ECMWF Data Assimilation Training Course 2019
Coupled Data Assimilation

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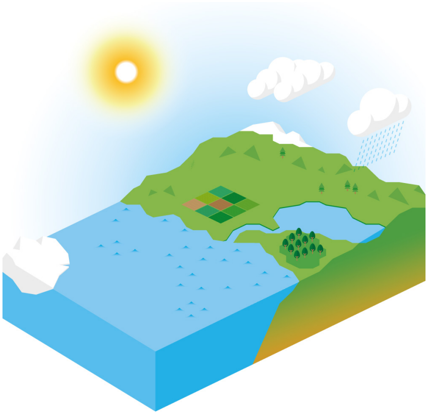
15 March 2019

ECMWF

Components of ECMWF forecasts



Components of ECMWF's Earth system.

Along with the atmosphere, there are the
ocean, wave, sea ice, land surface, snow, and lake models.

Introduction and basis coupled assimilation

Mathematical and computational challenges in coupled data assimilation

Coupled Assimilation terminology

Physical and practical challenges in coupled data assimilation

Coupled assimilation at ECMWF

Coupled assimilation configurations in reanalysis and future NWP

Overview and summary of coupled assimilation at ECMWF

Why do coupled assimilation?

Observation impact

Observations of one component of the system can updated another, e.g.

- Observing surface winds could directly impact on the land surface model, e.g. through updating both surface temperatures and evaporation rates
- Observations of passive (chemical) tracers can be used to update atmospheric winds

More consistent analyses

By treating components together they may become more *balanced*.

- This can lead to a reduction in fast adjustments at the start of forecasts, known as *initialisation shock*

Multivariate assimilation

One can write the 4D-Var cost function as

$$J(\boldsymbol{x}) = \frac{1}{2}(\boldsymbol{x_b} - \boldsymbol{x})^T P_b^{-1}(\boldsymbol{x_b} - \boldsymbol{x}) + \frac{1}{2}\sum_k (\boldsymbol{y}_k - \mathcal{G}_k(\boldsymbol{x}))^T R_k^{-1}(\boldsymbol{y}_k - \mathcal{G}_k(\boldsymbol{x}))$$

and its gradient

$$-\nabla J(\boldsymbol{x}) = P_b^{-1}(\boldsymbol{x_b} - \boldsymbol{x}) + \sum_k M_k^T H_k^T R_k^{-1}(\boldsymbol{y}_k - \mathcal{G}_k(\boldsymbol{x})).$$

Cycling of 4D-Var can be written as:

$$\boldsymbol{x}_b = \mathcal{M}(\boldsymbol{x}_a)$$

Question: which terms in these equations can transfer information from one component of $\boldsymbol{x}$ to another?

A simple example 1

Suppose we model the temperature in the room, but we spilt the room in half and have one temperature for each half; x_1 and x_2.
Now let us measure the temperature in each half of the room; y_1 and y_2.

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Uncoupled assimilation (3D-Var)

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Uncoupled assimilation (3D-Var)

$$\boldsymbol{x} = x_1, \boldsymbol{y} = y_1, H = 1, R = \sigma_{y_1}^2, P_b = \sigma_{x_1}^2$$

$$J_1(\boldsymbol{x}) = (x_{b_1} - x_1)\sigma_{x_1}^{-2}(x_{b_1} - x_1) + (y_1 - x_1)\sigma_{y_1}^{-2}(y_1 - x_1)$$

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$$\boldsymbol{x} = x_2, \boldsymbol{y} = y_2, H = 1, R = \sigma_{y_2}^2, P_b = \sigma_{x_2}^2$$

$$J_2(\boldsymbol{x}) = (x_{b_2} - x_2)\sigma_{x_2}^{-2}(x_{b_2} - x_2) + (y_2 - x_2)\sigma_{y_2}^{-2}(y_2 - x_2)$$

A simple example 2

Coupled assimilation (3D-Var)

$$\boldsymbol{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}, \boldsymbol{y} = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}, H = I, R = \begin{bmatrix} \sigma_{y_1}^2 & 0 \\ 0 & \sigma_{y_2}^2 \end{bmatrix}, P_b = \begin{bmatrix} \sigma_{x_1}^2 & \sigma_{x12}^2 \\ \sigma_{x12}^2 & \sigma_{x_2}^2 \end{bmatrix}$$

$$J(\boldsymbol{x}) = \begin{bmatrix} x_{b_1} - x_1 \\ x_{b_2} - x_2 \end{bmatrix}^T \begin{bmatrix} \sigma_{x_1}^2 & \sigma_{x12}^2 \\ \sigma_{x12}^2 & \sigma_{x_2}^2 \end{bmatrix}^{-1} \begin{bmatrix} x_{b_1} - x_1 \\ x_{b_2} - x_2 \end{bmatrix}$$
$$+(y_1 - x_1)\sigma_{y_1}^{-2}(y_1 - x_1) + (y_2 - x_2)\sigma_{y_2}^{-2}(y_2 - x_2)$$

A simple example 3

Suppose we stop observing y_2.

- In uncoupled 3D-Var, $x_2 = x_{b_2}$, i.e. nothing happens for this variable
- In coupled 3D-Var x_2 is still updated if $\sigma^2_{x_{12}} \neq 0$

A simple example 3

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- In uncoupled 3D-Var, $x_2 = x_{b_2}$, i.e. nothing happens for this variable
- In coupled 3D-Var x_2 is still updated if $\sigma^2_{x_{12}} \neq 0$

If we never observe y_2, the *cross-covariance* $\sigma^2_{x_{12}}$ allows us to constrain x_2.

Coupled assimilation 3D-Var

Recall the 3D-Var cost function:

$$J(\boldsymbol{x}) = \frac{1}{2}(\boldsymbol{x_b} - \boldsymbol{x})^T P_b^{-1}(\boldsymbol{x_b} - \boldsymbol{x}) + \frac{1}{2}(\boldsymbol{y} - \mathcal{H}(\boldsymbol{x}))^T R^{-1}(\boldsymbol{y} - \mathcal{H}(\boldsymbol{x}))$$

and its gradient

$$-\nabla J(\boldsymbol{x}) = P_b^{-1}(\boldsymbol{x_b} - \boldsymbol{x}) + H^T R^{-1}(\boldsymbol{y} - \mathcal{H}(\boldsymbol{x}))$$

There are two ways x_2 can influence x_1:

- H is a function of both x_1 and x_2
- $P_{b12} \neq 0$

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Reminder: 4D-Var equations

One can write the 4D-Var cost function as

$$J(\boldsymbol{x}) = \frac{1}{2}(\boldsymbol{x_b} - \boldsymbol{x})^T P_b^{-1}(\boldsymbol{x_b} - \boldsymbol{x}) + \frac{1}{2}\sum_k (\boldsymbol{y}_k - \mathcal{G}_k(\boldsymbol{x}))^T R_k^{-1}(\boldsymbol{y}_k - \mathcal{G}_k(\boldsymbol{x}))$$

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Cycling of 4D-Var can be written as:

$$\boldsymbol{x}_b = \mathcal{M}(\boldsymbol{x}_a)$$

Why coupled assimilation and not just multivariate assimilation?

- P_b — background error covariance coupling
- $\mathcal{G} = \mathcal{H}(\mathcal{M})$
  - $\mathcal{H}$ — observation operator coupling
  - $\mathcal{M}$ — coupled nonlinear trajectories
- M^T — coupled TL/AD
- H^T — coupled Jacobian (of observation operator)
- R — coupled observation error covariance matrix
- $\mathcal{M}$ — coupled model for cycling the analyses

Why coupled assimilation and not just multivariate assimilation?

- P_b — background error covariance coupling
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- R — ~~coupled observation error covariance matrix~~
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Coupled assimilation challenges 1: The state vector

$$\boldsymbol{x} = \begin{bmatrix} \boldsymbol{x}_1 \\ \boldsymbol{x}_2 \end{bmatrix}$$

The components $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$ can

- Be on different grids
- Have different representations (eg. spectral vs grid point)
- Stored on different processors
- Stored in very different places in the code (i.e. different modules)
- Not even represented in the same code!

So there can be huge technical challenges to overcome before one can even write down a coupled state vector.

Coupled assimilation challenges 2: Background error coupling

$$P_b = \begin{bmatrix} P_{11} & P_{12} \\ P_{12} & P_{22} \end{bmatrix}$$

Assuming we can specify P_{11} and P_{22}, then we have to specify the cross covariance terms P_{12}.

We have all the same problems as for the state vector: grids, storage, etc.

P_b also needs to be a covariance matrix, i.e. be positive definite.

These problems go away if $P_{12} = \mathbf{0}$.

Ensemble methods for representing P_{12} are promising.

Coupled assimilation challenges 3: Observation operator coupling

$$\mathcal{H} = \mathcal{H}\left(\begin{bmatrix}\boldsymbol{x}_1\\ \boldsymbol{x}_2\end{bmatrix}\right)$$

If the problems of the state vector can be solved, then a coupled observation operator should be possible.
This then requires H^T, a coupled Jacobian, which is a technical exercise to ensure its availability.

Coupled assimilation challenges 4: Coupled nonlinear evolution

$$\mathcal{M} = \mathcal{M}\left(\begin{bmatrix}\boldsymbol{x}_1 \\ \boldsymbol{x}_2\end{bmatrix}\right)$$

This is typically the *easiest* form of coupling to use in coupled data assimilation. This is because the model is generally developed before the assimilation technique is put in place.
We will return to this later on.

Coupled assimilation challenges 5: TL/AD coupling

$$M = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix} \quad \text{i.e.} \quad M\boldsymbol{x} = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix} \begin{bmatrix} \boldsymbol{x}_1 \\ \boldsymbol{x}_2 \end{bmatrix} = \begin{bmatrix} M_{11}\boldsymbol{x}_1 + M_{12}\boldsymbol{x}_2 \\ M_{21}\boldsymbol{x}_1 + M_{22}\boldsymbol{x}_2 \end{bmatrix}$$

$$M^T = \begin{bmatrix} M_{11}^T & M_{21}^T \\ M_{12}^T & M_{2}^T \end{bmatrix} \quad \text{i.e.} \quad M^T\boldsymbol{x} = \begin{bmatrix} M_{11}^T & M_{21}^T \\ M_{12}^T & M_{22}^T \end{bmatrix} \begin{bmatrix} \boldsymbol{x}_1 \\ \boldsymbol{x}_2 \end{bmatrix} = \begin{bmatrix} M_{11}^T\boldsymbol{x}_1 + M_{21}^T\boldsymbol{x}_2 \\ M_{12}^T\boldsymbol{x}_1 + M_{22}^T\boldsymbol{x}_2 \end{bmatrix}$$

The coupled TL/AD terms M_{12} and M_{21} may not be implemented.

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- **Coupled Assimilation terminology**
- Physical and practical challenges in coupled data assimilation
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Timing of observation impact

Recall the gradient of the 4D-Var cost function

$$-\nabla J(\boldsymbol{x}) = P_b^{-1}(\boldsymbol{x_b} - \boldsymbol{x}) + \sum_k M_k^T H_k^T R_k^{-1}(\boldsymbol{y}_k - \mathcal{G}_k(\boldsymbol{x})).$$

Then if any of P_b, M, H, or $\mathcal{G} = \mathcal{H}(\mathcal{M})$ have coupling terms then an observation in one component will modify the state of the other *within the assimilation cycle*.

Timing of observation impact

Recall the gradient of the 4D-Var cost function

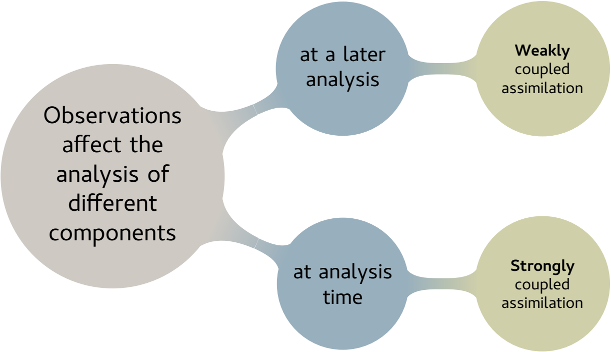
$$-\nabla J(\boldsymbol{x}) = P_b^{-1}(\boldsymbol{x_b} - \boldsymbol{x}) + \sum_k M_k^T H_k^T R_k^{-1}(\boldsymbol{y}_k - \mathcal{G}_k(\boldsymbol{x})).$$

Then if any of P_b, M, H, or $\mathcal{G} = \mathcal{H}(\mathcal{M})$ have coupling terms then an observation in one component will modify the state of the other *within the assimilation cycle*. Suppose none of these terms have coupling terms, but the model which cycles the analysis,

$$\boldsymbol{x}_b = \mathcal{M}(\boldsymbol{x}_a),$$

is coupled. The an observation in one component will modify the state of the other *in the next the assimilation cycle*.

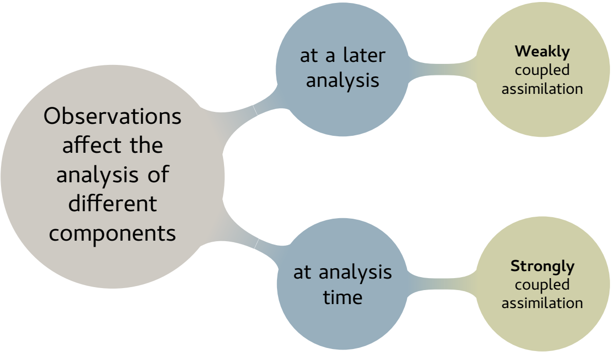
Coupled DA categories



Formal definitions are available in

Stephen G Penny et al. (2017). *Coupled Data Assimilation for Integrated Earth System Analysis and Prediction: Goals, Challenges and Recommendations*. Tech. rep. World Meteorological Organisation

Coupled DA categories



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Note that these are only broad categorisations, they tell you nothing about which terms are coupled.

Coupled assimilation in the ensemble Kalman filter

One can write the EnKF update as

$$\begin{aligned}\boldsymbol{x}_t^a =& \boldsymbol{x}_t^b + P^b H^T (HP^bH^T + R)^{-1}(y - \mathcal{H}(\boldsymbol{x}_t^b)) \\ =& \mathcal{M}(\boldsymbol{x}_{t-1}^a) + P^b H^T (HP^bH^T + R)^{-1}(y - \mathcal{H}(\mathcal{M}(\boldsymbol{x}_{t-1}^a)))\end{aligned}$$

1. If the observation operator is coupled then we have immediate cross component impact.
2. If the observation operator is not coupled then for an observation to have immediate cross component impact P^b must have nonzero diagonal terms.
3. If neither of these conditions hold then the nonlinear model $\mathcal{M}$ will mix the information as the ensemble members are propagated from one analysis time to the next.

Hence (1) and (2) are a form of strongly coupled assimilation.
The case (3) would fall under weakly coupled assimilation.
Note that localisation methods across the different components need to be specified!

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Long assimilation windows

- ☺ The longer the assimilation window, the more observations we get to put into our systems
- ☺ The longer the assimilation window, the more flow dependence we obtain in our solution - i.e. we become less reliant on the background error covariance that we specify at $t = 0$.
- ☹ The longer the assimilation window, the more nonlinearities make the tangent linear approximation worse.

Timescales in the Earth System

▸ Microscale turbulence	minutes
▸ Mesoscale storms (tornadoes/thunderstorms)	hours
▸ Synoptic scale cyclones	days
▸ Planetary waves/blocking structures	weeks
▸ Intraseasonal features	months
▸ Seasonal cycles/ENSO	years

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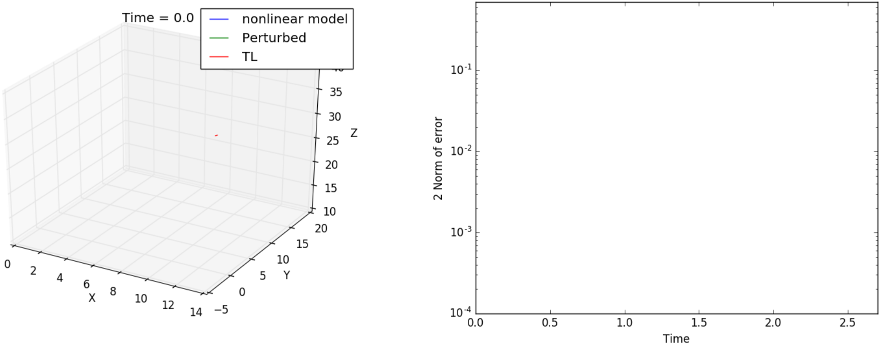
▸ Internal waves	hours
▸ Tides	days
▸ Mesoscale eddies	weeks/months
▸ ENSO	years
▸ Thermohaline circulation	centuries

Tangent linear model and approximation



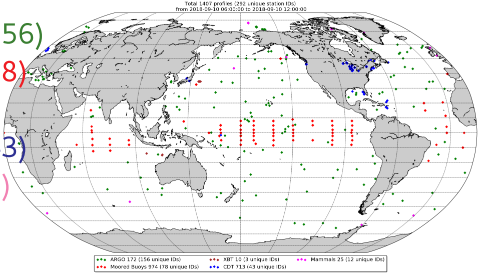
Different observation networks and infrastructure

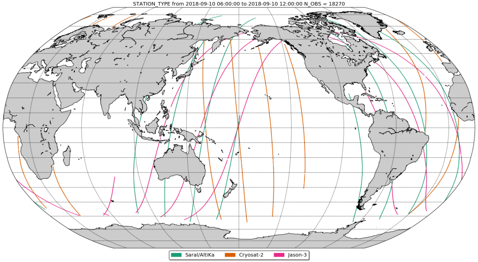
- Observations of one system may not be available within the assimilation window for the faster components.
- You won’t get impact from observations that have not arrived.

Ocean observation latency

49 hour cut-off

172 (156)
974 (78)
10 (3)
713 (43)
25 (12)

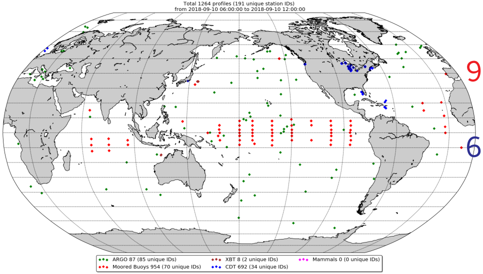


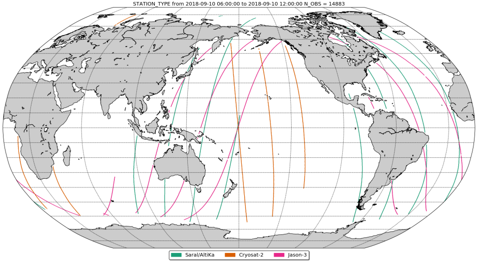


18270

1 hour cut-off

87 (85)
954 (70)
8 (2)
692 (34)
0 (0)





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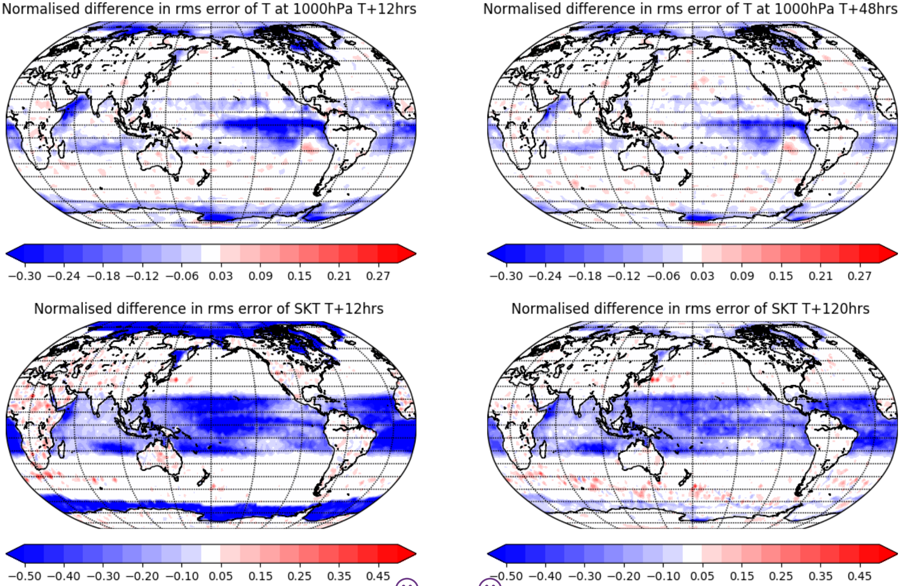
Weakly coupled assimilation

- The concept of weakly coupled assimilation is very flexible.
- It allows different components to be assimilated separately and information mixed by the model.
- It also allows for different assimilation techniques to be used for each component.
- It doesn't actually require the assimilation windows of each component to be aligned.

We use 2D-OI for the wave analysis and snow depth analysis.
We use 1D-OI for the soil temperature analysis and the SEKF for soil moisture analysis.
We use 3D-Var FGAT for the sea ice analysis and a simpled nudging for the SST analysis (see next slides).

WCDA maps of surface temperature forecast errors



New possible biases with coupled assimilation

- If a coupled $\mathcal{M}$ has different biases compared to the uncoupled version, then these can be passed between the components of the analysis.
- In our ocean model we have more *effective* resolution in the tropics (due to latitudinal variability of the Rossby radius of deformation) than the extratropics.
- As such the model performs less well in the extratropics, and so to not degrade the atmospheric analysis we do not couple the ocean and atmosphere here.

Philip A Browne et al. (2019). "Weakly Coupled Ocean-Atmosphere Data Assimilation in the ECMWF NWP System". In: *Remote Sensing* 11.234, pp. 1–24. DOI: 10.3390/rs11030234

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Outer loop coupling (1)

One approach is known as outer loop coupling 4D-Var in which $\mathcal{M}$ is coupled, i.e. we use coupled trajectories and the coupled model to cycle the analysis.
We neglect all coupling terms in the TL and AD:

$$M = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix} := \begin{bmatrix} M_{11} & 0 \\ 0 & M_{22} \end{bmatrix} \quad \text{i.e.} \quad M\boldsymbol{x} = \begin{bmatrix} M_{11} & 0 \\ 0 & M_{22} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} M_{11}x_1 \\ M_{22}x_2 \end{bmatrix}$$

$$M^T = \begin{bmatrix} M_{11}^T & M_{21}^T \\ M_{12}^T & M_{22}^T \end{bmatrix} := \begin{bmatrix} M_{11}^T & 0 \\ 0 & M_{22}^T \end{bmatrix} \quad \text{i.e.} \quad M^T\boldsymbol{x} = \begin{bmatrix} M_{11}^T & 0 \\ 0 & M_{22}^T \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} M_{11}^T x_1 \\ M_{22}^T x_2 \end{bmatrix}$$

Outer loop coupling (2)

Recall the linearisation state $\boldsymbol{x}^{(m)}$ such that

$$\boldsymbol{x} = \boldsymbol{x}^{(m)} + \delta\boldsymbol{x}^{(m)}$$

Then the cost function becomes

$$\begin{aligned} J(\delta\boldsymbol{x}^{(m)}) =& \tfrac{1}{2}(\boldsymbol{x}_b - \boldsymbol{x}^{(m)} - \delta\boldsymbol{x}^{(m)})^T P_b^{-1}(\boldsymbol{x}_b - \boldsymbol{x}^{(m)} - \delta\boldsymbol{x}^{(m)}) \\ &+ \tfrac{1}{2}(\boldsymbol{d}^{(m)} - G\delta\boldsymbol{x}^{(m)})^T R^{-1}(\boldsymbol{d}^{(m)} - G\delta\boldsymbol{x}^{(m)}) \end{aligned}$$

where $\boldsymbol{d}^{(m)} = \boldsymbol{y} - \mathcal{G}(\boldsymbol{x}^{(m)})$

Outer loop coupling (3)

If we do not specify background error coupling terms (i.e. P_b block diagonal), and the TL/AD is not coupled, then the cost function is separable:

$$J(\delta \boldsymbol{x}^{(m)}) = J\left(\begin{bmatrix}\delta \boldsymbol{x}_1^{(m)} \\ \delta \boldsymbol{x}_2^{(m)}\end{bmatrix}\right) = J_1(\delta \boldsymbol{x}_1^{(m)}) + J_2(\delta \boldsymbol{x}_2^{(m)})$$

Exercise: show this!

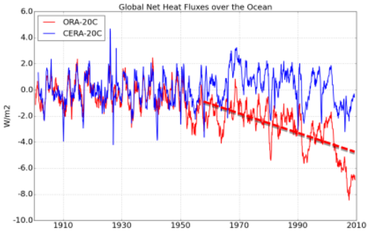
Thus the interaction between components happens though $\mathcal{G}$ each outer loop of the minimisation.

This method formed the basis of the CERA system which produced the CERA-20C and CERA-SAT reanalyses.

Patrick Laloyaux et al. (2018). "CERA-20C: A Coupled Reanalysis of the Twentieth Century". In: *Journal of Advances in Modeling Earth Systems* 10.5, pp. 1172–1195. DOI: 10.1029/2018MS001273

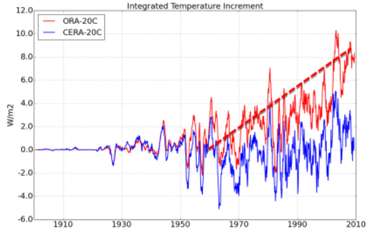
Dinand Schepers et al. (2018). "CERA-SAT: A coupled satellite-era reanalysis". In: *ECMWF Newsletter* 155, pp. 32–37. DOI: 10.21957/sp619ds74g

Balanced ocean-atmosphere analysis



Global net air-sea fluxes toward the ocean in CERA-20C and ORA-20C.

- Spurious trend in ORA-20C probably due to shift in wind forcing in ERA-20C (heat lost)



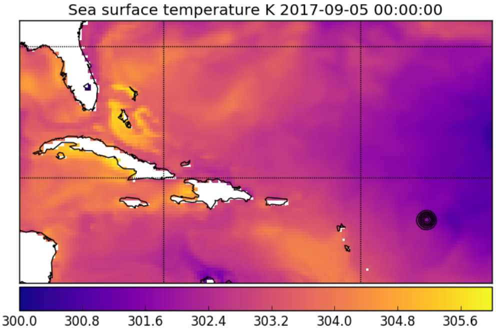
Ocean temperature increment in CERA-20C and ORA-20C.

- Increment in ORA-20C is trying to compensate for the heat lost
- CERA-20C fluctuates around zero suggesting a more balanced air-sea interface

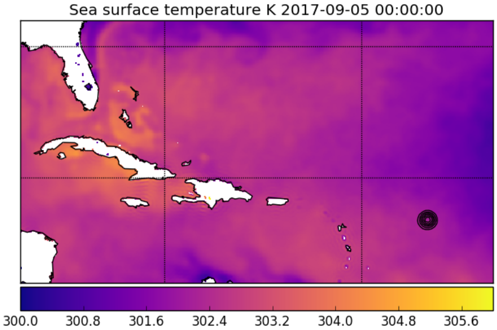
Courtesy of E. de Boisséson

Outer loop coupling for Hurricanes Irma and Jose

Coupled assimilation



Uncoupled analysis (OSTIA)



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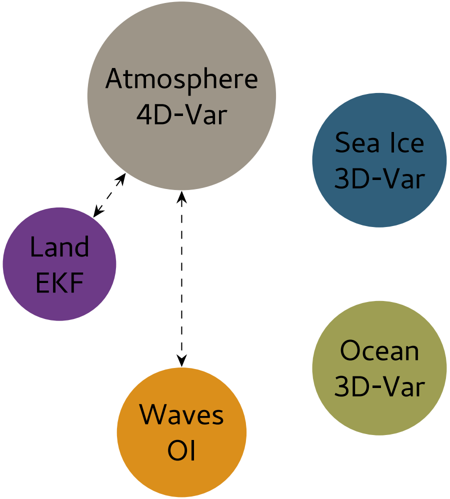
ECMWF
THE STRENGTH OF A COMMON GOAL
A ROADMAP TO 2025

"ECMWF has started to explore a new coupled assimilation system to initialise the numerical weather forecast in a more comprehensive and balanced manner. Such an approach has the potential to better use satellite measurements and to improve the quality of our forecasts. It will generate a reduction of initialisation shocks in coupled forecasts by fully accounting for interactions between the components. It will also lead to the generation of a consistent Earth-system state for the initialisation of forecasts across all timescales",
ECMWF Roadmap to 2025

ECMWF (2016). *The Strength of a Common Goal: A Roadmap To 2025*. Tech. rep. ECMWF. URL: https://www.ecmwf.int/sites/default/files/ECMWF{_}Roadmap{_}to{_}2025.pdf

Components of the Earth System Analyses

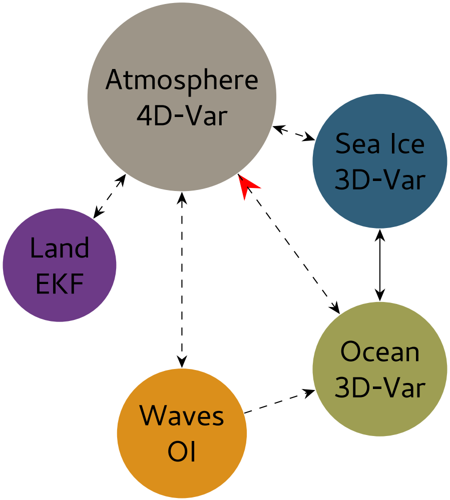
Coupled Assimilation in ERA5



- ERA5: land and waves weakly coupled

Components of the Earth System Analyses

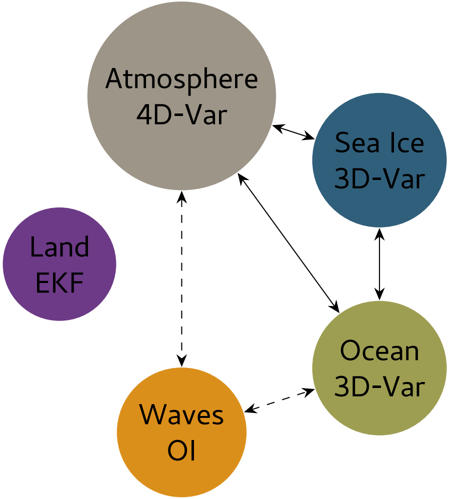
Coupled Assimilation in NWP



- HRES NWP, EDA
- Planned for CY46R1 in June 2019

Components of the Earth System Analyses

Coupled Assimilation in reanalyses and NWP research



- CERA-20C: outer loop coupling for atm-ocean, sea ice

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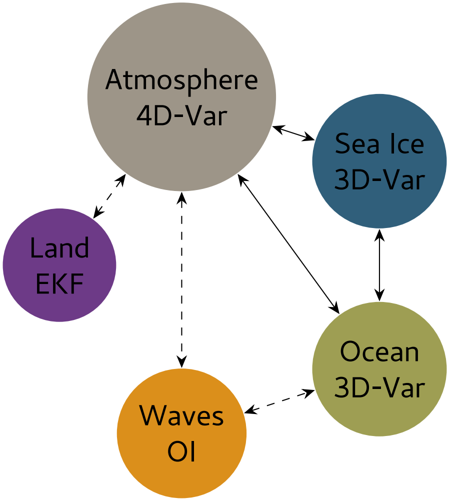

- CERA-20C: outer loop coupling for atm-ocean, sea ice
- CERA-SAT with also land-atm weak coupling and full observing system

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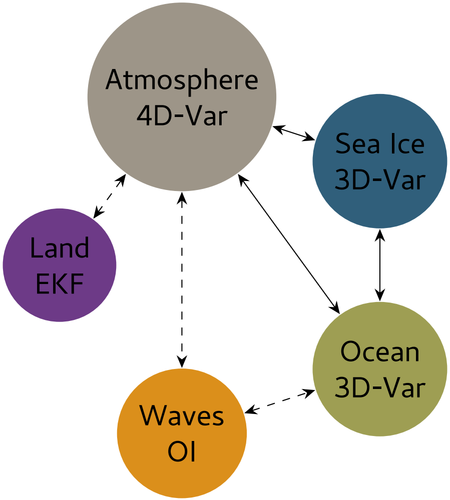
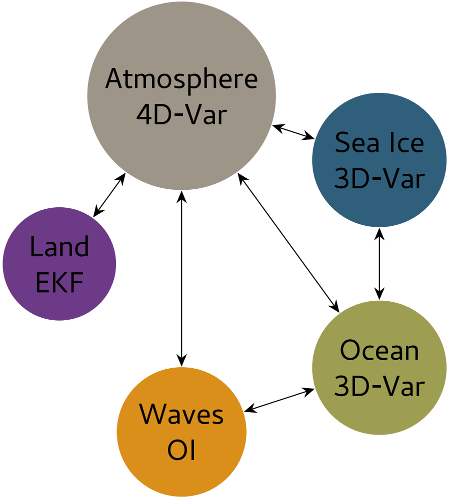


- CERA-20C: outer loop coupling for atm-ocean, sea ice
- CERA-SAT with also land-atm weak coupling and full observing system
- Hence different coupling strategies are used for the different configurations

Towards an Earth System Approach

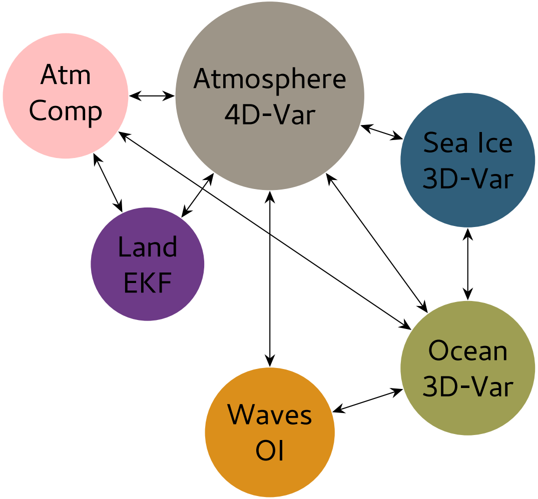
Coupled Assimilation - CERAv3?



- Consistency of the coupling approaches across the different components of the Earth system
- Comprehensive Earth system approach; atmosphere, land, ocean, sea ice, waves

Towards an Earth System Approach

Coupled Assimilation - CERAv3?



- Consistency of the coupling approaches across the different components of the Earth system
- Comprehensive Earth system approach; atmosphere, land, ocean, sea ice, waves, atmospheric composition

Summary

- Coupled data assimilation is, in theory, the same as multivariate DA
- Coupled data assimilation can improve balance in analyses and can increase the use of, and information gained from, observations
- Issues arise from:
  - Varying timescales in the different components - leads to poor TL approximation for “long” windows
  - Various components of the Earth system running separate models/executables - the full adjoint is not always available
  - Observation availability for all the components
- Strongly coupled assimilation: observations can impact multiple components at **that** analysis
- Weakly coupled assimilation: observations can impact multiple components at **a later** analysis
- ECMWF is regularly doing coupled assimilation:
  - Which components are coupled depends on the system
  - We continue to increase the amount and strength of coupling between the Earth system components
- Specifying cross-covariances is a big future challenge

References

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