3D-4D Variational Data Assimilation

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# 3D and 4D variational data assimilation

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### **Historical perspective**

- · Motivation for the development of 3D-Var
  - Improve our capacity to use new types of observations particularly satellite radiances (Eyre, 1989; Thépaut and Moll, 1990)
  - New background-error statistics models without data selection
  - Extension to 4D-Var (Talagrand and Courtier, 1987)
- NCEP (1992), ECMWF (1996), Météo-France and CMC (1997), MetOffice (1999)

## **Historical perspective (2)**

- Dual 3D-Var (Courtier, 1997)
  - NASA's Global Modeling and Assimilation Office (GMAO) (Cohn et al., 1998)
  - Naval Research Laboratory (Daley and Barker, 2000)
- 4D-Var
  - ECMWF (1997), Météo-France (2000), MetOffice (2004), JMA (2005), Meteorological Service of Canada (2005), NRL (2009)

# **Plan of presentation**

#### • 3D-Var

- Introduction of the incremental formulation
- First-Guess at Appropriate Time (FGAT)
- 4D-Var
  - Extension from 3D to 4D-Var
  - Incremental formulation
  - Evaluation of the impact of the first implementation of 4D-Var at the Meteorological Service of Canada
- Current issues
  - Comparaison of 4D-Var with the Ensemble Kalman filter
  - Hybrid formulation
  - Taking into account model error: the weak-constraint 4D-Var

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2

true value

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# **3D-Var: variational formulation of the statistical estimation problem**

Minimization of the cost function

$$J(\xi) = \frac{1}{2}\xi^{T}\xi + \frac{1}{2}(\mathbf{H}'\mathbf{B}^{1/2}\xi - \mathbf{y}')^{T}\mathbf{R}^{-1}(\mathbf{H}'\mathbf{B}^{1/2}\xi - \mathbf{y}')$$
  
with  $\delta \mathbf{x}_{a} = \mathbf{B}^{1/2}\xi^{*}$ ,  $\xi^{*}$  being min (J( $\xi$ ))  
where  $\delta \mathbf{x} = \mathbf{x} - \mathbf{x}_{b}$  : increment  
 $\mathbf{H}^{2} = \partial \mathbf{H}/\partial \mathbf{x}$  : tangent-linear of the observation operator  
 $\mathbf{y}' = \mathbf{y} - \mathbf{H}(\mathbf{x}_{b})$ : innovation vector (observation departure)  
(computed with respect to the high  
resolution background state)

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# Autocorrelation spectra of rotational and divergent components of backgrounderror















#### QC-Var

Definition of the cost function

$$J_{o}^{QC}(\mathbf{x}) \equiv J_{o}^{QC}(\hat{y}(\mathbf{x})) = -\ln p(y_{o} \mid H(\mathbf{x}))$$
where
$$= -\ln(P/D + C\exp(-J^{N}(\hat{y})))$$

$$J^{N}(\hat{y}(\mathbf{x})) = \frac{1}{2}\hat{y}^{T}\mathbf{R}^{-1}\hat{y} \equiv \frac{1}{2}\frac{(H(\mathbf{x}) - y_{o})^{2}}{\sigma_{o}^{2}}$$
16.







# **BIAS CORRECTION**

(from Auligné, McNally and Dee, QJ 2007)



#### **Static bias correction**

Modify the observation operator as

$$\tilde{H}(\mathbf{x},\boldsymbol{\beta}) = H(\mathbf{x}) + \sum_{i=0}^{N} \beta_{i} P_{i}(\mathbf{x})$$

• Find the coefficients  $\boldsymbol{\beta}$  by minimising

$$J(\boldsymbol{\beta}) = \frac{1}{2} \left( \mathbf{y} - \tilde{H}(\mathbf{x}_{b}, \boldsymbol{\beta}) \right)^{T} \left( \mathbf{y} - \tilde{H}(\mathbf{x}_{b}, \boldsymbol{\beta}) \right)$$

 The quantities P<sub>i</sub>(x) are the predictors which relate to the measurements

# **Predictors used for different satellite instruments** (Auligné, McNally and Dee, QJ 2007)

Instrument		Predictors		
AIRS	1000-300	200-50	10-1	50-5
ATOVS	1000-300	200-50	10-1	50-5
GEOS	1000-300	200-50	TCWV	
SSMI	Vs	Ts	TCWV	
<ul> <li>Geopo pressu</li> </ul>	otential thicknes res (in hPa)	ses for the layers	comprised betwe	een the

- TCWV: total content in water vaport
- V<sub>s</sub>: surface wind speed T<sub>s</sub>: skin temperature

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#### Adaptive online scheme: Var-BC

• Bias correction is incorporated within the assimilation scheme itself

$$J(\mathbf{x}, \beta) = \frac{1}{2} (\mathbf{y} - \tilde{H}(\mathbf{x}, \beta))^{T} \mathbf{R}^{-1} (\mathbf{y} - \tilde{H}(\mathbf{x}, \beta))$$
$$+ \frac{1}{2} (\beta - \beta_{b})^{T} \mathbf{B}_{\beta}^{-1} (\beta - \beta_{b})$$
$$+ \frac{1}{2} (\mathbf{x} - \mathbf{x}_{b})^{T} \mathbf{B}^{-1} (\mathbf{x} - \mathbf{x}_{b})$$

More apt to distinguish between model bias and observation biases.

# Comparison between VarBC and static bias correction (Auligné et al., 2007)



#### Summary up to now

- Variational assimilation made it possible to assimilate raw measurements, particularly those from satellite instruments
- Derived from a Bayesian perspective, the variational form is not restricted to Gaussian probability distributions
  - \* Non-Gaussian observation error distributions are used to perform implicitly the quality control of observations
- Online variational bias corrections is also a very convenient method to detect and correct systematic errors in the observations
- 3D-Var can be naturally extended to 4D-Var



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**Cost function** 

$$J(\xi) = \frac{1}{2}\xi^{T}\xi + \frac{1}{2}\left(\mathbf{H'L}(t_{o},t)\mathbf{B}^{1/2}\xi - \mathbf{y'}\right)^{T}\mathbf{R}^{-1}\left(\mathbf{H'L}(t_{o},t)\mathbf{B}^{1/2}\xi - \mathbf{y'}\right)^{T}$$

- Representation of the covariances contained within the change of variables  $\delta \bm{x}_{_0} = \bm{B}^{_{1/2}} \bm{\xi}$
- Each iteration of the minimization involves approximately 2-3 model integrations over the assimilation window (0 < t < T)</li>
- Incremental formulation allows to reduce the cost of 4D-Var by using a simplified model, the <u>tangent linear model</u> linearized around the current model trajectory (Courtier *et al.*, 1994)



Example	: the Lorenz (1963) model
Direct Model	$\frac{dX}{dt} = \sigma \left(-X + Y\right),$ $\frac{dY}{dt} = -XZ + rX - Y,$ $\frac{dZ}{dt} = XY - bZ,$
Tangent Linear Model (TLM)	$\frac{d}{dt} \begin{pmatrix} \delta X \\ \delta Y \\ \delta Z \end{pmatrix} = \begin{pmatrix} -\sigma & +\sigma & 0 \\ -Z_R(t) + r & -1 & -X_R(t) \\ Y_R(t) & X_R(t) & -b \end{pmatrix} \begin{pmatrix} \delta X \\ \delta Y \\ \delta Z \end{pmatrix}$
Adjoint Model	$\frac{d}{dt} \begin{pmatrix} \delta^* X \\ \delta^* Y \\ \delta^* Z \end{pmatrix} = - \begin{pmatrix} -\sigma & -Z_R(t) + r & Y_R(t) \\ +\sigma & -1 & X_R(t) \\ 0 & -X_R(t) & -b \end{pmatrix} \begin{pmatrix} \delta X \\ \delta Y \\ \delta Z \end{pmatrix}$



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Impact of 4D-Var in the Canadian operational assimilation and forecasting system

Results from Laroche et al. (2007), Environment Canada



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	Configurations				
Regional	Outer loop	Number of inner loops	Simplified physics	Low- resolution Analysis increments	High- resolution trajectory
3D-Var	1	~ 90	-	1.5º (T108) L58	~15 km L58
Global					
		00	DBI	1 = 0 (T100)	
4D-Var	1	30	-PBL	L58	(0.3° x 0.45°) L58

Observations	assim	ilateo	d at t	he CMC
Туре	Var	iables	6	Thinning
radiosonde/dropsonde	U, V, <sup>-</sup>	T, (T-T <sub>d</sub> ), p	D <sub>s</sub>	28 levels
Surface report	T, (T-T <sub>d</sub> ), p <sub>s</sub> ,	(U, V ove	r water)	1 report/6h
Aircraft (BUFR, AIREP, AMDAR, ADS)	L	J, V, T		1º x 1º x 50 hPa
ATOVS		Ocean	Land	250 km x 250 km
NOAA , AQUA	AMSU-A	3-10	6-10	
Water vapor channel GOES	Амзо-в (	IM3 6.7 μ)	3-4	2° x 2°
AMV (Meteosat, GOES, MTSAT)	(IR, WV,	U,V VI chann	els)	1.5º x 1.5º
MODIS (Aqua, Terra)		U,V		1.5º x 1.5º
Profiler (NOAA Network)		U,V		(750 m) Vertical



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Туре	Outer loops	Simplified Physics	Temporal thinning
3D-Var	1	-	3D
3D-Var (FGAT)	1	-	3D
4D-Var (1 loop)	1	(simpler)	4D
4D-Var simpler)	2	(simpler, simpler)	4D
4D-Var 3D-thin)	2	(simpler, better)	3D
4D-Var	2	(simpler, better)	4D





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# Assimilated radiances: major input in Strato-2b from new data and increased thinning

Number of radiance observations assimilated February 1st, 2009 (4 analyses):

Instrument	Platform	Strato 2a	Strato 2b	% Change
AIRS	AQUA	392 554	659 751	+ 68%
IASI	Metop-2	0	500 783	New
AMSU-A	NOAA-15	121 875	338 194	+ 178%
	NOAA-18	170 773	472 474	+ 177%
	AQUA	119 805	331 557	+ 177%
AMSUB	NOAA-15	14 762	41 350	+ 180%
	NOAA-16	30 082	84 341	+ 180%
	NOAA-17	32 965	92 609	+ 181%
MHS	NOAA-18	34 671	96 025	+ 177%
SSMI	DMSP-13	37 965	60 761	+ 60%
SSMIS	DMSP-16	0	39 330	New
GOES Imager	GOES-11	11 813	34 967	+ 196%
	GOES-12	10 024	41 919	+ 318%
SEVERI	MSG-2	0	69 183	New
MVIRI	Meteosat-7	0	41 882	New
GMS MTSAT	MTSAT-1	0	20 612	New
All Radi	iances:	977 289	2 925 788	+ 199%



### Experimental Systems (Buehner et al., 2010,a-b)

Modifications to configurations operational during summer 2008

- 4D-Var
  - incremental approach: ~35km/150km grid spacing, 58 levels, 10hPa top → Increased horizontal resolution of inner loop to 100km to match EnKF
- EnKF
  - 96 ensemble members: ~100km grid spacing, 28 levels, 10hPa top → Increased number of levels to 58 to match 4D-Var
- Same observations assimilated in all experiments:
  - radiosondes, aircraft observations, AMVs, US wind profilers, QuikSCAT, AMSU-A/B, surface observations
  - eliminated AIRS, SSM/I, GOES radiances from 4D-Var
  - quality control decisions and bias corrections extracted from an independent 4D-Var experiment

### **Experimental Configurations**

- Variational data assimilation system:
  - 3D-FGAT and 4D-Var with **B** matrix nearly like operational system: NMC method
  - 3D-FGAT and 4D-Var with flow-dependent B matrix from EnKF at middle or beginning of assimilation window (same localization parameters as in EnKF)
  - Ensemble-4D-Var (En-4D-Var): use 4D ensemble covariances to produce 4D analysis increment without TL/AD models (most similar to EnKF approach)
- EnKF:
  - Deterministic forecasts initialized with EnKF ensemble mean analysis (requires interpolation from ~100km to ~35km grid)

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### **Forecast Results – Precipitation**











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#### Forecast Results: En-4D-Var vs. 4D-Var-Benkf



## Summary

- Major future improvements of 4D-Var would require significant effort:
  - optimization/reformulation of GEM TL/AD and development of linearized physics
  - improved background-error covariances by using EnKF ensemble
     → requires synchronized development of 4D-Var and EnKF
  - significant redesign of variational code to facilitate major future changes to model (vertical co-ord, yin-yang, icosahedral etc.)
- Use of En-4D-Var (without GEM TL/AD):
  - advantages of a variational analysis could be preserved by using a variational solver within EnKF
  - allows use of some alternative approaches for modelling covariances: e.g. averaged covariances
  - allows use of var QC and Var-BC
  - requires further research to determine if it can be made sufficiently computationally efficient (in progress)

## Ensemble Kalman filter

Basic equations of a Kalman filter

$$\mathbf{X}_{n}^{a} = \mathbf{X}_{n}^{f} + \mathbf{K}_{n} \left( \mathbf{y}_{n} - \mathbf{H}_{n} \mathbf{X}_{n}^{b} \right) \qquad \mathbf{P}_{n}^{a} = \left( \mathbf{I} - \mathbf{K}_{n} \mathbf{H}_{n} \right) \mathbf{B}_{n}$$
$$\mathbf{K}_{n} = \mathbf{B}_{n} \mathbf{H}_{n}^{T} \left( \mathbf{R}_{n} + \mathbf{H}_{n} \mathbf{B}_{n} \mathbf{H}_{n}^{T} \right)^{-1} \qquad \mathbf{X}_{n+1}^{f} = F \left( \mathbf{X}_{n}^{a} \right)$$
$$\mathbf{B}_{n} = R \mathbf{P}^{a} R^{T} + \mathbf{Q}$$

• Ensemble Kalman filter  $\partial \mathbf{x}_{f}^{(i)}(t_{F}) = \mathcal{N}(\mathbf{X}_{a}^{(i)}) - \mathcal{N}(\mathbf{X}_{a})$ 

$$\mathbf{B}(t_F) \cong \left\langle \left( \partial \mathbf{x}_f^{(i)} \right) \left( \partial \mathbf{x}_f^{(i)} \right)^T \right\rangle = \frac{1}{(N-1)} \sum_{i=1}^N \left( \partial \mathbf{x}_f^{(i)} \right) \left( \partial \mathbf{x}_f^{(i)} \right)^T$$

The MSC EnKF solves explicitly

$$\left(\mathbf{R} + \mathbf{H}\mathbf{B}\mathbf{H}^{T}\right)^{-1}\left(\mathbf{y} - \mathbf{H}\left(\mathbf{x}_{b}^{(i)}\right)\right) = \mathbf{w}^{(i)}$$



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## Sequential algorithm (Houtekamer and Mitchell)

- In the EnKF, batches of p<sub>max</sub> (~1000) neighbouring observations are assimilated using a sequential algorithm.
- Allows use of a direct solution method (Cholesky decomposition) for solving the analysis equation.
- Computational cost increases as p<sub>max</sub><sup>3</sup> and approximately linearly with number of batches.
- In practice, then, more observations implies more batches.

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# Impact of having larger volumes of data

- The EnKF algorithm behaves poorly when the number of observations exceeds the number of degrees of freedom of the model state
- The sequential algorithm then shows a large dependence to the order in the observation processing and the ensemble then lacks dispersion
- To allow for small scale structures, with the current algorithm, it would be necessary to localize even more (at the expense of the larger scales) or increase the number of members.
- High resolution reference member should be used instead of the ensemble mean (incremental EnKF)

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## Conclusion

- Variational formulation of the statistical estimation problem allows
  - Take into account non-Gaussian error distributions
  - Quality control of observations can be embedded within the variational problem
  - Online bias correction of observations is very useful to detect and correct faulty observations and prevent them from altering the analysis
- Extension to 4D-Var
  - All forms of variational assimilation can be expressed in a similar form (e.g., 3D/4D-Var, strong and weak constraint 4D-Var) (Courtier, 1997)
  - Additional penalty term can be added to enforce balance constraints (Gauthier and Thépaut, 2001)



# • Intercomparison of EnKF and 4D-Var and the impact of flow dependent background-error covariances

- 4D-Var with operational **B** and EnKF ensemble mean analyses have comparable quality
  - $\rightarrow$  4D-Var better in extra-tropics at short-range, EnKF better in the medium range and tropics
- Largest impact (~9h gain at day 5) in southern extratropics for 4D-Var with flow-dependent EnKF B vs. 4D-Var with operational B and also better in tropics
- Use of 4D ensemble B in variational system (i.e. En-4D-Var):
  - improves on 3D-FGAT, but inferior to 4D-Var (both with 3D ensemble B), least sensitive to covariance evolution in tropics
  - comparable with EnKF

## Conclusion

- Weak-constraint 4D-Var offers both promises and challenges
  - Provides information about model error that can be used to diagnose and correct deficiencies in the model
  - Improving the model is a requirement to improve the forecasts
  - Computational issues need to be addressed before a full fledge weak-constraint 4D-Var can be envisioned
  - ... but already implemented at ECMWF