

UNDERSTANDING & SEPARATING THE ROLES OF DYNAMICS & STATISTICS IN DATA ASSIMILATION

Malaquias Pena¹ and Zoltan Toth

Environmental Modeling Center
NCEP/NWS/NOAA

¹ SAIC at EMC/NCEP/NOAA

Acknowledgements:

Mozheng Wei, Takemasa Miyosi, & Roman Krzysztofowicz

DA Workshop
4-8 February 2008, Banff, Canada

OUTLINE / SUMMARY

- **STATE ESTIMATION**
 - Bayesian fusion of
 - New observations
 - Prior
- **PRIOR**
 - Dynamical forecast
 - Effect of all prior observations included
 - Dynamical constraints
- **FUSION**
 - Propagate information from observations to all state variables
 - Error covariance crucial
- **COVARIANCE ESTIMATION**
 - Climatological sample
 - Large sample BUT
 - Not representative of particular cases
 - Case dependent sample
 - Ensembles
 - How to reduce effect of sampling errors?
- **ENSEMBLE DA**
 - “Fully ensemble-based DA”
 - Analysis & forecast steps share full error covariance
 - Inflation/localization noise cycled => negative impact?
 - **ET + 3DVAR**
 - *Analysis step feeds error variance into forecast step*
 - *Forecast step feeds error correlation into analysis step*
 - *Noise from regularization in analysis step not cycled => better covariance => better state estimates?*

BACKGROUND ON DA

- **Goal**
 - Assess state of under-observed dynamical systems
- **Needed when**
 - Observations are
 - Erroneous
 - How to reduce errors in observational data?
 - Scarce
 - How to fill in gaps in observational data?
- **Types of constraints** used in DA
 - Past observational data
 - Climatology
 - Conditional climatology
 - Persistence
 - *Dynamics*
 - Laws of nature

USE OF DYNAMICS IN DA

- **Concept**
 - Introduce dynamical constraint
 - Based on laws of nature
 - A priori info
- **Methodologies**
 - Use balance etc constraints
 - Use short range Numerical Prediction (NP)
- **“Vicious” cycle**
 - Prepare analysis
 - Needed as initial state for forecast
 - Run forecast
 - Needed to prepare analysis
- **Consequence**
 - Worry about convergence of DA cycles (not one step)
 - If & how fast convergence is?
 - How stable DA cycles are?
- **Practical solution**
 - *DA cycled with Numerical Prediction* (NP)
 - Forecast carries information from past
 - Ideally, all past info folded in?

DA CYCLED WITH NP

- **Components**

- “First Guess” (FG) or Background
 - Short range numerical prediction
 - Prior information
- Observations
 - To update prior information

- **Methodology**

- Statistical combination of components
 - Bayesian principles

- **Algorithm**

- Based on point-wise comparison of FG & observations
 - How to spread information in space?
 - *Background error covariance* (B)

HOW TO DEFINE BACKGROUND ERROR COVARIANCE?

- **Climatologically** – statistics of
 - Perceived error in FG (truth not known)
 - Laden with noise (due to noise in analysis)
 - Difference between lagged forecasts verifying at same time
 - “NMC method”
- **Dynamically** – statistics of
 - *Ensemble forecasts*
 - Case dependent estimate
 - May help even in cases of linear error growth

PROCESS OF ENSEMBLE-BASED DA

- Project state into future
 - Numerical prediction
 - Cycles state estimate
 - Any noise in initial condition hurts state estimate
- Project initial info on covariance into future
 - Run ensemble
 - Cycles error covariance estimate
 - *Any noise in initial info hurts covariance estimate*
- Estimate forecast error covariance
 - Based on finite sample of ensemble forecasts
 - Typically small sample due to high cost =>
 - *How to limit noise in covariance estimate?*
- Collect new observations
 - Estimate observational error
- Combine FG & observations using error estimates
 - Noise in either projected state or covariance info hurts analysis

Dynamics

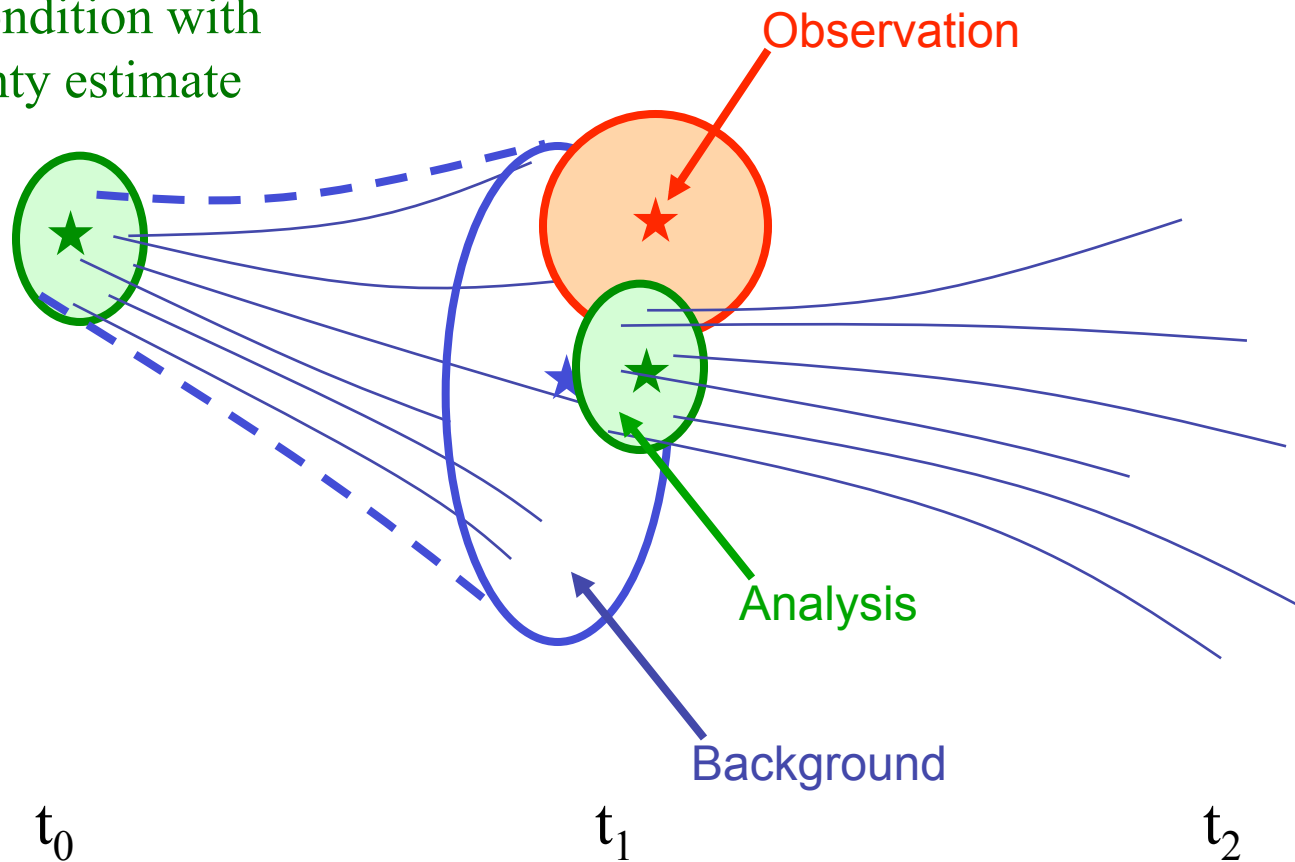
Statistics

ERROR COVARIANCE ESTIMATION

- Ingredients
 - Ensemble forecasts
 - Dynamical projection of prior covariance info
 - Statistical estimation
 - Small sample leads to filter divergence
- Methodology
 - Ensemble-based DA – ETKF-type methods
 - Modulate ens perts to avoid filter divergence
 - Covariance inflation – introduce noise
 - Localization
 - Cycle noisy covariance estimate
- Result
 - Noisy state and covariance estimates?
- Solution
 - ***Divorce dynamics from statistics***
 - Et + 3DVAR

Ensemble-based DA Experiments

Initial condition with uncertainty estimate



How well the ensemble forecasts sample the background uncertainty? How much information the observations add?

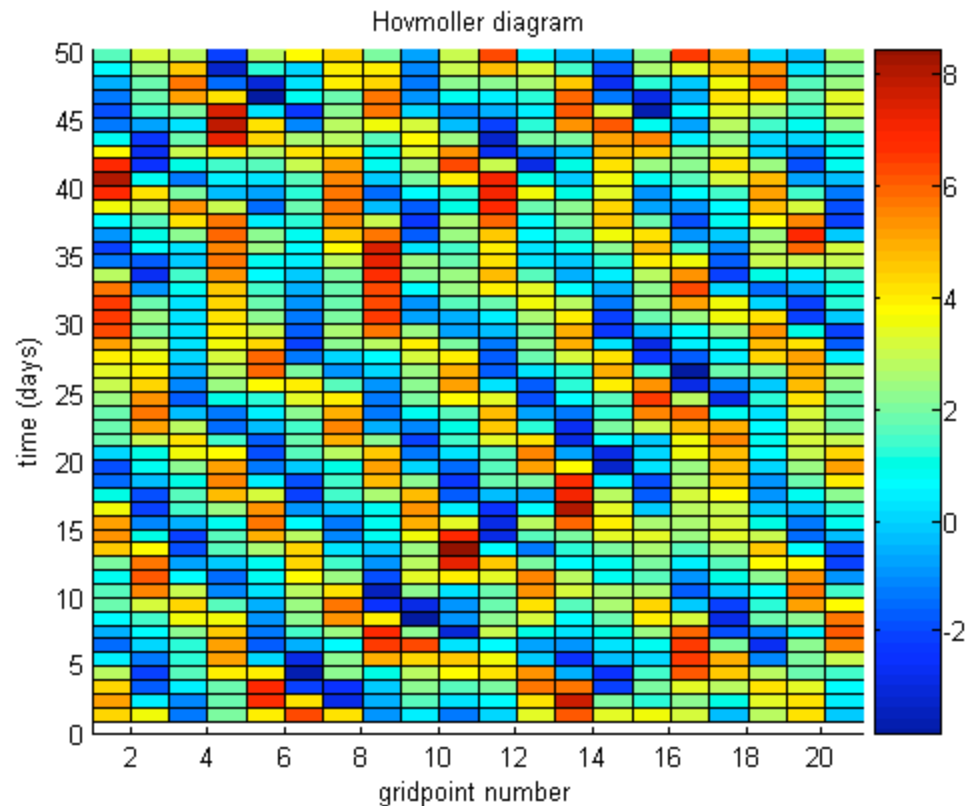
Lorenz 96 Model (with '07 pars)

$$\frac{d\mathbf{x}_m}{dt} = (\mathbf{x}_{m+1} - \mathbf{x}_{m-2})\mathbf{x}_{m-1} - \mathbf{x}_m + \mathbf{F}$$

Where $F = 5.1$ and $m = 1, \dots, 21$

Experimental setting:

- Perfect model scenario
- One observation per grid-point
- Observational error: uncorrelated normally distributed random noise with unit variance ($R=I$)
- 6-hr assimilation cycle



3DVar DA - Benchmark

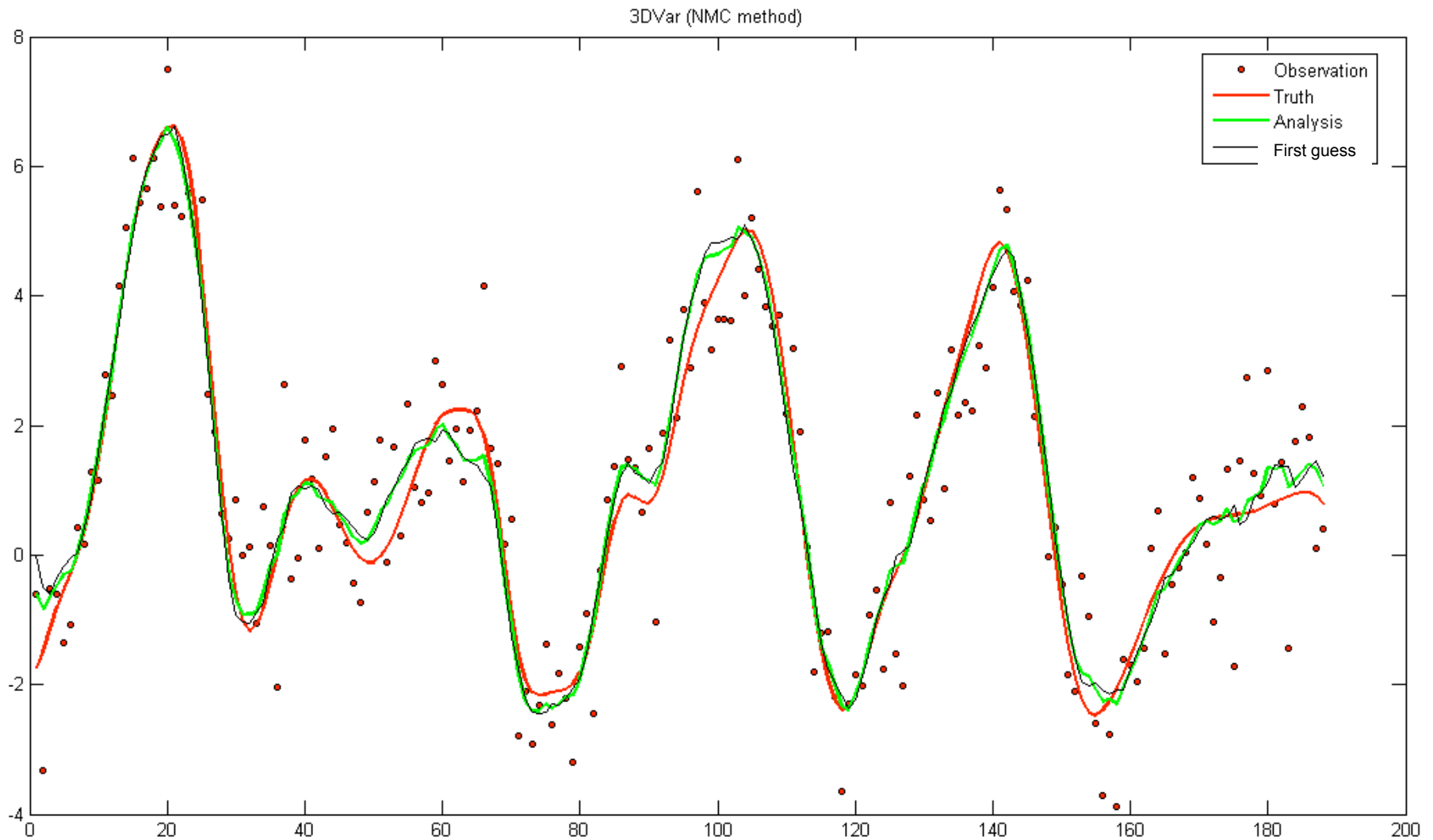
- Minimizing the following cost function

$$\mathbf{J}(\mathbf{x}) = \frac{1}{2} [(\mathbf{x} - \mathbf{x}^b) \mathbf{B}^{-1} (\mathbf{x} - \mathbf{x}^b) + (\mathbf{y}^o - \mathbf{H}\mathbf{x})^T \mathbf{R}^{-1} (\mathbf{y}^o - \mathbf{H}\mathbf{x})]$$



Inverse of background error covariance

Time series at one grid-point



Background error covariance: $B = \alpha B_0$, where B_0 is obtained from climatology and α a tuning parameter. $\alpha = 0.05$

ETKF

- $Z_a = Z_f T C^T$
 - $T = C(G + I)^{-1/2}$
- C, G eigenvector and eigenvalues of $Z_f^T H^T R^{-1} H Z_f$
(H=I used)
- $B = Z_f Z_f^T$
 - $A = Z_a Z_a^T = Z_f T (Z_f T)^T$
 - Full covariance shared between state & covariance update steps
 - Covariance inflation and/or localization of B **cycled**

Z is an $M \times K$ matrix whose columns are the K ensemble perturbations (departure from ensemble average) and M is the dimension of the state vector. Subindex a refers to analysis and f to forecast

ETKF

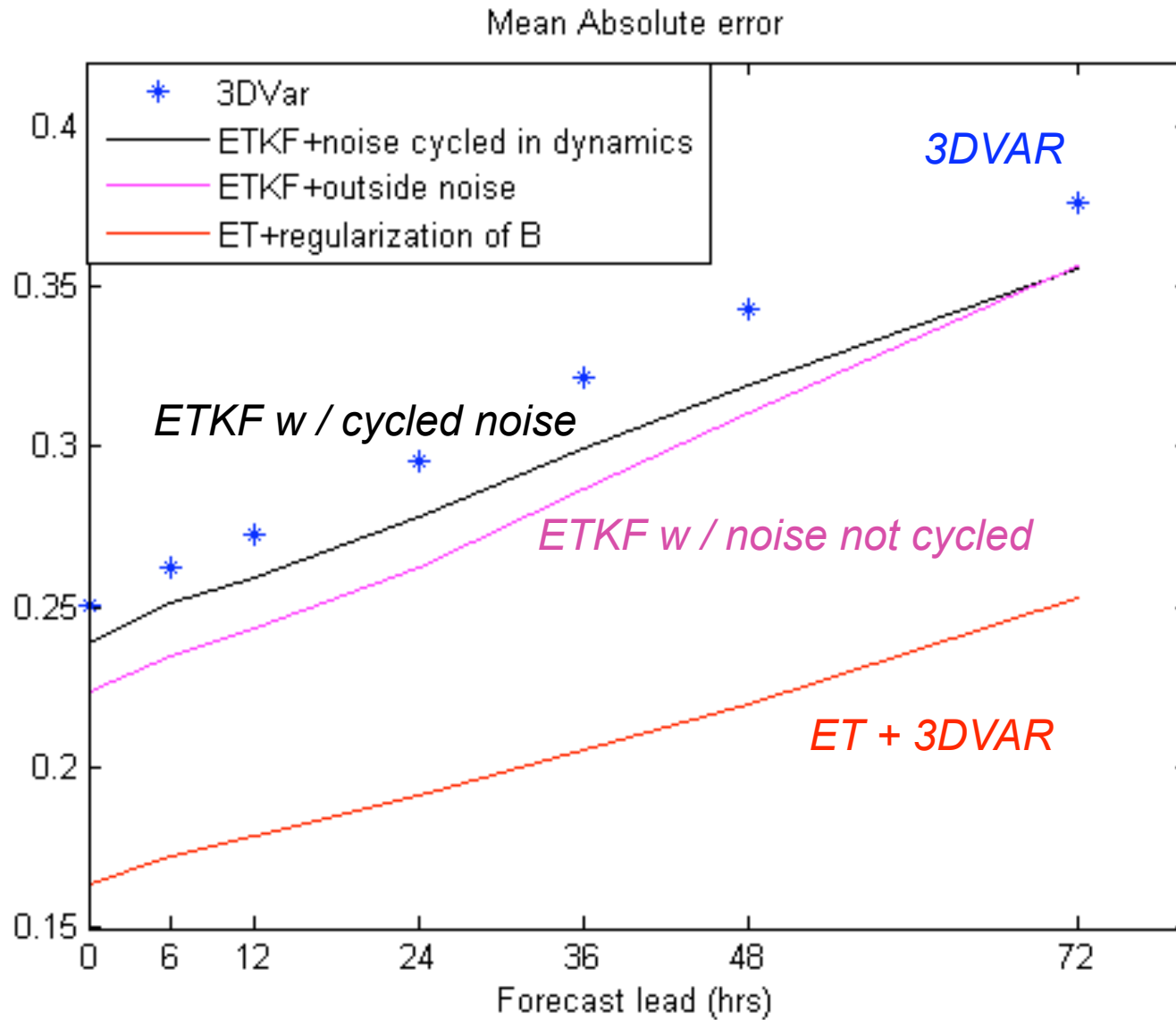
- $Z_a = Z_f T C^T$
 - $T = C(G+I)^{-1/2}$
- C, G eigenvector and eigenvalues of $Z_f^T H^T R^{-1} H Z_f$
(H=I used)
- $B = Z_f Z_f^T$
 - $A = Z_a Z_a^T = Z_f T (Z_f T)^T$
 - Full covariance shared between state & covariance update steps
 - Covariance inflation and/or localization of B **cycled**

ET + 3DVAR

- $Z_a = Z_f T C^T$
 - $T = C G^{-1/2}$
- C and G are eigenvector and eigenvalues of $Z_f^T A^{-1} Z_f$
- $B = Z_f Z_f^T$ fed into analysis step
 - $A^{-1} = B^{-1} + R^{-1}$ fed into ens pert generation step
 - No noise is added into ens. perts. - “pure” dynamics
 - Statistical manipulation of B not fed back into covariance – only variance affected

Z is an $M \times K$ matrix whose columns are the K ensemble perturbations (departure from ensemble average) and M is the dimension of the state vector. Subindex a refers to analysis and f to forecast

EFFECT OF SEPARATING ROLES OF DYNAMICS & STATISTICS

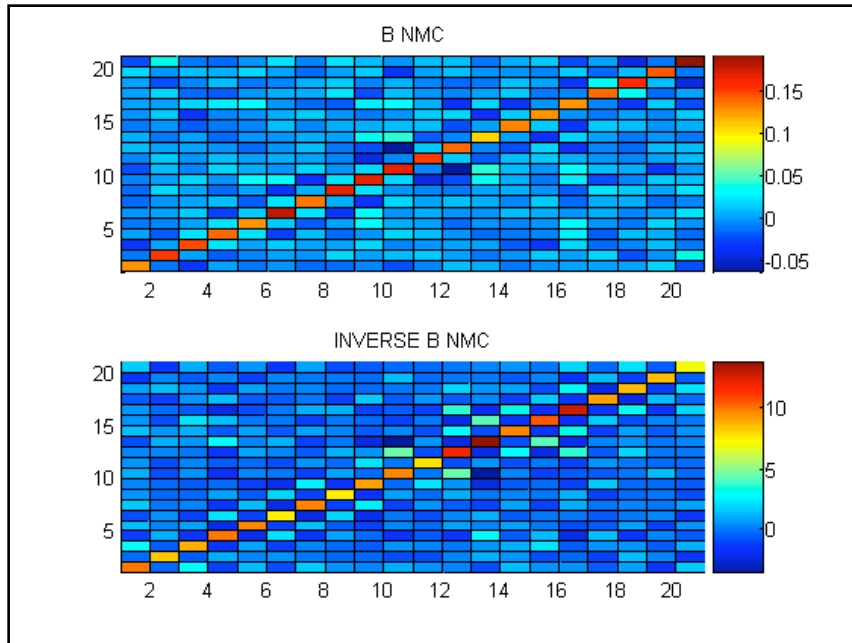


ETKF & other Ensemble-based DA methods

- Ensemble-based statistics of B are rank deficient and subject to sampling error
- Statistical regularization techniques to remedy problem
 - Add noise to analysis perturbations to avoid underestimation of B - Miller et al (1994) and Corazza et al (2002)
 - Blend ensemble B and 3DVar B – “hybrid” method - Hamill and Snyder (2000)
 - Localize effect of covariance
 - Shur product – Houtekamer et al
 - LETKF – Ott, Szunyogh et al., 2003
 - Addition of noise used here with ETKF

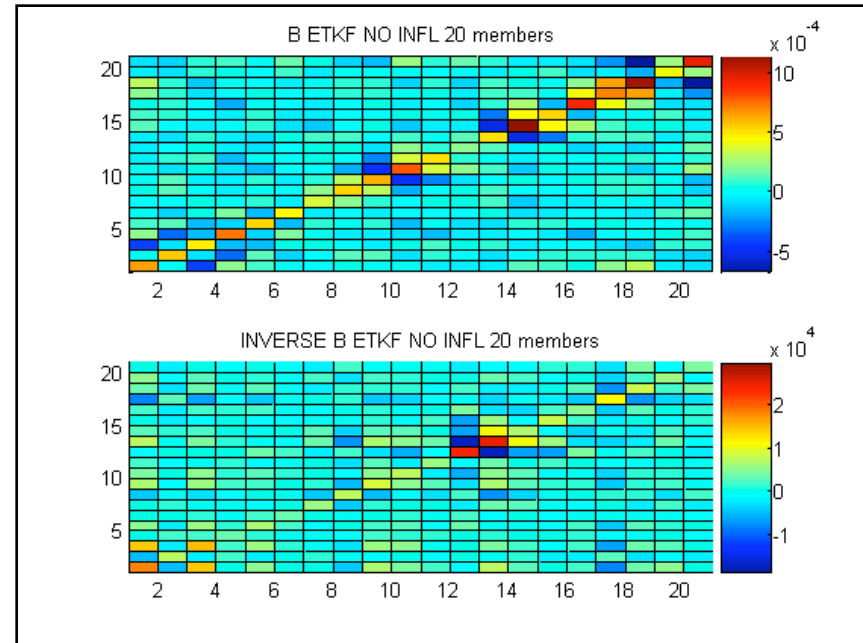
Snapshot of B and B⁻¹

3DVAR – NMC method



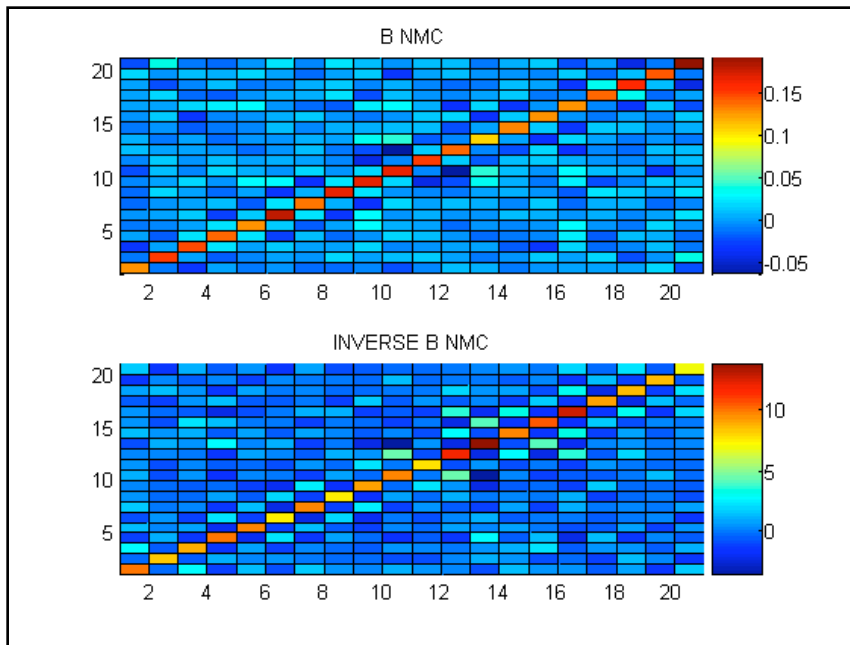
↑
Well-conditioned, stable

ETKF without inflation:

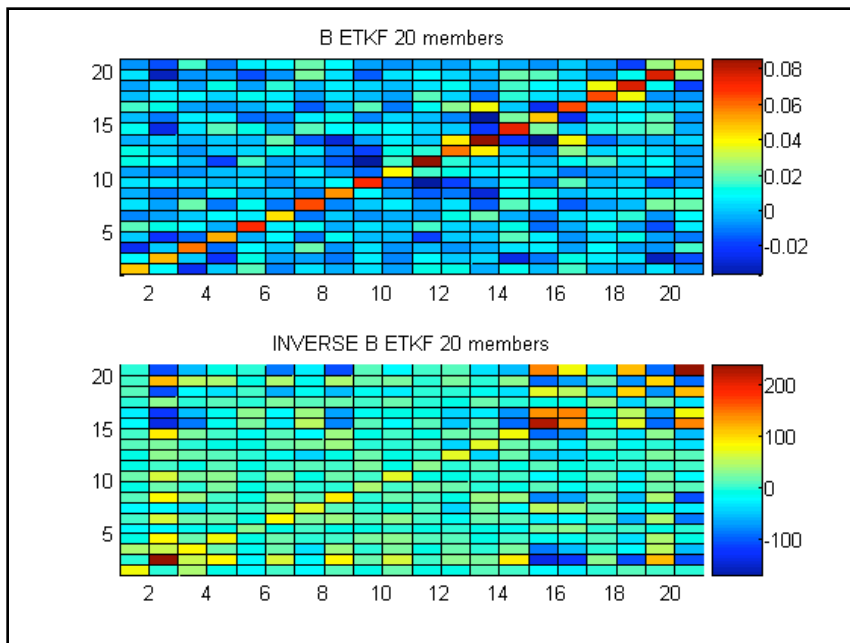
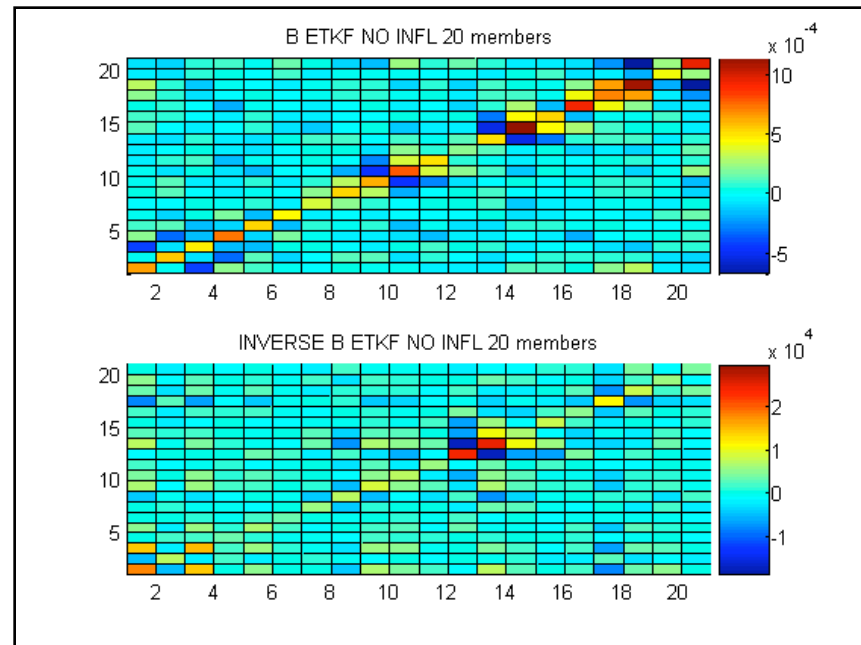


↑
Very unstable

NMC method

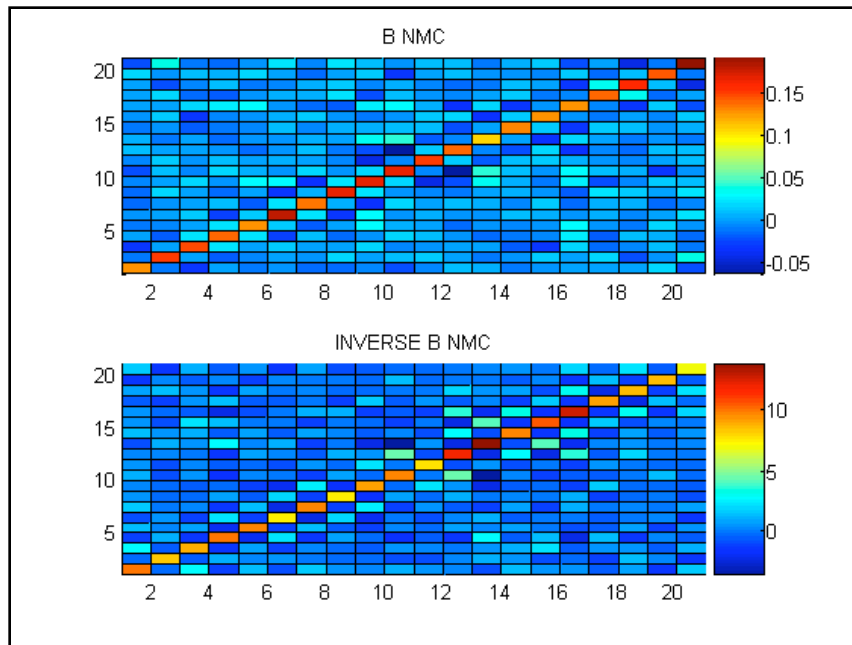


ETKF, no inflation

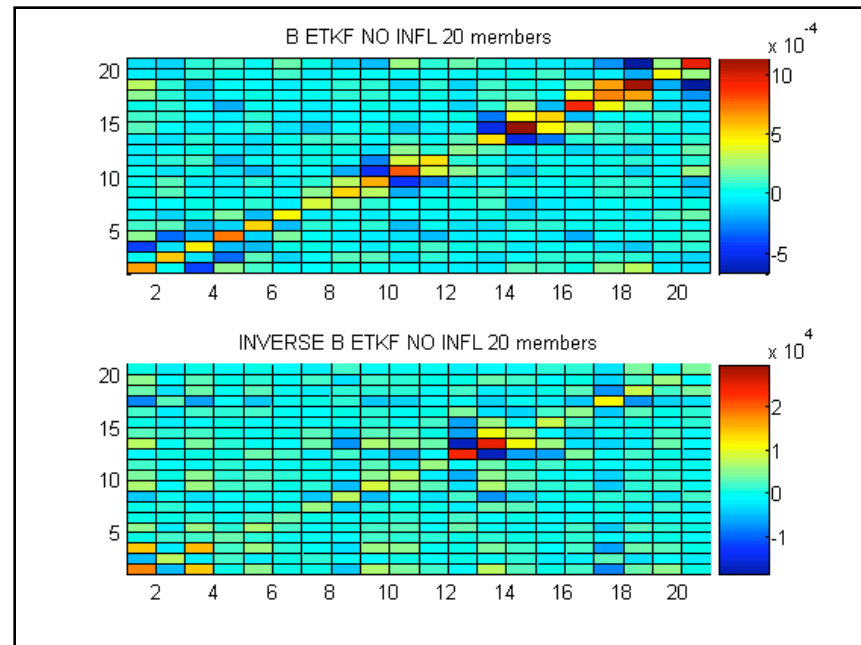


← ETKF with random perturbations added. Inverse becomes stable; However, noise cycled

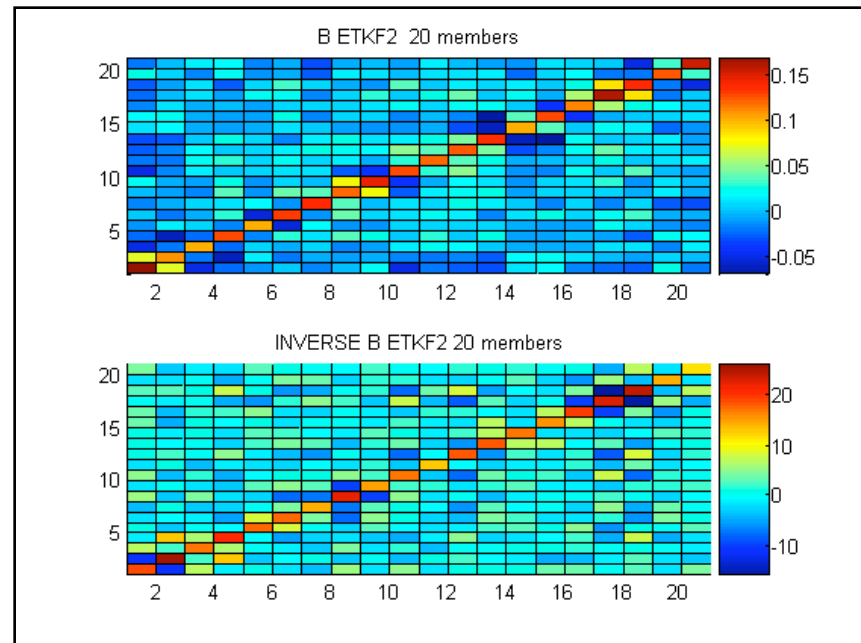
NMC method



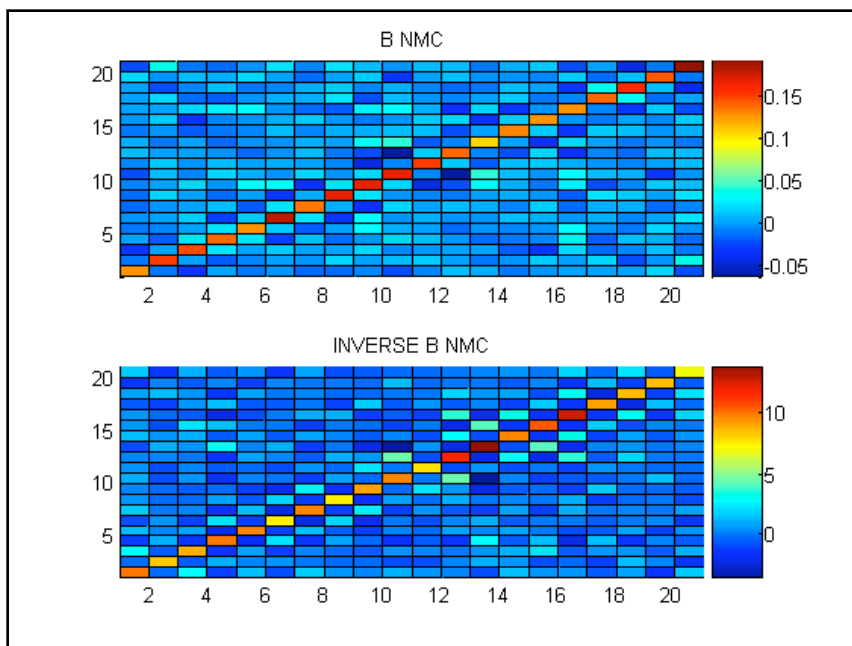
ETKF, no inflation



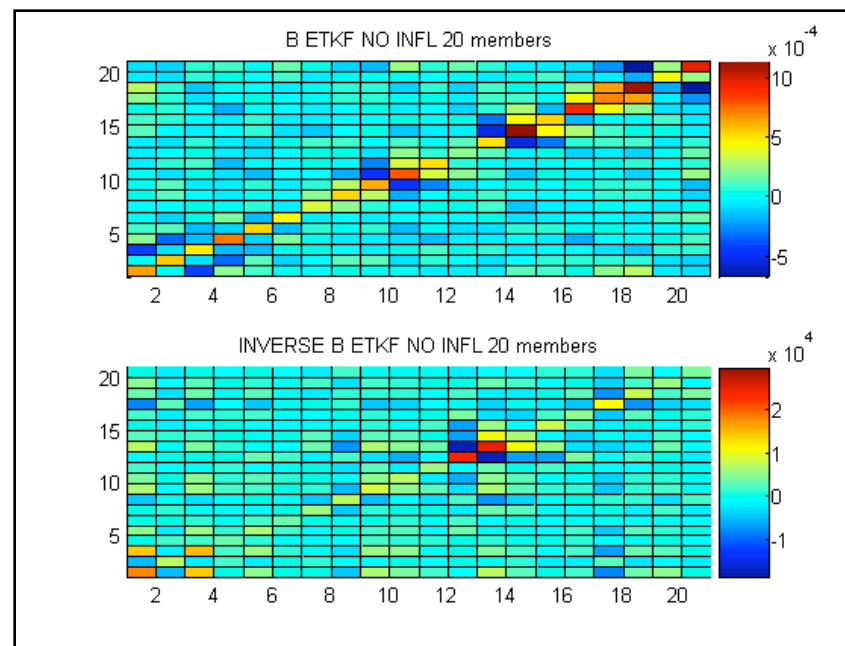
Two ensembles run with ETKF, one with (used for estimating B – regularization, then discarded), another without addition of noise (used for cycling covariance); Noise still impacts initial perturb



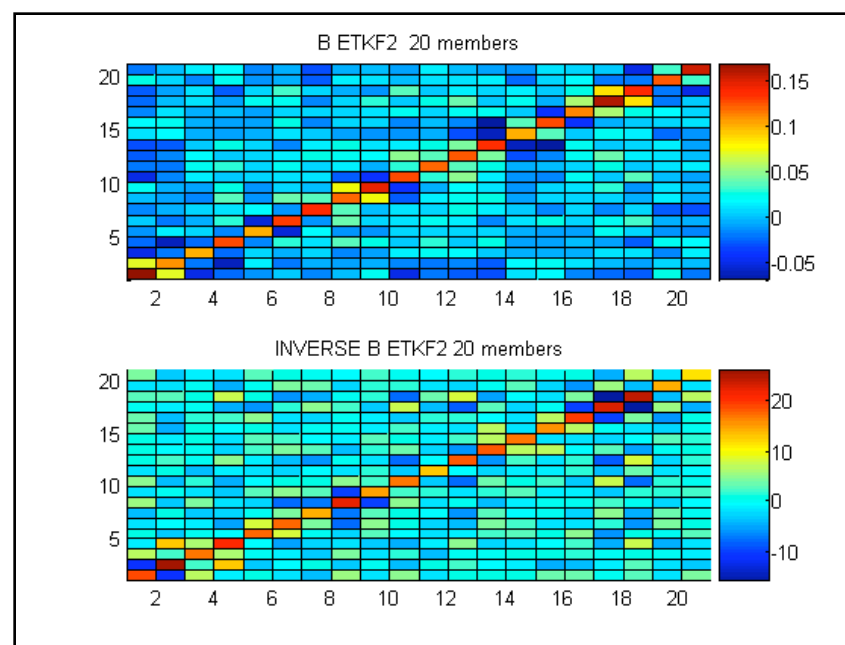
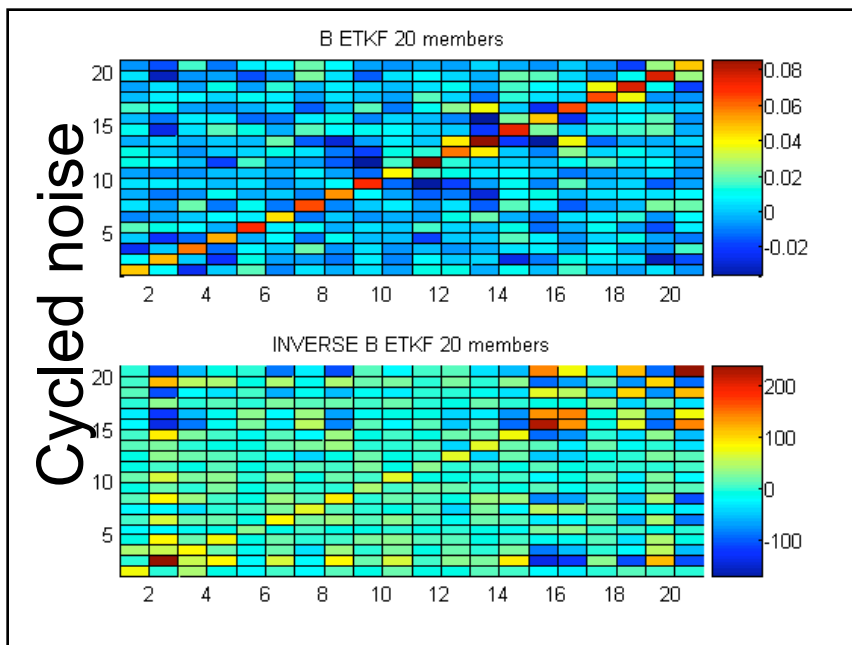
NMC method



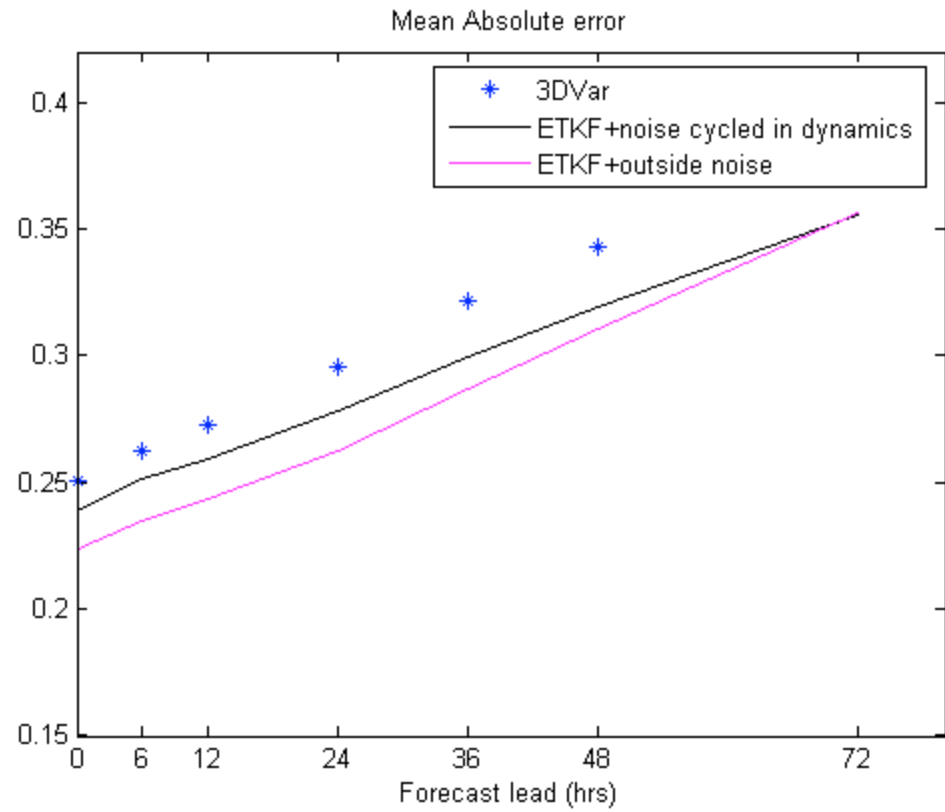
ETKF, no inflation



Cycled noise



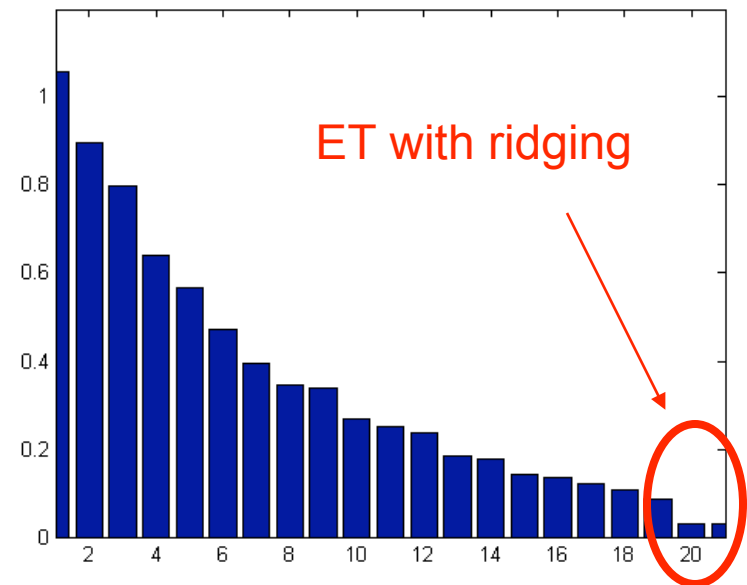
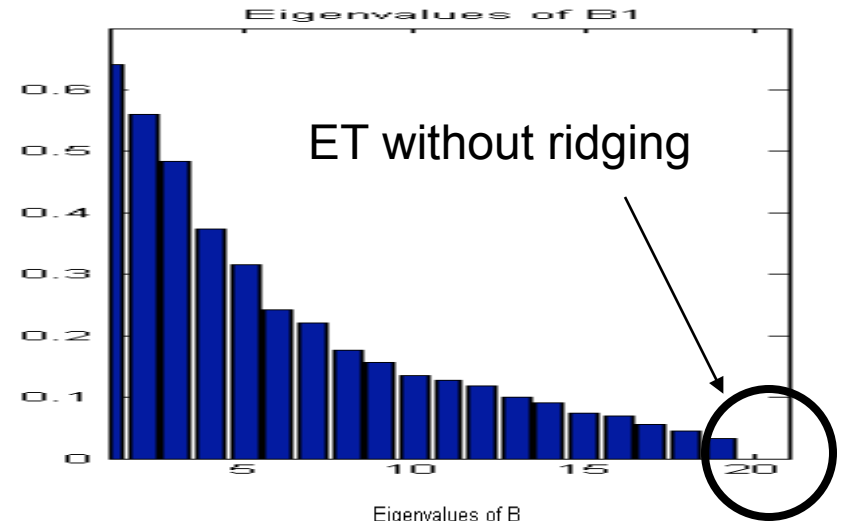
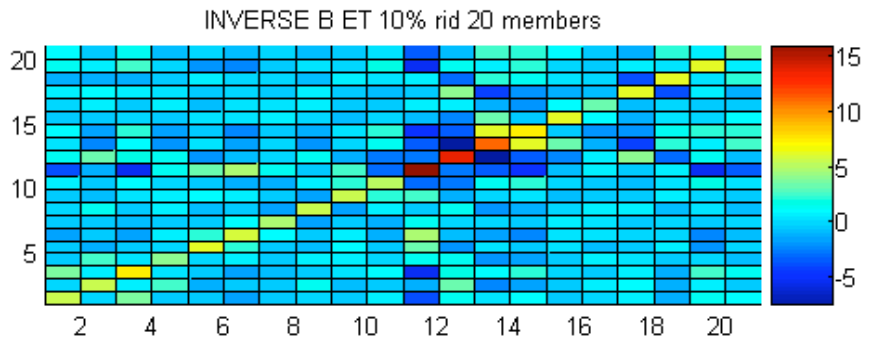
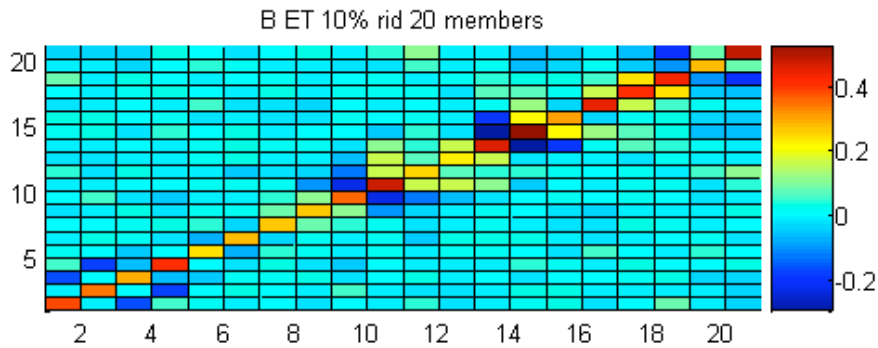
Noise for B only



Ridging procedure in ET + 3DVAR

Statistics

Add small (10%) value to diagonal of B



OUTLINE / SUMMARY

- **STATE ESTIMATION**
 - Bayesian fusion of
 - Prior
 - New observations
- **PRIOR**
 - Dynamical forecast
 - Effect of all prior observations included
 - Dynamical constraints
- **FUSION**
 - Propagate information from observations to all state variables
 - Error covariance crucial
- **COVARIANCE ESTIMATION**
 - Climatological sample
 - Large sample BUT
 - Not representative of particular cases
 - Case dependent sample
 - Ensembles
 - How to reduce effect of sampling errors?
- **ENSEMBLE DA**
 - “Fully ensemble-based DA”
 - Analysis & forecast steps share full error covariance
 - Inflation/localization noise cycled => negative impact?
 - **ET + 3DVAR**
 - *Analysis step feeds error variance into forecast step*
 - *Forecast step feeds error correlation into analysis step*
 - *Noise from regularization in analysis step not cycled => better covariance => better state estimates?*

BACKGROUND

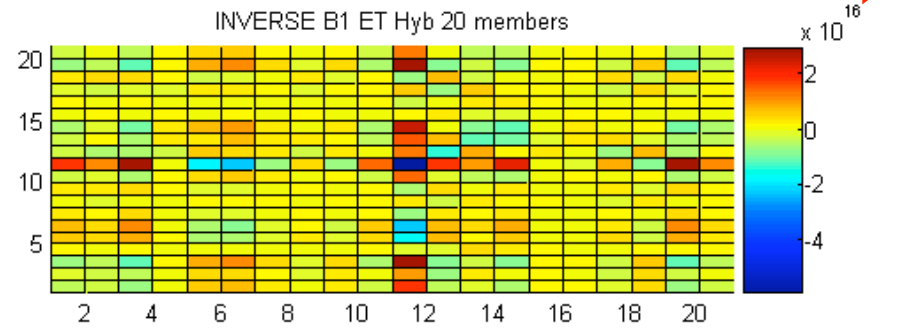
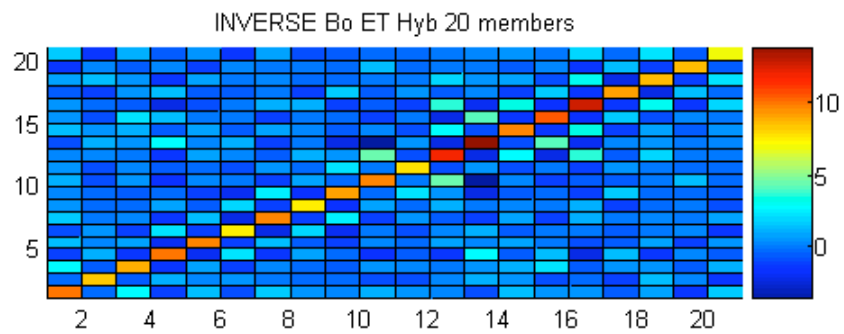
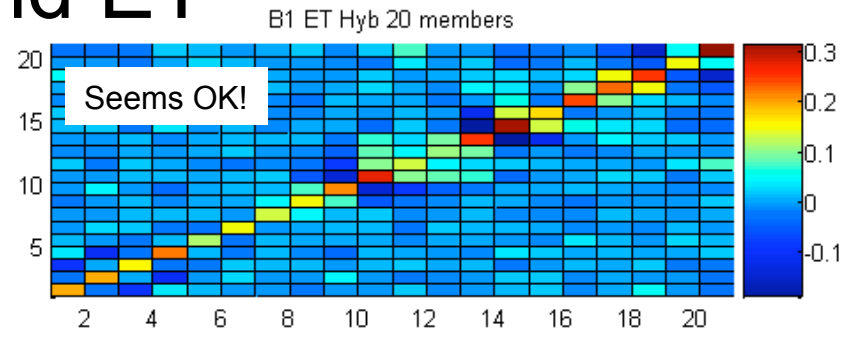
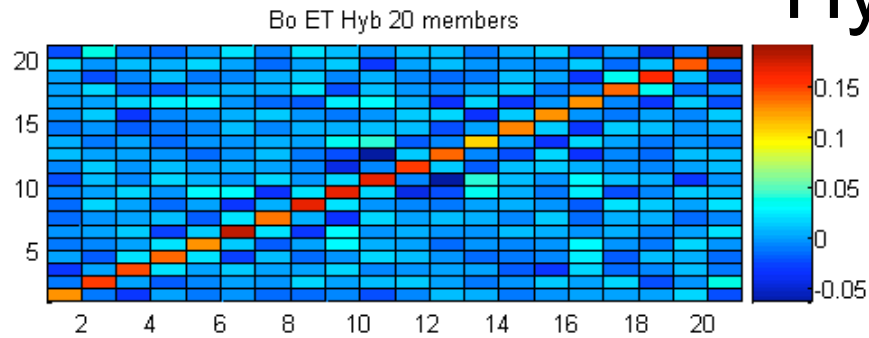
USE OF ENSEMBLES IN DA

- Error covariance estimation
 - Needed even in quasi-linear regime?
- State projection
 - Moderately non-linear regime
 - Use ensemble mean for estimating future state
 - Highly non-linear regime
 - Particle filtering needed?
 - Future study

IMPERFECT NUMERICAL MODELS

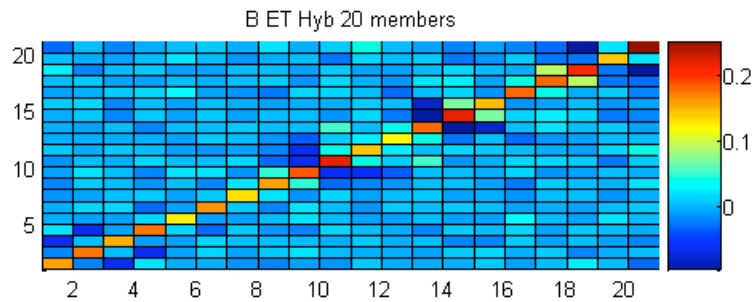
- Inconsistency between real & model systems
 - Transitional behavior if model started with real initial state
 - “Mapping paradigm” for reducing noise related to model drift
 - Physica D paper – Toth & Pena 2007

Hybrid ET

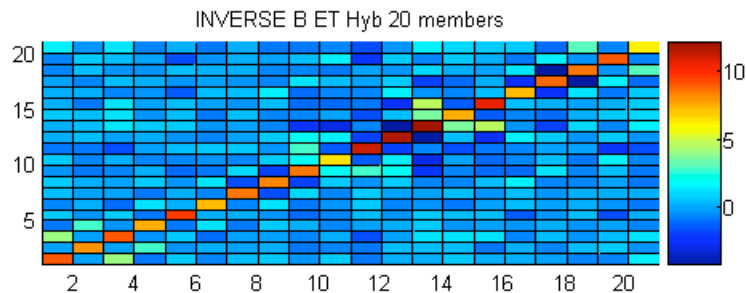


Bo From 3DVar

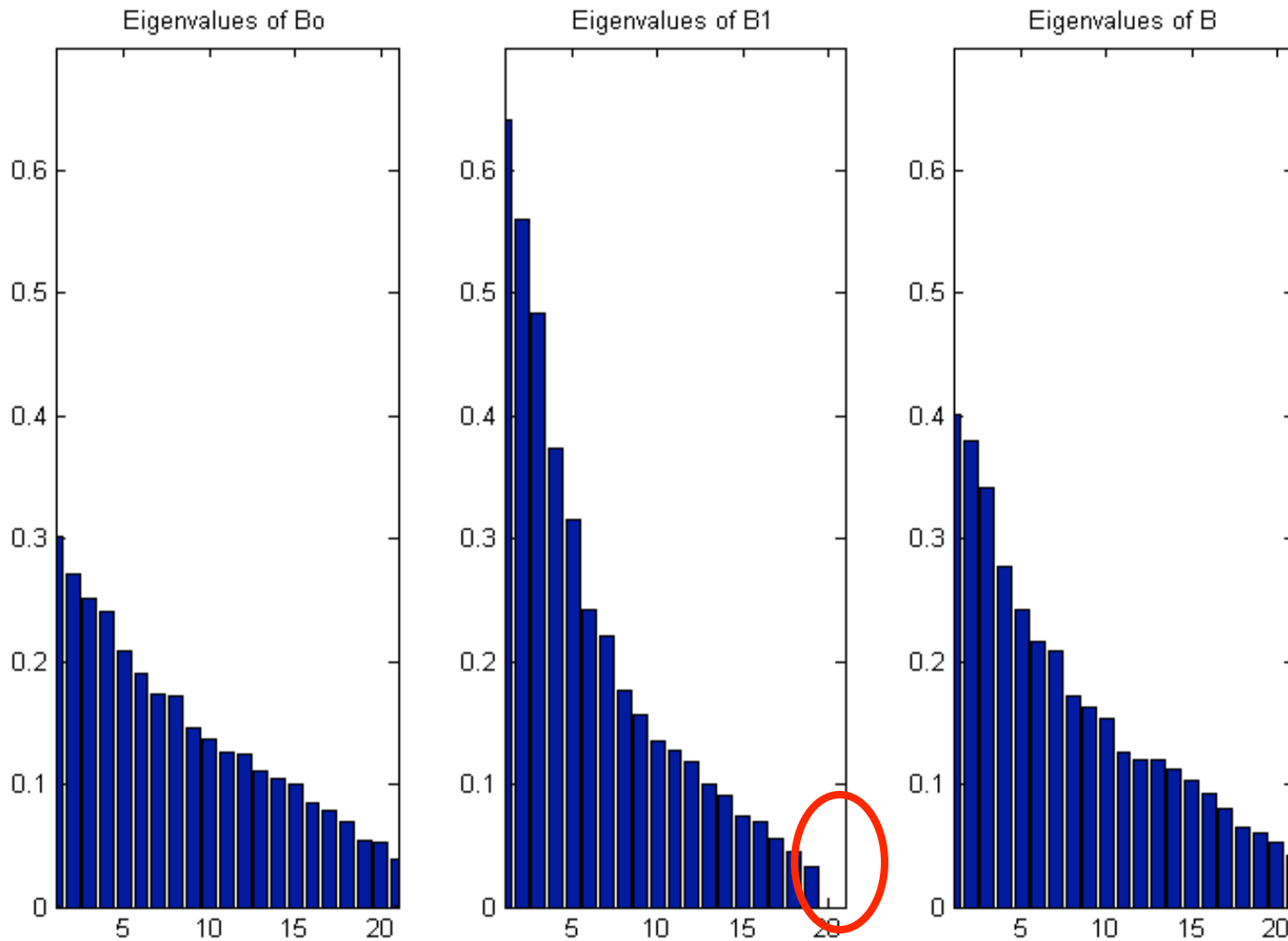
$$B = (B_0 + B_1) / 2$$



B1 from ET



Singular Value Decomposition of B_0 , B_1 and B :



Last 2 eigenvalues of B_1 are zero! B_1 is ill-conditioned

Is the hybrid approach a regularization strategy?

VARIANTS OF ENSEMBLE-BASED DA

- Perturbed observations
 - Represent all sources of forecast error at its source
 - Add noise to data representing observational uncertainty
 - Large amount of noise needed to avoid filter divergence
 - Cycling of noise makes state & error covariance estimates noisy
 - » Houtekamer, Anderson, etc, late 1990s
- ETKF & related methods
 - Reduce noise by eliminating perturbed observations
 - Covariance inflation needed to avoid filter divergence
 - Add noise to initial ensemble perturbations =>
 - Noisy covariance estimate
 - Cycle noisy covariance estimate
 - Negative effect on analysis state?
 - Anderson, Bishop, Szunyogh, Whitaker, etc, 2000+