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Overview of Observational Aspects of Data Assimilation

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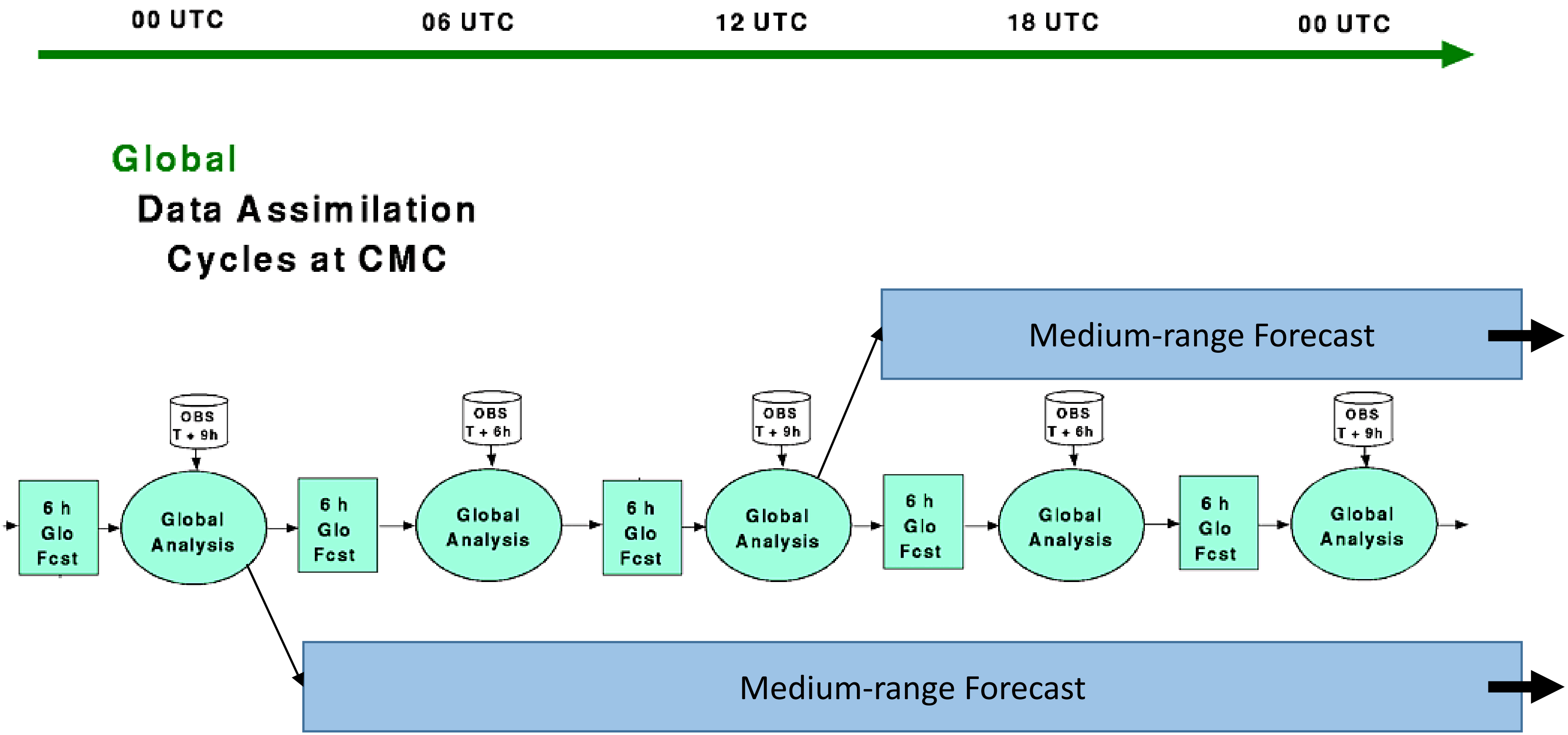
Introduction: Use of observations in DA

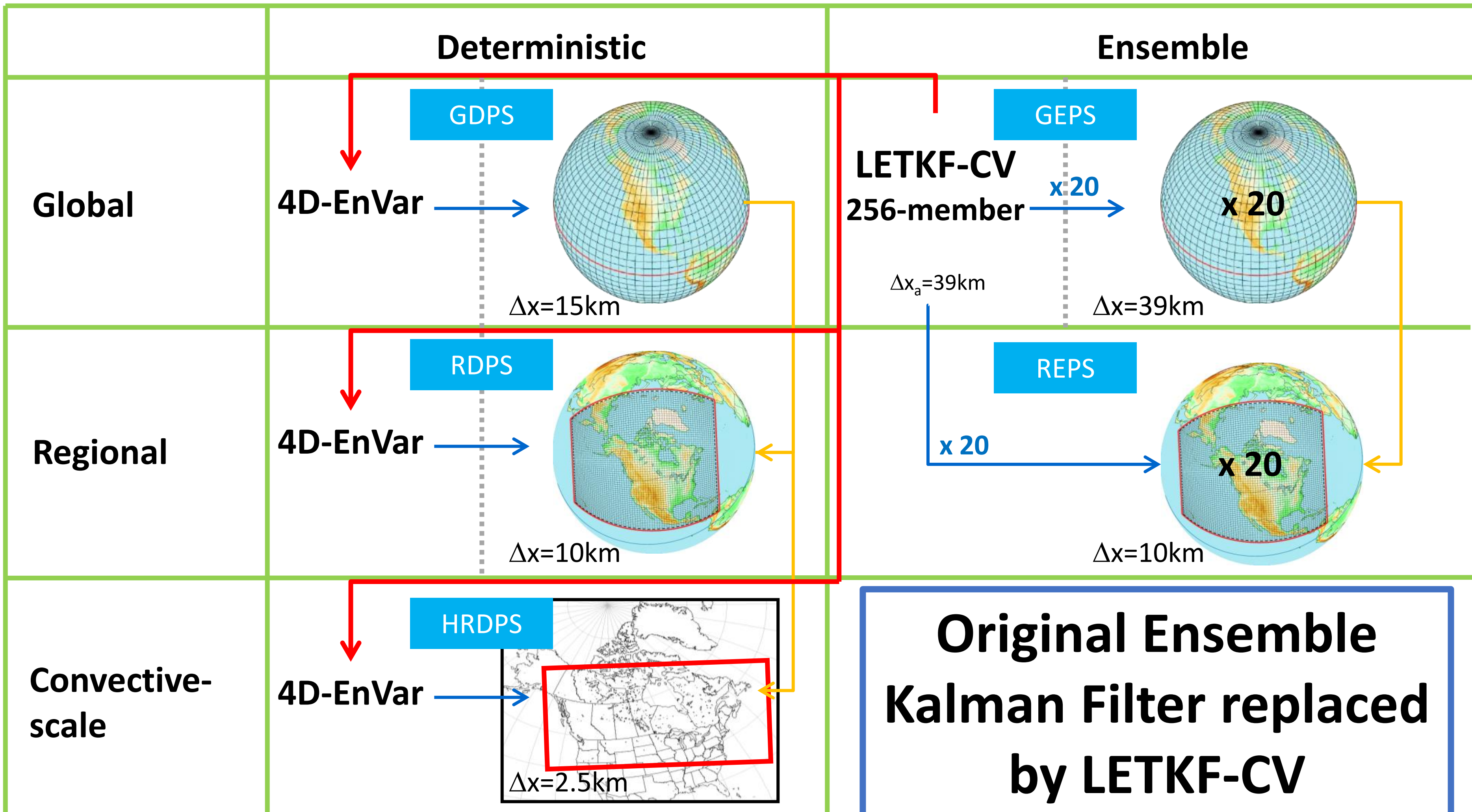
- Various data assimilation (DA) algorithms used for NWP, ocean/sea-ice prediction, and other Earth system components
- Approaches can be derived from Bayes theorem $[p(x|y) \propto p(y|x)p(x)]$ by applying specific simplifying assumptions about errors and models
- Goal is to repeatedly correct short-term forecast (i.e. background state) as best as possible using all available observations
- Deterministic DA produces single "best estimate"; ensemble DA produces ensemble of estimates, approximating probability distribution
- Any observation can be used, even if noisy, biased, indirect, but:
  - Their "optimal" use requires perfect knowledge of both the observation <u>and</u> background error statistics
  - Also requires accurate model of the observing process (i.e. observation operator) and associated uncertainties
  - Incorrect assumptions about observation or background error statistics (bias, covariances, Gaussianity) can result in degraded accuracy from assimilation

Example: Global Deterministic Prediction System



Data Assimilation: Goal is to correct a short-term forecast using information from all available observations

NWP systems at ECCC



Kalman filter – basis of most DA approaches

- The Kalman Filter equations describe the analysis update of the mean and covariance in the case of unbiased Gaussian errors and linear observation operator:

$$\boldsymbol{x}_a = \boldsymbol{x}_b + \mathbf{K}(\boldsymbol{y} - \mathbf{H}x_b)$$
$$\mathbf{P}_a = (\mathbf{I} - \mathbf{KH})\mathbf{P}$$
$$\mathbf{K} = \mathbf{PH}^T(\mathbf{HPH}^T + \mathbf{R})^{-1}$$

$\mathbf{K}$: Kalman gain matrix
$\mathbf{P}$: Background error cov.
$\mathbf{R}$: Observation error cov.
$\mathbf{H}$: Observation operator

- For a single, directly observed, variable:

$$x_a = (1 - k)x_b + (k)y$$
$$\sigma_a^2 = (1 - k)\sigma_b^2$$
$$k = \frac{\sigma_b^2/\sigma_o^2}{\sigma_b^2/\sigma_o^2 + 1} \quad (\text{i.e. between 0 and 1})$$

- Therefore, result of DA is just a weighted average of the background and observation; assimilation always reduces the apparent uncertainty
- Weighting (i.e. k) only depends on ratio of σ_b^2/σ_o^2
- Assumes we know the true background and observation error covariances (which we generally don't)

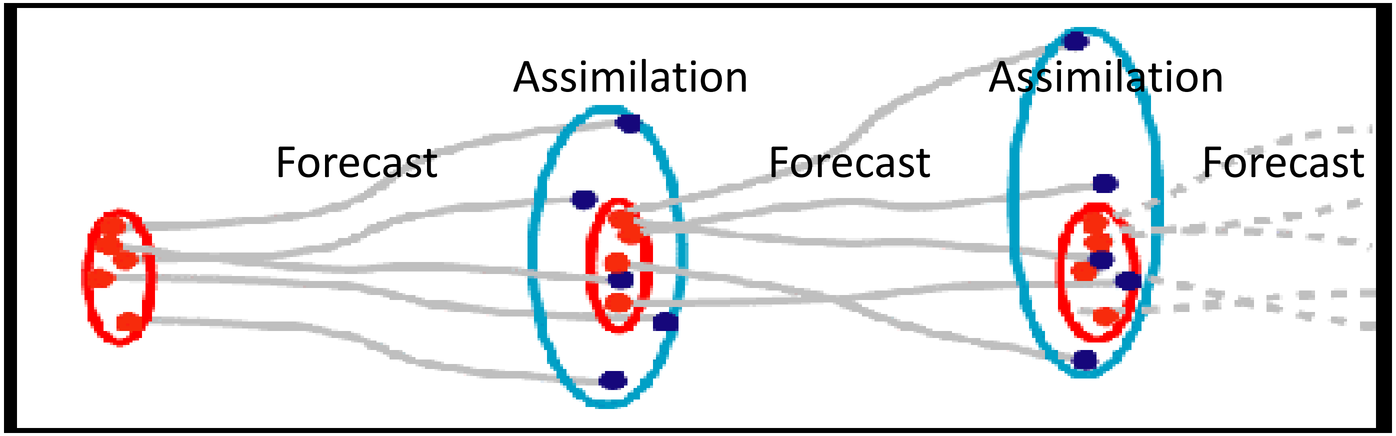
Ensemble Kalman filter: EnKF

- In the EnKF, ensemble of model states are propagated through the forecast-analysis cycle to approximate probability distributions → <u>error of ensemble mean should be consistent with ensemble spread</u>
- Ensemble of short-term forecasts used to approximate the background-error covariances; all members updated during assimilation step to correct mean state and reduce ensemble spread
- Many EnKF flavours; all flavours require "localization" of background-error covariances; original "perturbed obs" EnKF applies the KF equation to each member to assimilate randomly perturbed obs:

$$\mathbf{x}_a^n = \mathbf{x}_b^n + \mathbf{K}_{enkf}(\mathbf{y} + \boldsymbol{\varepsilon}_{obs}^n - H(\mathbf{x}_b^n))$$

$$\mathbf{K}_{enkf} = \mathbf{L} \circ \mathbf{P}_{ens}\mathbf{H}^T(\mathbf{L} \circ \mathbf{H}\mathbf{P}_{ens}\mathbf{H}^T + \mathbf{R})^{-1}$$

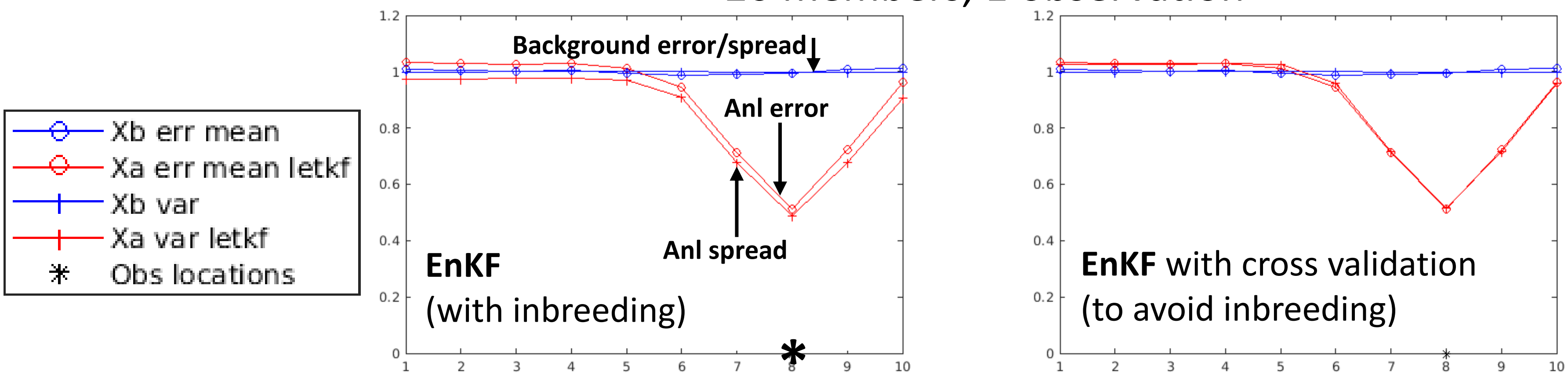
$\boldsymbol{\varepsilon}_{obs}^n$: Random obs perturbation
$\mathbf{L}$: Localization matrix
$\mathbf{P}_{ens}$: Ensemble-based background error cov.



Inbreeding during EnKF analysis

- Most EnKF algorithms do not account for “inbreeding”, caused by dependence between ensemble perturbation being updated and perturbations used to estimate $\mathbf{P}_{ens}$
- Produces too much ensemble spread reduction in assimilation step
- Cross-validation allows inbreeding to be mostly eliminated by using an independent set of perturbations to estimate $\mathbf{P}_{ens}$ for each member update – e.g. use other 19 members to update each of 20 members

20 members, 1 observation



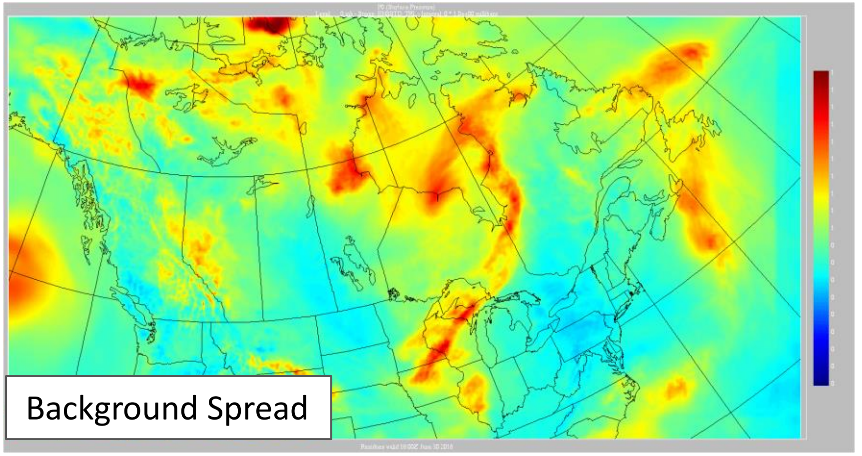
$$\mathbf{x}_a^n = \mathbf{x}_b^n + \mathbf{K}_{enkf}^n(\mathbf{y} + \boldsymbol{\varepsilon}_{obs}^n - \boldsymbol{H}(\mathbf{x}_b^n))$$

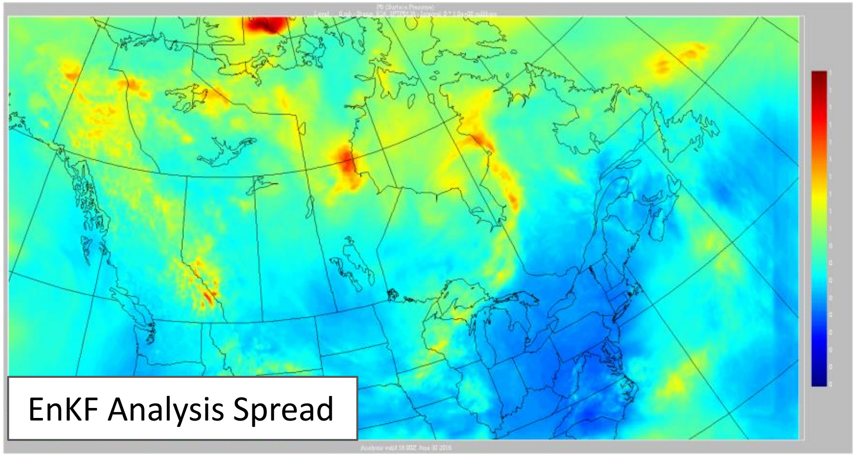
$$\mathbf{K}_{enkf}^n = \mathbf{L} \circ \mathbf{P}_{ens}^n \mathbf{H}^T (\mathbf{L} \circ \mathbf{H}\mathbf{P}_{ens}^n \mathbf{H}^T + \mathbf{R})^{-1}$$

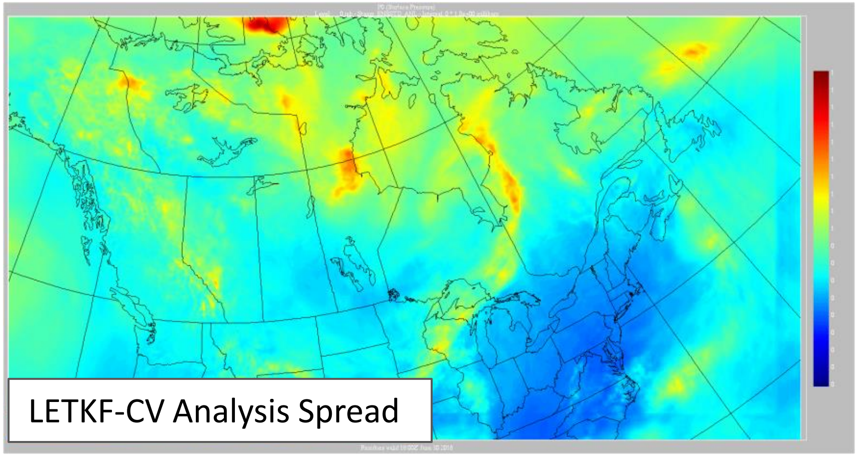
doesn’t use *n*th member

Application of cross-validation to LETKF

- Until now, cross validation only applied to perturbed-observation EnKF, but also possible using "gain form" of LETKF (Bishop et al. 2017)
- Figures show surface pressure ensemble spread (from Buehner 2020)
- Without cross validation, LETKF needed additional multiplicative inflation to maintain reasonable spread (RTPS, α=0.8)
- At ECCC, LETKF-CV is about to replace EnKF in operations







Ensemble-Variational approach: EnVar

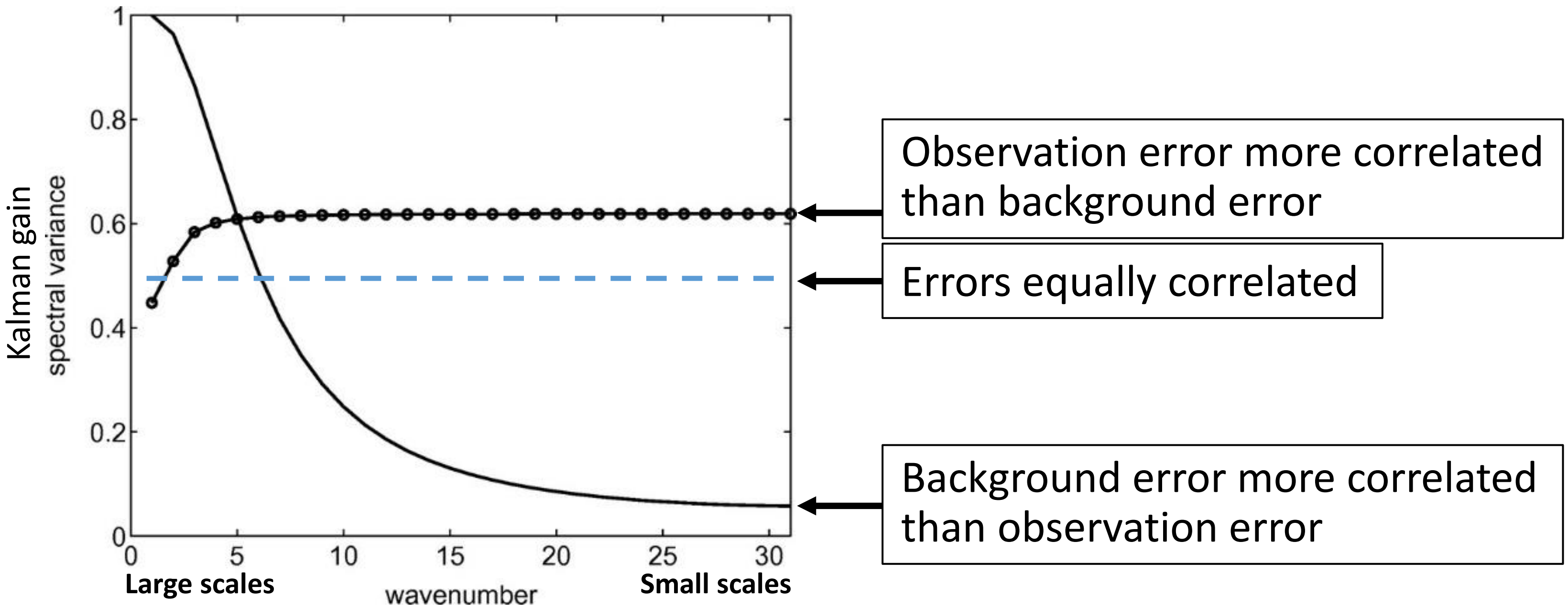
- Ensembles from EnKF also used to specify background-error covariances for deterministic DA with 4D-EnVar
- Similar to EnKF, but unique features of 4D-EnVar approach:
  - Very large number of observations can be assimilated (overall cost not directly related to number of observations)
  - Can use hybrid covariances, blending climatological covariances with ensemble-based covariances, though currently moving away from its use
  - Spatial covariance localization applied in model-space, not observation space → more appropriate for non-local observations (e.g. radiances)
  - Scale-dependent localization (SDL) can be used to better simultaneously fit wide range of scales (Caron and Buehner 2018)
- Analysis obtained by minimizing the pre-conditioned cost function:

$$J(\mathbf{v}) = \frac{1}{2}\mathbf{v}^T\mathbf{v} + \frac{1}{2}[\mathbf{y} - \boldsymbol{H}(\mathbf{x}_b) - \mathbf{H}\Delta\mathbf{x}(\mathbf{v})]^T\,\mathbf{R}^{-1}[\mathbf{y} - \boldsymbol{H}(\mathbf{x}_b) - \mathbf{H}\Delta\mathbf{x}(\mathbf{v})]$$

$$\Delta\mathbf{x}(\mathbf{v}) = \sum_{n=1\rightarrow N_{ens}} \frac{(\mathbf{x}_b^n - \overline{\mathbf{x}_b})}{\sqrt{N_{ens} - 1}} \circ \mathbf{L}^{1/2}\mathbf{v}^n$$

Kalman gain in spectral space

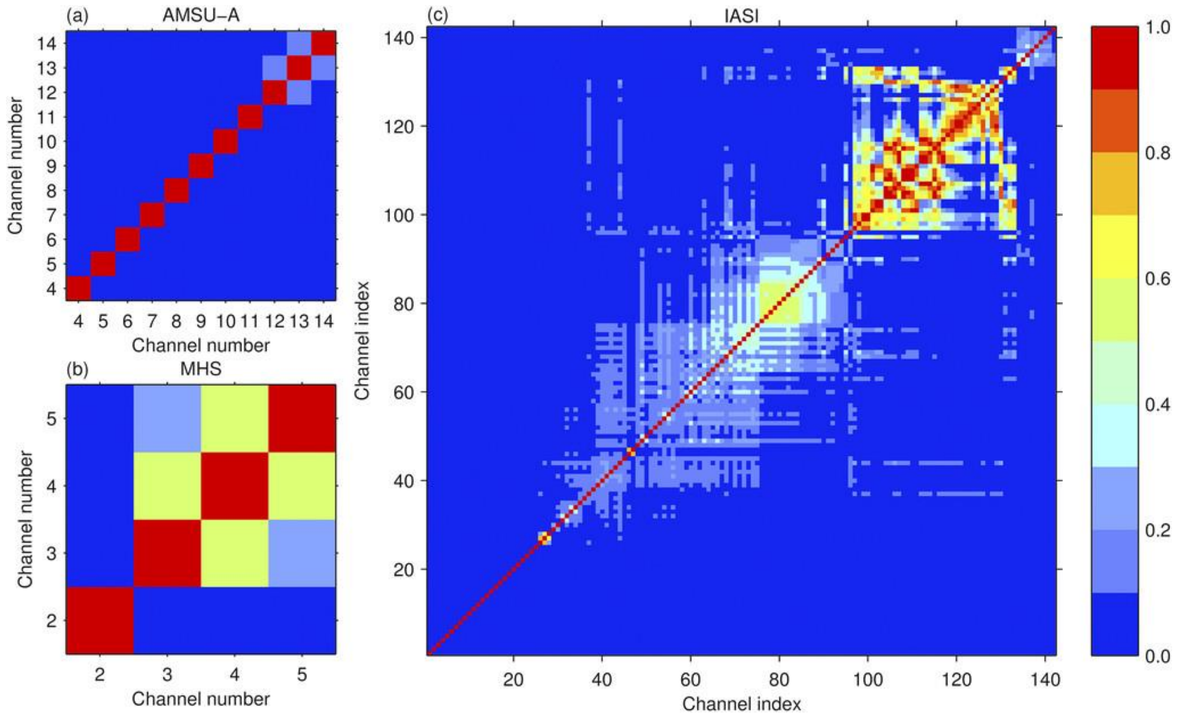
- When considering multiple observations distributed over space/time, error **correlations** can influence weighting as much as variances
- Figure (from Stonebridge et al. 2018) shows Kalman gain ($\mathbf{K}$) for different amounts of observation and background error correlation



- Ignoring real observation error correlations results in giving too much weight to observations at large scales and too little at small scales

Accounting for obs-error correlations

- Can be technically challenging to fully account for observation-error correlations in DA algorithms (requires large matrix inversions)
- Vertical or inter-channel error correlations easier to include than horizontal correlations due to smaller number of observations involved
- Figure shows example of inter-channel radiance error correlations used in ECCC deterministic DA systems



Mis-specified obs error statistics

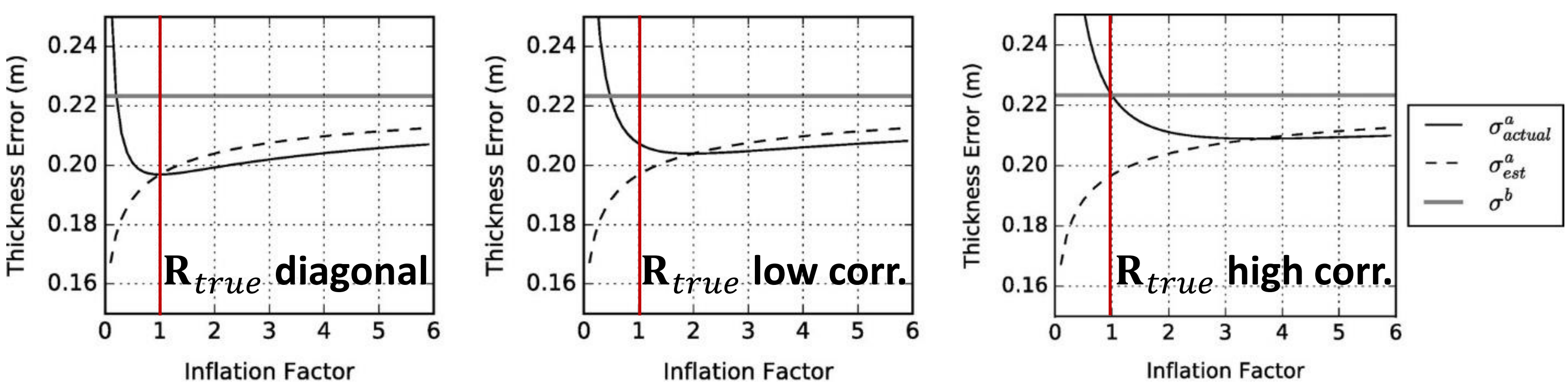
- If $\mathbf{R}$ is mis-specified, the <u>real</u> analysis error covariance is:

$$\mathbf{P}_a = (\mathbf{I} - \mathbf{KH})\mathbf{P}(\mathbf{I} - \mathbf{KH})^T + \mathbf{KR}_{true}\mathbf{K}^T$$

- Instead of the normal <u>estimated</u> value:

$$\mathbf{P}_a = (\mathbf{I} - \mathbf{KH})\mathbf{P}$$

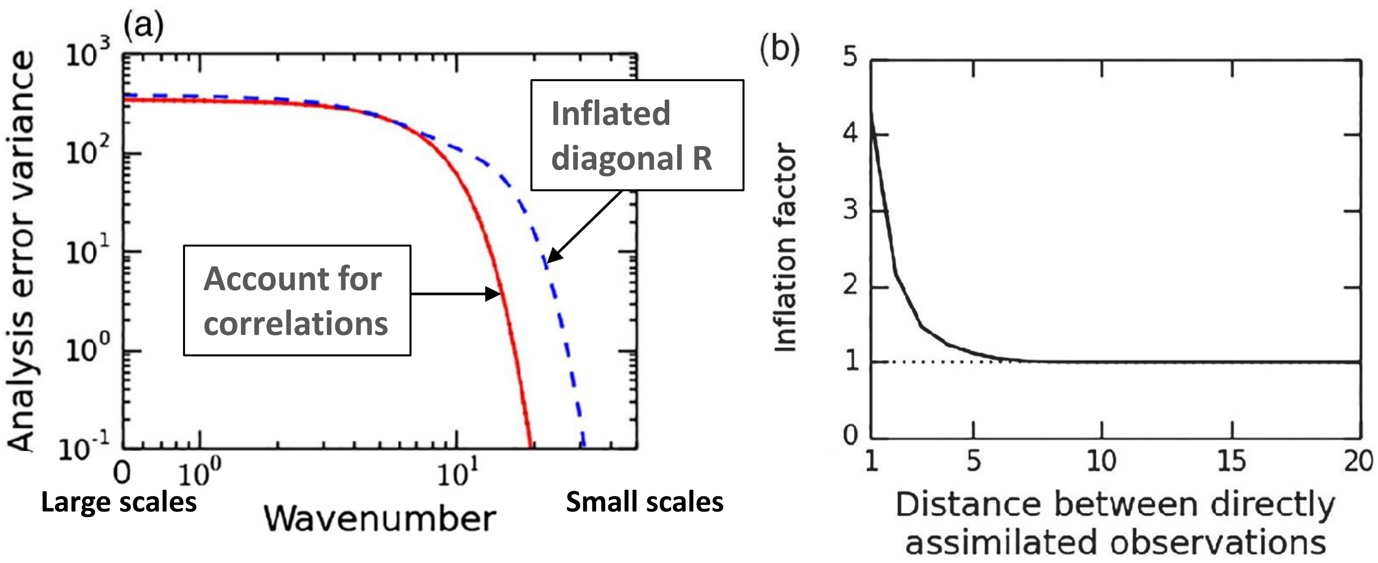
- Common to inflate observation error variance to avoid overfitting large scales from neglecting observation error correlations
- Figure (Stonebridge et al. 2018) shows <u>real</u> and <u>estimated</u> analysis error stddev as a function of inflation factor applied to a diagonal $\mathbf{R}$



- Inflating diagonal $\mathbf{R}$ can reduce both the real analysis error and underestimation of analysis error (e.g. via analysis ensemble spread)

Mis-specified obs error correlations

- Inflation avoids over-fitting large scales, but further under-fits small scales
- Alternatively, spatial thinning of obs can be used to avoid overfitting; also neglects observational information at small scales



(a) Analysis error when assimilating obs with correlated error when either accounting for correlations (red) or using inflated diagonal **R** (blue)

(b) Optimal obs error inflation factor for different amounts of spatial thinning

(Idealized numerical experiments from Bédard and Buehner 2019)

Thinning vs. error inflation in real NWP

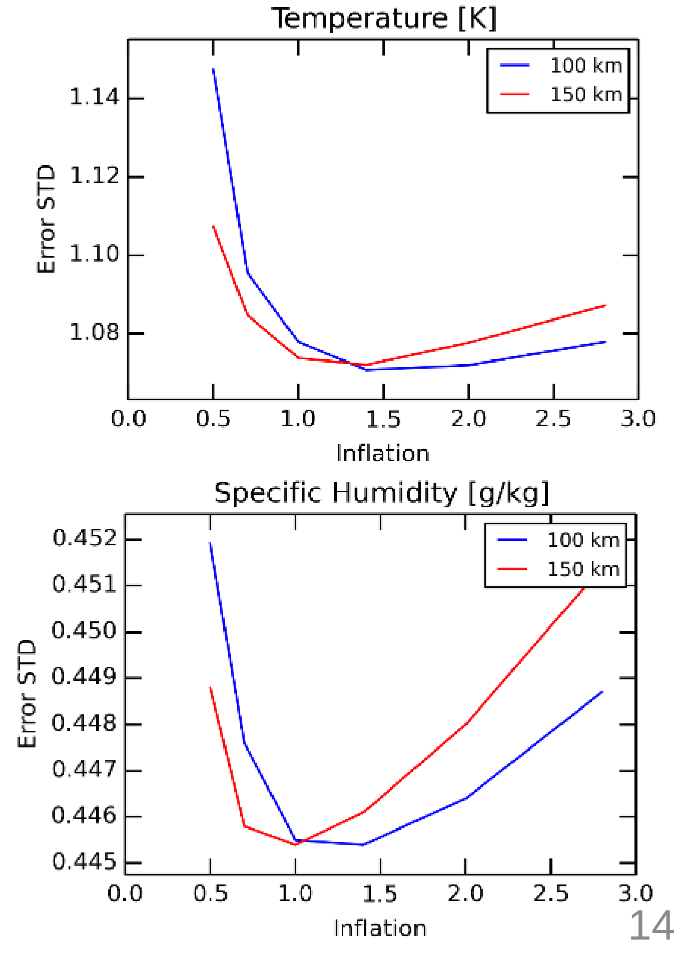
- Series of experiments performed varying both the inflation of the error variance and the spatial thinning for all types of radiance observations

- Decreasing thinning without changing inflation can result in forecast degradation

- Beneficial to increase inflation when thinning reduce from **150km** to **100km**

- However, optimal inflation likely not equal for all sensor types or channels (e.g. humidity vs. temperature sensitive)

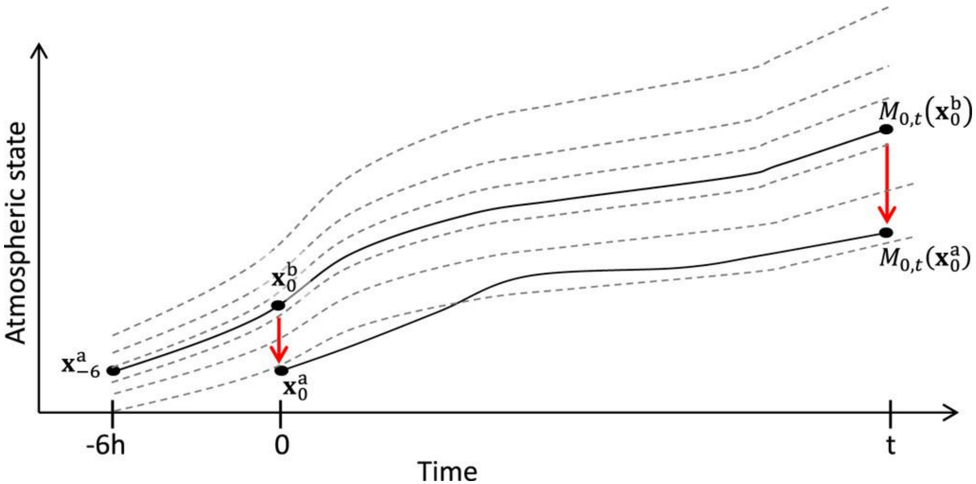
Average global 48h forecast scores (1000 to 1 hPa):



(Courtesy: Joël Bédard and Alain Beaulne)

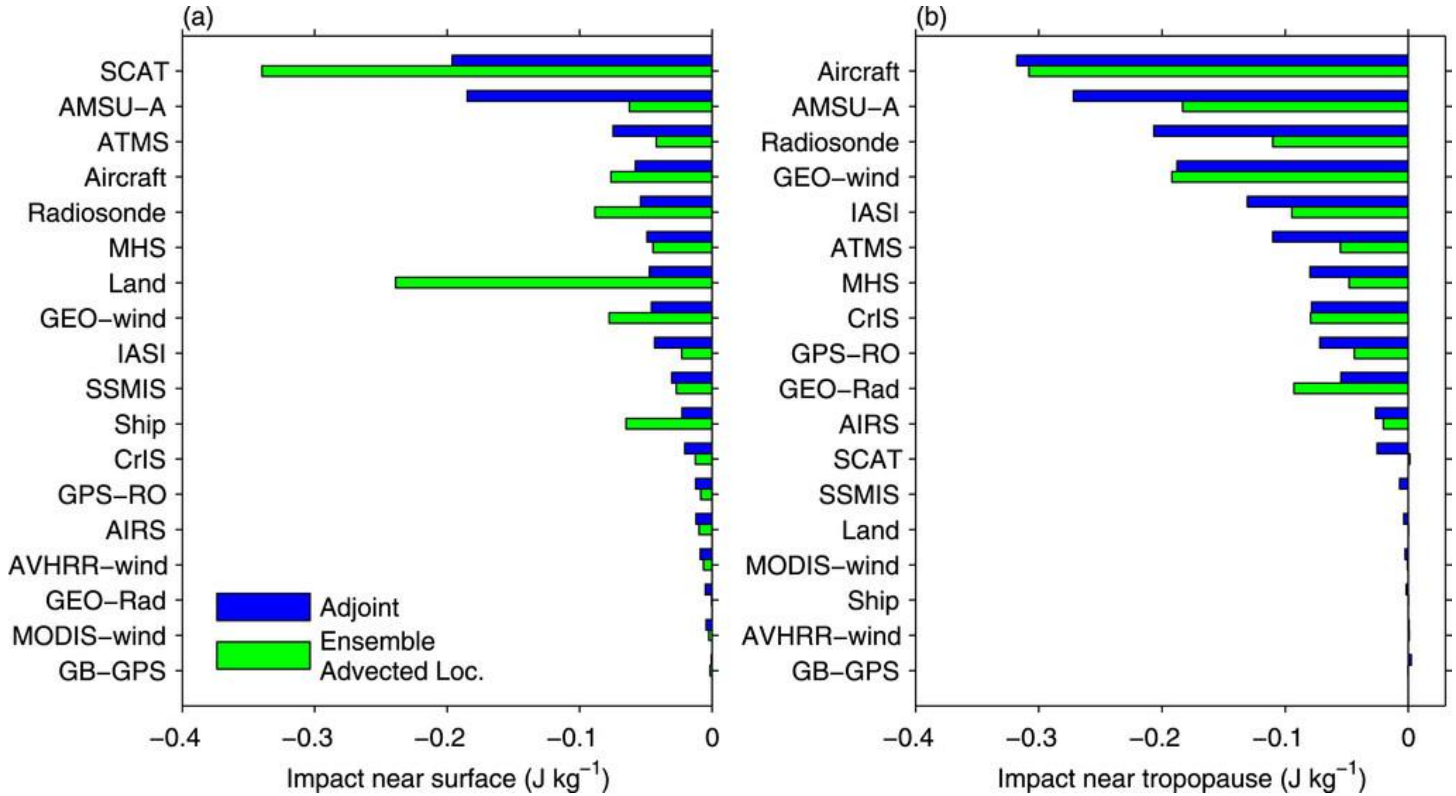
Estimating observation impact

- Modern NWP DA systems are highly complex; measuring the impact of currently assimilated or future hypothetical observations through OSEs or OSSEs can be very costly (and OSSEs difficult to do correctly)
- Several alternative approaches exist for estimating the impact of observation subsets on the analysis or forecast error, including:
  - Impact should be related to change in ensemble spread, which depends on $\mathbf{H}$, $\mathbf{R}$, and $\mathbf{P}_{ens}$, not actual observed values → can be used to estimate impact of new hypothetical observations for observation network design
  - FSOI approximates contribution of currently used observations to error reduction in short-term forecasts by propagating sensitivities from forecast to analysis time using either an adjoint model or ensembles



Estimating observation impact: FSOI

- Estimated relative impact of major observation groups varies with approach used to propagate sensitivity from forecast to analysis time
- Choice of scalar measure of forecast error also affects relative impact, for example: near surface (left) vs. near tropopause (right)



(Figure from Buehner et al. 2018)

The challenge of Earth system DA

- Forecast models are becoming increasingly coupled – e.g., the ECCC medium-range deterministic forecasts include coupled components:
  - Atmosphere
  - Land
  - Ocean
  - Sea ice
  - Ozone
- Forecast model for generating the background state, only couples Atmosphere + Land + Ozone → i.e. *partially* weakly coupled DA
- Data assimilation systems for all components are nearly independent, only some *ad hoc* coupling included where essential
- Use of separate DA systems for each component makes it challenging to obtain consistent analyses for initializing coupled forecasts
- Strongly coupled DA also challenging as it requires all components use same DA system/algorithm, temporal frequency, obs. cutoff time

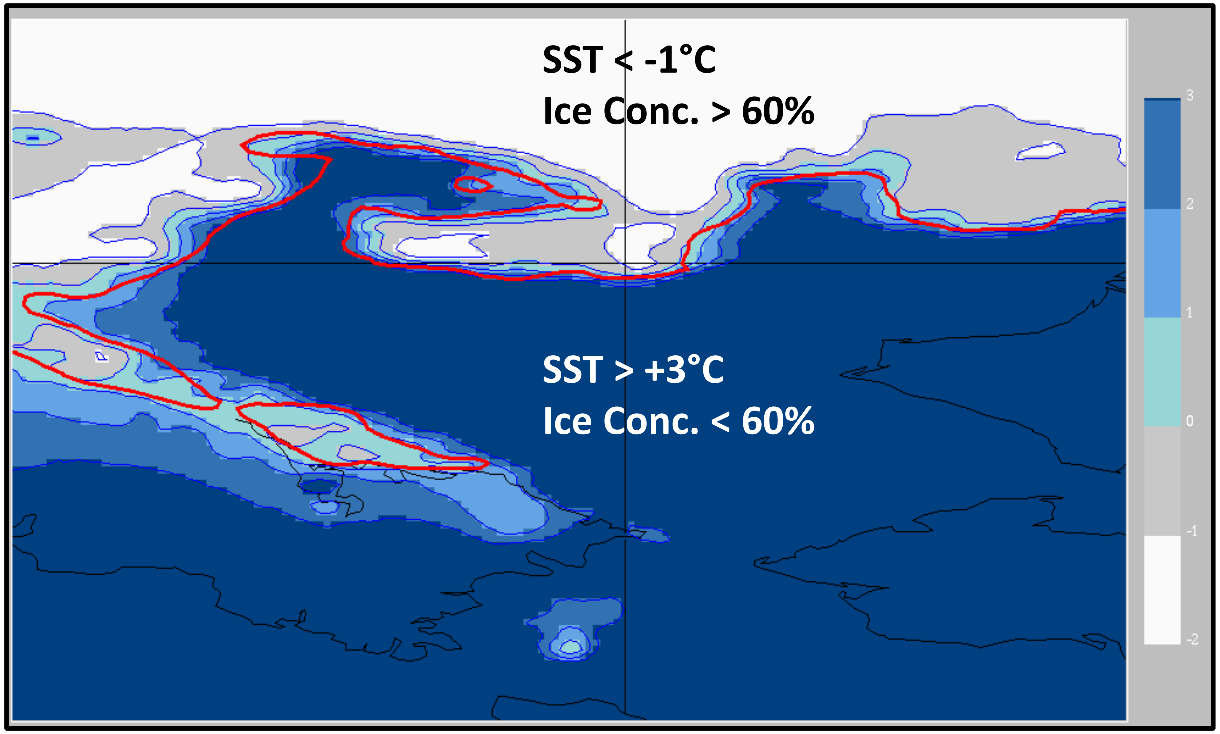
Atmosphere-ice-ocean initial conditions

- Initial condition consistency is required between Atmosphere, Ice and Ocean components to avoid initial shocks and forecast degradations
- Example: ice analysis indicates high concentration, but background state has no ice and SST above freezing → ice added by DA will rapidly melt during subsequent forecast
- Analyses of SST and Ice concentration currently produced with DA systems that cycle through time without using a forecast model
- Since DA components at ECCC are currently separate, *ad hoc* approaches needed to impose consistency:

    1. Consistency between <u>Atmosphere and Ocean</u> from using same gridded SST analysis in both – assimilated in ocean with high weight, specifies lower boundary for atmosphere
    2. Consistency between <u>Ocean and Ice</u> from bogus freezing point SST observations where ice analysis > 60% concentration and remove ice in analysis where SST analysis > 4°C

SST and ice concentration analyses

- Example of analyses of SST (shading) and Ice Concentration (red contour: 60% concentration) in the Bering Sea (July 9, 2021)

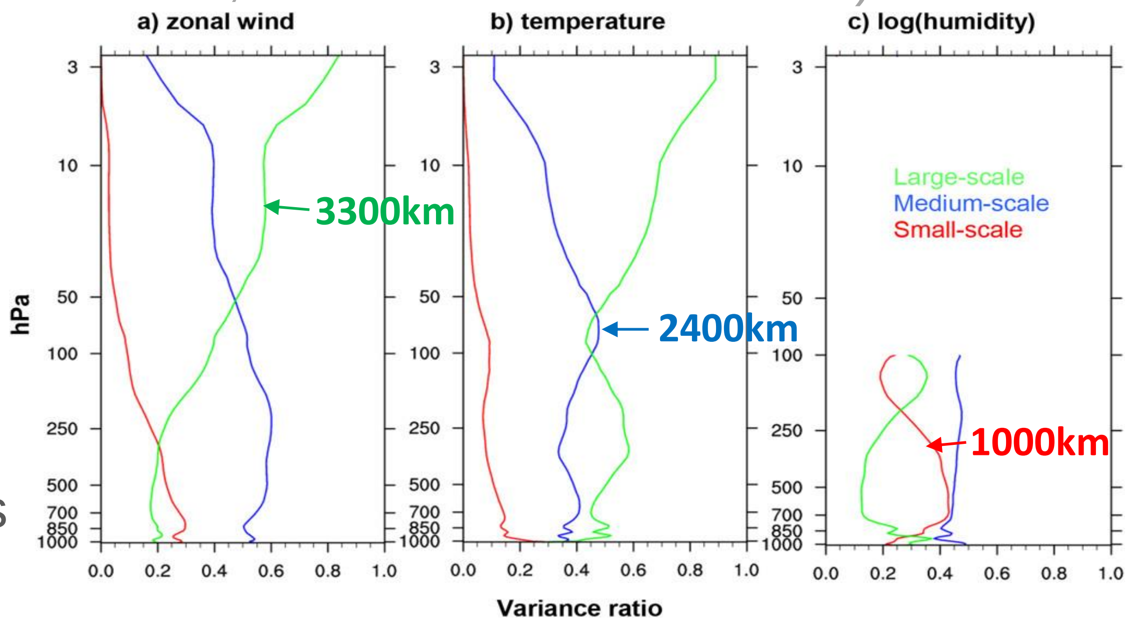


Wide range of spatial scales

- Earth system components may have dominant background errors at very different spatial scales, e.g. in ECCC operational systems:
    - Sea ice 3D-Var correlation scale: **10km** (e-folding distance)
    - SST Optimal Interpolation correlation scale: **85km** to **136km** (e-folding distance)
    - 3D ocean localization scale applied to ensemble of climatological anomalies: **200km** (cut-off radius)
    - Land surface “pseudo-analysis” screen-level Optimal Interpolation correlation scale: **239km**($T\text{-}T_d$) and **425km**(T) (e-folding distance)
    - Atmospheric 4D-EnVar localization scale: **2800km** (zero distance)
- Special treatment required to correctly include between-component cross-covariances with component-dependent length scales
- 4D-EnVar now uses Scale-Dependent Localization with length scales: 1000km, 2400km, 3300km, depending on horizontal scale → significantly improved medium-range forecasts

Scale-dependent localization

- Method: Decompose ensemble perturbations according to specified ranges of horizontal scale and apply different amount of localization to each (Buehner and Shlyaeva 2015; Caron and Buehner 2018)
- Naturally provides varying amount of localization that depends on variable, vertical level, local conditions, etc.
- Figure shows relative amount of ensemble variance in 3 wave bands (Caron & Buehner 2018)



- So far, only use for horizontal-scale-dependent horizontal localization, could also apply to vertical-scale-dependent vertical localization
- If applied to strongly coupled 4D-EnVar with multiple components, also provides component-dependent localization to multi-component ensemble (cross-)covariances while ensuring positive-definite matrix

Overview of MIDAS

- MIDAS: Modular and Integrated Data Assimilation System
- Purpose: provide platform for efficient collaborative development of DA systems at ECCC for various applications and **facilitate future research on strongly coupled DA**
- A set of Fortran programs and modules that implement DA algorithms (3D-Var, EnVar and LETKF) and related procedures
- Evolved out of original variational DA code; never separate from code for operational systems; code improved/refactored *as needed*
- Development is an open collaboration; single code repository managed with *gitlab work flow*: feature/release branches, issues, etc.
- Fortran modules are fairly general, and becoming increasingly so, to facilitate increasing number of applications and scientific innovations
- EnVar and LETKF share a lot of code (e.g. obs operators, file I/O), so when new application is implemented for one, the other is much easier

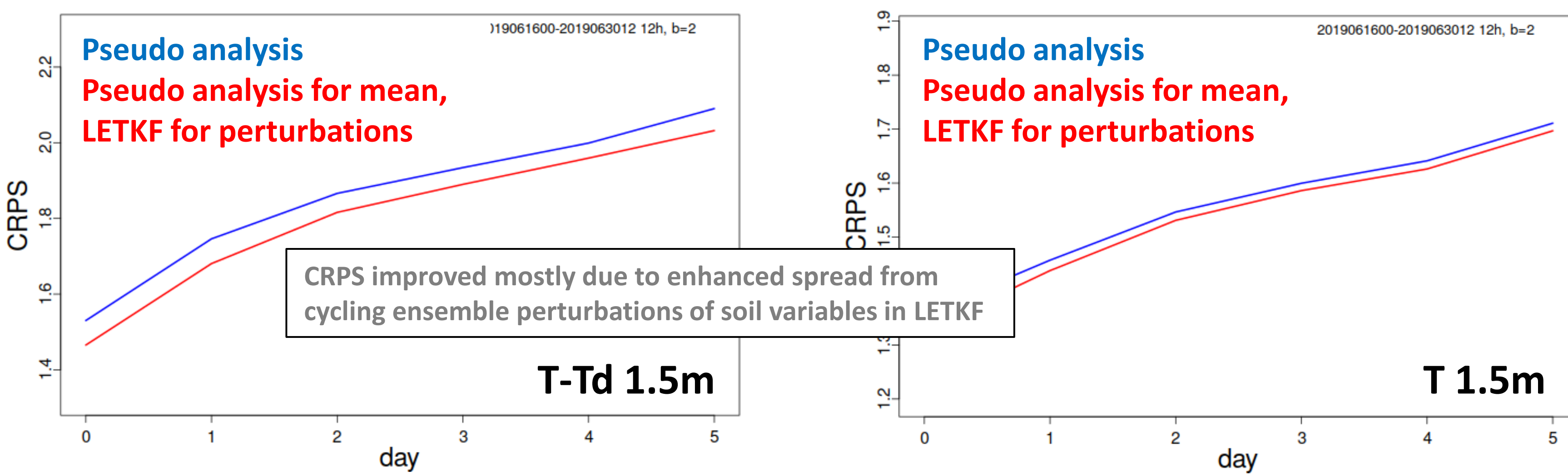
Earth system DA at ECCC

- Currently many separate (uncoupled) DA systems for initializing Earth system components, including atmosphere, land, ocean, sea-ice
- MIDAS used for operational NWP (4D-EnVar, LETKF, Observation QC, thinning and bias correction, soon FSOI)
- Integration in MIDAS of DA for more Earth system components facilitates collaboration on common DA tools/algorithms and essential for research on strongly coupled DA
- Currently testing both sea-ice and SST analysis systems using MIDAS-based 3D-Var (diffusion operator for horizontal correlations)
- Technical work also begun on MIDAS-based DA for the 3D ocean and land surface → starting with LETKF is easiest
- Goal is to first implement in MIDAS stand-alone DA for each Earth system component before exploring strong coupling strategies in LEKTF and 4D-EnVar

Initial experiments for coupled land DA

- Operational “pseudo analysis” produces analysis increments for soil variables based on analysis increments for screen-level temperature and humidity – all ensemble members initialized with same analysis
- Atmospheric LETKF assimilates screen-level temperature and humidity; atmosphere and land-surface models already coupled
- Easy to include soil variables in LETKF analysis → ensemble cov. between soil and atmospheric variables produces soil increments
- Cycling coupled atmosphere-land ensembles, recentered on pseudo analysis, improves screen-level ensemble forecasts in short tests

Screen-level CRPS scores for North America, June 16-30, 2019



ECCC Future directions and challenges

- Remove technical obstacles by developing MIDAS such that it can be used effectively for uncoupled DA of sea-ice, ocean, land, etc.
- Explore pragmatic approaches for strongly coupling DA of selected Earth system components within LETKF and 4D-EnVar
- Related scientific innovations:
  - Address model uncertainty at interface of coupled Earth system models: reduce biases, simulate random errors in ensembles
  - Apply SDL to coupled ensemble covariances of multiple Earth system components with very different length scales
  - Address observation gaps by assimilating obs at interface of Earth system components: e.g. surface-sensitive radiances over land/ice/snow