

NASDAC project

This research was born during the NASDAC project, funded by the European Community. As PI of NASDAC I invited mathematicians from Argonne National Laboratory (namely, Dr. Emil Constantinescu) to collaborate with Dr. Andrey Moore of University of Santa Cruz in California, in the redesigning of DA algorithms for Ocean Circulation models (namely the Regional Ocean Modeling System Data Assimilation software framework).

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The focus has been on designing **scalable mathematical models** exploiting space-and-time parallelism (DD - PINT Framework) by introducing decomposition from the beginning of the math-stack.

PINT-DD FRAMEWORK: a two level decomposition

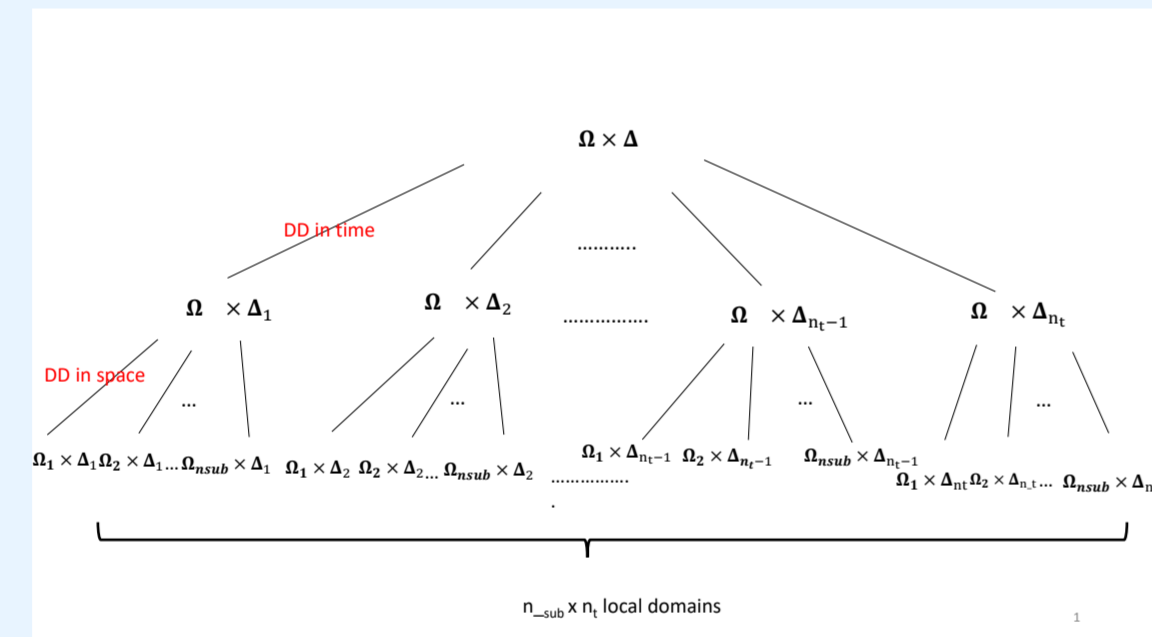


Figure 1. Two Level Domain Decomposition

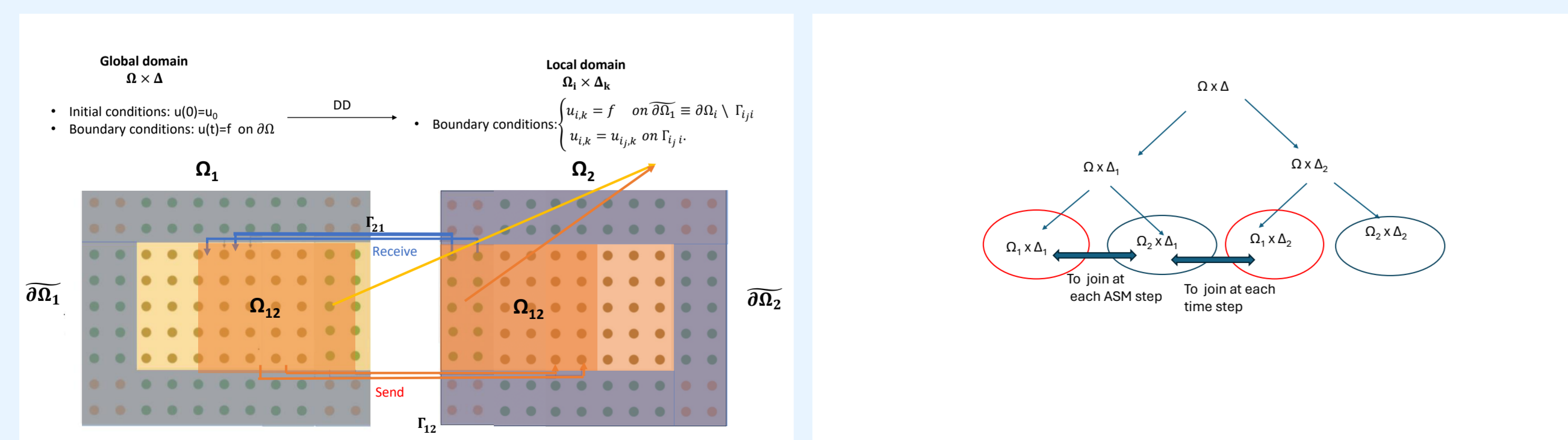
Reduced Model

- In Time:** Similarly to PinT methods, we use **DA as coarse predictor** for the local PDE-based model, providing the initial approximations needed for locally solving the initial value problems on each time subinterval, whereas the **PDE model serves as a fine corrector**, on each time interval, iteratively improving the prediction.

- In Space:** Similarly to Additive Schwarz methods we use the approximation of the numerical solution computed on the interfaces between adjacent spatial subdomains as boundary conditions of local PDE-models. Local communications along the overlapping regions allow to calculate local solutions that connect each other ensuring smoothness and uniqueness of the global solution (information bridge)

Regularized DA operator:

- Starting from the reduced functional, which is obtained by simply applying the restriction operator, we add a **regularization constraint**. This regularization is introduced to enforce the continuity of each solution of the local problem along the overlapping region between adjacent subdomains.



Schwarz boundary conditions

joining condition wrt space and time

DD-KF: local computational scheme on two spatial subdomains (Ω_i and Ω_j) for each time subinterval Δ_s ($\Delta = \cup_{s=1,L} \Delta_s$)

- Predictor phase.** Computation of local estimates:

$$x_{i,k+1} = M_i \hat{x}_{i,k} + b_k|_{\Omega_i} + b_{i,k}; \quad (1)$$

where $b_{i,k}$ is the contribution of $x_{j,k}$ restricted to $\partial\Omega_i \cap \Omega_j$ (according to the Additive Schwarz Method) while, as initial value, we consider the estimate computed at the previous step in the adjacent time sub interval $x_{i,k+1}^{\Delta_j} = x_{i,k+1}^{\Delta_{j-1}}$.

$$P_i = M_i P_i M_i^T + P_{\Omega_i \leftrightarrow \Omega_j} + Q_{i,k}, \quad (2)$$

where

$$\begin{aligned} P_{\Omega_i \leftrightarrow \Omega_j} &= M_{i,j} P_{j,i} M_i^T + M_i P_{j,i} M_{i,j}^T + M_{i,j} P_j M_{i,j}^T \\ P_{i,j} &= M_i P_{i,j} M_j^T + C_{\Omega_i \leftrightarrow \Omega_j} \\ C_{\Omega_i \leftrightarrow \Omega_j} &= M_i P_i M_{j,i}^T + M_{i,j} P_{j,i} M_{j,i}^T + M_{i,j} P_j M_{j,i}^T \end{aligned} \quad (3)$$

- Corrector phase.**

$$K_i = (P_i H_{k+1}|_{\Omega_i}^T + P_{i,j} H_{k+1}|_{\Omega_j}^T) \cdot F; \quad (4)$$

where

$$\begin{aligned} F &= (H_{k+1}|_{\Omega_i} P_i H_{k+1}|_{\Omega_i}^T + H_{k+1}|_{\Omega_j} P_j H_{k+1}|_{\Omega_j}^T + R_{i,j} + R_{k+1})^{-1} \\ R_{i,j} &= (H_{k+1}|_{\Omega_j} P_{j,i} H_{k+1}|_{\Omega_i}^T + H_{k+1}|_{\Omega_i} P_{i,j} H_{k+1}|_{\Omega_j}^T) \\ P_i &= (I - K_i H_{k+1}|_{\Omega_i}) P_i - K_i H_{k+1}|_{\Omega_j} P_{j,i} \end{aligned} \quad (5)$$

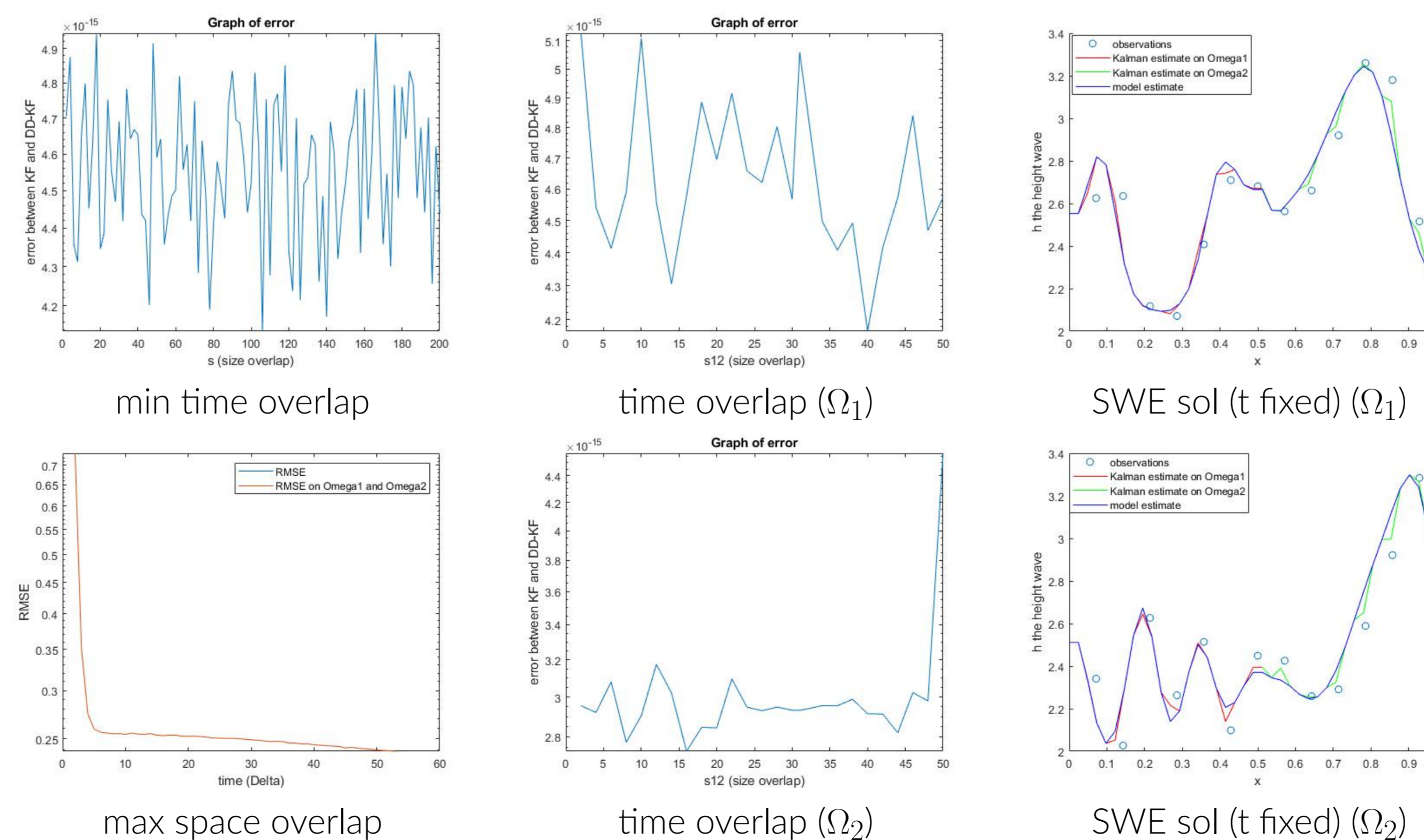
update local estimate of covariance matrices

$$P_{i,j} = (I - K_i H_{k+1}|_{\Omega_i}) P_{i,j} - K_i H_{k+1}|_{\Omega_j} P_{j,i}. \quad (6)$$

Update DD-KF estimates:

$$\hat{x}_{i,k+1} = x_{i,k+1} + K_i [y_{k+1} - (H_{k+1}|_{\Omega_i} x_{i,k+1} + H_{k+1}|_{\Omega_j} x_{j,k+1})] + \dots \quad (7)$$

Some results to the initial boundary problem of SWEs....



The local concurrent algorithm in $\Delta_s \times (\Omega_i, \Omega_j)$

for $k = 1, k_{local}$ %loop over (local) time steps in Δ_s

Define predicted covariance matrices: $P_{i,i}, P_{j,i}$

Compute Kalman gains: $K_{i,i}, K_{j,i}$

Update covariance matrices: $P_{i,i}, P_{j,i}$

repeat % ASM loop over n

Send and Receive data values among adjacent sets

Compute Kalman estimate

$$\hat{x}_{i,k}^{n+1} = x_{i,k}^n + K_{i,k} \left[(y_k - H_k|_{\Omega_j} x_{j,k}^n) - H_k|_{\Omega_i} x_{i,k}^n \right] + \beta \underbrace{\mathcal{O}_{i,j}(\hat{x}_{i,k}^n|_{\Omega_i}, \hat{x}_{j,k}^n|_{\Omega_j})}_{\text{joint cond in space}}$$

until $\|\hat{x}_{i,k}^{n+1} - \hat{x}_{j,k}^n\| < TOL$

Send and Receive data values among adjacent sets

Update Kalman estimate $\hat{x}_{i,k}^{n+1} = \hat{x}_{i,k}^{n+1} + \alpha \underbrace{\mathcal{R}_{i,j}(\hat{x}_{i,k}^n, \hat{x}_{j,k-1}^n)}_{\text{joint cond in time}}$

endfor

- communications along the overlapping regions allow to calculate local solutions that connect each other ensuring smoothness, uniqueness of the global solution and the propagation of local information along the sub domains in order to face with the issues of information transfer of non local observations
- following a predictor-corrector approach, we initially use DA background values as coarse predictor for the initial conditions in each subinterval, then iteratively, the model itself serves as fine correction
- localization is implemented by multiplying the sample covariance between observation and model state priors and the sample covariance between observation and observation priors by a distance-dependent function (Houtekamer and Mitchell 2001; Hamill et al. 2001), which is called observation space localization. By using the forward error analysis (FEA), we derive the number of conditions of DD-DA. We find that DD-DA actually reduces the number of conditions of DA, revealing that it is much more appropriate than the standard approach that is usually implemented in most operative software;
- in order to facilitate shared/distributed communication we assign nearby domains that communicate often to shared memory. this is why DD in space is implemented at the finest level.

Future work

DD-KF could be applied to EnKF by changing the filter, as it is performed in DD-KF. Specifically, in order to enforce the matching of local solutions on adjacent regions, local problems should be slightly modified by adding the smoothness-regularization constraint to the correction phase on local solutions; such term keeps track of contributions of adjacent domains to ensembles regions. The same modification should be done on the covariance matrices.

References

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