:

$$J^k(\delta\mathbf{x}^{(k)}) = \left(\delta\mathbf{x}^{(k)} + \sum_{l=1}^{(k-1)} \delta\mathbf{x}^{(l)}\right)^T \mathbf{B}^{-1} \left(\delta\mathbf{x}^{(k)} + \sum_{l=1}^{(k-1)} \delta\mathbf{x}^{(l)}\right) + \sum_{i=0}^{N} \left(\mathbf{H}_{t_i}^{(k-1)}\tilde{\mathbf{M}}_{t_i}^{(k-1)}\delta\mathbf{x}^{(k)} - \mathbf{d}_{t_i}^{(k-1)}\right)^T \mathbf{R}_{t_i}^{-1} \left(\mathbf{H}_{t_i}^{(k-1)}\tilde{\mathbf{M}}_{t_i}^{(k-1)}\delta\mathbf{x}^{(k)} - \mathbf{d}_{t_i}^{(k-1)}\right)$$

How good our approximation of the "true" $\mathbf{F}$ (i.e. $\mathbf{HM}$) is?
For 3D-Var ($\tilde{\mathbf{M}} = \mathbf{I}$) and 4D-Var ($\tilde{\mathbf{M}}$ includes some approximations as well)?

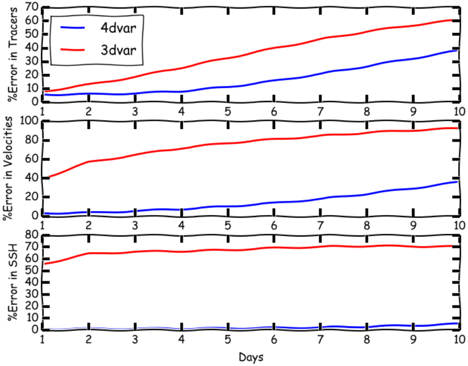
incremental 4Dvar vs incremental 3Dvar

ORCA1



Approximation in the linear propagator

incremental 4Dvar vs incremental 3Dvar
ORCA25

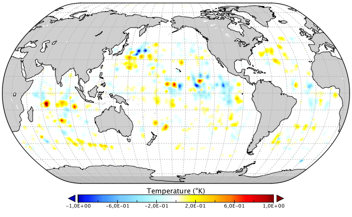


Approximation in the linear propagator

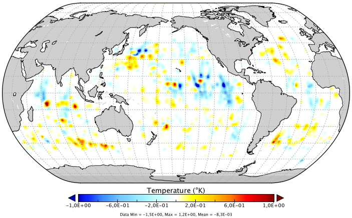
incremental 4Dvar vs incremental 3Dvar

ORCA 025, One day assimilation window, T,S and SSH assimilation

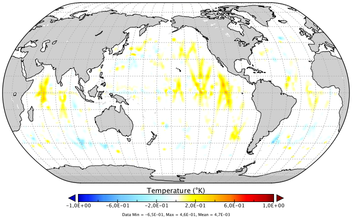
4Dvar (1 day) T300 increment



3Dvar (1 day) T300 increment



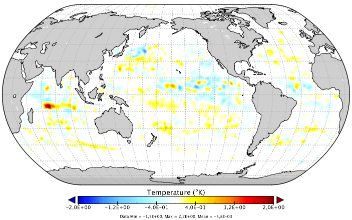
4Dvar - 3Dvar (1 day) T300 increment difference



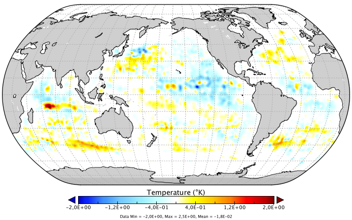
incremental 4Dvar vs incremental 3Dvar

ORCA 025, 5 day assimilation window, T,S and SSH assimilation

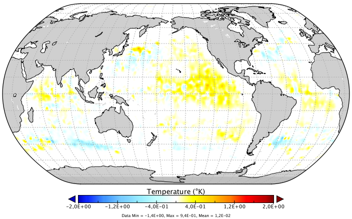
4Dvar (5 days) T300 increment



3Dvar (5 days) T300 increment



4Dvar - 3Dvar (5 days) T300 increment difference



There are potential interest to use 4DVar for longer assimilation windows / higher resolution, but it comes at a cost:

Orca1, 10 iteration, 1 node:

1day:

4dvar: 12mn (17mn)
3dvar: 6mn (11mn)

10days:

4dvar: 48mn (1h)
3dvar: 6mn (16mn)

Orca025, 5 iteration, 6 nodes:

5 day:

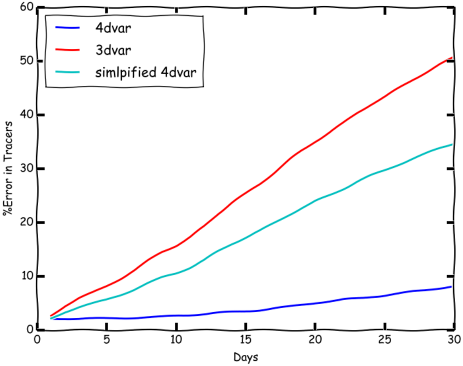
4dvar: 7h (9h)
3dvar: 45mn (2h45)

Simplified 4Dvar

Do we really need a full tangent model?

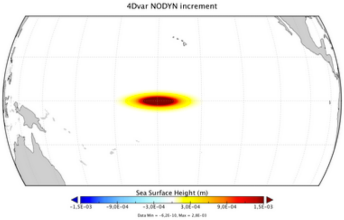
$$\frac{\partial \delta T}{\partial t} = -\nabla.(\delta T \mathbf{U}) + \delta D^{vT}$$

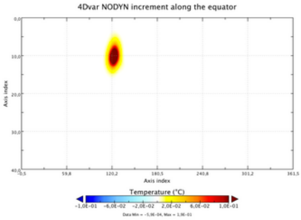
$$\delta D^{vT} = \frac{\partial}{\partial z}\left(A^{vT}\frac{\partial \delta T}{\partial z}\right)$$

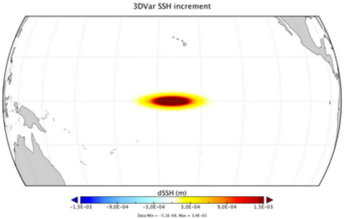


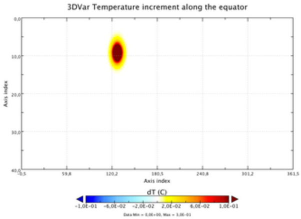
Simplified 4Dvar

Single temperature observation (10d assimilation window)



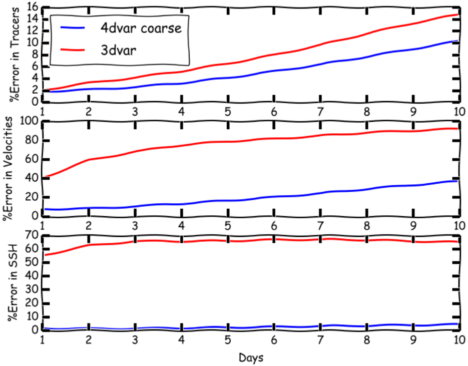






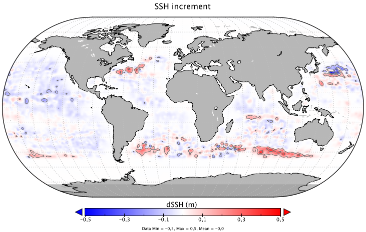
ORCA025 for the direct model, ORCA1 for the tangent model. Perturbations generated at coarse resolution.

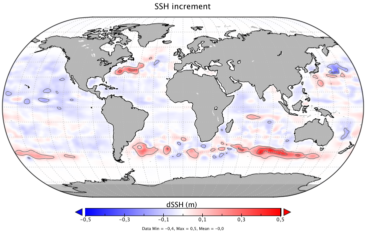
Interpolation: observation operator simplification: its weighted ajoint.

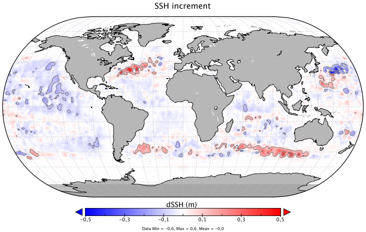


Approximation in the linear propagator

Multi incremental 4Dvar







5 day:

4dvar: 7h (9h)

3dvar: 45mn (2h45)

5day, ORCA1 (Z42) in the inner loop:

4dvar: 45mn

3dvar: 2mn

Back to the second question

Can we improve coupled consistency through data assimilation?

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the answer is yes, probably ...

Back to the second question

Can we improve coupled consistency through data assimilation?

the answer is yes, probably ...

but at a cost ...

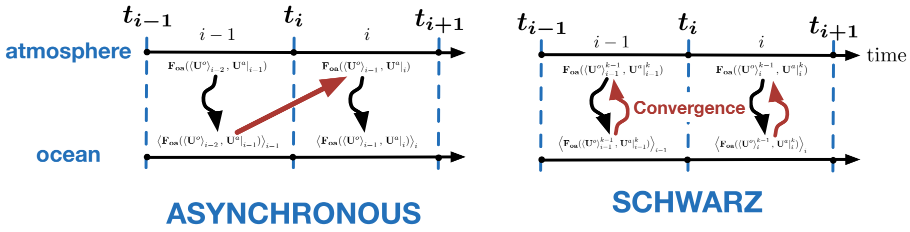
Ocean atmosphere coupling

OA coupling is a complex matter with many sources of uncertainties

- time/space non-confomity
- interfaces may actually not be represented by any component
- multi physics with different characteristics.
- highly parameterised interface (Bulk formulae)
- coupling methods
- ...

Some of theses uncertainties are unavoidable, some others are linked to the way we implement things.
Coupled DA is an opportunity to account for or reduce them

Focus on flux consistency



The SWR algorithm reads :

$$\begin{cases} \mathcal{L}_a(u_a^k) = f_a & \text{on } \Omega_a \times T_W \\ u_a^k(z,0) = u_0(z) & z \in \Omega_a \\ \mathcal{C}_a(u_a^k) = \mathcal{F}_{oa}(u_a^k, u_o^{k-1}) & \text{on } \Gamma \times T_W \end{cases} \quad \begin{cases} \mathcal{L}_o(u_o^k) = f_o & \text{on } \Omega_o \times T_W \\ u_o^k(z,0) = u_0(z) & z \in \Omega_o \\ \mathcal{C}_o(u_o^k) = \mathcal{F}_{oa}(u_a^k, u_o^k) & \text{on } \Gamma \times T_W \end{cases}$$

where $T_W = [t_i; t_{i+1}]$

- At convergence, it provides a flux consistent solution : $\mathcal{C}_a(u_a) = \mathcal{C}_o(u_o)$ on $\Gamma \times T_W$

For a fistful of algorithms

- Fully coupled models. $\mathbf{x} = u_0(z),\ z \in \Omega$

$$J_{FCM}(\mathbf{x}) = \left(\mathbf{x} - \mathbf{x}^b\right)^T \mathbf{B}^{-1} \left(\mathbf{x} - \mathbf{x}^b\right) + \sum_{i=0}^{N} \left(\mathcal{H}_{t_i}(\mathcal{M}_{t_i}(\mathbf{x})) - \mathbf{y}^o_{t_i}\right)^T \mathbf{R}^{-1}_{t_i} \left(\mathcal{H}_{t_i}(\mathcal{M}_{t_i}(\mathbf{x})) - \mathbf{y}^o_{t_i}\right)$$

- Partially coupled models. $\mathbf{x}_0 = (u_0(z), u_o^0(0,t))^T,\ z \in \Omega,\ t \in [0,T]$

$$J_{PCM}(\mathbf{x}) = J^b(\mathbf{x}) + \sum_{i=0}^{N} \left(\mathcal{H}_{t_i}(\mathcal{M}^{trunc}_{t_i}(\mathbf{x})) - \mathbf{y}^o_{t_i}\right)^T \mathbf{R}^{-1}_{t_i} \left(\mathcal{H}_{t_i}(\mathcal{M}^{trunc}_{t_i}(\mathbf{x})) - \mathbf{y}^o_{t_i}\right) + J^s(\mathbf{x})$$

- Weakly coupled models. $\mathbf{x}_0 = (u_0(z), u_o^0(0,t), u_a^0(0,t))^T,\ z \in \Omega,\ t \in [0,T]$

$$J_{WCM}(\mathbf{x}) = J^b_a(\mathbf{x}_a) + J^b_o(\mathbf{x}_o) + J^o_a(\mathbf{x}_a) + J^o_o(\mathbf{x}_o) + J^s(\mathbf{x})$$

- and obviously CERA (uncoupled in the inner loop). $\mathbf{x} = u_0(z),\ z \in \Omega$

$$J^s(\mathbf{x}) = \gamma \|\mathcal{C}_a(u_a(0,t)) - \mathcal{C}_o(u_o(0,t))\|^2_{[0,T]}.$$

Stand-alone SCM

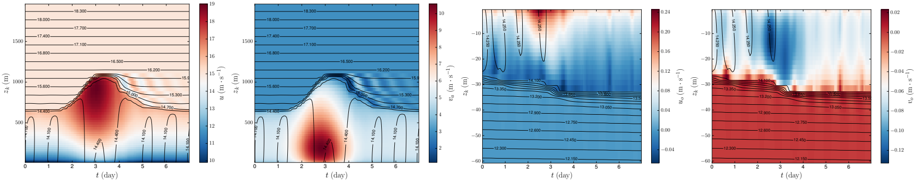


Figure: Colors represent zonal (a,c) and meridional (b,d) atmosphere wind and ocean current velocities components and black isolines represent temperatures.

$$\frac{\partial \mathbf{u}_\beta(z,t)}{\partial t} = -f\mathbf{k}\times\mathbf{u}_\beta(z,t) + \frac{\partial}{\partial z}\left(K_m^\beta(z)\frac{\partial \mathbf{u}_\beta(z,t)}{\partial z}\right) + F_{\mathbf{u}_\beta}(z,t) \quad \text{sur } \Omega_\beta\times[0,T]$$

$$\frac{\partial \mathbf{t}_\beta(z,t)}{\partial t} = \frac{\partial}{\partial z}\left(K_s^\beta(z)\frac{\partial \mathbf{t}_\beta(z,t)}{\partial z}\right) + F_{\mathbf{t}_\beta}(z,t) \quad \text{sur } \Omega_\beta\times[0,T]$$

$$\rho_a K_m^a(z^+)\left.\frac{\partial \mathbf{u}_a}{\partial z}\right|_\Gamma = \rho_o K_m^o(z^-)\left.\frac{\partial \mathbf{u}_o}{\partial z}\right|_\Gamma = \mathcal{F}_{oa}^m(\mathbf{u}_a,\mathbf{u}_o,\mathbf{t}_a,\mathbf{t}_o) \quad \text{sur } \Gamma\times[0,T]$$

$$\rho_a K_s^a(z^+)\left.\frac{\partial \mathbf{t}_a}{\partial z}\right|_\Gamma = \rho_o K_s^o(z^-)\left.\frac{\partial \mathbf{t}_o}{\partial z}\right|_\Gamma = \mathcal{F}_{oa}^s(\mathbf{u}_a,\mathbf{u}_o,\mathbf{t}_a,\mathbf{t}_o) \quad \text{sur } \Gamma\times[0,T]$$

where $\beta = a, o$ refer to atmosphere and ocean variables respectively. Both models use the same structure and differ from their forcing terms F_*, their interface conditions and the computation of their turbulent viscosity and diffusivity coefficients K_m^β and K_s^β.

Results summary

Algorithm	γ	k_{max}	# of minimisation iterations	Computing cost (relative to CERA)	Interface imbalance indicator	RMSE improvement (in %)
FCM-F	—	k_{cvg}	26	3.8	$2.\,10^{-12}$	74
CERA-F	—	k_{cvg}	24	1.1	$5.8\,10^{-12}$	24
CERA-1	—	1	26	1	1.6	40
CERA-1-SWR	—	1	26	1	$5\,10^{-2}$	45
PCM-1	0.1	1	25	0.96	$4.\,10^{-3}$	60
WCM	0.1	0	31	1.2	$6.\,10^{-3}$	57

Table: Result summary for the SCM system (limited to 2 outer loops)

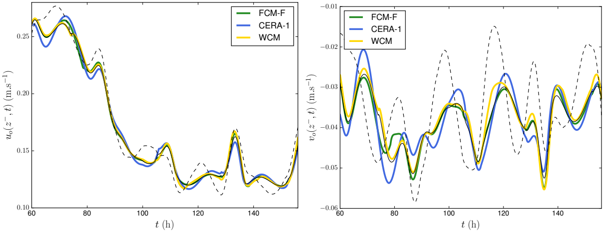
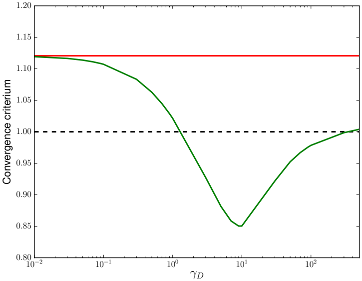


Figure: Forecast of SSU and SSV from FCM-F, CERA-1 and WCM analysis. Dashed and plain black lines are background and truth evolutions respectively

Convergence criteria

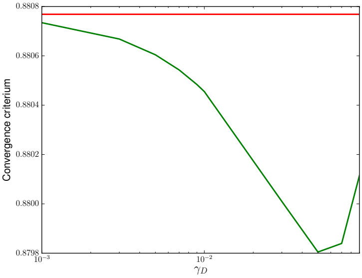
In the previous frame, we were limited to 2 outer loops, due to non convergence of CERA. Adding the J^s term sorts this out



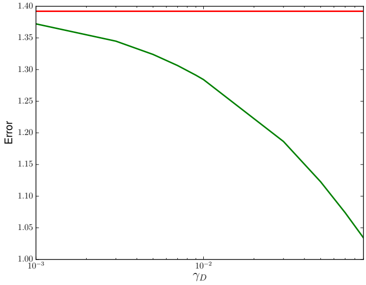
$$\left\|\left(\widetilde{\mathbf{F}}^T\widetilde{\mathbf{F}}\right)^{-1}\left(\widetilde{\mathbf{F}}^T\mathbf{F}\right)\right\|_2$$

Convergence criteria

In the previous frame, we were limited to 2 outer loops, due to non convergence of CERA. Adding the J^s term sorts this out But we can inflate **B** to make CERA converge



$$\left\| \left(\widetilde{\mathbf{F}}^T\widetilde{\mathbf{F}}\right)^{-1}\left(\widetilde{\mathbf{F}}^T\mathbf{F}\right)\right\|_2$$



$$\|\tilde{\mathbf{x}}_0 - \mathbf{x}_0\|$$

Outcome

The outer/inner loop framework allows for approximation

- their impact can be studied theoretically
- they can (should?) be specific for a given application
- they can be (partially) accounted for by modifying the cost function

In addition to deliverables

- 4DVar, simplistic 4DVar and multigrid 4DVar are available in Nemovar repository
- a stand alone single column will soon be available along with its OOPs interfaces