4DEnVar: link with 4D state formulation of variational assimilation and different possible implementations

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Introduction

- 4D-Var

  ✓ Simplified description of $\mathbf{B}_0$ at initial time t_0.

  ➢ Ensemble of perturb. 4D-Vars (Météo-France (MF), ECMWF): dynamics of
  - error variances (MF, 2008)
  - and correlat. (MF, 2013), with wavelet $\mathbf{B}_0$ (Fisher, 2003; Varella et al, 2011).

  ✓ Difficult development and maintenance of TL/AD.

  ✓ Poor scalability of TL/AD at low resolution.

- 4D-Var based on a 4D ensemble: 4DEnVar

  ✓ Keeps benefits of 4D-Var (global analysis, additional terms, outer-loop, …)

  ✓ Localization of the raw covariances made in model space.

  ✓ Minimization cost similar to 3D-Var, parallelization properties.

4D state formulation of variational assimilation

- Minimization of

$$J(\delta \mathbf{x}_0, \ldots, \delta \mathbf{x}_K) = \delta \mathbf{x}_0^T \mathbf{B}_0^{-1} \delta \mathbf{x}_0 + \Sigma_{k=1,K} (\delta \mathbf{x}_k - \mathbf{M}_k \delta \mathbf{x}_{k-1})^T \mathbf{Q}_k^{-1} (\delta \mathbf{x}_k - \mathbf{M}_k \delta \mathbf{x}_{k-1})$$
$$+ \Sigma_{k=0,K} (\mathbf{H}_k \ \delta \mathbf{x}_k - \mathbf{d}_k)^T \mathbf{R}_k^{-1} (\mathbf{H}_k \ \delta \mathbf{x}_k - \mathbf{d}_k).$$

$$\delta \underline{\mathbf{x}} = \begin{pmatrix} \delta \mathbf{x}_0 \\ \delta \mathbf{x}_1 \\ \\ \delta \mathbf{x}_K \end{pmatrix} \quad \underline{\mathbf{D}} = \begin{pmatrix} \mathbf{B}_0 & & & \\ & \mathbf{Q}_1 & & \\ & & & \\ & & & \mathbf{Q}_K \end{pmatrix} \quad \underline{\mathbf{F}}^{-1} = \begin{pmatrix} \mathbf{I} & & & \\ -\mathbf{M}_1 & \mathbf{I} & & \\ & & & \\ & & -\mathbf{M}_K & \mathbf{I} \end{pmatrix} \quad \underline{\mathbf{F}} = \begin{pmatrix} \mathbf{I} & & & \\ \mathbf{M}_0^1 & \mathbf{I} & & \\ & & & \\ \mathbf{M}_0^K & \mathbf{M}_1^K & & \mathbf{I} \end{pmatrix}$$

$$J(\delta \underline{\mathbf{x}}) = \delta \underline{\mathbf{x}}^T \underline{\mathbf{F}}^{-T} \underline{\mathbf{D}}^{-1} \underline{\mathbf{F}}^{-1} \delta \underline{\mathbf{x}} + (\underline{\mathbf{H}} \ \delta \underline{\mathbf{x}} - \underline{\mathbf{d}})^T \underline{\mathbf{R}}^{-1} (\underline{\mathbf{H}} \ \delta \underline{\mathbf{x}} - \underline{\mathbf{d}}).$$

(Courtier, 1997; Trémolet, 2006; Fisher, 2013)

- Also equivalent to the minimization of

$$J(\delta \underline{\mathbf{x}}) = \delta \underline{\mathbf{x}}^T \underline{\mathbf{B}}^{-1} \delta \underline{\mathbf{x}} + (\underline{\mathbf{H}} \ \delta \underline{\mathbf{x}} - \underline{\mathbf{d}})^T \underline{\mathbf{R}}^{-1} (\underline{\mathbf{H}} \ \delta \underline{\mathbf{x}} - \underline{\mathbf{d}}), \qquad \text{with } \underline{\mathbf{B}} = \underline{\mathbf{F}} \ \underline{\mathbf{D}} \ \underline{\mathbf{F}}^T.$$

4DEnVar formulation

- Minimization of

$$J(\underline{\delta \mathbf{x}}) = \underline{\delta \mathbf{x}}^T \underline{\mathbf{B}}^{-1} \underline{\delta \mathbf{x}} + (\underline{\mathbf{d}} - \underline{\mathbf{H}}\ \underline{\delta \mathbf{x}})^T \underline{\mathbf{R}}^{-1} (\underline{\mathbf{d}} - \underline{\mathbf{H}}\ \underline{\delta \mathbf{x}}), \text{ with}$$

$$\underline{\mathbf{B}} = \underline{\mathbf{X}}^b (\underline{\mathbf{X}}^b)^T,$$

$\underline{\mathbf{X}}^b = (\underline{\mathbf{x}}^{b'}_1, \ldots, \underline{\mathbf{x}}^{b'}_L)$, $\underline{\mathbf{x}}^{b'}_l = \underline{\mathbf{x}}^b_l - \langle \underline{\mathbf{x}}^b \rangle / (L-1)^{1/2}$, $l=1,L$, and L ensemble size.

(Liu et al, 2008, 2009; Buehner et al, 2010; Lorenc, 2012)

- 4DEnVar without/with model error perturbations:

$\underline{\mathbf{x}}^{b'}_l = \underline{\mathbf{F}}\ \underline{\mathbf{D}}^{1/2}\ \underline{\eta}_l / (L-1)^{1/2}$, where $\underline{\eta}_l$ is a 4D random vector.

Link with previous 4D formulation of variational assimilation.

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Implementations of 4DEnVar

- *Formulation 1:*
  $\underline{\delta \mathbf{x}} = \underline{\mathbf{B}}^{1/2} \chi = (\underline{\mathbf{X}}^b(\underline{\mathbf{X}}^b)^T \circ \underline{\boldsymbol{C}})^{1/2} \chi = (\underline{\mathbf{X}}^b(\underline{\mathbf{X}}^b)^T \circ \underline{1}\, \boldsymbol{C}\, \underline{1}^T)^{1/2} \chi = \Sigma_{l=1,L}\, \underline{\mathbf{x}}^{b'}{}_l \circ (\boldsymbol{C}^{1/2} \chi_l)$

  $J^b(\chi) = \Sigma_{l=1,L}\, \chi_l^T \chi_l$, dim $\chi = N(N_c)xL$.

  Conjugate Gradient (CG) with $\underline{\mathbf{B}}^{1/2}$ change of variables.

  (Buehner, 2005, 2010)

- *Formulation 2:*
  $\underline{\delta \mathbf{x}} = \Sigma_{l=1,L}\, \underline{\mathbf{x}}^{b'}{}_l \circ \alpha_l$, with $\alpha_l = \boldsymbol{C}^{1/2} \chi_l$

  $J^b(\alpha) = \Sigma_{l=1,L}\, \alpha_l^T \boldsymbol{C}^{-1} \alpha_l$, dim $\alpha = N(N_c)xL$ (Lorenc, 2003).

  Double Preconditioned CG (DPCG) with $\boldsymbol{C}$ preconditioning.

  (Wang et al, 2007; Wang, 2010)

Possible alternative implement. of 4DEnVar: 4D B preconditioning

- *Formulation 3:*

DPCG, with 4D covariance matrix $\underline{\mathbf{B}}$: BCG

(Derber and Rosati, 1989; El Akkraoui et al, 2012; Gürol et al, 2012)

In this case, the dimension of the control variable $\underline{\delta \mathbf{x}}$ is (K+1)xMxN.

$$\underline{\mathbf{d}}_{-1} = \underline{\mathbf{e}}_{-1} = \mathbf{0}$$
$$\beta_{-1} = 0$$
$$\underline{\delta \mathbf{x}}_0 = \mathbf{0}$$
$$\underline{\mathbf{g}}_0 = \underline{\mathbf{H}}^T \underline{\mathbf{R}}^{-1} \underline{\mathbf{d}}$$
$$\underline{\mathbf{h}}_0 = \underline{\mathbf{B}}\, \underline{\mathbf{g}}_0$$

for i = 0 : I - 1

$$\underline{\mathbf{d}}_i = \underline{\mathbf{h}}_i + \beta_{i-1} \underline{\mathbf{d}}_{i-1}$$
$$\underline{\mathbf{e}}_i = \underline{\mathbf{g}}_i + \beta_{i-1} \underline{\mathbf{e}}_{i-1}$$
$$\underline{\mathbf{f}}_i = \underline{\mathbf{e}}_i + \underline{\mathbf{H}}^T \underline{\mathbf{R}}^{-1} \underline{\mathbf{H}}\, \underline{\mathbf{d}}_i$$
$$\alpha_i = \underline{\mathbf{g}}_i^T \underline{\mathbf{h}}_i \,/\, \underline{\mathbf{d}}_i^T \underline{\mathbf{f}}_i$$
$$\underline{\delta \mathbf{x}}_{i+1} = \underline{\delta \mathbf{x}}_i + \alpha_i \underline{\mathbf{d}}_i$$
$$\underline{\mathbf{g}}_{i+1} = \underline{\mathbf{g}}_i - \alpha_i \underline{\mathbf{f}}_i$$
$$\underline{\mathbf{h}}_i = \underline{\mathbf{B}}\, \underline{\mathbf{g}}_i$$
$$\beta_i = \underline{\mathbf{g}}_{i+1}^T \underline{\mathbf{h}}_{i+1} \,/\, \underline{\mathbf{g}}_i^T \underline{\mathbf{h}}_i$$

end

Multiplication by $\underline{\mathbf{B}}$

- Application of DPCG : $\underline{\mathbf{h}} = \underline{\mathbf{B}}\,\underline{\mathbf{g}}$

- $\underline{\mathbf{B}} = (\,\underline{\mathbf{X}}^{b'} (\underline{\mathbf{X}}^{b'})^T \circ \underline{\mathbf{1}}\, \mathbf{C}\, \underline{\mathbf{1}}^T)$

  $\mathbf{C} = \mathbf{S}^{-1}\, \mathbf{C}^s\, \mathbf{S}$

- $\mathbf{h}_{k,m} = \Sigma_{l=1,L}\, \Sigma_{k'=1,K}\, \Sigma_{m'=1,M}\, \mathbf{x}^{b'}{}_{l,k,m} \circ S^{-1} (\, \mathbf{C}^s\ S\ (\ \mathbf{x}^{b'}{}_{l,k',m'} \circ \mathbf{g}_{k',m'}\ )\,)$,

  k and k' time indices,
  m and m' variable indices.

- Compact and meaningful expression of the application of $\underline{\mathbf{B}}$.

- No need of extra variables (α_l or χ_l , with $\alpha_l = \mathbf{C}^{1/2} \chi_l$).

- Can be parallelized.

Possible alternative implement. of 4DEnVar: 4D B preconditioning in dual space

- *Formulation 4:*

BCG in observation space : RBCG (Gratton and Tshimanga, 2009; Gürol, 2012, 2013).

Similar to previous BCG but with $\underline{\mathbf{h}}_i = \underline{\mathbf{H}}\,\underline{\mathbf{B}}\,\underline{\mathbf{H}}^T\,\underline{\mathbf{g}}_i$.

In this case, the dimension of the control variable $\delta\underline{\mathbf{y}}$ is P (number of observations).

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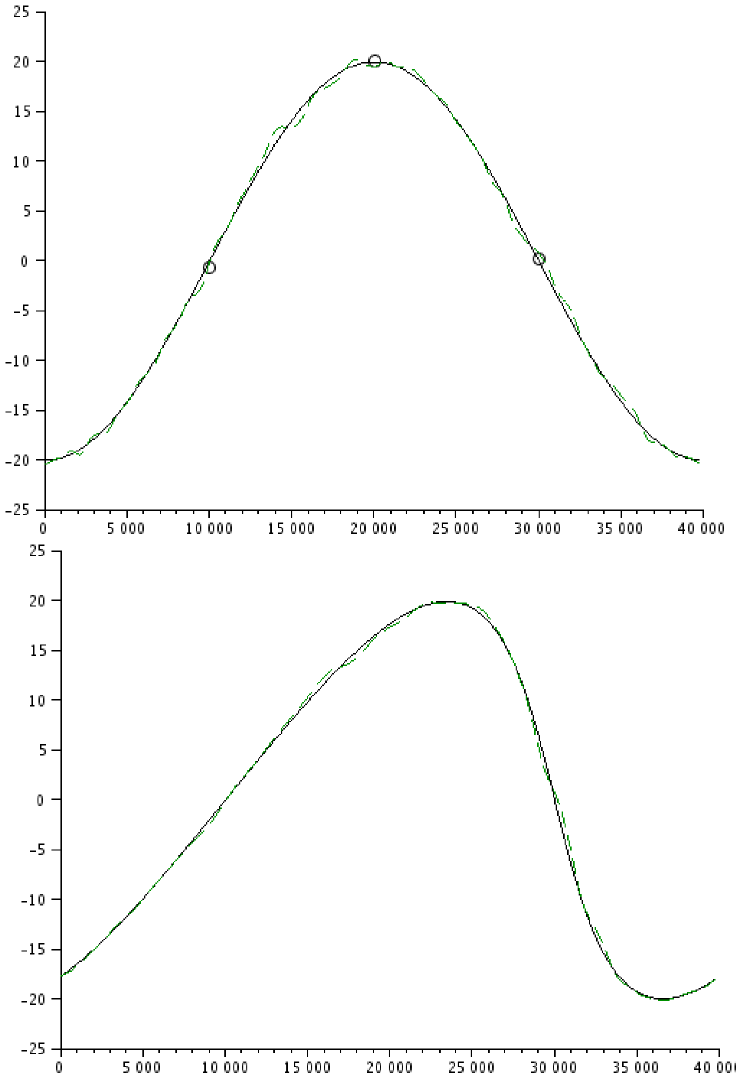
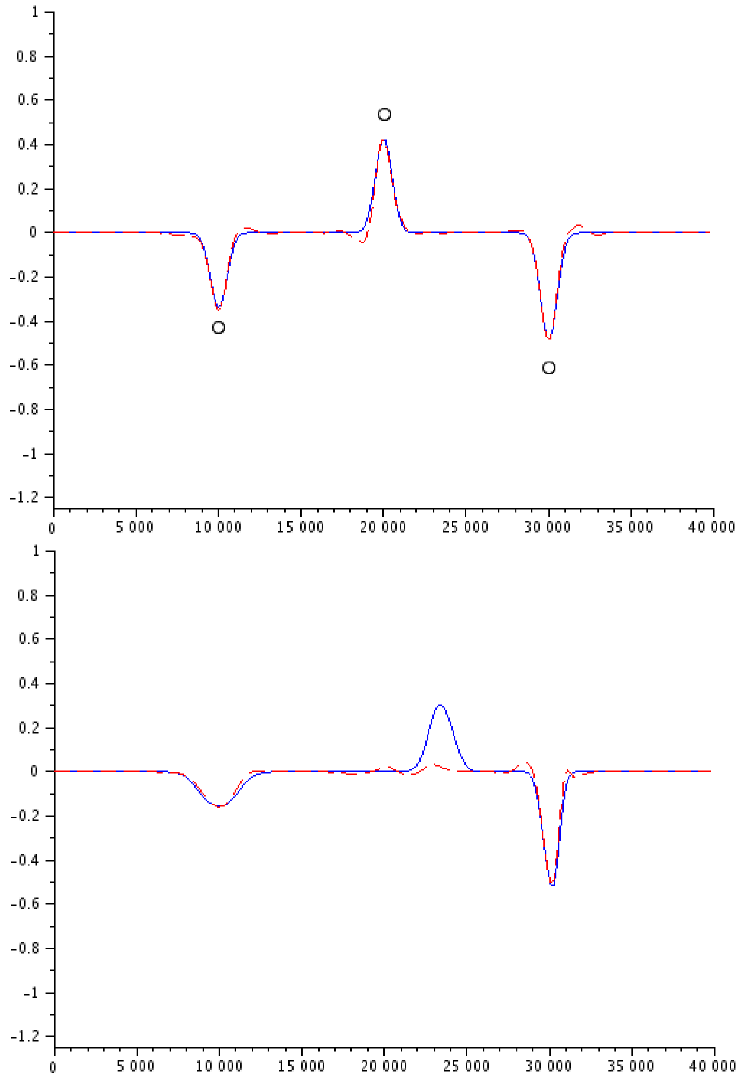
4D-Var / 4DEnVar comparison
Burgers' model



t_0

t_f = 48h



True wind field $\mathbf{x}^t$

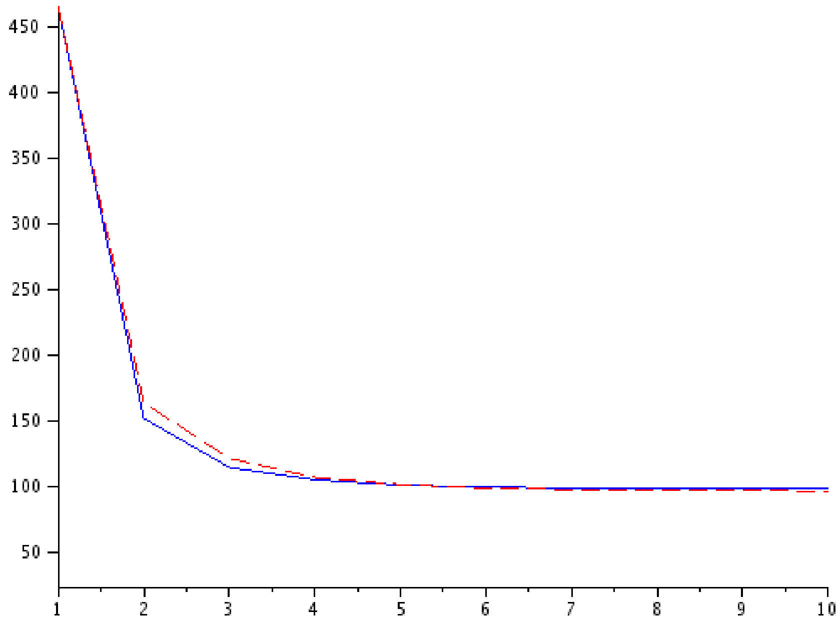
Bg wind field $\mathbf{x}^b$

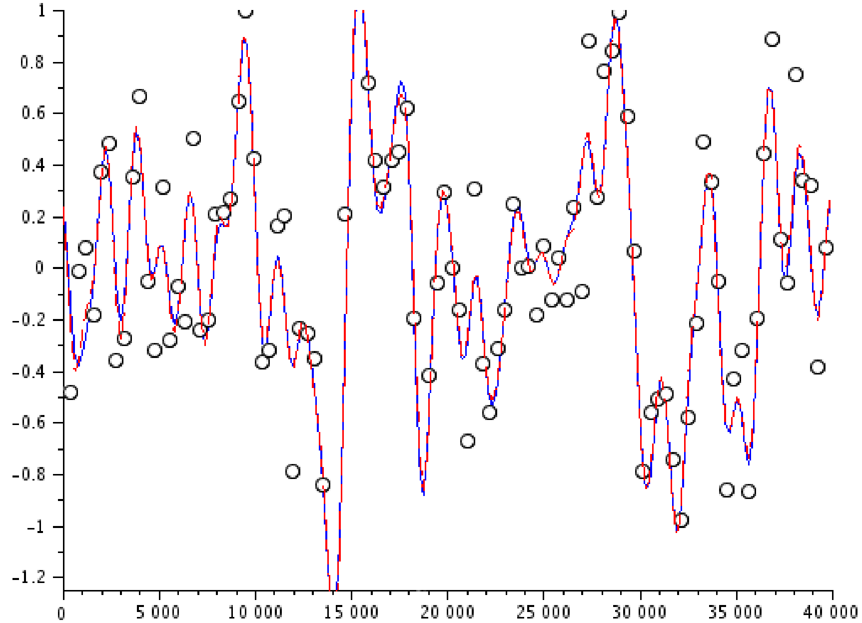
$\delta\mathbf{x}^a$ 4D-Var

$\delta\mathbf{x}^a$ 4DEnVar, L =100, L^c=1500km

4D-Var / 4DEnVar convergence
Burgers' model

time t0





J 4D-Var
J 4DEnVar

$\underline{\delta \mathbf{x}}^a$ 4D-Var
$\underline{\delta \mathbf{x}}^a$ 4DEnVar, L=100, L^c=1500km, t_f=6h

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Hybrid formulation

- Hybrib $\underline{\mathbf{B}}^h$ matrix :

$\underline{\mathbf{B}}^h = \gamma^{s2}\,\underline{\mathbf{B}}^s + (1-\gamma^{s2})\,\underline{\mathbf{B}}^e$ $\qquad\qquad$ $\underline{\mathbf{B}}^{h1/2} = (\ \gamma^s\,\underline{\mathbf{B}}^{s1/2} \quad (1-\gamma^{s2})^{1/2}\,\underline{\mathbf{B}}^{e1/2}\ )$

(Hamill and Snyder, 2000)

- Type and size of control variable(s) depend on the formulation:
  - ✓ *Formulation 1:* $J(\chi^s, \chi^e)$
  - ✓ *Formulation 2:* $J(\delta\mathbf{x}^s, \alpha)$
  - ✓ *Formulation 3:* $J(\underline{\delta\mathbf{x}})$
  - ✓ *Formulation 4:* $J(\underline{\delta\mathbf{y}})$

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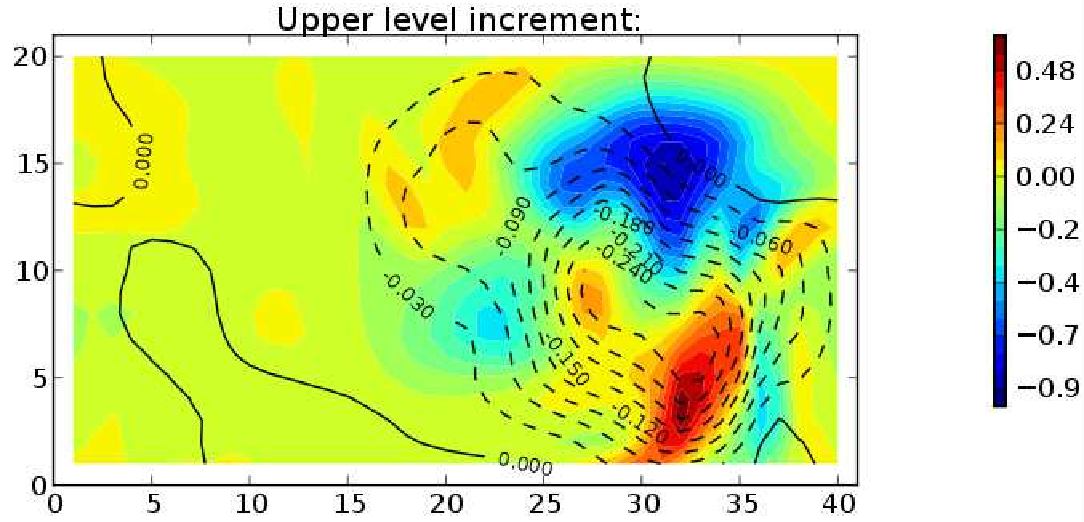
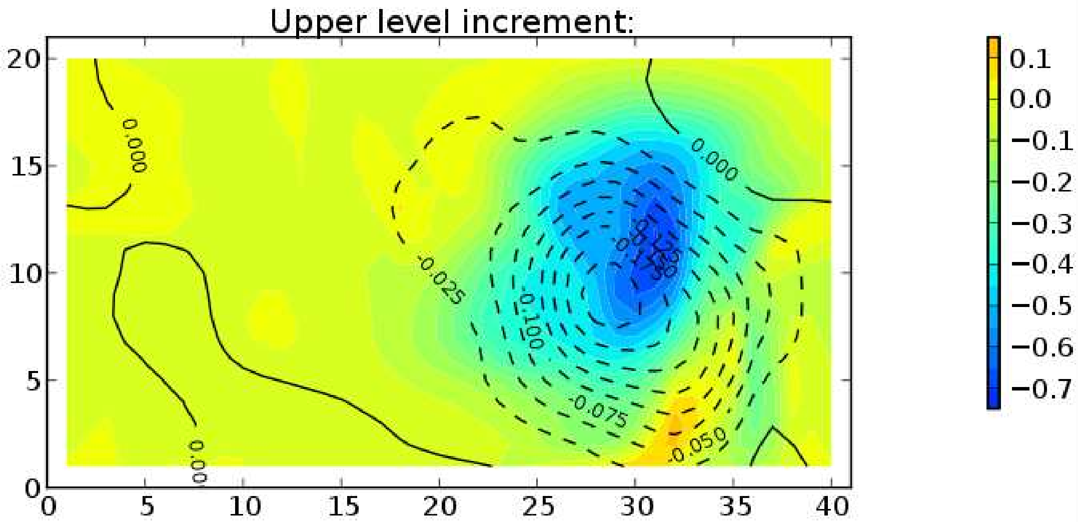
Hybrid formulation
Two-layer quasi-geostrophic model



4DEnVar $\delta\mathbf{x}$, using BCG

dashed line : ψ
shaded : q



Hybrid 4DEnVar $\delta\mathbf{x}$, using BCG

Developed (Arbogast, 2013) in OOPS (Trémolet and Fisher, 2013)

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Conclusion and future work

- Conclusion
  - ✓ Link of 4DEnvar with 4D state formulation of variational assimilation.
  - ✓ Efficient preconditioning available relying on **B**.
  - ✓ BCG with **B** matrix, and RBCG in dual space: possible implementations.
- Future work
  - ✓ Define a reasonable and efficient localization in space and time.
  - ✓ Memory and IO issues.
  - ✓ Ensemble of 4DEnVars?