Sampling strategies and SQRT analysis schemes for the EnKF

Geir Evensen

Norsk Hydro Research Centre, Bergen, Norway

Based on Evensen 2004, submitted to Ocean Dynamics

Background

- EnKF/EnKS in native formulation are pure Monte Carlo methods.
- Uses Monte Carlo sampling for initial ensemble, model noise and measurement perturbations.
- Uses stochastic equation for ensemble integration.
- Computes analysis based on ensemble perturbations and measurement perturbations.
- Review by Evensen (2003), Ocean Dynamics, 53, 343–367.

Part one: Outline

Sampling errors can be reduced by:

- Wise sampling of initial ensemble and model noise as motivated by
  - Pham (2001), MWR.
  - Nerger et al (to appear 2004), MWR.
- Elimination of measurement perturbations in the analysis scheme is possible by use of “square root” algorithms as shown by
  - Andersen (2001), MWR.
  - Bishop et al (2001), MWR.
  - Whitaker and Hamill (2002) MWR.
  - Tippett et al (2003) MWR.

EnKF: Ensemble representation

- Define the ensemble matrix

$$\boldsymbol{A} = (\boldsymbol{\psi}_1, \boldsymbol{\psi}_2, \ldots, \boldsymbol{\psi}_N) \in \Re^{n \times N}.$$

- The ensemble mean is (defining $\mathbf{1}_N \in \Re^{N \times N} \equiv 1/N$)

$$\overline{\boldsymbol{A}} = \boldsymbol{A}\mathbf{1}_N.$$

- The ensemble perturbations becomes

$$\boldsymbol{A}' = \boldsymbol{A} - \overline{\boldsymbol{A}} = \boldsymbol{A}(\boldsymbol{I} - \mathbf{1}_N).$$

- The ensemble covariance matrix $\boldsymbol{P}_\mathrm{e} \in \Re^{n \times n}$ becomes

$$\boldsymbol{P}_\mathrm{e} = \frac{\boldsymbol{A}'(\boldsymbol{A}')^\mathrm{T}}{N-1}$$

EnKF: Measurement perturbations

- Given a vector of measurements $\boldsymbol{d} \in \Re^m$, define

$$\boldsymbol{d}_j = \boldsymbol{d} + \boldsymbol{\epsilon}_j, \qquad j = 1, \ldots, N,$$

stored in

$$\boldsymbol{D} = (\boldsymbol{d}_1, \boldsymbol{d}_2, \ldots, \boldsymbol{d}_N) \in \Re^{m \times N},$$

- The ensemble perturbations are stored in

$$\boldsymbol{E} = (\boldsymbol{\epsilon}_1, \boldsymbol{\epsilon}_2, \ldots, \boldsymbol{\epsilon}_N) \in \Re^{m \times N},$$

thus, the measurement error covariance matrix becomes

$$\boldsymbol{R}_\mathrm{e} = \frac{\boldsymbol{E}\boldsymbol{E}^\mathrm{T}}{N-1}.$$

EnKF: Analysis equation

- The analysis equation can now be written

$$\boldsymbol{A}^{\mathrm{a}} = \boldsymbol{A} + \boldsymbol{P}_{\mathrm{e}}\boldsymbol{H}^{\mathrm{T}}(\boldsymbol{H}\boldsymbol{P}_{\mathrm{e}}\boldsymbol{H}^{\mathrm{T}} + \boldsymbol{R}_{\mathrm{e}})^{-1}(\boldsymbol{D} - \boldsymbol{H}\boldsymbol{A}).$$

- Defining the innovations $\boldsymbol{D}' = \boldsymbol{D} - \boldsymbol{H}\boldsymbol{A}$ and using previous definitions:

$$\begin{aligned}\boldsymbol{A}^{\mathrm{a}} =& \boldsymbol{A} + \boldsymbol{A}'\boldsymbol{A}'^{\mathrm{T}}\boldsymbol{H}^{\mathrm{T}}\left(\boldsymbol{H}\boldsymbol{A}'\boldsymbol{A}'^{\mathrm{T}}\boldsymbol{H}^{\mathrm{T}} + \boldsymbol{E}\boldsymbol{E}^{\mathrm{T}}\right)^{-1}\boldsymbol{D}' \\ =& \boldsymbol{A} + \boldsymbol{A}'\boldsymbol{S}^{\mathrm{T}}\boldsymbol{C}^{-1}\boldsymbol{D}', \\ =& \boldsymbol{A}\boldsymbol{X}\end{aligned}$$

where $\boldsymbol{S} = \boldsymbol{H}\boldsymbol{A}'$ and $\boldsymbol{C} = (\boldsymbol{S}\boldsymbol{S}^{\mathrm{T}} + \boldsymbol{E}\boldsymbol{E}^{\mathrm{T}})$ and

$$\boldsymbol{X} = \boldsymbol{I} + \boldsymbol{S}^{\mathrm{T}}\boldsymbol{C}^{-1}\boldsymbol{D}'$$

EnKF with linear exact model

- Linear noise free model

$$\boldsymbol{A}_k = \boldsymbol{F}^k \boldsymbol{A}_0$$

- EnKF with linear noise free model

$$\boldsymbol{A}_k = \boldsymbol{F}^k \boldsymbol{A}_0 \prod_{i=1}^{k} \boldsymbol{X}_i$$

- With rank$(\boldsymbol{F}) = n$ and rank$(\boldsymbol{X}_i) = N$, the quality of the EnKF solution is dependent on the rank and conditioning of the initial ensemble $\boldsymbol{A}_0$.

Improved sampling: Introduction

- Full covariance

$$\boldsymbol{P} = \boldsymbol{Z}\boldsymbol{\Lambda}\boldsymbol{Z}^{\mathrm{T}}$$

- Ensemble covariance

$$\begin{aligned}\boldsymbol{P}_{\mathrm{e}} =& \frac{1}{N-1}\boldsymbol{A}'(\boldsymbol{A}')^{\mathrm{T}} \\ =& \frac{1}{N-1}\boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^{\mathrm{T}}\boldsymbol{V}\boldsymbol{\Sigma}^{\mathrm{T}}\boldsymbol{U}^{\mathrm{T}} = \frac{1}{N-1}\boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{\Sigma}^{\mathrm{T}}\boldsymbol{U}^{\mathrm{T}}\end{aligned}$$

- When $N \to \infty$

$$\boldsymbol{P}_e = \frac{1}{N-1}\boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{\Sigma}^{\mathrm{T}}\boldsymbol{U}^{\mathrm{T}} \to \boldsymbol{P} = \boldsymbol{Z}\boldsymbol{\Lambda}\boldsymbol{Z}$$

or $\boldsymbol{U} \to \boldsymbol{Z}$ and $\boldsymbol{\Sigma}\boldsymbol{\Sigma}^{\mathrm{T}}/(N-1) \to \boldsymbol{\Lambda}$.

Improved sampling: Approach

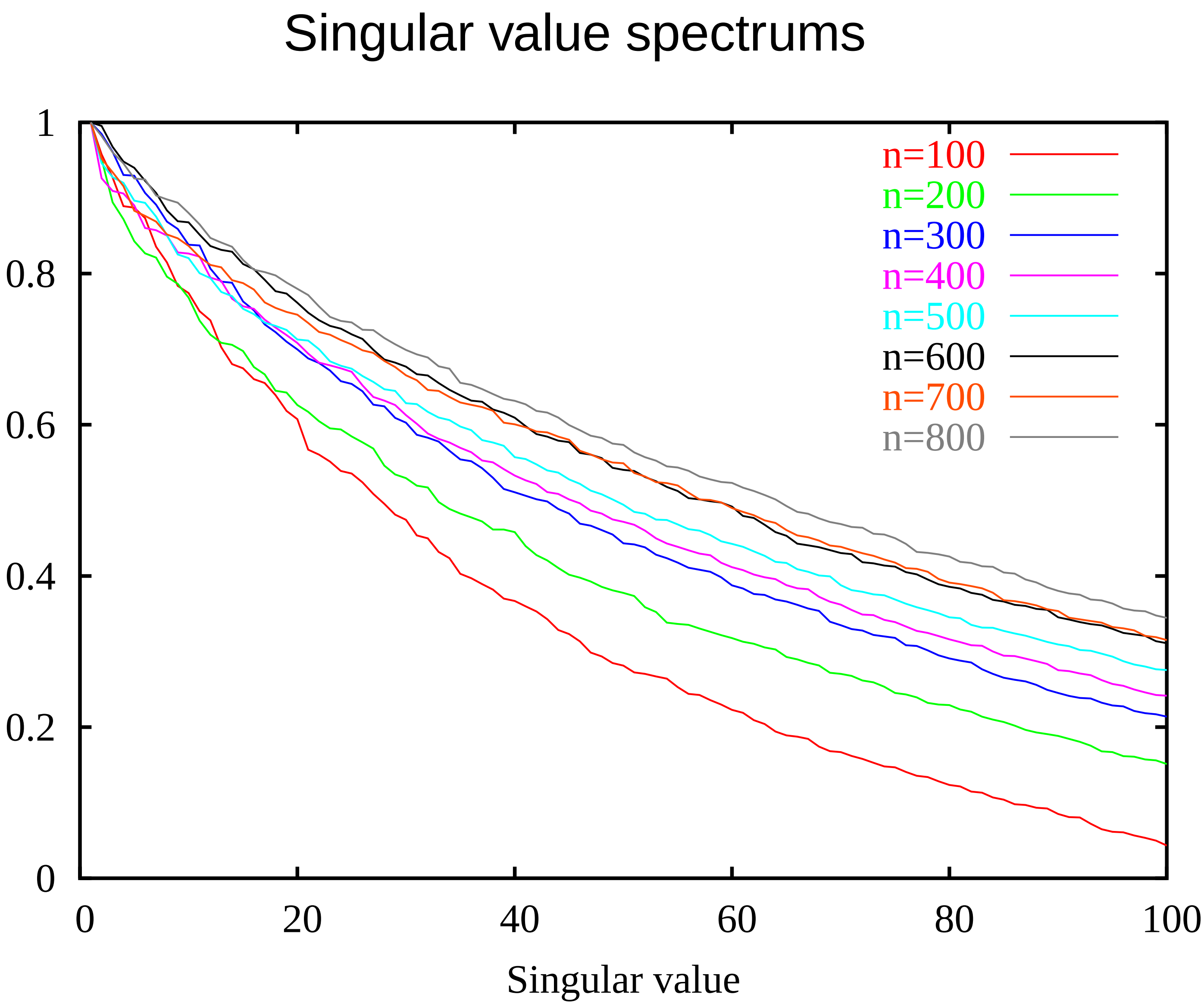
- Generate an ensemble which best possibly represents $\boldsymbol{P}$.
- Should be constructed using the first N eigenvectors of $\boldsymbol{P}$ but these are too expensive to compute.
- Approximate eigenvectors $\boldsymbol{Z}$ by singular vectors $\boldsymbol{U}$ computed from a large ensemble of perturbations:

$$\widehat{\boldsymbol{A}}' = \widehat{\boldsymbol{U}}\widehat{\boldsymbol{\Sigma}}\widehat{\boldsymbol{V}}^{\mathrm{T}} \in \Re^{n\times\alpha N}.$$

- Store first N singular vectors of $\widehat{\boldsymbol{U}}$ in $\boldsymbol{U}_1$.
- Store N dominant singular values of $\widehat{\boldsymbol{\Sigma}}$ in $\boldsymbol{\Sigma}_1$.
- Generate a random orthogonal matrix $\boldsymbol{V}_1^{\mathrm{T}} \in \Re^{N\times N}$.
- Compute

$$\boldsymbol{A}' = \boldsymbol{U}_1 \alpha^{-1} \boldsymbol{\Sigma}_1 \boldsymbol{V}_1^{\mathrm{T}}$$

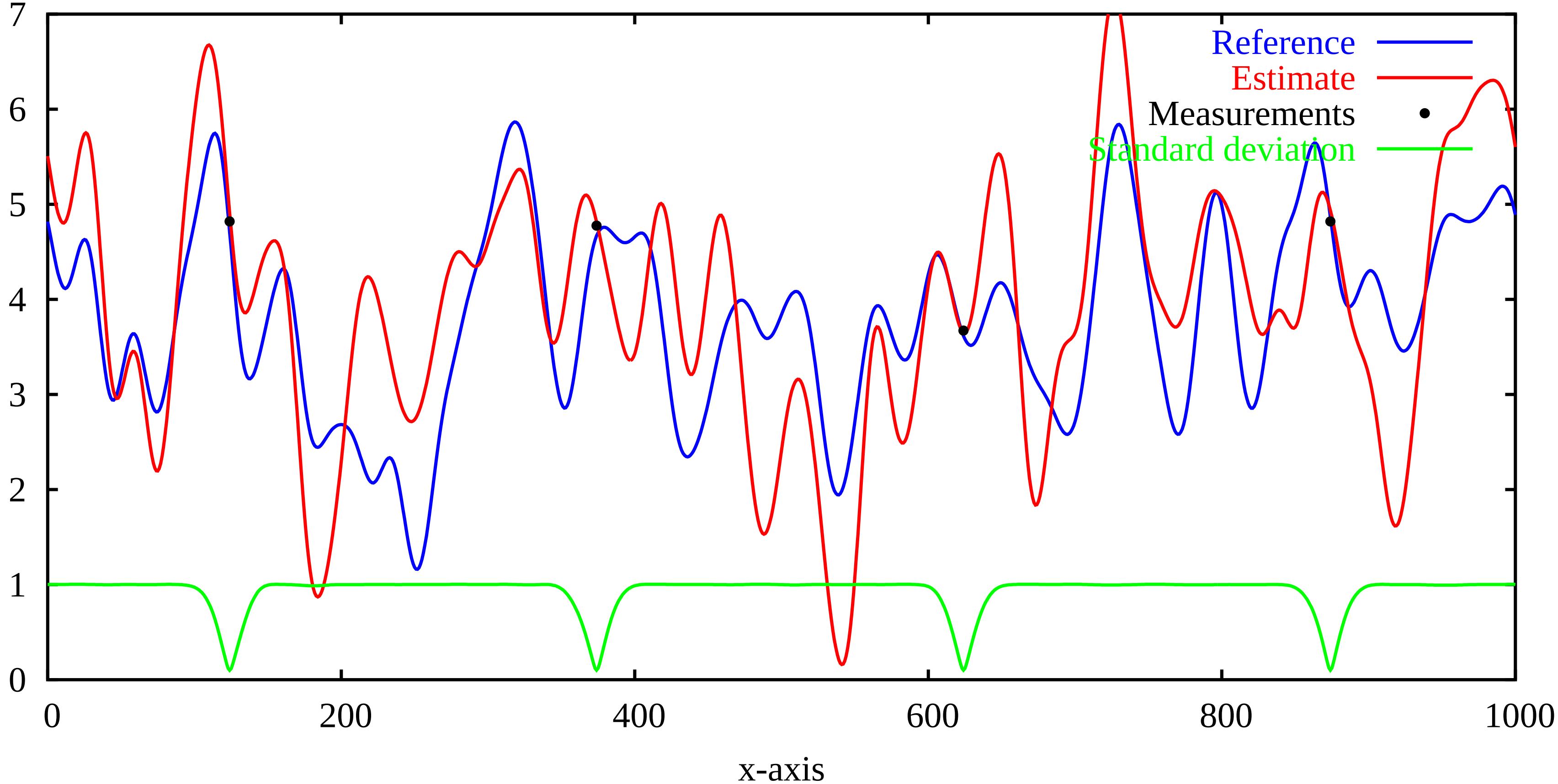
Improved sampling: Conditioning



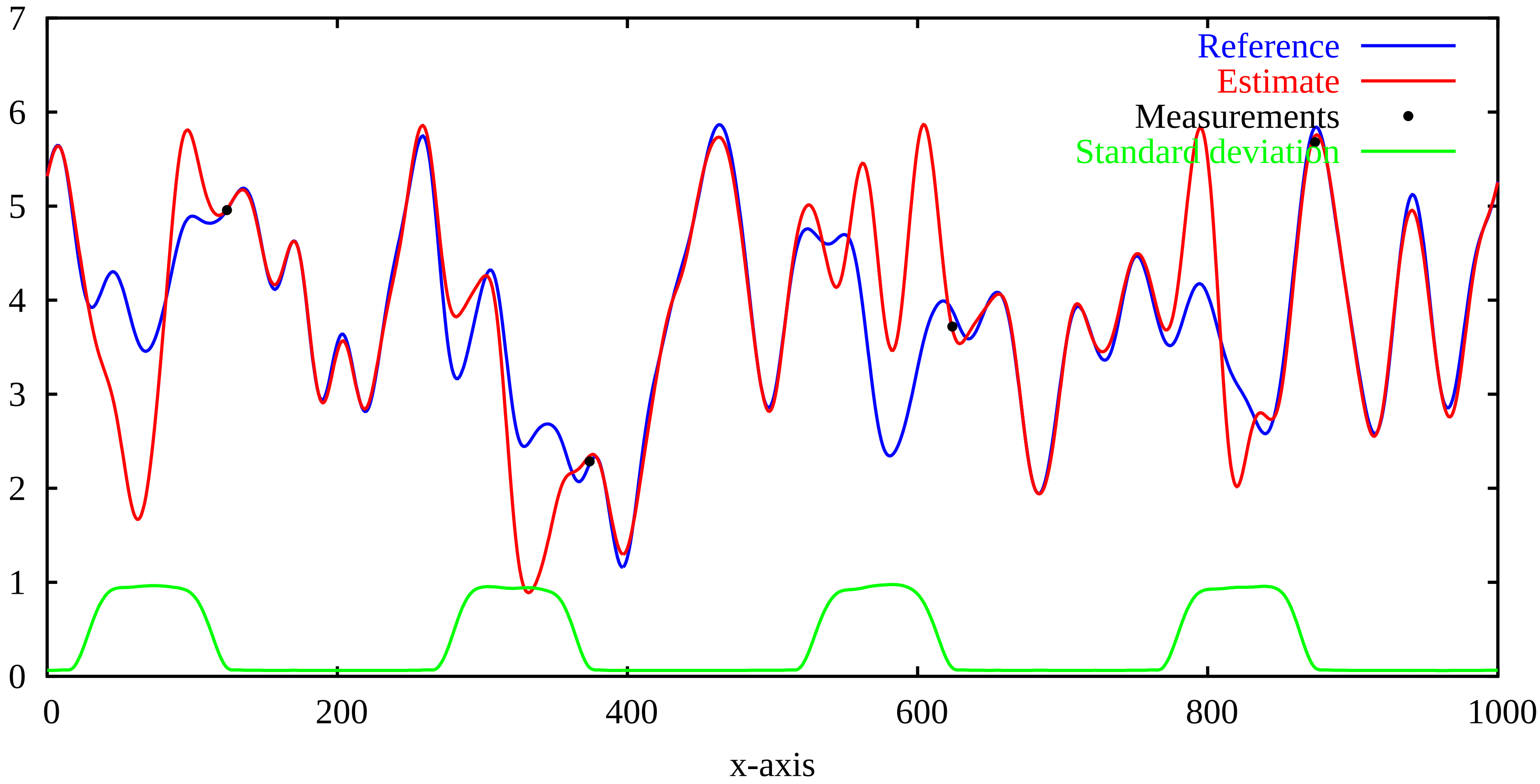
Example: Model

- Linear one-dimensional “exact” advection model on periodic domain.
- Advection speed is 1.0, $\Delta x = 1.0$ and time step is $\Delta t = 1.0$.
- True initial condition sampled from the distribution Φ which has mean equal to zero, variance equal to one and spatial decorrelation length 20.
- First guess is true state pluss another sample drawn from Φ, thus initial variance is assumed to be one.
- Initial ensemble is generated by adding samples drawn form Φ, to the first guess.
- Four measurements every 5th time step with std. dev. 0.1.
- Integration length is 300 time units.

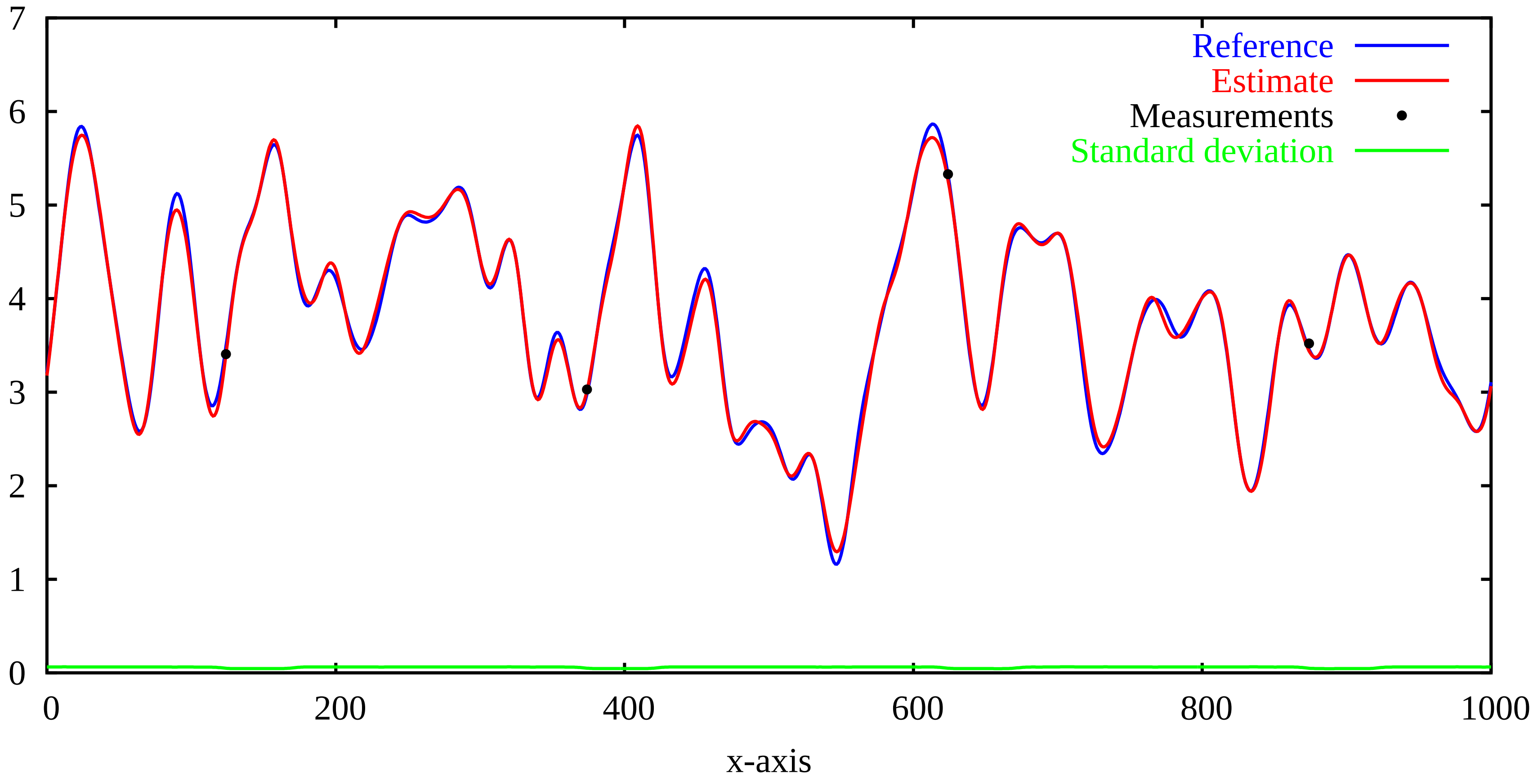
Example (Time t=3)



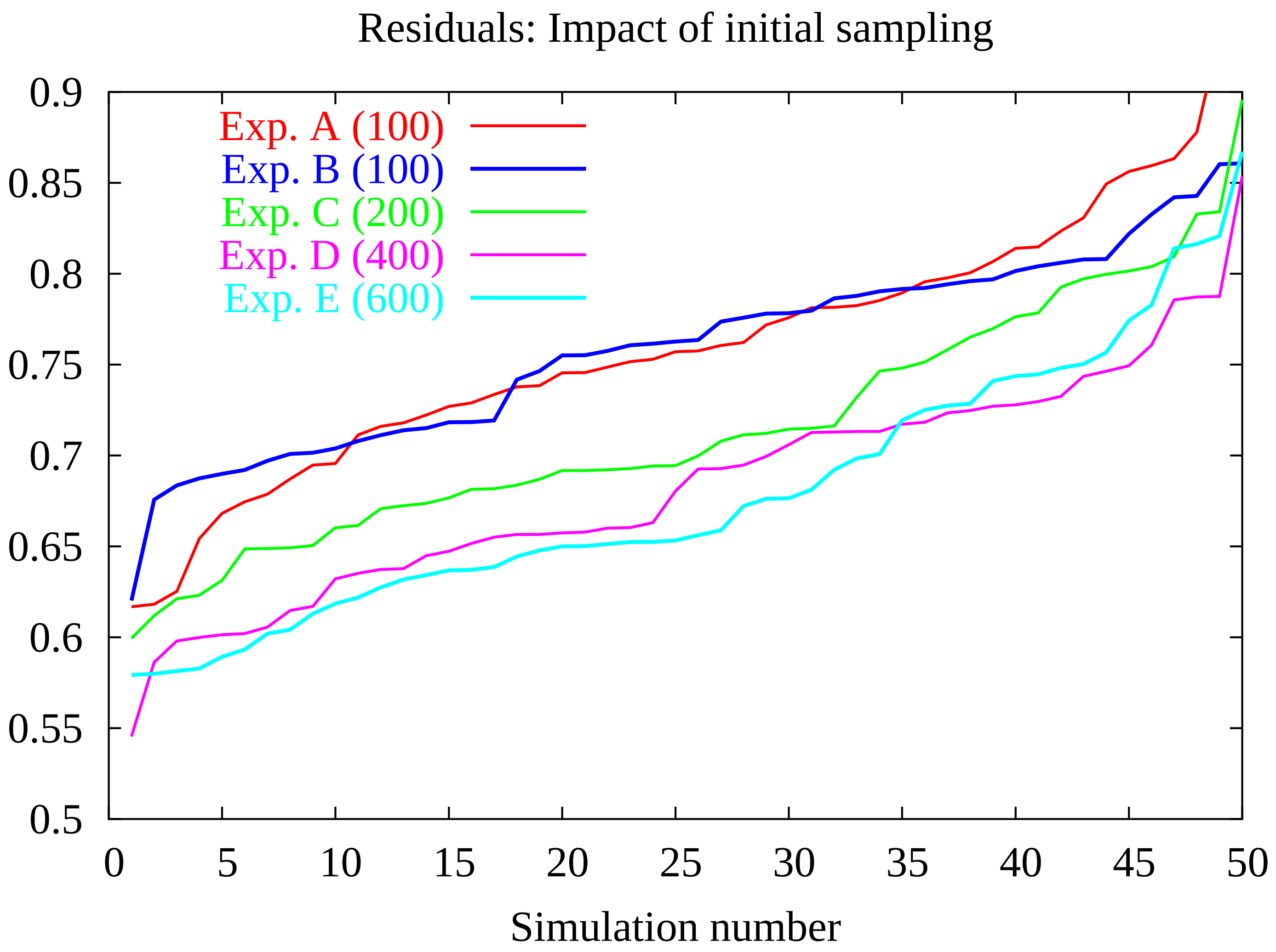
Example (Time t=121)



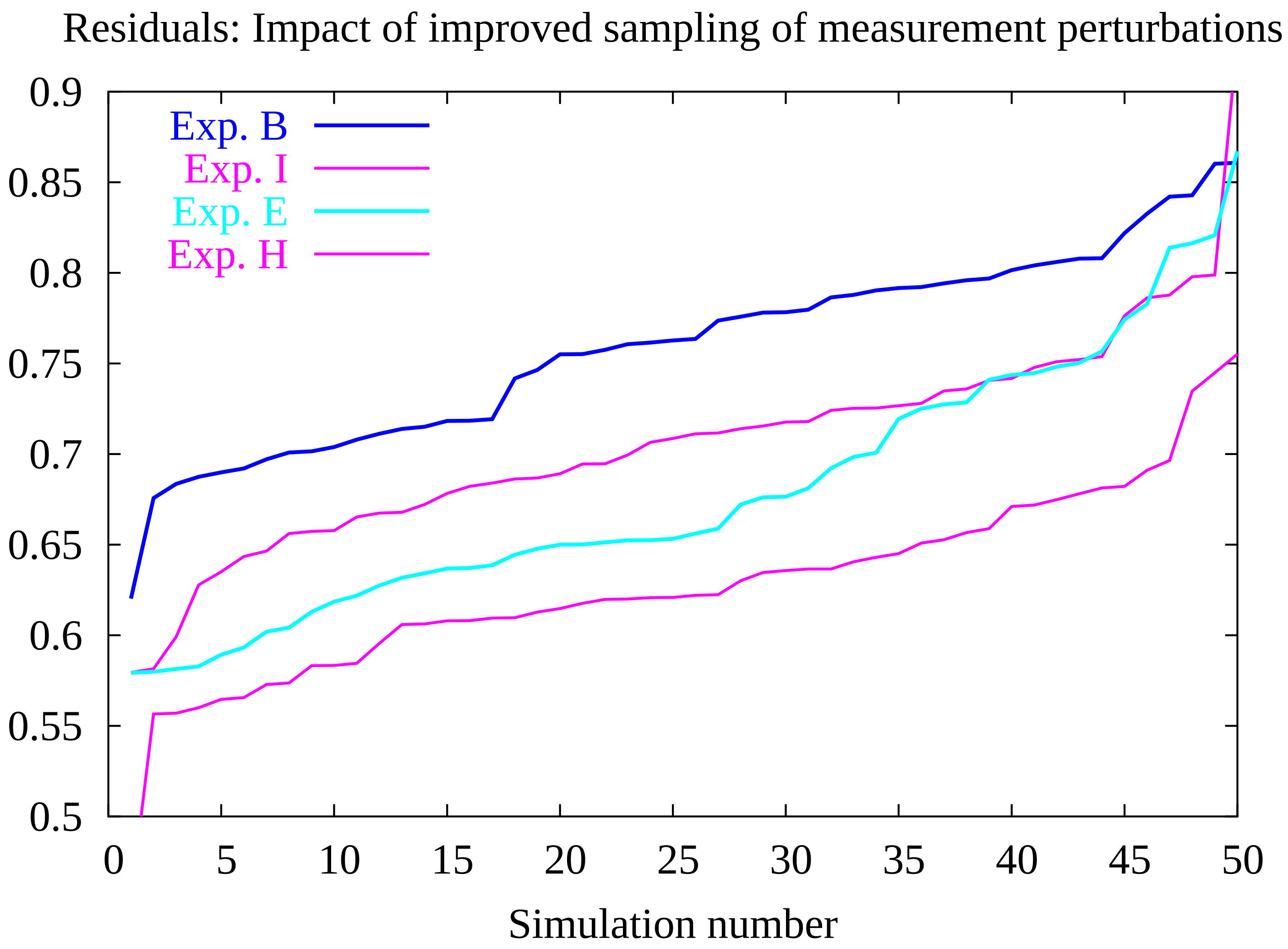
Example (Time t=241)



Improved sampling: Initial ensemble



Improved sampling: Measurements



A square root analysis scheme (1)

- The ensemble mean can be updated from

$$\overline{\boldsymbol{\psi}}^{\mathrm{a}} = \overline{\boldsymbol{\psi}}^{\mathrm{f}} + \boldsymbol{A}'\boldsymbol{S}^{\mathrm{T}}\boldsymbol{C}^{-1}(\boldsymbol{d} - \boldsymbol{H}\overline{\boldsymbol{\psi}}^{\mathrm{f}}).$$

- The analysis covariance is defined as

$$\boldsymbol{P}^{\mathrm{a}} = \boldsymbol{P}^{\mathrm{f}} - \boldsymbol{P}^{\mathrm{f}}\boldsymbol{H}^{\mathrm{T}}(\boldsymbol{H}\boldsymbol{P}^{\mathrm{f}}\boldsymbol{H}^{\mathrm{T}} + \boldsymbol{R})^{-1}\boldsymbol{H}\boldsymbol{P}^{\mathrm{f}},$$

  or, in ensemble notation

$$\boldsymbol{A}^{\mathrm{a}\prime}\boldsymbol{A}^{\mathrm{a}\prime\mathrm{T}} = \boldsymbol{A}'\left(\boldsymbol{I} - \boldsymbol{S}^{\mathrm{T}}\boldsymbol{C}^{-1}\boldsymbol{S}\right)\boldsymbol{A}'^{\mathrm{T}}.$$

- Inverse of $\boldsymbol{C}$

$$\boldsymbol{C} = \boldsymbol{Z}\boldsymbol{\Lambda}\boldsymbol{Z}^{\mathrm{T}} \Rightarrow \boldsymbol{C}^{-1} = \boldsymbol{Z}\boldsymbol{\Lambda}^{-1}\boldsymbol{Z}^{\mathrm{T}}$$

A square root analysis scheme (2)

- We get

$$
\begin{aligned}
\boldsymbol{A}^{a\prime}\boldsymbol{A}^{a\prime\mathrm{T}} &= \boldsymbol{A}'\left(\boldsymbol{I} - \boldsymbol{S}^{\mathrm{T}}\boldsymbol{Z}\boldsymbol{\Lambda}^{-1}\boldsymbol{Z}^{\mathrm{T}}\boldsymbol{S}\right)\boldsymbol{A}'^{\mathrm{T}} \\
&= \boldsymbol{A}'\left(\boldsymbol{I} - \left(\sqrt{\boldsymbol{\Lambda}^{-1}}\boldsymbol{Z}^{\mathrm{T}}\boldsymbol{S}\right)^{\mathrm{T}}\left(\sqrt{\boldsymbol{\Lambda}^{-1}}\boldsymbol{Z}^{\mathrm{T}}\boldsymbol{S}\right)\right)\boldsymbol{A}'^{\mathrm{T}} \\
&= \boldsymbol{A}'\left(\boldsymbol{I} - \boldsymbol{X}_2{}^{\mathrm{T}}\boldsymbol{X}_2\right)\boldsymbol{A}'^{\mathrm{T}},
\end{aligned}
$$

with the SVD of $\boldsymbol{X}_2$ defined as

$$
\boldsymbol{U}_2\boldsymbol{\Sigma}_2\boldsymbol{V}_2^{\mathrm{T}} = \boldsymbol{X}_2 = \sqrt{\boldsymbol{\Lambda}^{-1}}\boldsymbol{Z}^{\mathrm{T}}\boldsymbol{S}.
$$

A square root analysis scheme (3)

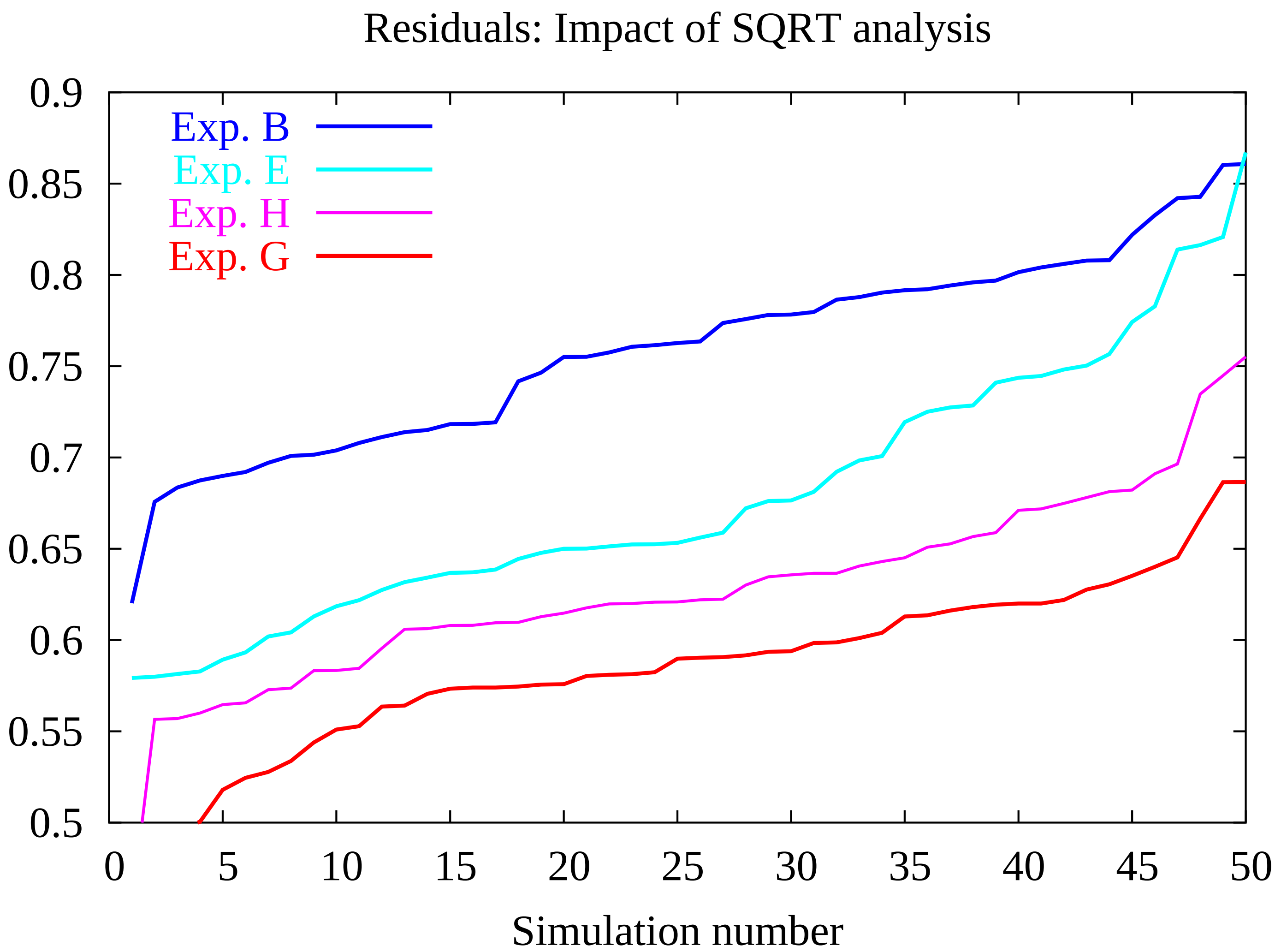
- We then get

$$
\begin{aligned}
\boldsymbol{A}^{\mathrm{a}\prime}\boldsymbol{A}^{\mathrm{a}\prime\mathrm{T}} &= \boldsymbol{A}'\left(\boldsymbol{I} - [\boldsymbol{U}_2\boldsymbol{\Sigma}_2\boldsymbol{V}_2^{\mathrm{T}}]^{\mathrm{T}}[\boldsymbol{U}_2\boldsymbol{\Sigma}_2\boldsymbol{V}_2^{\mathrm{T}}]\right)\boldsymbol{A}'^{\mathrm{T}} \\
&= \boldsymbol{A}'\left(\boldsymbol{I} - \boldsymbol{V}_2\boldsymbol{\Sigma}_2^{\mathrm{T}}\boldsymbol{\Sigma}_2\boldsymbol{V}_2^{\mathrm{T}}\right)\boldsymbol{A}'^{\mathrm{T}} \\
&= \boldsymbol{A}'\boldsymbol{V}_2\left(\boldsymbol{I} - \boldsymbol{\Sigma}_2^{\mathrm{T}}\boldsymbol{\Sigma}_2\right)\boldsymbol{V}_2^{\mathrm{T}}\boldsymbol{A}'^{\mathrm{T}} \\
&= \left(\boldsymbol{A}'\boldsymbol{V}_2\sqrt{\boldsymbol{I} - \boldsymbol{\Sigma}_2^{\mathrm{T}}\boldsymbol{\Sigma}_2}\right)\left(\boldsymbol{A}'\boldsymbol{V}_2\sqrt{\boldsymbol{I} - \boldsymbol{\Sigma}_2^{\mathrm{T}}\boldsymbol{\Sigma}_2}\right)^{\mathrm{T}}.
\end{aligned}
$$

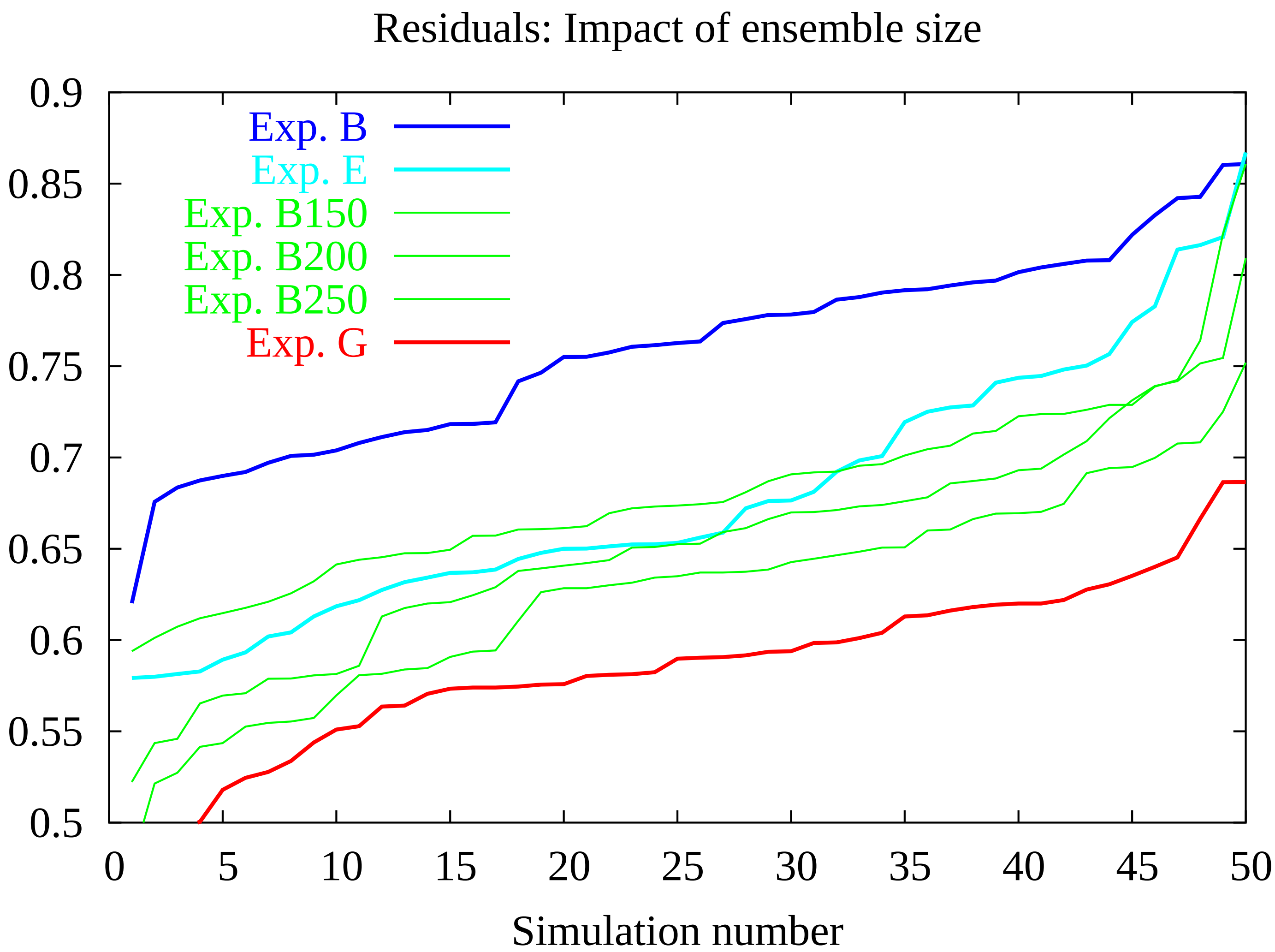
- The analysis equation becomes

$$
\boldsymbol{A}^{\mathrm{a}\prime} = \boldsymbol{A}'\boldsymbol{V}_2\sqrt{\boldsymbol{I} - \boldsymbol{\Sigma}_2^{\mathrm{T}}\boldsymbol{\Sigma}_2}.
$$

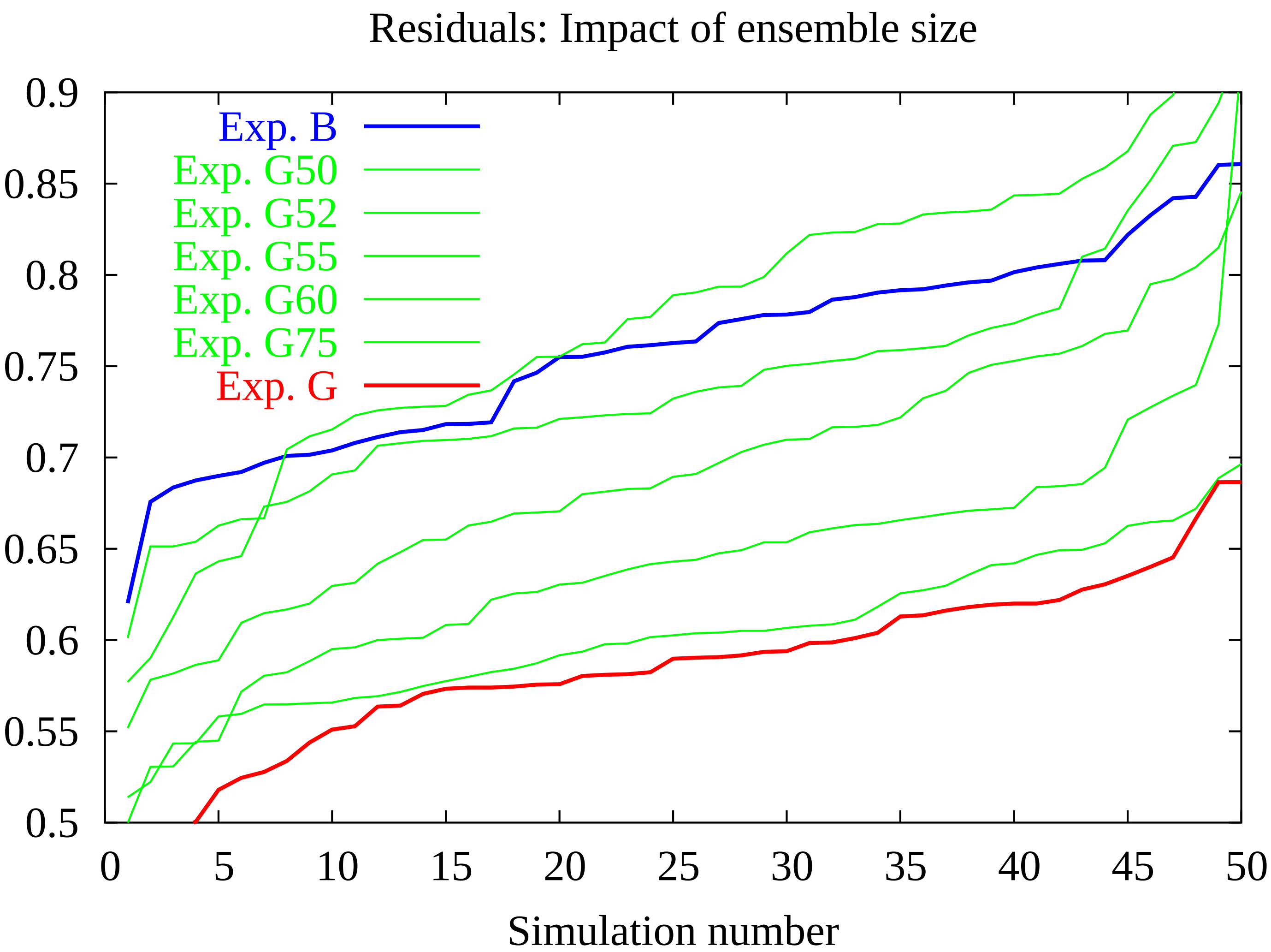
A square root analysis scheme (4)



Impact of ensemble size (1)



Impact of ensemble size (2)



Summary: Part one

- Size matters!
- With the right technique size is not all!
  - Sampling of initial ensemble (and model noise).
  - Square root formulation for analysis scheme.
- Details in Evensen 2004, Ocean Dynamics.
- F90 code for new routines available from http://www.nersc.no/∼geir/EnKF