A stable and accurate Variational Kalman Filter

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Overview

- Desirable properties of assimilation methods
- Variational methods and Ensemble Kalman filters
- Deterministic Kalman filters:
  - Classical Extended Kalman filter
  - Variational reformulation of the Kalman filter
- Quasi-Geostrophic model: integration and implementation
- Parallelization concerns
- Conclusions

Desirable properties of assimilation methods

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- Assimilation methods should be
- Accurate
    - No bias
- Precise
    - Use all available information in an optimal fashion
    - Provide for dynamic error covariances
- Parallelizable
- Simple
    - Tangent linear and adjoint models difficult to maintain
- All these criteria are difficult to meet simultaneously

Variational methods and Ensemble Kalman Filters

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- Optimum Interpolation
  - Unbiased
  - Parallelizable by domain decomposition
  - Not precise – static error covariances
  - No tangent linear or adjoint model

- 4DVAR
  - Precise, but static error covariances
  - Potentially biased – because of strong model constraint
  - Not very parallelizable
  - Tangent linear and adjoint models

Variational methods and Ensemble Kalman Filters

- Weak constraint 4DVAR
  - Precise, partially dynamic error covariance
  - Potentially biased
  - Computationally expensive – big control vector dimension
  - Parallelizable – by domain decomposition in time ?
  - Tangent linear and adjoint models

- Ensemble Kalman Filters
  - Potentially unbiased
  - Efficiently parallelizable
  - Dynamic error covariance
  - Not precise – ensemble small compared to state space dimension
  - No tangent linear or adjoint models

Extended and Variational Kalman Filters

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Kalman Filters:
Extended Kalman Filter

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Input: $x_k, y_{k+1}, C_k, Q_{k+1}, R_{k+1}, M_{k+1}, K_{k+1}.$

1. $x^p_{k+1} := M_{k+1} x_k$
2. $C^p_{k+1} := M_{k+1} C_k M'_{k+1} + Q_{k+1}$
3. $G_{k+1} := C^p_{k+1} K'_{k+1} \left(K_{k+1} C^p_{k+1} K'_{k+1} + R_{k+1} \right)^{-1}$
4. $x_{k+1} := x^p_{k+1} + G_{k+1} \left(y_{k+1} - K_{k+1} x^p_{k+1} \right)$
5. $C_{k+1} := C^p_{k+1} - G_{k+1} K_{k+1} C^p_{k+1}$

Output: x_{k+1}, C_{k+1}

Where: C_k, Q_{k+1}, R_{k+1} are covariance matrices of $x_k, \varepsilon^p_{k+1}, \varepsilon^o_{k+1}$ respectively.

Extended Kalman Filter: drawbacks

- Covariance error matrix propagation requires $O(n^3)$ flops
- Covariance storage requires to store n^2 floating-point or double-precision values
- In the case of weather simulation dynamical systems $n \approx 10^{17}$, which makes the basic formulations impossible to implement

Solution: provide a low-memory matrix approximation supporting efficient matrix-vector multiplications

Variational Kalman Filter VKF

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- Variational Kalman Filter
  - Precise – equivalent to EKF, hence dynamic error covariance
  - Guaranteed to be stable
  - Bias can be kept under control
  - Not very parallelizable
  - Tangent linear and adjoint models inherited from 4DVAR

Low-memory matrix approximations

- Consider an arbitrary matrix A
- The task is to compute its “smallest” update D in terms of Frobenius norm such that $(A + D)v = y$, where v and y is known pair of vectors and v is nonzero.

$$Dv = y - Av = r, \|D\|_{Fr}^2 \to min$$

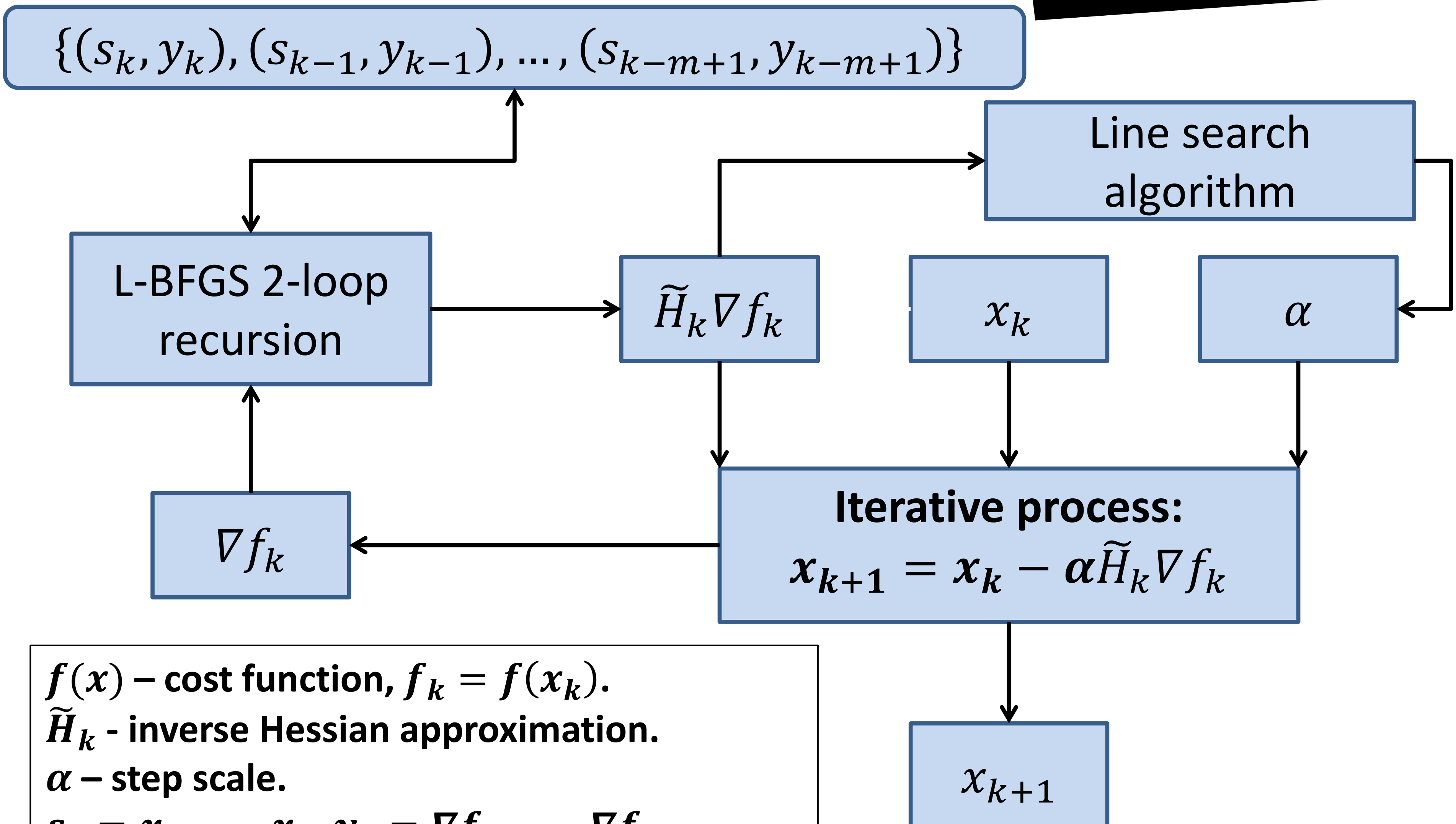
- Consider a pair of vectors v and y.
- The task is to find a symmetric positive definite matrix which maps v to y.

Low-memory matrix approximations: BFGS update

Theorem. Let L_C be a nonsingular matrix, $H_C = L_C L_C^T$. Let y and v be an arbitrary pair of vectors where v is nonzero. There is a symmetric positive definite matrix H_+, such that $(H_C + H_+)v = y$, if and only if $y^T v > 0$. If there is such a matrix , then $H_+ = J_+ J_+^T$, where

$$J_+ = L_C + \frac{\left(y - \sqrt{\frac{y^T v}{v^T H_C v}} H_C v\right)\left(L_C^T v\right)^T}{\sqrt{\frac{y^T v}{v^T H_C v}} v^T H_C v}$$

Low-memory matrix approximations: BFGS update



$f(x)$ – cost function, $f_k = f(x_k)$.
$\widetilde{H}_k$ - inverse Hessian approximation.
α – step scale.
$s_k = x_{k+1} - x_k$, $y_k = \nabla f_{k+1} - \nabla f_k$.

Variational Kalman Filter

Input: $x_k, y_{k+1}, C_k, Q_{k+1}, (R_{k+1})^{-1}, M_{k+1}, K_{k+1}.$

1. $x_{k+1}^p := M_{k+1}(x_k)$
2. *Compute L-BFGS approximation* B_{k+1}^* *of* $\left(C_{k+1}^p\right)^{-1}$,
   where $C_{k+1}^p := M_{k+1} C_k M_{k+1}' + Q_{k+1}.$
3. *Minimize with L-BFGS*
   $$l(x) = (y_{k+1} - K_{k+1}x)'(R_{k+1})^{-1}(y_{k+1} - K_{k+1}x) + \left(x - x_{k+1}^p\right)' B_{k+1}^* \left(x - x_{k+1}^p\right)$$
4. *Define* x_{k+1} *to be the minimizer from step 3 and* C_{k+1} *to be the L-BFGS approximation of inverse Hessian of the problem on step 2.*

Use of LBFGS in stabilized VKF

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Assume that an approximation $B^{\#}_{k-1}$ for covariance C^{est}_{k-1} is available. Then the EKF formulas can be approximated directly, which leads to the following algorithm:

1. Compute prediction $x^p_k = \mathcal{M}_k(x^{est}_k)$.

   Define prediction covariance $C^p_k = M_k B^{\#}_{k-1} M^T_k + C_{\varepsilon^p_k}$.

   Define $A = K_k C^p_k K^T_k + C_{\varepsilon^o_k}$, $b = y_k - K_k x^p_k$.
2. Solve optimization problem $\frac{1}{2} x^T A x - b^T x \to min$ with respect to x and compute a low-memory approximation $B^* \approx A^{-1}$.
3. Compute state estimate $x^{est}_k = x^p_k + C^p_k K^T_k x^*$, where x^* is solution for the optimization problem from step 2.
4. Compute a low-memory approximation $B^{\#}_k$ for the estimate covariance $C^{est}_k = C^p_k - C^p_k K^T_k B^* K_k C^p_k$.

Matrix $\boldsymbol{C^{est}_k = C^p_k - C^p_k K^T_k B^* K_k C^p_k}$ is not guaranteed to remain positive definite. Therefore, numerical instability may occur in some cases.

Stabilized VKF

- Setting $B^* = A^{-1}$ we get

$$C_k^{est} = C_k^p - C_k^p K_k^T (2I - B^* A) B^* K_k C_k^p = C_k^p - C_k^p K_k^T A^{-1} K_k C_k^p = C_k^p - G_k K_k C_k^p,$$

which is the exact formula from the EKF. Therefore, the Stabilized VKF still mimics the basic EKF formulas.

Quasigeostrophic 2-layer model

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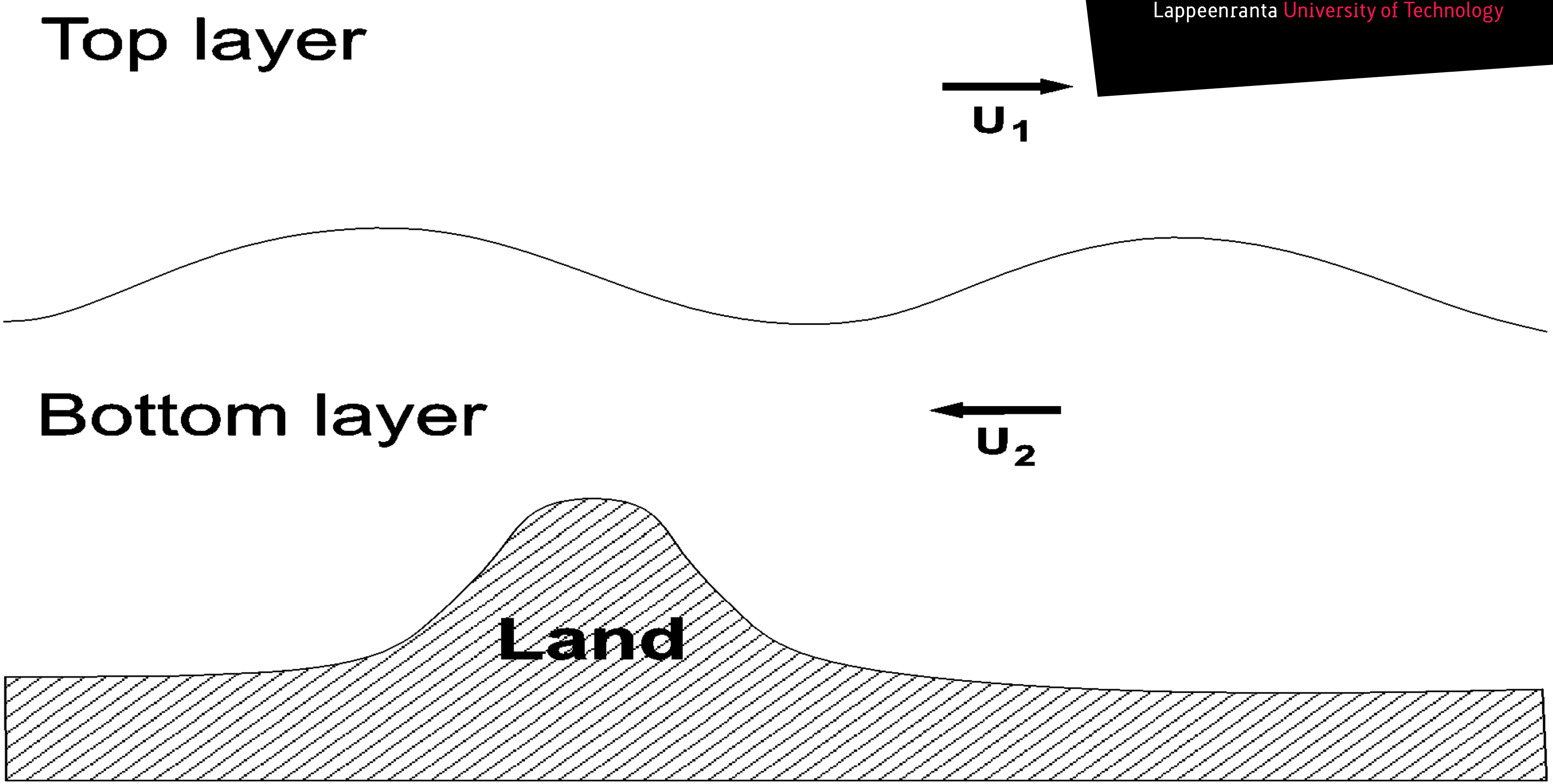
Quasi-Geostrophic model: review



U_1 - constant zonal flow in the top layer.

U_2 - constant zonal flow in the bottom layer.

D_1 - undisturbed depth of the top layer.

D_2 - undisturbed depth of the bottom layer.

$S(x, y)$ - orography term.

f_0 - Coriolis parameter.

Quasi-Geostrophic model: review

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$$\acute{g} = g\frac{\Delta\theta}{\bar{\theta}}, F_1 = \frac{f_0^2 L^2}{\acute{g} D_1}, F_2 = \frac{f_0^2 L^2}{\acute{g} D_2},$$

$$R_s = \frac{f_0 L S(x,y)}{U D_2}, \beta = \beta_0 \frac{L}{U}.$$

$$\frac{D_1 q_1}{Dt} = \frac{D_2 q_2}{Dt} = 0;$$

$$q_1 = \nabla^2 \psi_1 - F_1(\psi_1 - \psi_2) + \beta y,$$

$$q_2 = \nabla^2 \psi_2 - F_2(\psi_2 - \psi_1) + \beta y + R_s.$$

$$\frac{D_i \cdot}{Dt} = \frac{\partial \cdot}{\partial t} + u_i \frac{\partial \cdot}{\partial x} + v_i \frac{\partial \cdot}{\partial y},$$

$$\nabla \psi_i = (v_i, -u_i)$$

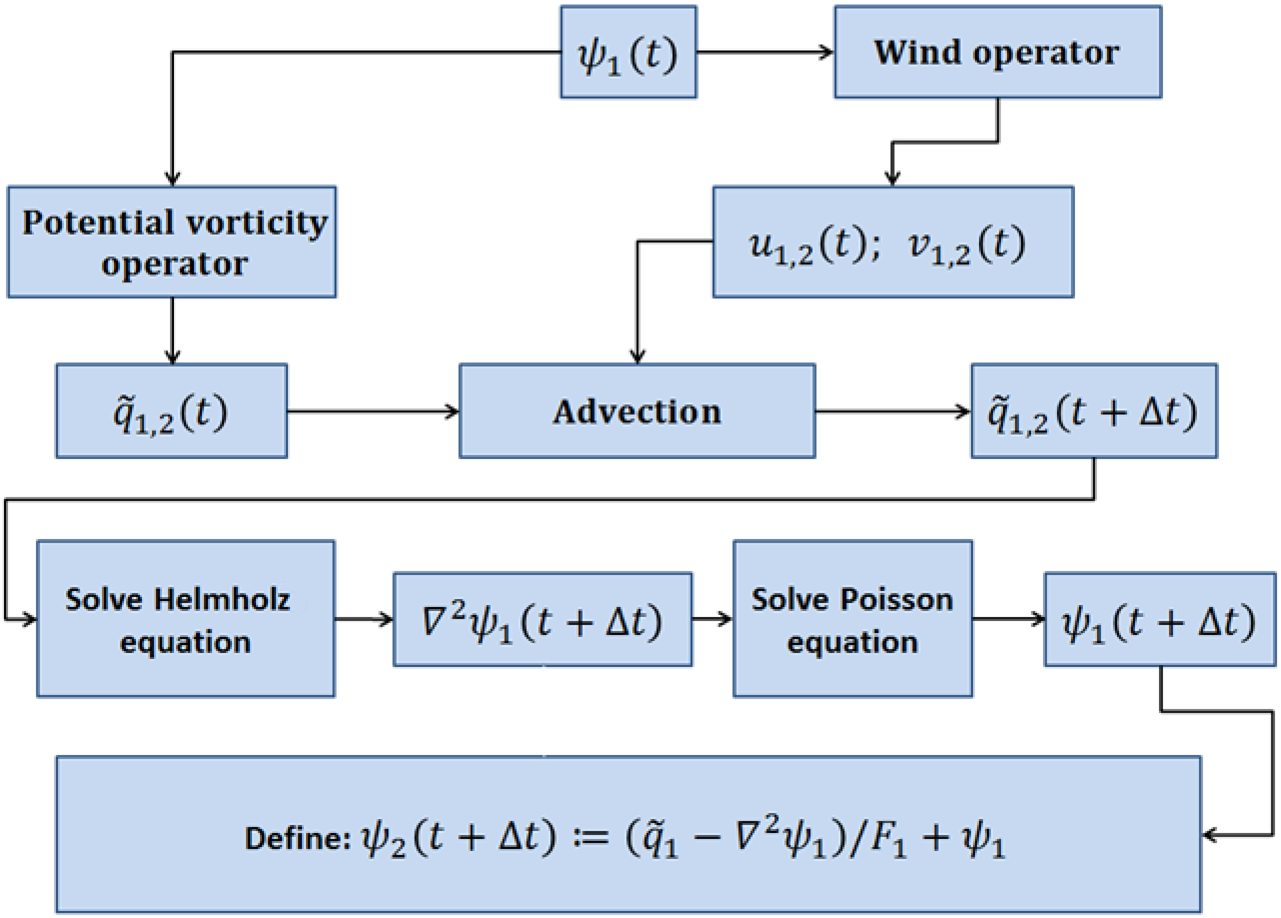
Quasi-Geostrophic model: review

$$\frac{D_1 q_1}{Dt} = \frac{D_2 q_2}{Dt} = 0,$$
$$q_1 = \nabla^2 \psi_1 - F_1(\psi_1 - \psi_2) + \beta y,$$
$$q_2 = \nabla^2 \psi_2 - F_2(\psi_2 - \psi_1) + \beta y + R_s,$$
$$\frac{D_i \cdot}{Dt} = \frac{\partial \cdot}{\partial t} + u_i \frac{\partial \cdot}{\partial x} + v_i \frac{\partial \cdot}{\partial y},$$
$$\nabla \psi_i = (v_i, -u_i)$$

Apply ∇^2 to the equation for q_1, subtract F_1 times equation for q_1 and F_2 times equation for q_2:

$$\nabla^2(\nabla^2 \psi_1) - (F_1 + F_2)(\nabla^2 \psi_1) =$$
$$\nabla^2(q_1 - \beta y) - F_2(q_1 - \beta y) - F_1(q_2 - \beta y - R_s)$$

Quasi-Geostrophic model: integration pipeline



Wind operator:

$$\nabla\psi_i = (v_i, -u_i)$$

Experimental Design: simulation model

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- **Two-layer Quasi-Geostrophic model solved on a cylindrical 40x20 domain**
- **Spatial discretization steps** $\triangle x = \triangle y = 300km$
- **Time discretization step** $\triangle t = 21600s$
- **Layer depths** $D_1 = 6000m$, $D_2 = 4000m$
- **Orography term:**
  - **Gaussian hill**
  - **2000m high, 1000km wide at grid vertex** $(0, 15)$
- **Domain 12000km x 6000km**

Experimental Design: orography component

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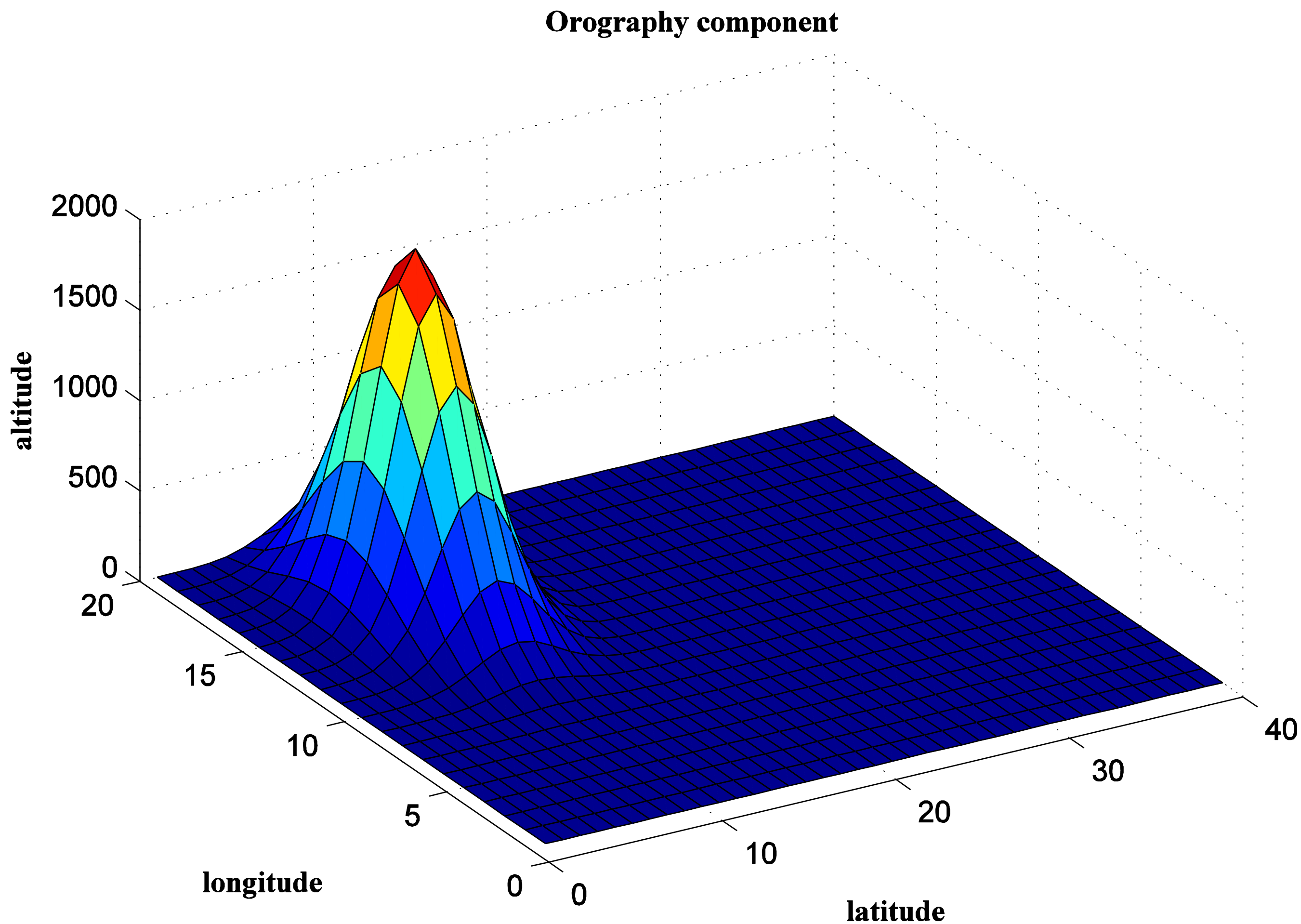

Experimental Design: assimilation with a biased model

- **Assimilation model, and tangent linear and adjoint models:**
  - **The same settings as for simulation model**
  - **Different layer depths $D_1 = 5500m$, $D_2 = 4500m$**
- **Initial state:**
  - **Propagate assimilation and "truth" models for two weeks with one hour time step**
- **Observation concept:**
  - **Observe sparse set of 100 grid vertices at every assimilation step**
  - **Selection of the vertices observed at every assimilation step remains unchanged**

Experimental Design: model error

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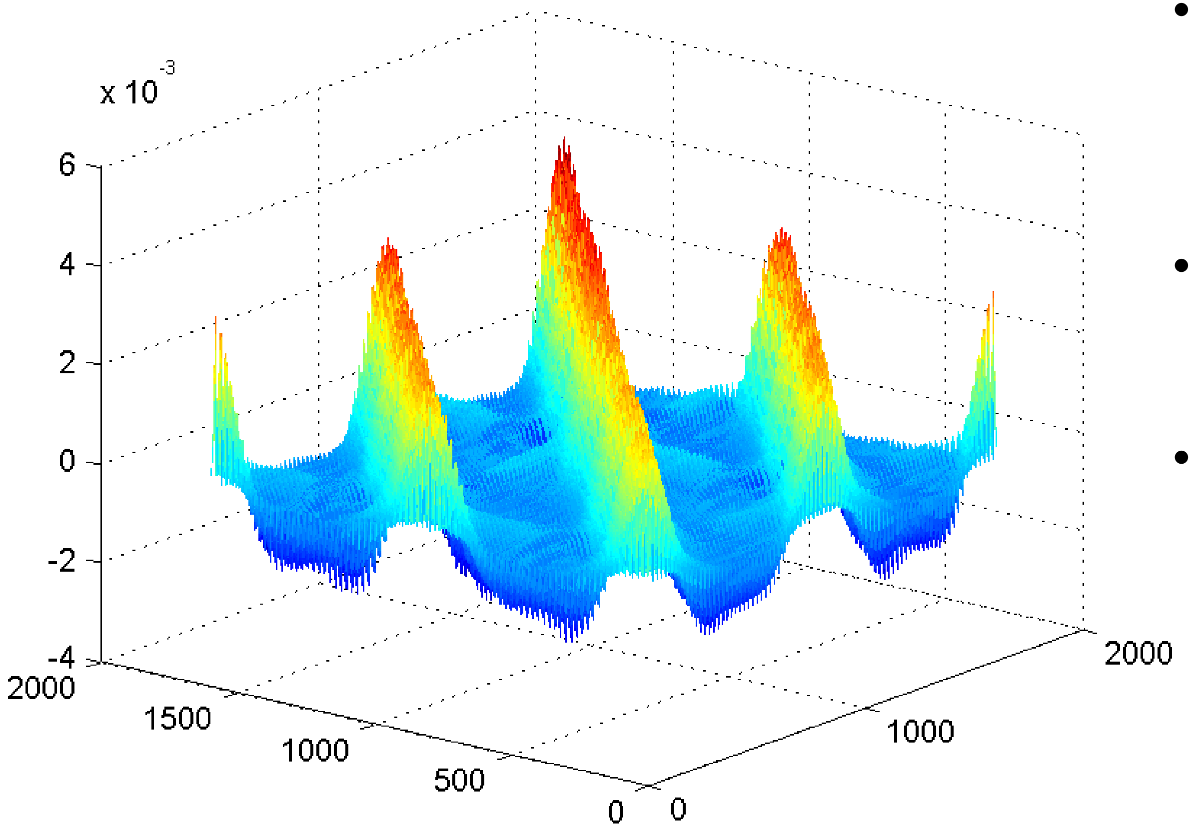

- Main diagonal hill corresponds to in-layer correlations between the vertices.
- Off diagonal hills correspond to cross-layer correlations
- Small hills near the corners reveal model's periodical nature

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Assimilation results

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Parallelization concerns with VKF

Parallelization concerns with VKF

- With respect to parallelization, VKF is similar to 4DVAR
- This means it is an inherently serial algorithm
- Both
  - L-BFGS itself,
  - the alternating serial calls to the tangent linear and adjoint models, and
  - the alternation between 3DVAR-like purely spatial observation processing and 4DVAR-like error covariance update process
- are all serial

Parallelization concerns with VKF

- On the other hand, the serial complexity of VKF is almost identical to that of 4DVAR, and it may be even less: it consists of the same operations as 4DVAR, organized in a different manner
- So instead of a variational form of EKF, VKF can also be seen as an efficient way to provide 4DVAR with
  - A dynamic error covariance matrix
  - A way to counter model bias without covariance inflation
- But VKF can be run - just like 4DVAR - in an Ensemble of Data Assimilations EDA
- This will yield as ensemble from the right posterior distribution

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Conclusions

Conclusions

- Assimilation methods should be
  - Accurate
  - Precise
  - Parallelizable
  - Simple
- Stabilized Variational Kalman Filter is
  - Accurate
  - Precise
  - Not very parallelizable – but serves well in EDA
  - Simple, if 4DVAR has been in use before

Conclusions

- VKF has been implemented in the Lappeenranta version of ECMWF OOPS, dubbed LOOPS
- **Integration with IFS is possible once it is brought into OOPS – see the talk by Yannick and Mike in Session 11 tomorrow ☺**

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Thank You!