Stabilized approximate Kalman filter and its extension towards parallel implementation

An example of two-layer Quasi-Geostrophic model + CUDA-accelerated shallow water

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Data assimilation at glance

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- Consider coupled system of stochastic equations:

$$x_{k+1} = \mathcal{M}_k(x_k) + \varepsilon_k,$$
$$y_{k+1} = \mathcal{H}_{k+1}(x_{k+1}) + \eta_{k+1},$$

where $x_k (\in \mathbb{R}^n)$ describes system state at time instance k,

$y_{k+1} (\in \mathbb{R}^m)$ is observed data obtained at time instance $k+1$,

$\mathcal{M}_k$ is state transition operator, and $\mathcal{H}_{k+1}$ is observation mapping describing how system state relates to the observed data at a certain time instance,

ε_k and η_{k+1} are random terms that model prediction and observation uncertainties.

- The task: given the estimate x_k^{est} of state x_k and observation y_{k+1} derive estimate x_{k+1}^{est}.

Approximating the EKF

- Denote $C_k = Cov(x_k)$, $C_{\varepsilon_k} = Cov(\varepsilon_k)$, $C_{\eta_{k+1}} = Cov(\eta_{k+1})$
- Recall formulation of the Extended Kalman filter:
  1. Run the forecast model: $x_{k+1}^{p} = \mathcal{M}_k(x_k)$,
  2. Estimate forecast covariance: $C_{k+1}^{p} = Cov\left(x_{k+1}^{p}\right) = M_k^{TL} C_k M_k^{AD} + C_{\varepsilon_k}$,
  3. Compute the Kalman gain: $G_{k+1} = C_{k+1}^{p} H_{k+1}^{AD} \left(H_{k+1}^{TL} C_{k+1}^{p} H_{k+1}^{AD} + C_{\eta_{k+1}}\right)^{-1}$,
  4. Compute state estimate: $x_{k+1}^{est} = x_{k+1}^{p} + G_{k+1}\left(y_{k+1} - H_{k+1}^{TL} x_{k+1}^{p}\right)$,
  5. Find covariance of the estimate: $C_{k+1}^{est} = C_{k+1}^{p} - G_{k+1} H_{k+1}^{TL} C_{k+1}^{p}$.
- <u>Problem:</u> Large dimension of state x_k induces issues at covariance matrix storage
- <u>Solution:</u> approximate problematic matrices the same way as it is done for Hessians of large-scale optimization problems

EKF approximation based on BFGS*

1. Run forecast model: $x_{k+1}^{p} = \mathcal{M}_k(x_k)$,
2. At the code level define operator implementing forecast covariance matrix:
$$C_{k+1}^{p} = M_k^{TL} x_{k+1}^{p} M_k^{AD} + C_{\varepsilon_k},$$
3. Apply L-BFGS minimization to auxiliary quadratic cost function:
$$f(x) = x^T A x - x^T b,$$

where $A = H_{k+1}^{TL} C_{k+1}^{p} H_{k+1}^{AD} + C_{\eta_{k+1}}$, and $b = y_{k+1} - H_{k+1}^{TL} x_{k+1}^{p}$,

4. Assign x^* to the minimizer of $f(x)$ and B^* to approximation of Hessian matrix A produced as part of output from L-BFGS
5. Compute state estimate: $x_{k+1}^{est} = x_{k+1}^{p} + C_{k+1} H_{k+1}^{AD} x^*$
6. Approximate covariance matrix of the estimate by applying L-BFGS minimization to a quadratic cost function with Hessian defined as follows:
$$C_{k+1}^{p} - C_{k+1}^{p} H_{k+1}^{AD} B^* H_{k+1}^{TL} C_{k+1}^{p}$$

*See H. Auvinen et. al. “The variational Kalman filter and an efficient implementation using limited memory BFGS”

BFGS EKF: Instability problem

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- Approximate estimate covariance matrix $C_{k+1}^{p} - C_{k+1}^{p} H_{k+1}^{AD} B^{*} H_{k+1}^{TL} C_{k+1}^{p}$ may have "non-physical" negative eigenvalues as B^{*} is itself approximation of prior covariance projected onto the observation space:

$$B^{*} \approx \left(H_{k+1}^{TL} C_{k+1}^{p} H_{k+1}^{AD} + C_{\eta_{k+1}}\right)^{-1}$$

- L-BFGS on the other hand relies on the eigenvalues of Hessian being non-negative
- We correct this problem by injecting "stabilizing correction", i.e. we replace B^{*} by $(2I - B^{*}A)B^{*}$.
- Let us denote $C_{k+1}^{p} - C_{k+1}^{p} H_{k+1}^{AD} (2I - B^{*}A) B^{*} H_{k+1}^{TL} C_{k+1}^{p}$ as $\hat{C}_{k+1}^{est}$.

Lemma. For any symmetric matrix B^{*}, the matrix $\hat{C}_{k+1}^{p}$ is non-negative. Moreover, as $B^{*} \to A^{-1}$ necessarily $\hat{C}_{k+1}^{est} \to C_{k+1}^{est}$ and the following inequalities hold:

$$\left\|\hat{C}_{k+1}^{est} - C_{k+1}^{est}\right\|_{Fr} \leq \|A\| \left\|H_{k+1}^{TL} C_{k+1}^{p}\right\|_{Fr}^{2} \|B^{*} - A^{-1}\|^{2},$$

$$\left\|\hat{C}_{k+1}^{est} - C_{k+1}^{est}\right\| \leq \|A\| \left\|H_{k+1}^{TL} C_{k+1}^{p}\right\|^{2} \|B^{*} - A^{-1}\|^{2}.$$

Current toy-case: the QG-model*

- The current test case for DA testing purposes is provided by Two-Layer Quasi-Geostrophic model:
  - Simulates “slow” wind motions
  - Resides on cylindrical surface vertically divided into two layers
  - The boundary conditions are periodic in zonal direction and fixed at the top and at the bottom of the cylinder
- The model is chaotic, dimension can be adjusted by changing resolution of the spatial grid
- Provides a neat toy-case, which can be run with no special hardware

*See C.Fandry and L.Leslie, “A two-layer quasi-geostrophic model of summer trough formation in the Australian subtropical easterlies”.

Current toy-case: the QG-model

- Governing equations with respect to unknown stream function $\psi_i(x, y)$

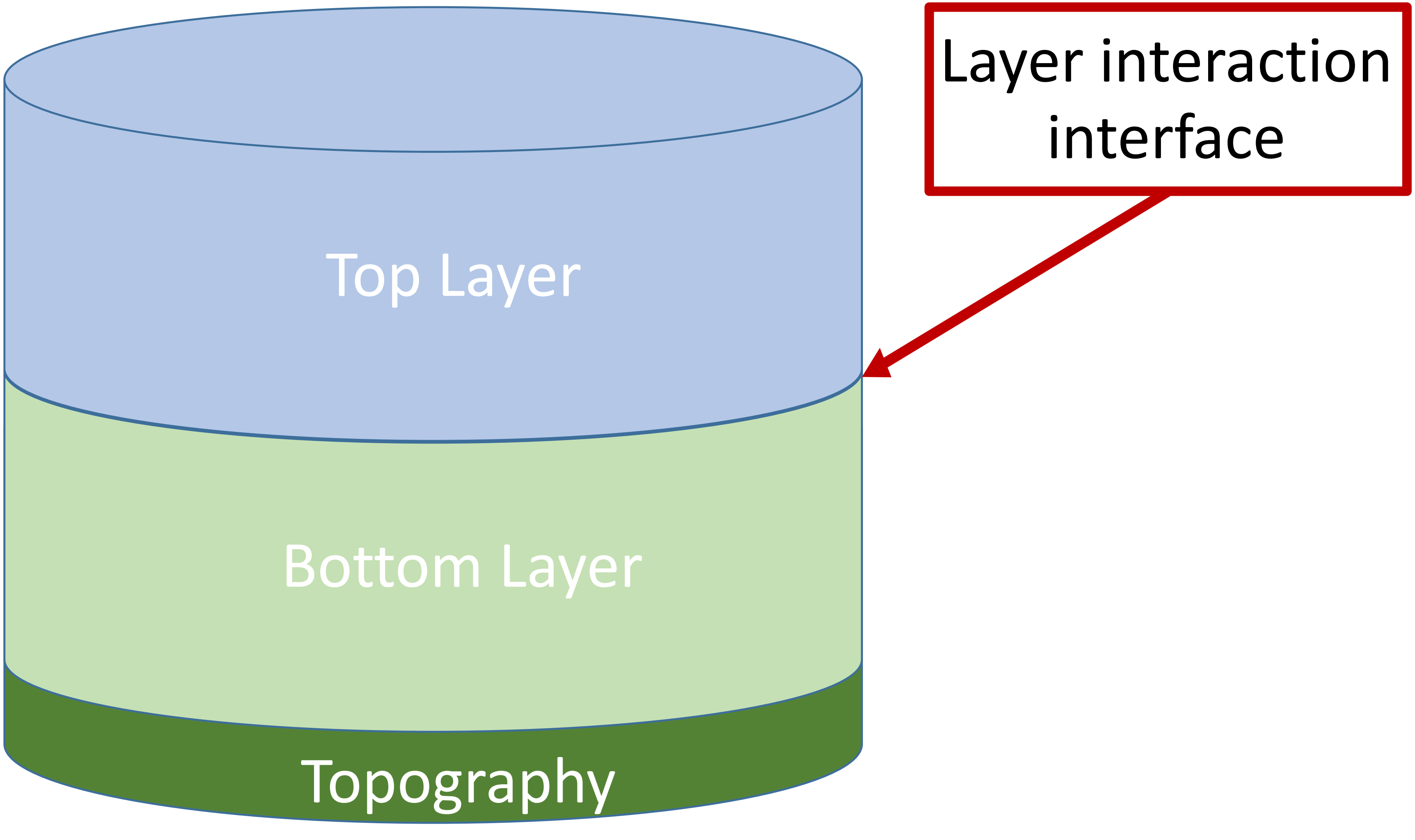
$$q_1 = \nabla^2\psi_1 - F_1(\psi_1 - \psi_2) + \beta y,$$
$$q_2 = \nabla^2\psi_2 - F_2(\psi_2 - \psi_1) + \beta y + R_s,$$
$$\frac{D_1 q_1}{Dt} = \frac{D_2 q_2}{Dt} = 0,$$

  where $R_s = R_s(x, y)$ is orography surface,

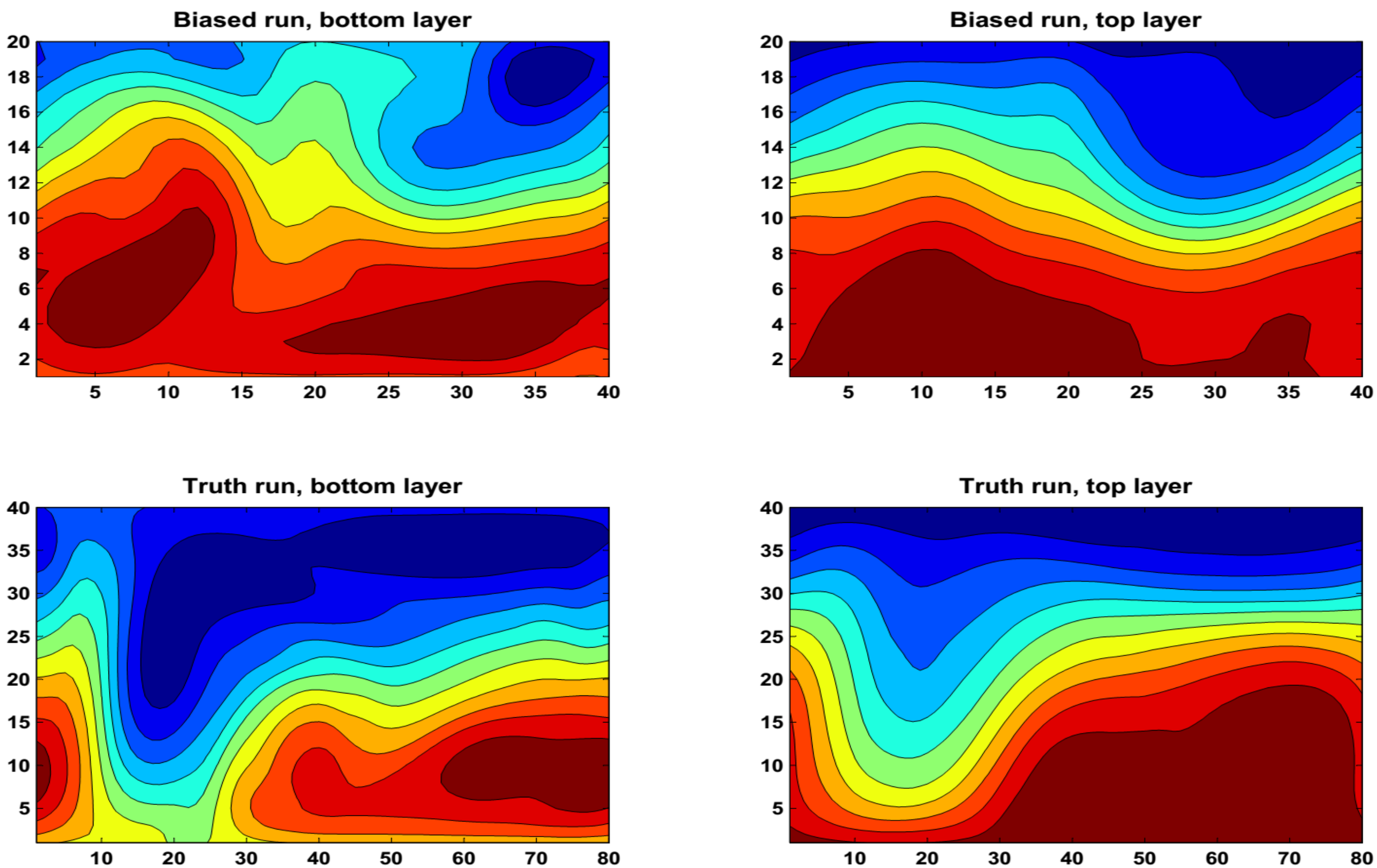
  $\frac{D_i \cdot}{Dt} = \frac{\partial \cdot}{\partial t} + u_i \frac{\partial \cdot}{\partial x} + v_i \frac{\partial \cdot}{\partial y}$ and $\nabla\psi_i = (v_i, -u_i)$.

- The equations are numerically solved by combining finite-difference approximation of derivatives with semi-Lagrangian advection

Current toy-case: the QG-model



QG-model: chaotic behavior



Numerical experiments: the QG-model

- Data assimilation performance was tested in emulated environment: we ran two instances of the qg-model at different resolutions and used one to emulate observations and the other to make predictions
- Observations were collected from a sparse subset of the state vector elements
- Predictions were made at lower resolution then the “truth” and the values of the depths of the model layers were biased
- Sources of incoming observations were interpolated onto the spatial grid of lower-resolution model by bilinear interpolation
- Estimation quality was measured by root mean square error
- We run several experiments at different resolutions and with different number of observations employing stabilized BFGS EKF, usual uncorrected BFGS EKF, weak-constraint 4D-VAR and the parallel filter

Convergence with and without the stabilizing correction

No.	Truth run res.	Biased run res.	Obs. num.	State dim.
1	10-by-10	9-by-9	50	162
2	15-by-15	12-by-12	85	288
3	80-by-40	40-by-20	500	1600

Table 1: Benchmark options depending on model resolution.

		Benchmark					
		I		II		III	
		BFGS-EKF	SA-EKF	BFGS-EKF	SA-EKF	BFGS-EKF	SA-EKF
BFGS vectors	5	0.5860	0.5508	–	0.6476	–	0.4102*
	10	0.5573	0.5445	0.7021	0.6718	–	0.4412
	15	0.4959	0.4788	0.5807	0.5690	–	0.3815
	20	0.4686	0.4695	0.5195	0.5152	0.3686	0.3656
EKF ref.		0.4247		0.4346		0.2694	

Table 2: Mean values of RMS error obtained from the benchmarks using varied capacity of the BFGS storage.

Parallel filter

- Consider combined state and observation vectors

$$\bar{x}_k = (x_{k-P+1}, x_{k-P+2}, \dots, x_k),$$
$$\bar{y}_k = (y_{k-P+2}, y_{k-P+3}, \dots, y_{k+1}).$$

- We extend transition and observation operators onto combined state space:

$$\bar{\mathcal{M}}_k(\bar{x}_k) = \big(\mathcal{M}_{k-P+1}(x_{k-P+1}), \mathcal{M}_{k-P+2}(x_{k-P+2}), \dots, \mathcal{M}_k(x_k)\big),$$
$$\bar{\mathcal{H}}_{k+1}(\bar{y}_k) = \big(\mathcal{H}_{k-P+2}(x_{k-P+2}), \mathcal{H}_{k-P+3}(x_{k-P+3}), \dots, \mathcal{H}_{k+1}(x_{k+1})\big).$$

- We call the data assimilation problem formulated for $\bar{\mathcal{M}}_k$ and $\bar{\mathcal{H}}_{k+1}$ the parallel filtering task.

Parallel filter: additional comments

- Model error covariance C_{ε_k} and observation error covariance $C_{\eta_{k+1}}$ can be extended to combined state and observation spaces as follows:

$$\bar{C}_{\varepsilon_k} = \begin{pmatrix} C_{\varepsilon_{k-P+1}} & \dots & O \\ \dots & \dots & \dots \\ O & \dots & C_{\varepsilon_k} \end{pmatrix},$$

$$\bar{C}_{\eta_{k+1}} = \begin{pmatrix} C_{\eta_{k-P+2}} & \dots & O \\ \dots & \dots & \dots \\ O & \dots & C_{\eta_{k+1}} \end{pmatrix}.$$

- Adding non zero off-diagonal terms into definition of $\bar{C}_{\varepsilon_k}$ and $\bar{C}_{\eta_{k+1}}$ allows to account for time-correlated prediction and observation errors, which relaxes one of the classical assumptions used by derivation of the Kalman filter formulae

Parallel filter: additional comments

- Allows to account for cross-time correlations between the states included into analysis
- Combines observations from several time steps, which should help in case of deficient observations
- Enables natural parallel implementation, as model propagations within combined state are executed independently
- Retrospective analysis of the older states are computed as part of the normal algorithm's output with no extra outlay

Main problem: parallel filtering task is extremely large scale, which means that a highly-compressed packaging of covariance data is required.

Solution: Use L-BFGS approximation with stabilization introduced earlier.

Relation to the Weak-Constraint 4D-Var*

- Consider combined transition operator $\bar{\mathcal{M}}_k$ and combined observation mapping $\bar{\mathcal{H}}_{k+1}$. Assume that x^b is a prior state estimate at time instance $k-P+1$. Then weak-constraint 4D-Var estimate is calculated by minimizing the following cost function with respect to x_k:

$$l\left(\bar{x}_k|\bar{y}_k, x^b\right) = \mathcal{R}_1(\bar{x}_k, \bar{y}_k) + \mathcal{R}_2(\bar{x}_k) + \mathcal{R}_3\left(x_{k-P+1}, x^b\right)$$

- $\mathcal{R}_1(\bar{x}_k, \bar{y}_k)$ defines measure for observation discrepancy:

$$\mathcal{R}_1(\bar{x}_k, \bar{y}_{k+1}) = \sum_{i=0}^{P-1} \|y_{k-P+1+i} - \mathcal{H}_{k-P+2+i}(x_{k-P+1+i})\|^2_{C^{-1}_{\eta_{k-P+1+i}}}.$$

- $\mathcal{R}_2(\bar{x}_k)$ smoothing part, accounts for prediction errors:

$$\mathcal{R}_2(\bar{x}_k) = \sum_{i=1}^{P-1} \|x_{k-P+1+i} - \mathcal{M}_{k-P+i}(x_{k-P+i})\|^2_{Q^{-1}_{k-P+i+1}}.$$

- $\mathcal{R}_3\left(x_{k-P+1}, x^b\right)$ penalizes discrepancy with the prior:

$$\mathcal{R}_3\left(x_{k-P+1}, x^b\right) = \left\|x_{k-P+1} - x^b\right\|^2_{B^{-1}}.$$

*See Y. Trémolet “Accounting for an imperfect model in 4D-Var”

Relation to the Weak-Constraint 4D-Var

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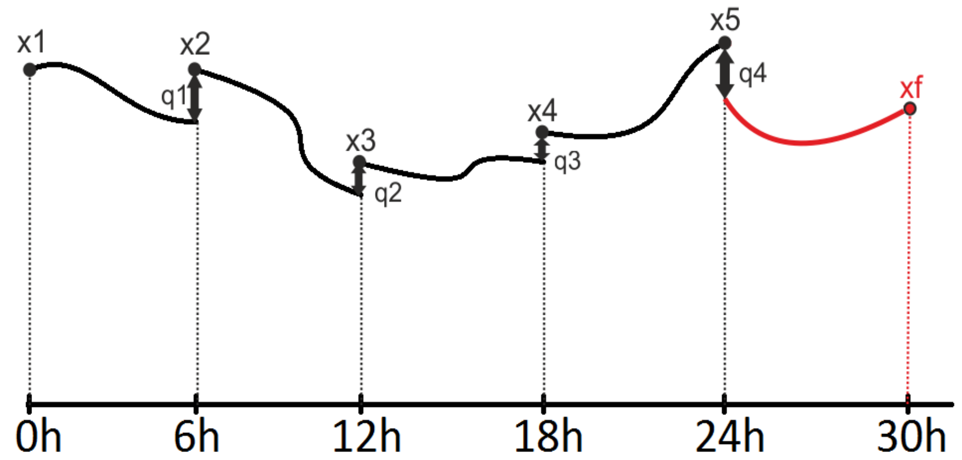
- Weak-constraint 4D-Var employs the concept of time window composed of a few consequent states.
- Propagations of each state over the time are performed independently from each other and thus can be executed in parallel.
- It is allowed to have a “jump” q_i between prediction $\mathcal{M}_i(x_i)$ and the next state x_{i+1}. This accounts for prediction error.
- Forecast is defined by prediction made from the state located at the end of the window



Relation to the Weak-Constraint 4D-Var

- Estimation task of the parallel filter can be reformulated in terms of the following cost function, which should be minimized with respect to $\bar{x}_k$:

$$l\left(\bar{x}_k | \bar{y}_k , \bar{x}_k^p\right) = \mathcal{R}_1(\bar{x}_k, \bar{y}_k) + \mathcal{R}_2\left(\bar{x}_k, \bar{x}_k^p\right).$$

- $\mathcal{R}_1(\bar{x}_k, \bar{y}_k)$ penalizes discrepancy between observation and the estimate:

$$\mathcal{R}_1(\bar{x}_k, \bar{y}_k) = \sum_{i=0}^{P-1} \| y_{k-P+1+i} - \mathcal{H}_{k-P+1+i}(x_{k-P+1+i}) \|^2_{C^{-1}_{\eta_{k-P+1+i}}},$$

- $\mathcal{R}_2\left(\bar{x}_k, \bar{x}_k^p\right)$ penalizes discrepancy between the estimate and the forecast:

$$\mathcal{R}_2\left(\bar{x}_k, \bar{x}_k^p\right) = \left\| \bar{x}_k - \bar{x}_k^p \right\|^2_{\left(\bar{C}^{est}_{k+1}\right)^{-1}}, \text{ where } \bar{x}_k^p = \bar{\mathcal{M}}_{k-1}(\bar{x}^{est}_{k-1}).$$

- If C^{est}_{k+1} is block-diagonal (it is usually not in practice), then $\mathcal{R}_2\left(\bar{x}_k, \bar{x}_k^p\right)$ can be reduced to the following sum:

$$\mathcal{R}_1(\bar{x}_k, \bar{y}_k) = \sum_{i=0}^{P-1} \left\| x_{k-P+1+i} - x^p_{k-P+1+i} \right\|_{\left(C^{est}_{k-P+1+i}\right)^{-1}}.$$

Relation to the Weak-Constraint 4D-Var

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- If $\bar{C}_{k+1}^{est}$ is block-diagonal then parallel filtering effectively reduces to weak-constraint 4D-Var with fixed predictions $x_i^p = \mathcal{M}_{i-1}(x_{i-1})$.
- If parameter $\bar{x}_i^p$ in the parallel filtering likelihood function is allowed to vary during minimization and $\bar{C}_{k+1}^{est}$ is block-diagonal, then parallel filtering becomes equivalent to the weak-constraint 4D-Var.
- <u>In parallel filtering we do not need to assume block-diagonal approximations of covariance matrices</u>, which enables cross-correlations between time sub-windows. In Weak-Constraint 4D-Var the same effect is achieved by unfixed value of x_i^p.
- Dimension of the data assimilation problem defined by parallel filtering can be effectively treated by low-memory approaches provided by L-BFGS EKF approximation with stabilizing correction.

Numerical experiments: the QG-model

- The total window comprised three 6-hour sub-windows (18-hour analysis)
- Dimension of combined state for 18-hour window was 4800
- BFGS storage capacity was set to 20 vectors
- Quality of obtained estimates was measured by root mean square error
- The results were compared against usual single-state SA-EKF and weak-constraint 4D-VAR
- Model used to simulate observations had spatial grid resolution 40-by-80 points in both layers
- Prediction model used 4-times smaller resolution of 20-by-40 points in both layers
- Integration time step was set to one hour of model time

Test of concept: 10 observations

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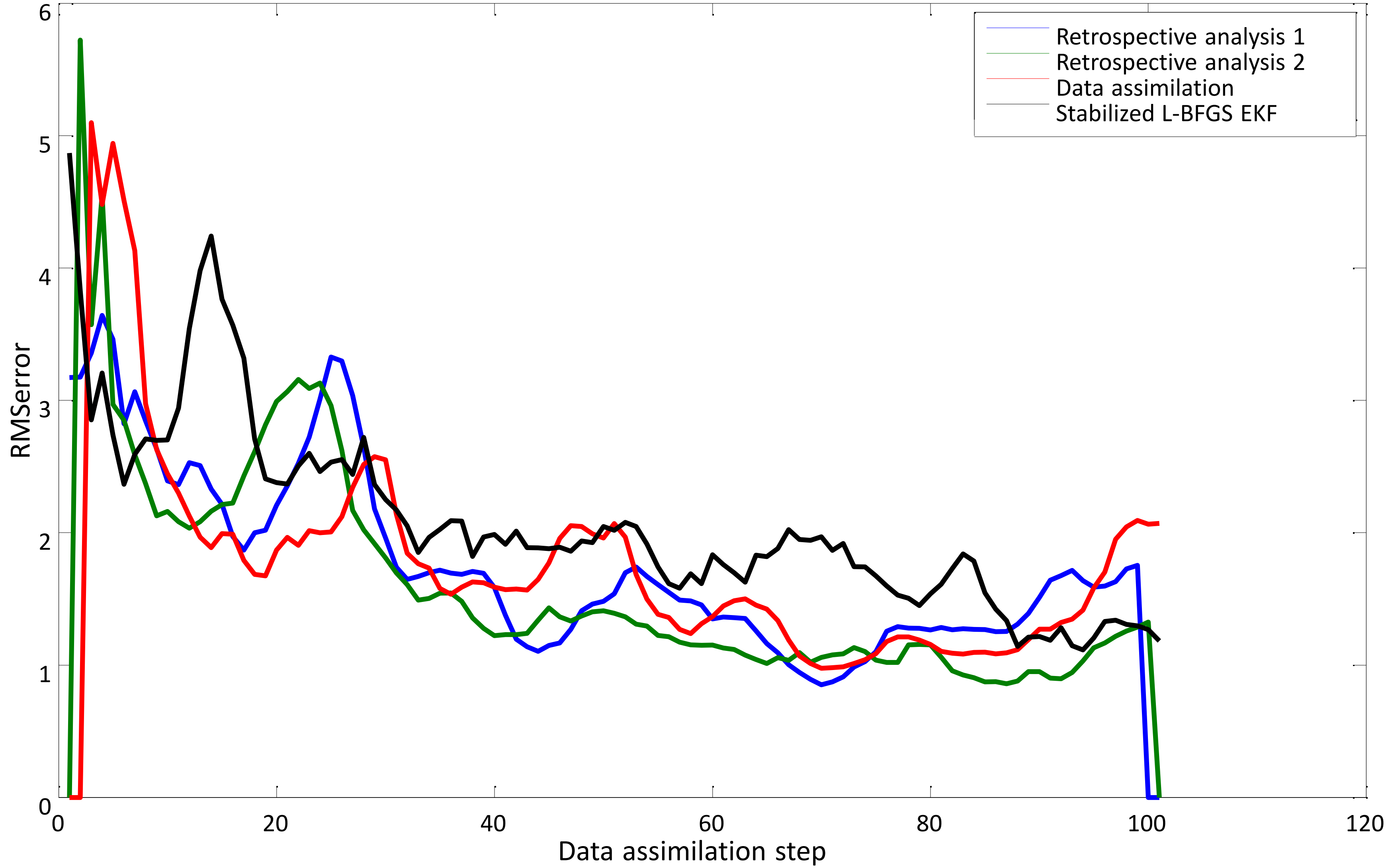

Test of concept: 20 observations

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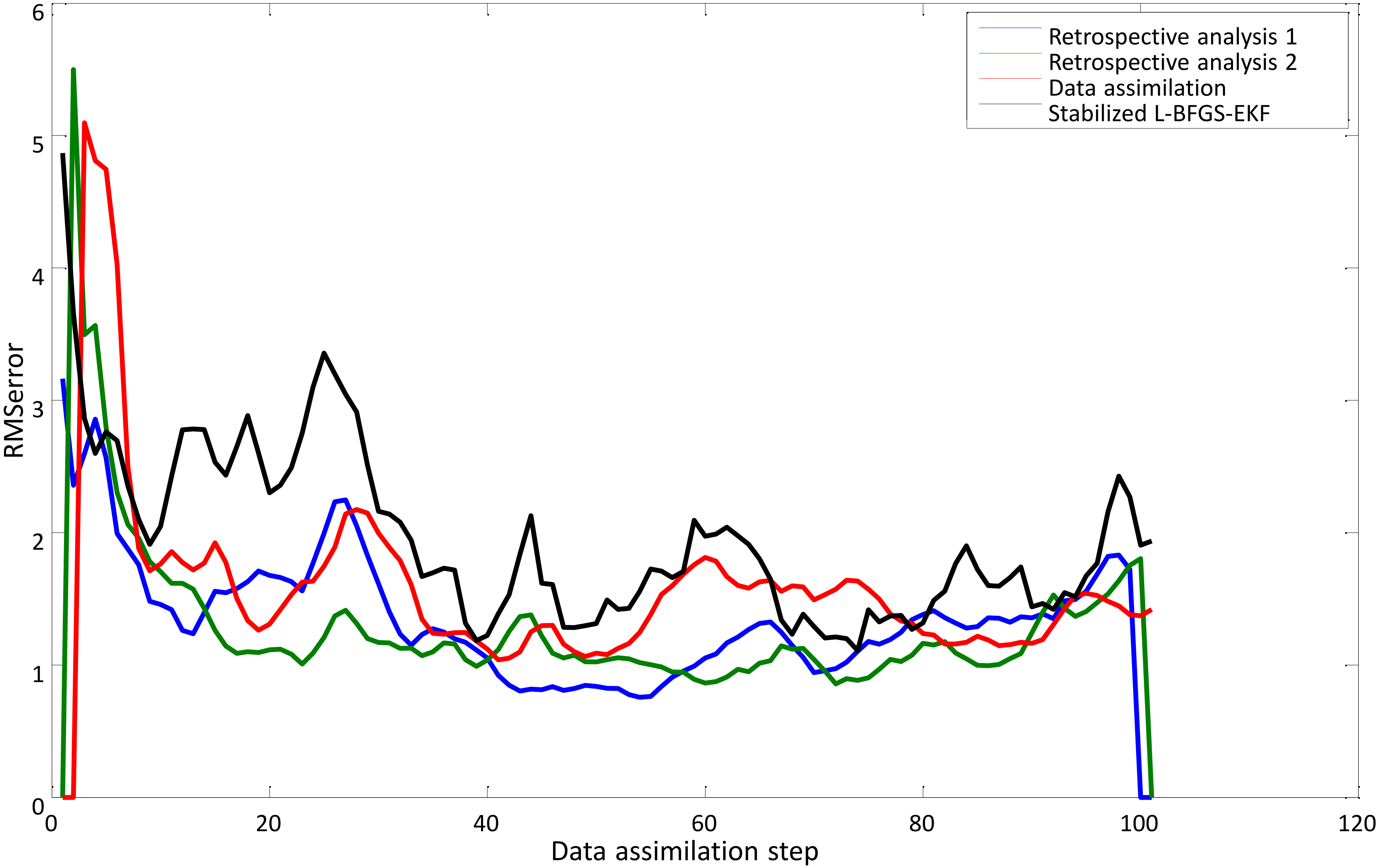
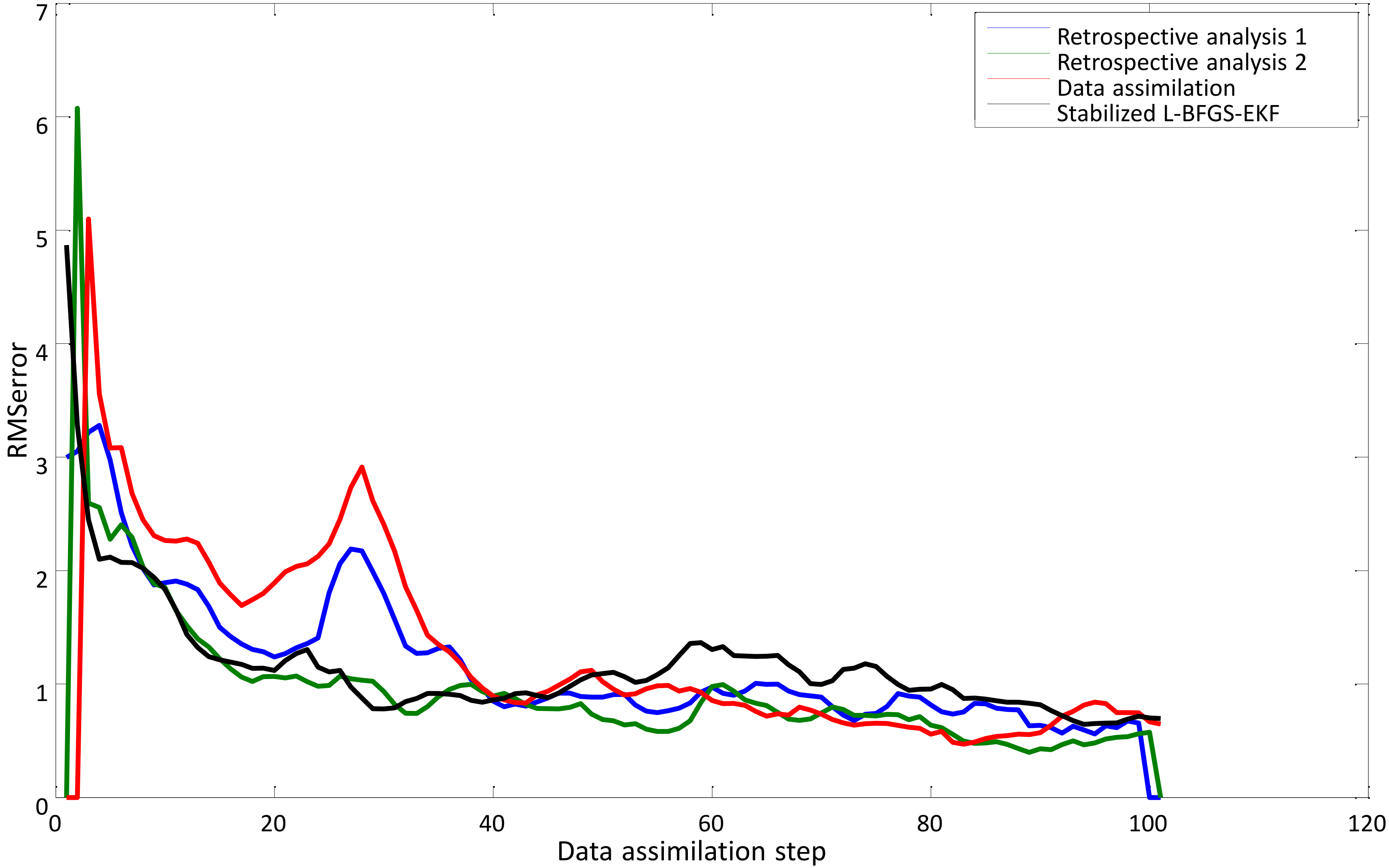
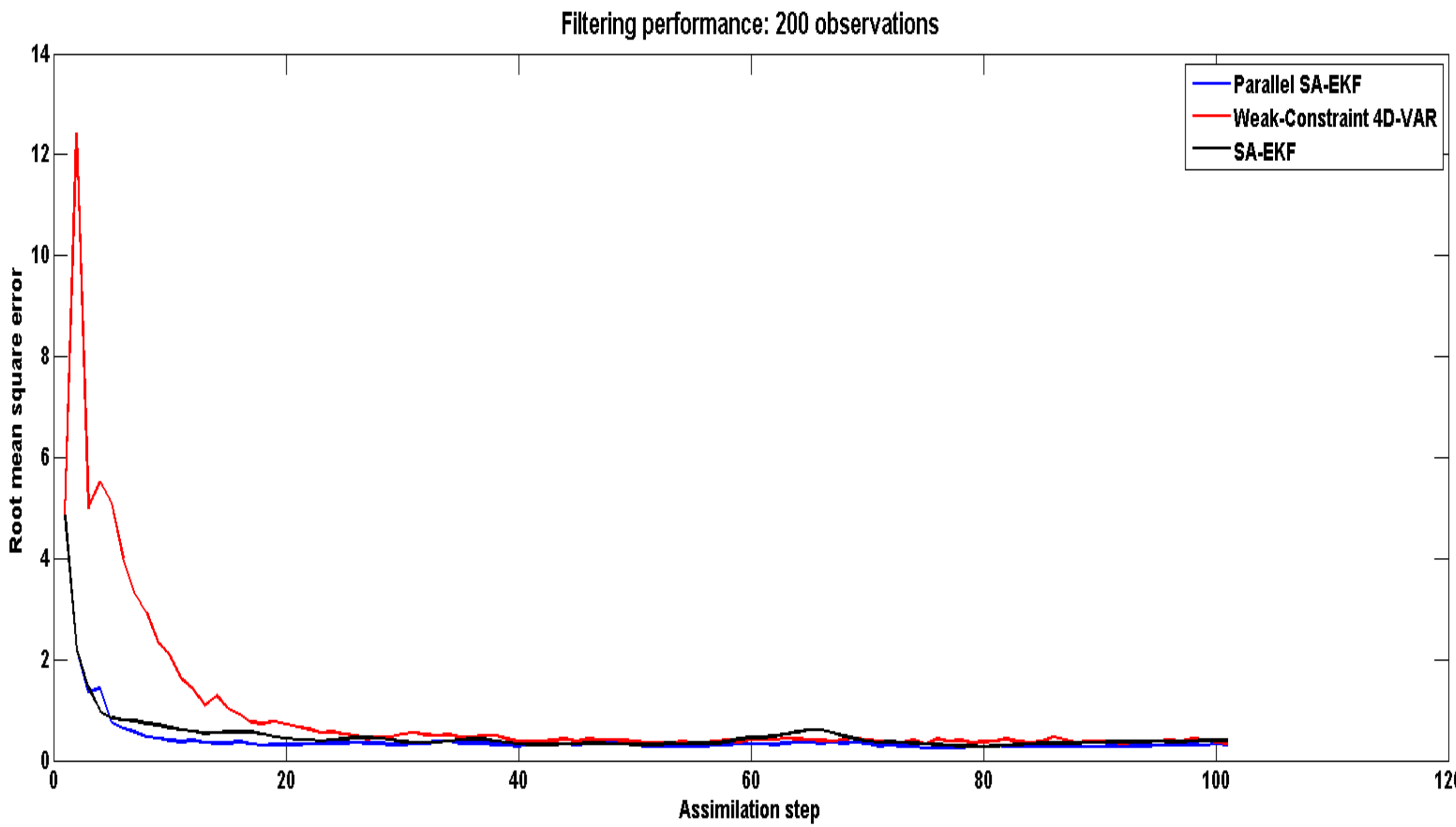


Test of concept: 30 observations



Test of concept: 200 observations



Future case: Large-Scale Shallow Water

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– $$\begin{cases} h_t + (hu)_x + (hv)_y = 0, \\ (hu)_t + \left(hu^2 + \frac{1}{2}gh^2\right)_x + (huv)_y = -ghB_x - gu\sqrt{u^2+v^2}/C_z^2, \\ (hu)_t + (huv)_x + \left(hu^2 + \frac{1}{2}gh^2\right)_y = -ghB_y - gv\sqrt{u^2+v^2}/C_z^2, \end{cases}$$

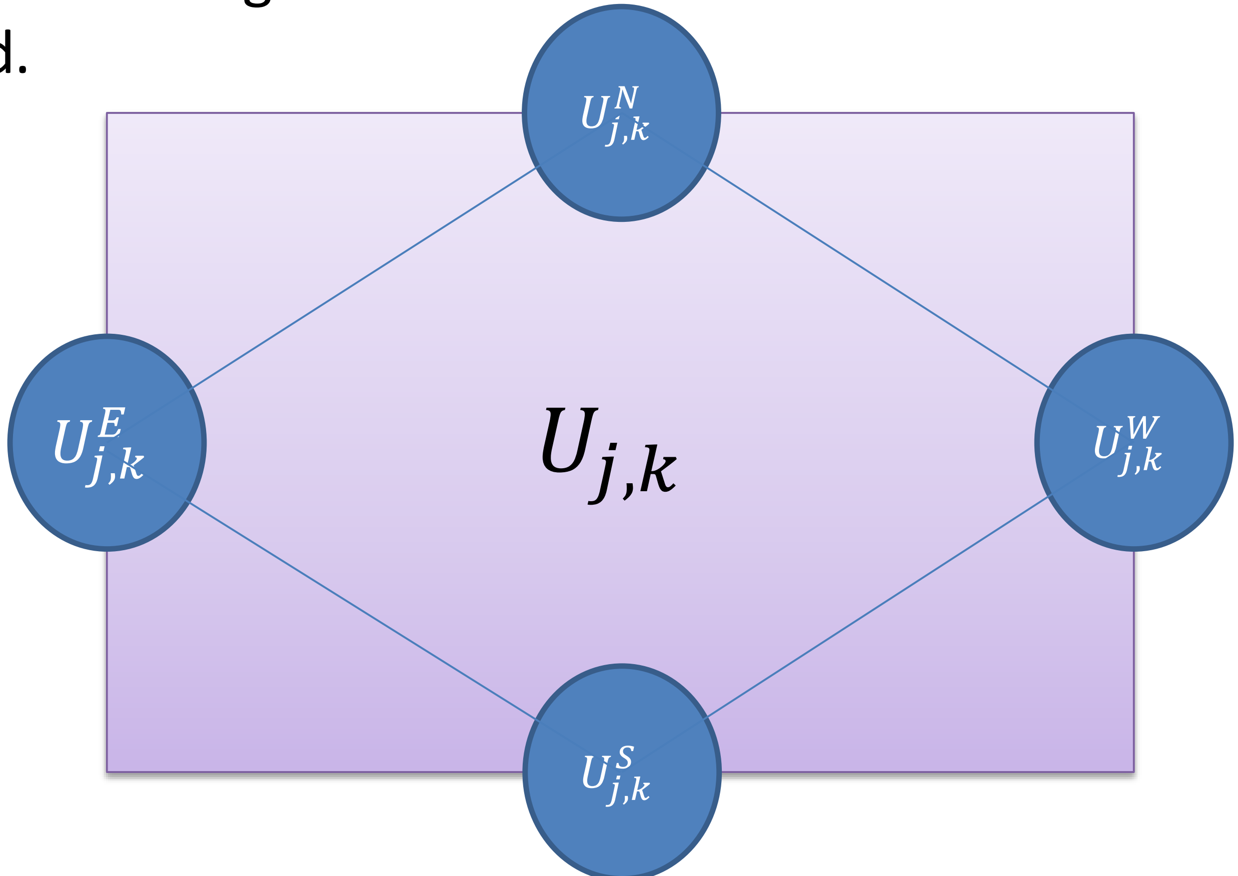
Here h denotes water elevation, u and v are horizontal and vertical velocity components, B_x and B_y denote gradient direction of the surface implementing topography, g is acceleration of gravity, C_z is the Chézy coefficient.

– It is possible to account for additional phenomena (e.g. wind stresses, friction etc.) by udjusting the right-hand-side part of the equations

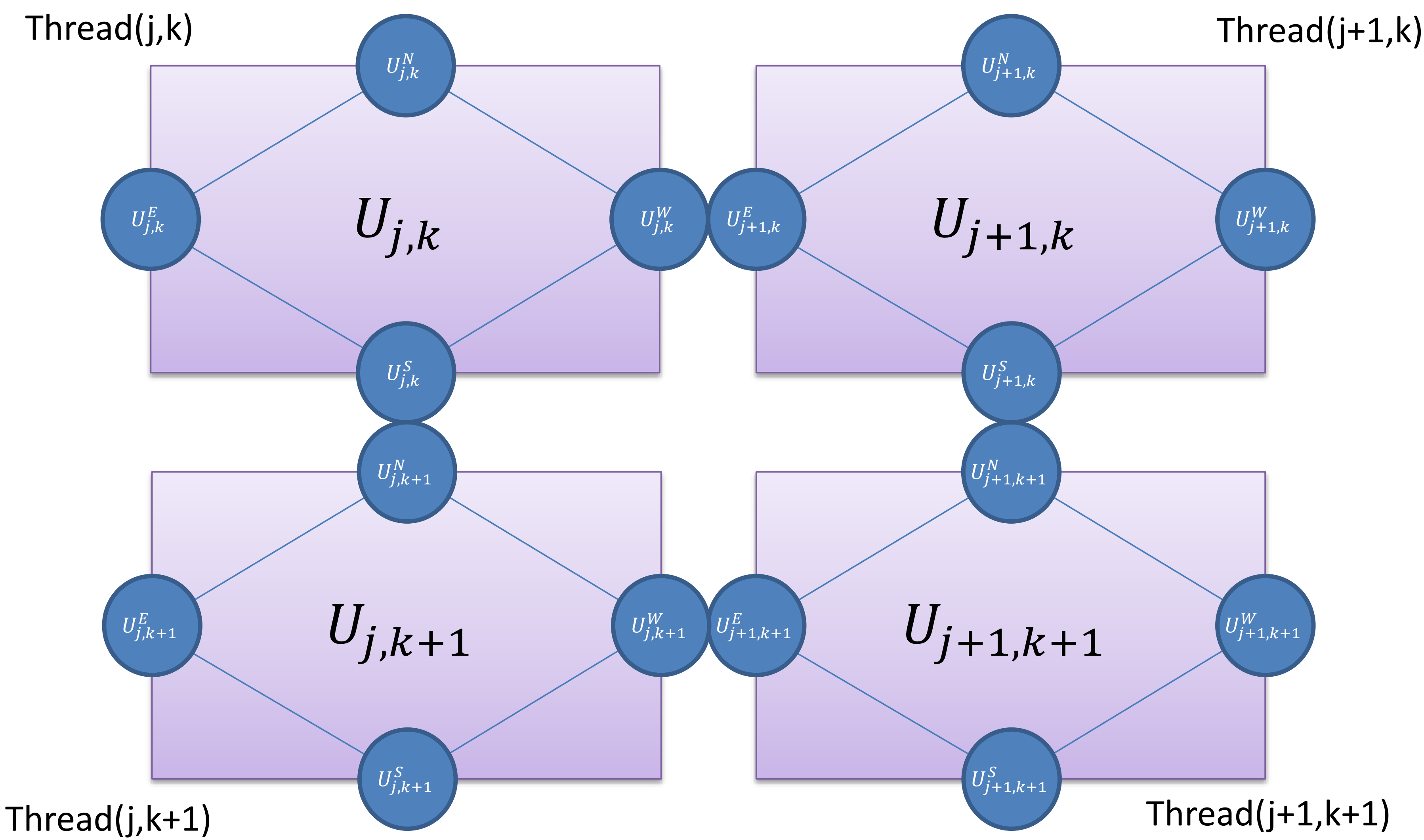
*See http://www.sintef.no/Projectweb/Heterogeneous-Computing/Research-Topics/Shallow-Water/ for details on practical application of the model

Numerics: Discretization by finite volumes

- Numerics: Kurganov-Petrova second-order well-balanced positivity preserving central-upwind scheme
- The problem is solved for a huge set of discretization cells that form a staggered grid.



Numerics:
fitting with GPU architecture



Roadmap of the GPU implementation

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- Single call to cudaMalloc(…) to allocate a huge linear block of memory. The needed part is then accessed by the offsets.
- Extensive use of the shared memory: neighboring cells propagate their "boundary conditions" between each other through the CUDA shared memory
- No intermediate transfers to the host: all computations are done on the GPU-side
- The grid is horizontally divided between all available GPUs. Pinned memory is used for data exchange to minimize the I/O workload (albeit, this part needs more testing)
- The serial part of the code is reduced to data initialization, hence the impact of the Amdahl's law is minimal → the code scales very good with growth of the spatial resolution (one can run up to 3 000 000 dimensional shallow water in very this laptop!)
- Under certain conditions we were able to reach 100x performance boost over CPU-hosted implementation based on intel MKL routines

Conclusion

- Presented an algorithm based on Kalman filter approximation, which is able to preserve stability when applied to large-scale dynamics
- A further improvement for the approach based on parallelization is introduced
- Both concepts are tested with a toy-case chaotic model, which can be made fairly large-scale by increasing spatial discretization
- A new test model, which can be run at a very high resolution on widely available hardware is implemented (thanks to CUDA!)

Thank you for attention!