Efficient Particle Filters for high-dimensional systems

Peter Jan van Leeuwen and Mel Ades
Data-Assimilation Research Centre DARC
University of Reading

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How is DA used today in geosciences?

Present-day data-assimilation systems are based on linearizations and state covariances are essential.

4DVar, Representer method (PSAS):

- Gaussian pdf's for the state, solves only for posterior mode, needs error covariance of initial state (B matrix)

(Ensemble) Kalman filter:

- assumes Gaussian pdf's for the state, approximates posterior mean and covariance, doesn't minimize anything in nonlinear systems, needs inflation and localisation

Combinations of these: hybrid methods (!!!)

Notation

- Prior knowledge, the Stochastic PDE:

$$x^n = f(x^{n-1}) + \beta^{n-1}$$

- Observations: y^n

- Relation between the two: $y^n = H(x^n) + \epsilon^n$

Nonlinear filtering: Particle filter

$$p(x|y) = \frac{p(y|x)p(x)}{\int p(y|x)p(x)\ dx}$$

↓ Use ensemble

$$p(x) = \sum_{i=1}^{N} \frac{1}{N}\delta(x - x_i)$$

$$p(x|y) = \sum_{i=1}^{N} w_i \delta(x - x_i)$$

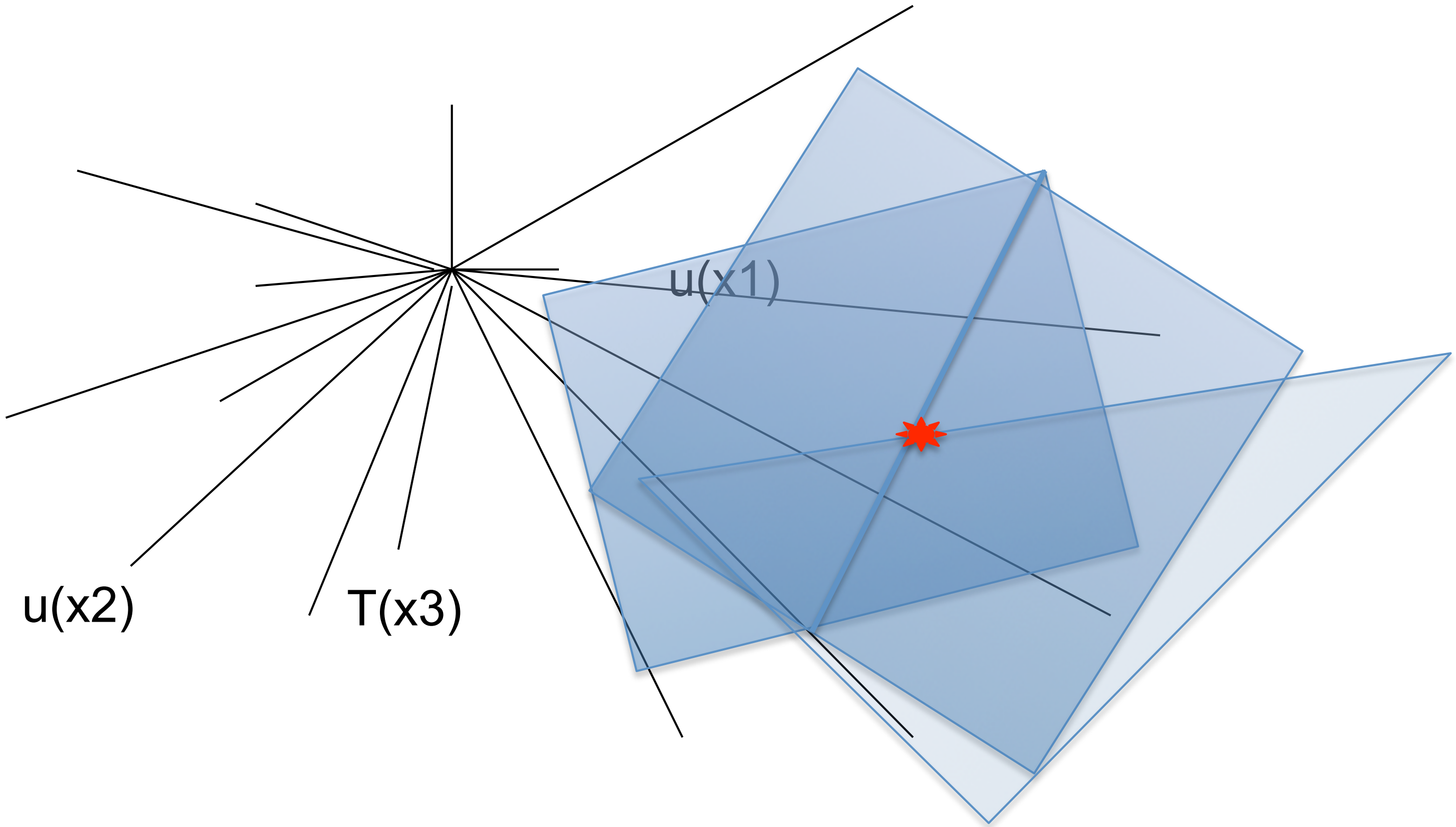
with

$$w_i = \frac{p(y|x_i)}{\sum_j p(y|x_j)}$$

the weights.

Why are particle filters degenerate I

Probability space in large-dimensional systems is 'empty': the curse of dimensionality



Why are Particle Filters degenerate II

- The volume of a hypersphere of radius *r* in an *M* dimensional space is

$$V \propto \frac{r^M}{\Gamma(M/2-1)}$$

- Taking for the radius $r \approx 3\sigma_y$ we find, using Stirling:

$$V \propto \left[\frac{9\sigma_y}{M/2}\right]^{M/2}$$

- So very small indeed.

Why are Particle Filters degenerate III

For the optimal proposal density we find, for Gaussian process model and Gaussian observation errors:

$$
\begin{aligned}
w_i &\propto p(y^n|x_i^{n-1}) \\
&\propto \exp\left[-\frac{1}{2}(y^n - Hf(x_i^{n-1}))(HQH^T + R)^{-1} \right. \\
&\qquad \left. \times (y^n - Hf(x_i^{n-1}))\right].
\end{aligned}
$$

Ignoring covariances we find:

$$
\mathrm{var}[-\log(w_i)] \propto \frac{M}{2}\left(\frac{V_x}{V_\beta + V_y}\right)^2 \left(1 + 2\left(\frac{V_y + V_\beta}{V_x}\right)\right)
$$

Why are Particle Filters degenerate?

- ‘Number of particles needed grows exponentially with dimension of the state vector (Bickel et al, 2007).’
- A slightly different view: degeneracy due to number of independent observations.
- This is related to the extremely narrow likelihood, a tiny move of a particle gives a completely different weight.

The statistics

- The Stochastic PDE: $x^n = f(x^{n-1}) + \beta^{n-1}$
- Observations: y^n
- Relation between the two: $y^n = H(x^n) + \epsilon^n$

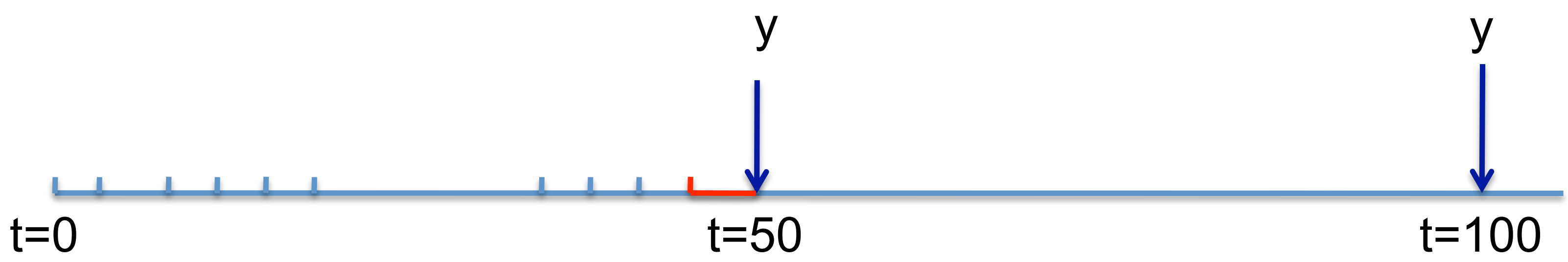
Assume: $\beta \sim N(0, Q)$

$\epsilon \sim N(0, R)$

H is linear

The Equivalent-Weights Particle Filter

- Use simple proposal at each time step, e.g. 'nudging'.
- Use different proposal at final time step to ensure that weights are very similar.



Proposal density between observations

We can explore the fact that the model needs several O(100) time steps between observations, e.g. by using a relaxation term in the proposal:

$$q(x^n | x_i^{n-1}, y^m) = N\left(f(x_i^{n-1}) + S\left(y^m - H(x_i^{n-1})\right), Q\right)$$

Corresponding to an evolution equation for each particle

$$x_i^n = f(x_i^{n-1}) + \hat{\beta}_i^n + S\left(y^n - H(x_i^{n-1})\right)$$

Proposal density between observations

- One could also use the ‘optimal proposal density’ between observations.

- This can be implemented as a minimization method for each particle, and is also known as the Implicit Particle Filter.

- This is related to a method called 4DVar in meteorology and oceanography, which explores only the mode of the joint-in-time pdf.

Proposal density at observation time:
the essence of the Equivalent-Weights Particle Filter

The proposal density depends on the maximum weight from a deterministic particle can achieve during the last time step:

$$q(x^n|x_i^{n-1},y^n) = \begin{cases} q_1(x^n|x_i^{n-1},y^n) & \text{if} \quad w_i^{max} > w^{target} \\ q_2(x^n|x_i^{n-1},y^n) & \text{if} \quad w_i^{max} < w^{target} \end{cases}$$

The target weight is set by the user, as e.g. the weight that 80% of the particles can achieve.

The maximum weights

1. We know:

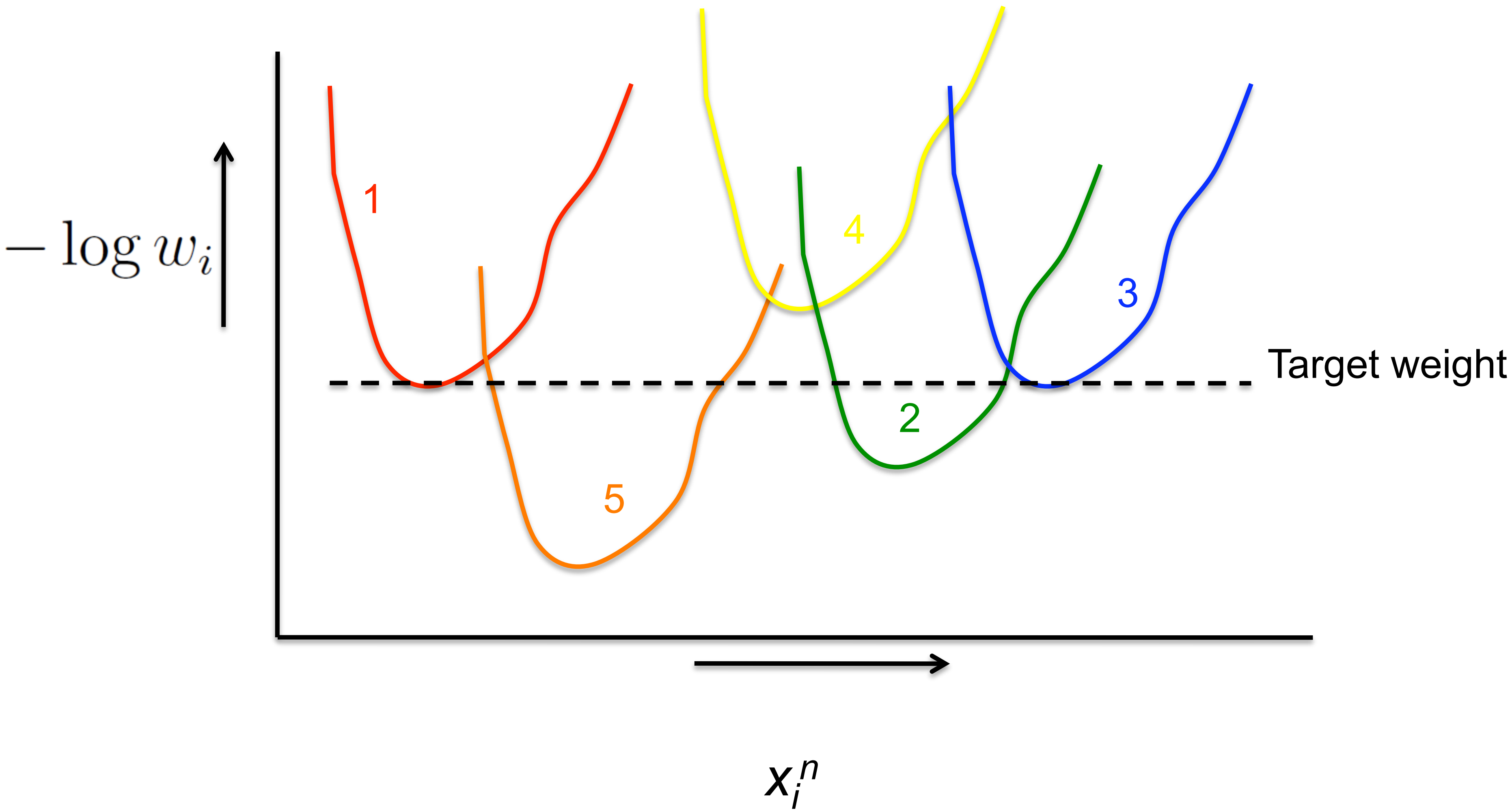
$$w_i = \frac{p(y^n|x_i^n)}{p(y^n)} \frac{p(x_i^n|x_i^{n-1})}{q(x_i^n|x_i^{n-1}, y^n)}$$

2. Write down expression for each weight ignoring proposal:

$$w_i \propto w_i^{rest} \exp \left[-\frac{1}{2}\left(x_i^n - f(x_i^{n-1})\right)^T Q^{-1}\left(x_i^n - f(x_i^{n-1})\right) - \frac{1}{2}(y^n - H(x_i^n))^T R^{-1}(y^n - H(x_i^n)) \right]$$

3. When H is linear this is a quadratic function in x_i^n for each particle. Otherwise linearize.

The target weight



The Equivalent-Weights Particle Filter

The proposal density is chosen as:

$$q(x^n|x_i^{n-1}, y^n) = \begin{cases} q_1(x^n|x_i^{n-1}, y^n) & \text{if} \quad w_i^{max} > w^{target} \\ q_2(x^n|x_i^{n-1}, y^n) & \text{if} \quad w_i^{max} < w^{target} \end{cases}$$

The target weight is set by the user, as e.g. the weight that 80% of the particles can achieve.

The two proposal densities

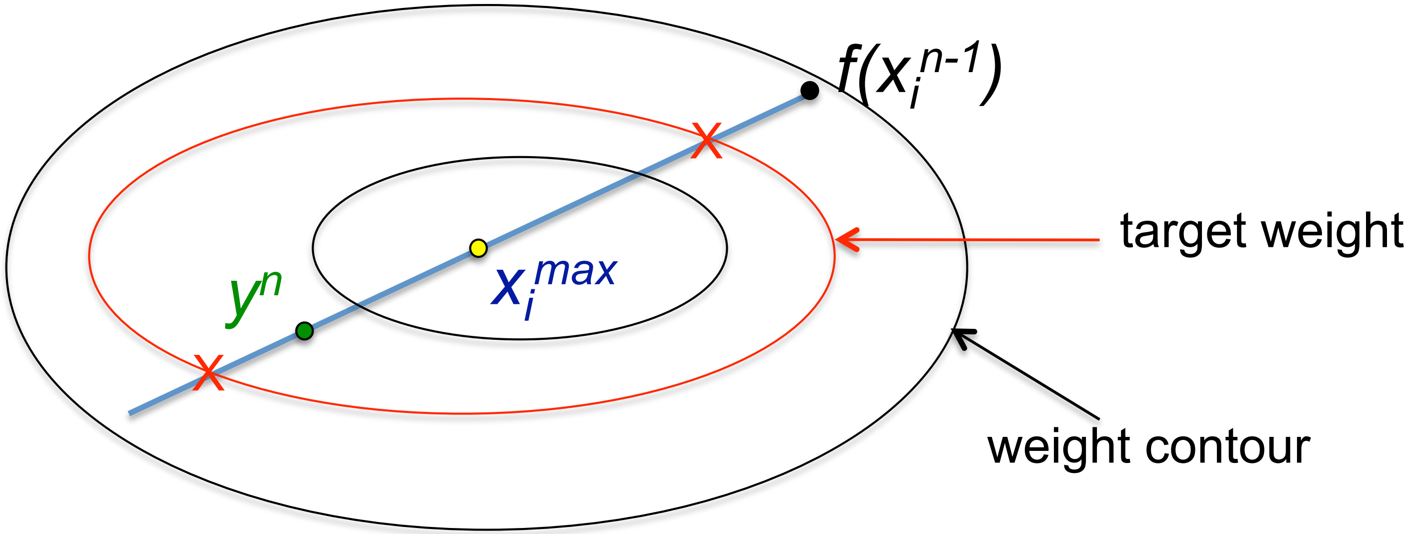
For particles that can reach the target weight we use:

$$q_1(x^n|x_i^{n-1}, y^m) = (1-\epsilon)U\left(\hat{x}_i - \gamma_U Q^{1/2}\mathbf{1}, \hat{x}_i + \gamma_U Q^{1/2}\mathbf{1}\right) + \epsilon \; N\left(\hat{x}_i, \gamma_N^2 Q\right)$$

For particles that cannot reach the target weight we use:

$$q_2(x^n|x_i^{n-1}, y^m) = N\left(f(x_i^{n-1}), Q\right)$$

The deterministic move



Determine α at crossing of line with target weight contour in:

$$\hat{x}_i = f(x_i^{n-1}) + \alpha_i K \left(y^n - H(f(x_i^{n-1})) \right)$$

with

$$K = QH^T(HQH^T + R)^{-1}$$

Equivalent-Weights Particle Filter

- Use relaxation-term proposal up to last time step
- Calculate w_i^{max} and target weight (e.g. 80%)
- Calculate deterministic moves for high-weight particles:

$$\hat{x}_i = f(x_i^{n-1}) + \alpha_i K \left(y^n - H(f(x_i^{n-1}))\right)$$

- Determine stochastic move

$$p(\hat{\beta}_i^{n-1}) \propto (1-a)U[-b,b] + aN(0,\hat{Q})$$

- Calculate new weights and resample 'lost' particles

How essential are Gaussian assumptions?

- Allows for analytical expressions.
- But no real need.
- w_i^{max} calculations do not have to be very accurate.
- Same for $w^{target.}$
- Deterministic move has to be very accurate, good iterative schemes should be used.

Application: the barotropic vorticity equation

- Stochastic barotropic vorticity equation:

$$\frac{\partial q}{\partial t} + u \cdot \nabla q = F$$

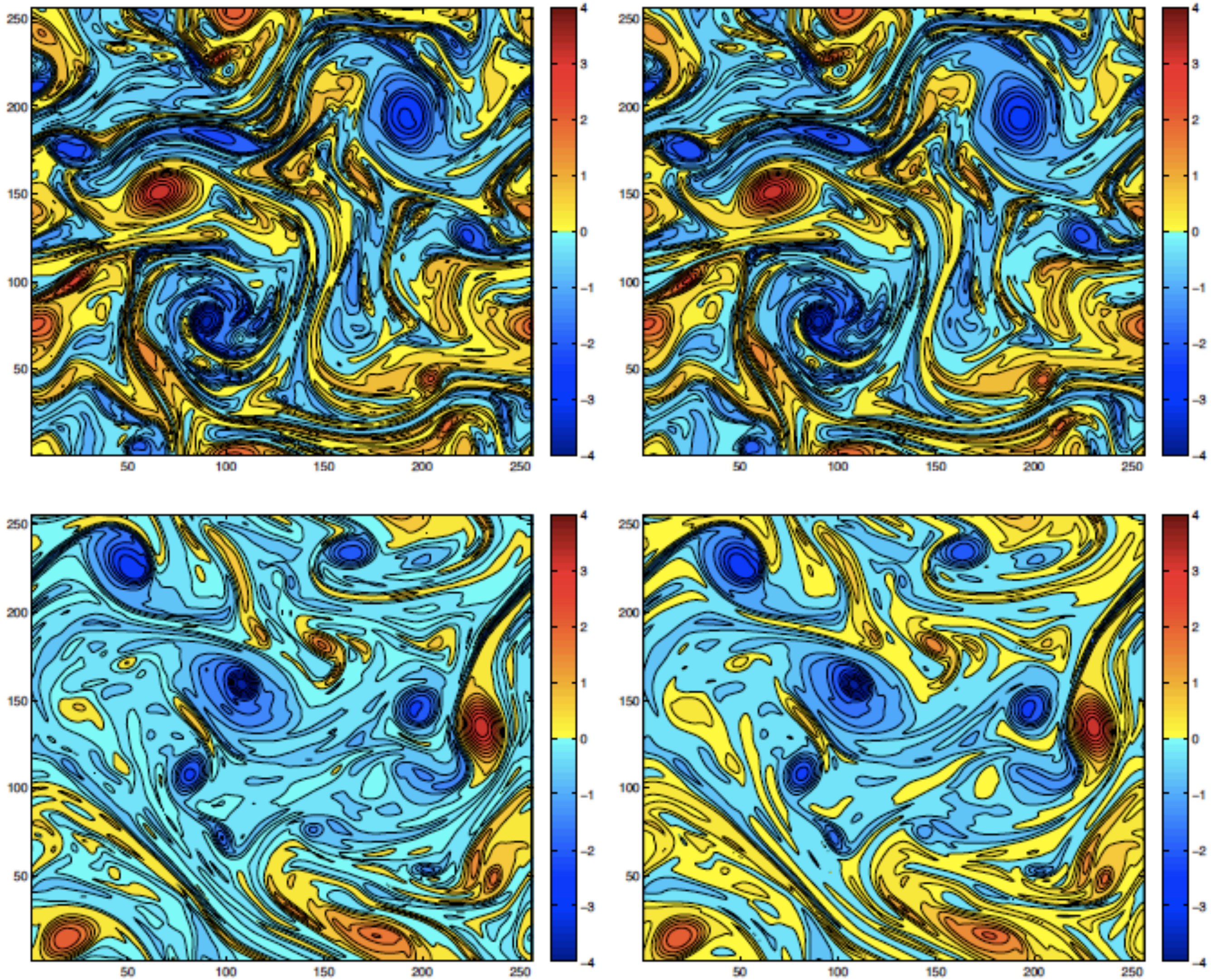
- 256 by 256 grid - 65,536 variables
- Doubly periodic boundary conditions
- Semi-Langrangian time stepping scheme
- Twin experiments
- Observations every 50 time steps – decorrelation time of 42
- 32 particles

Fully observed system

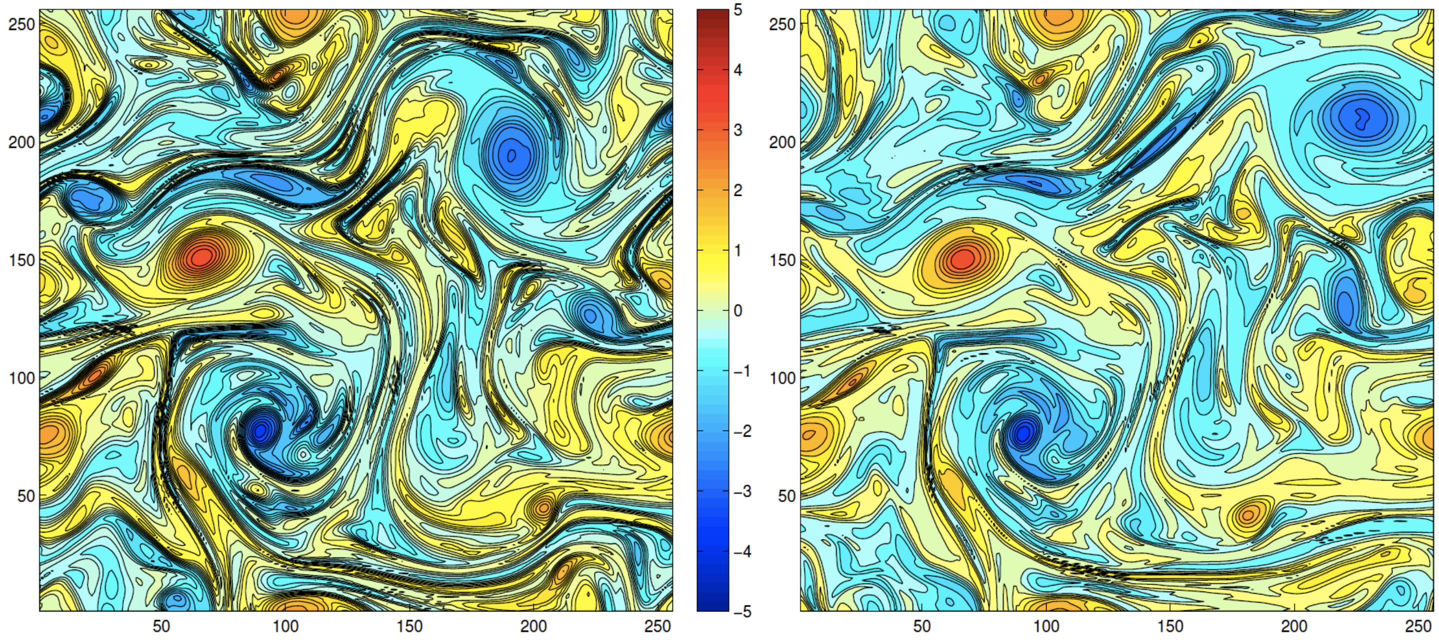
True model state | Mean of particles

Time step 600

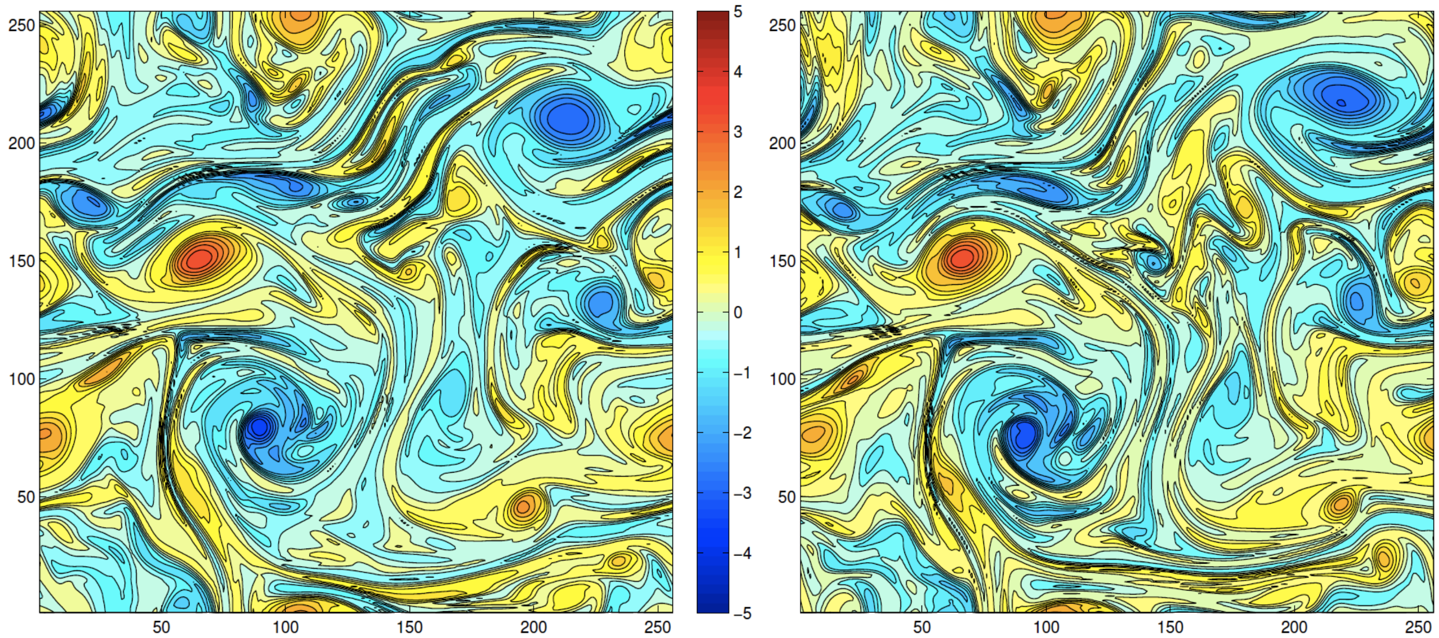
Time step 1150



Individual particles are not smooth.

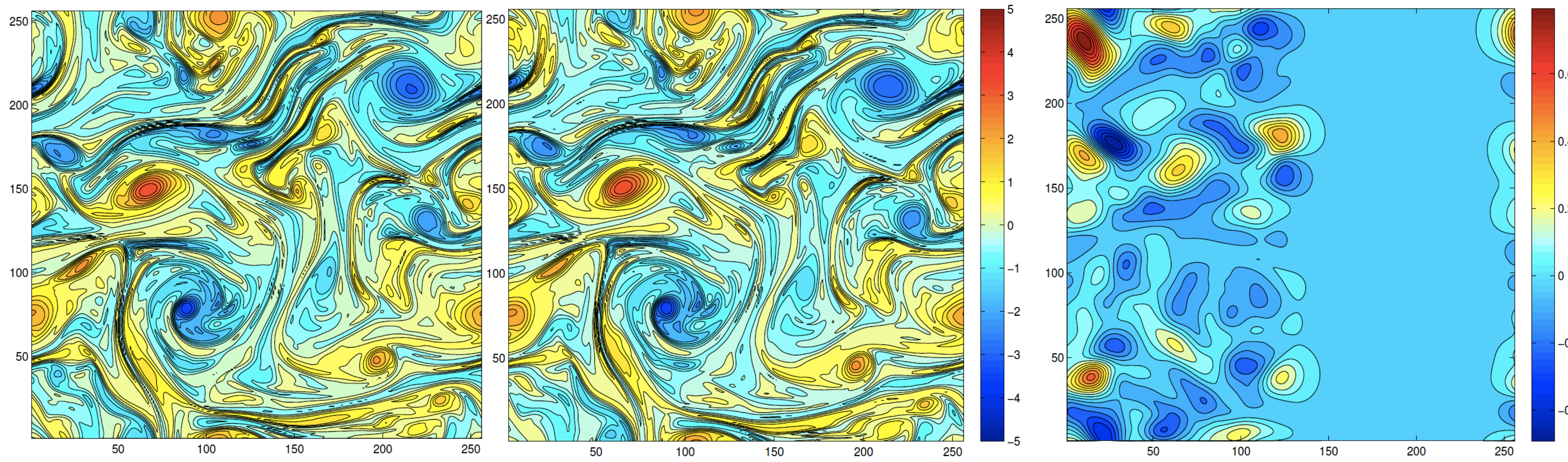


(a) truth (b) Particle 2



(c) Particle 23 (d) Particle 28

The update of the unobserved part

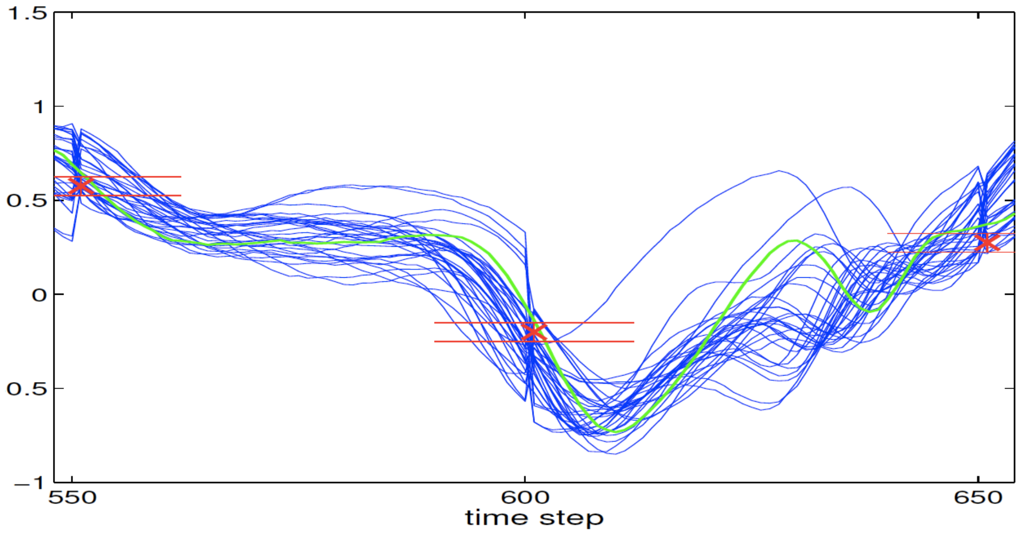


Particle 23 before update

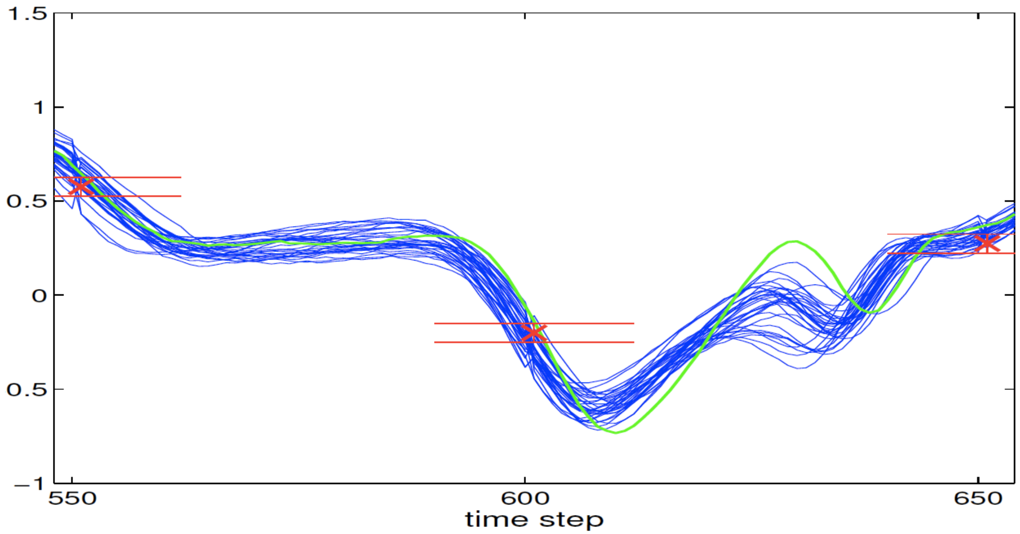
Particle 23 after update

Difference

Time evolution for different relaxation strengths

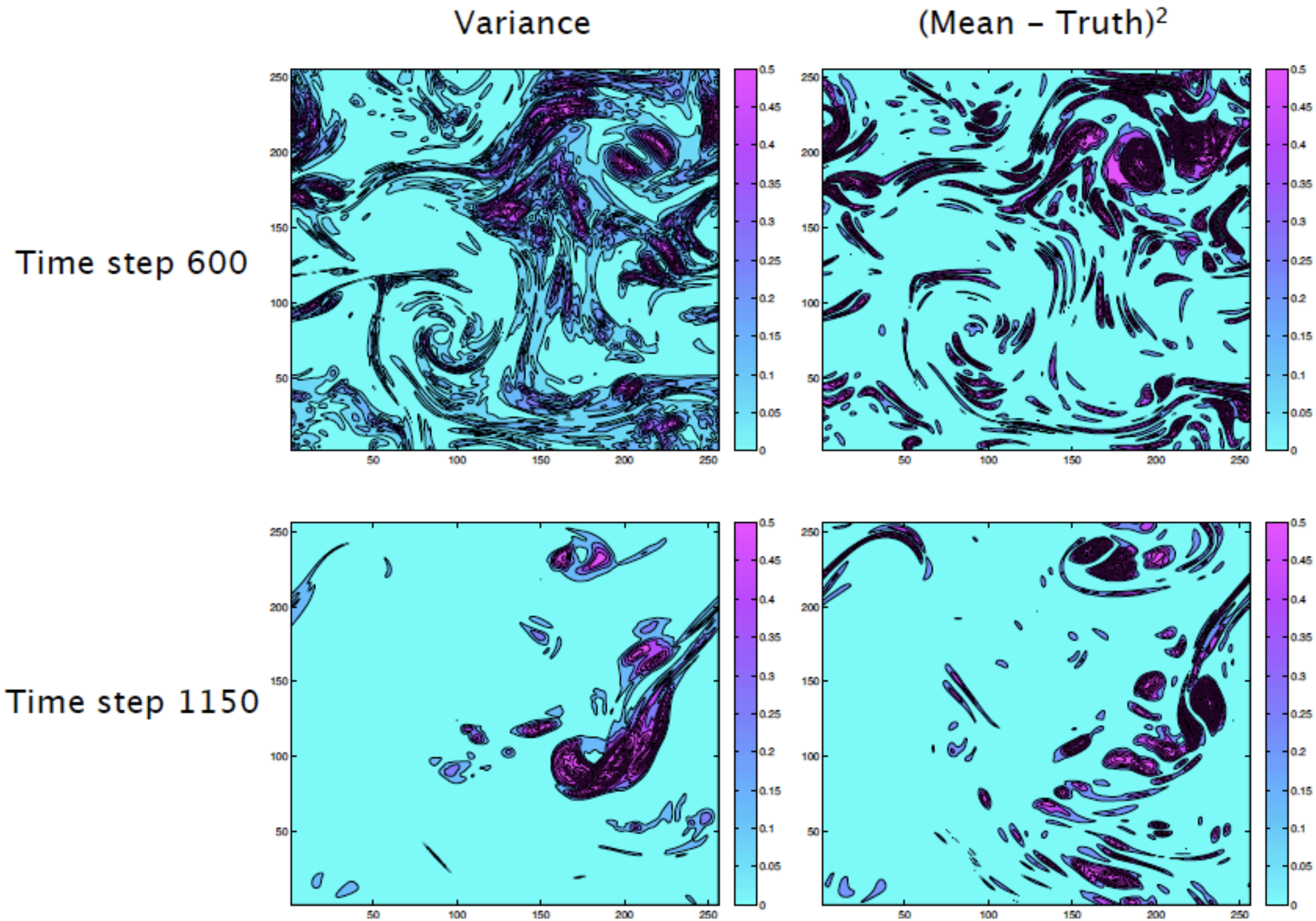


(a) $b = 1$

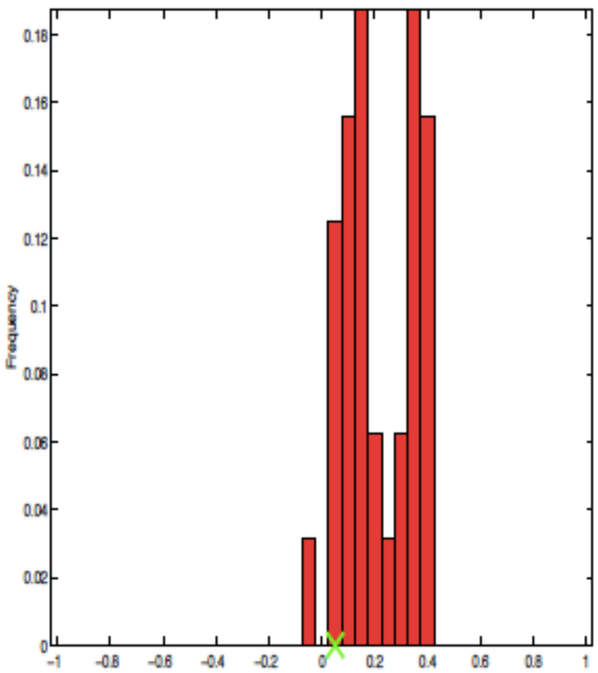


(b) $b = 8$

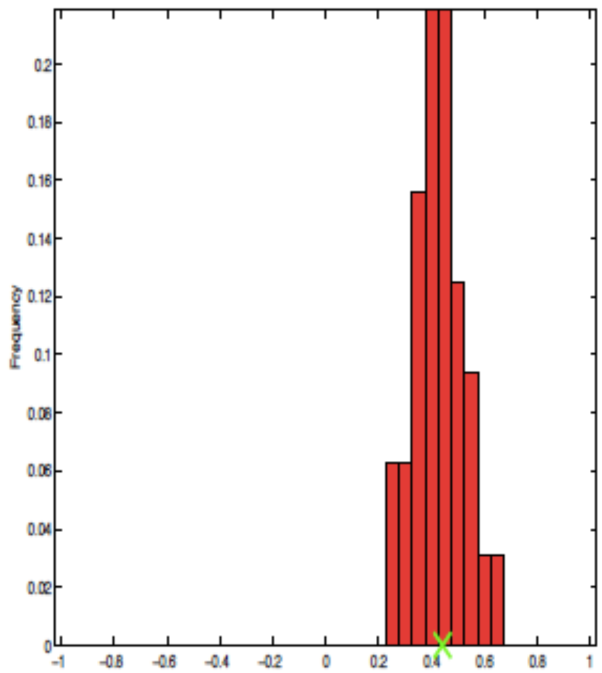
¼ observations over half of state



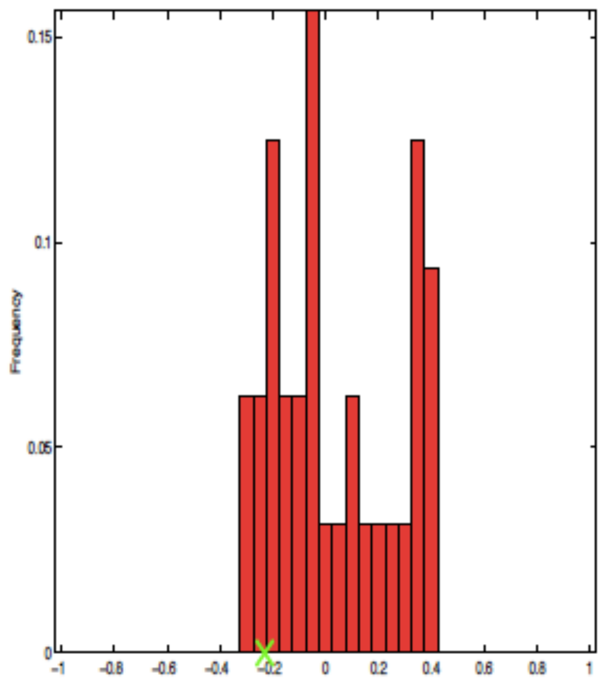
Marginal posterior probability densities



variable (20,64)

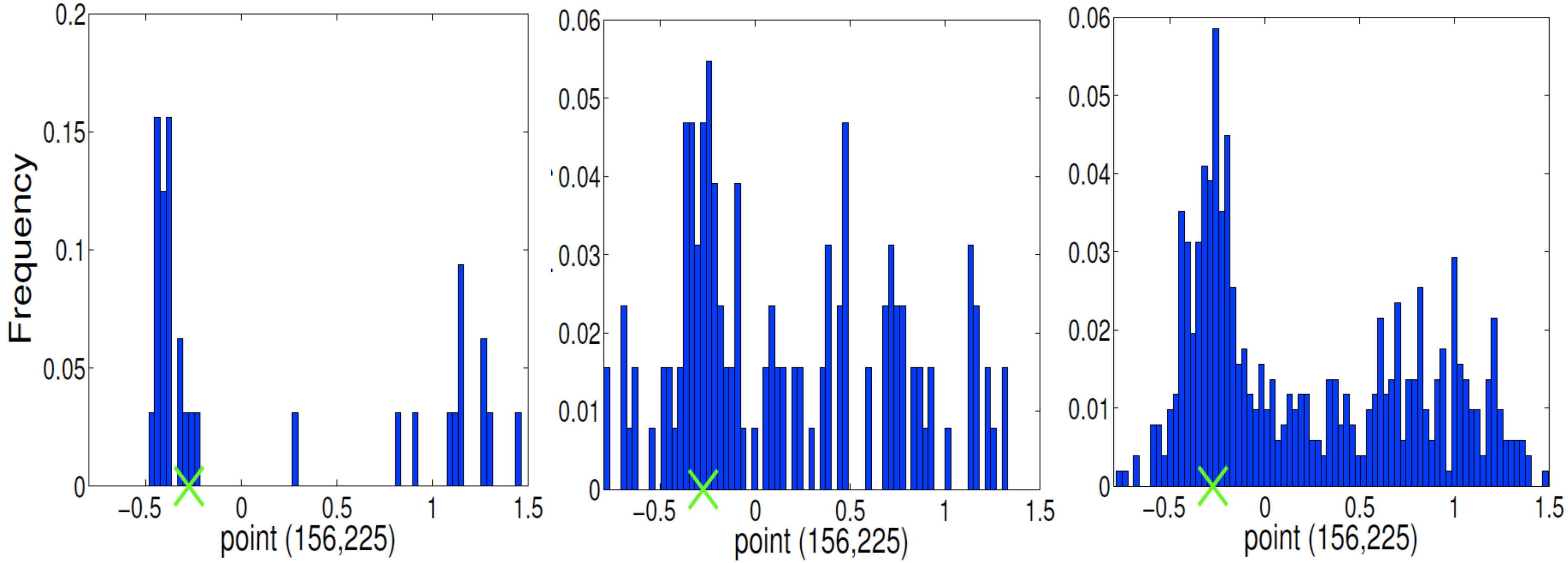


variable (56,64)



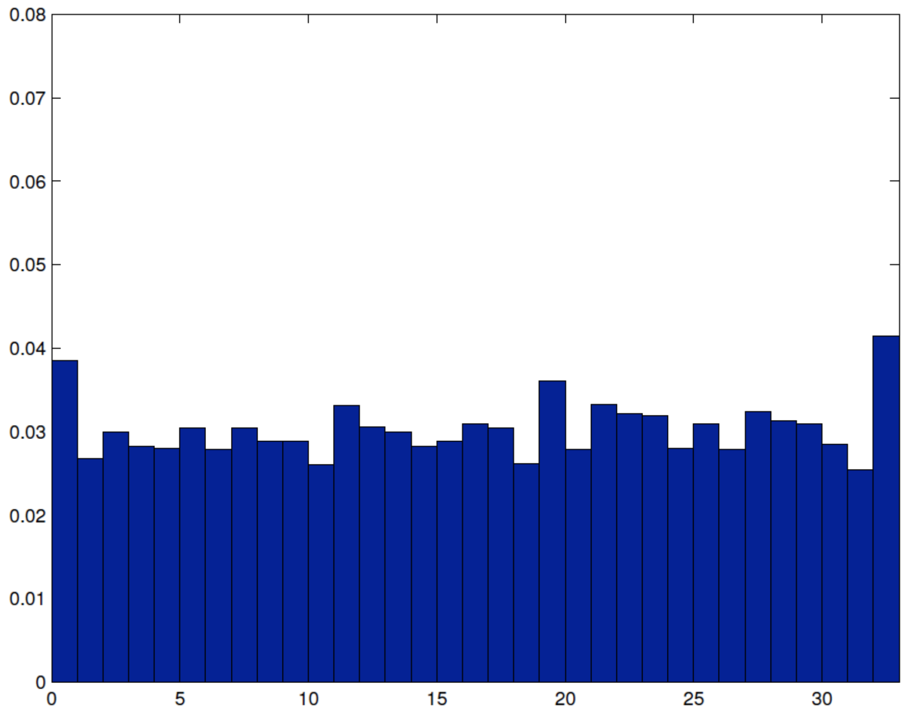
variable (197,64)

Convergence of the pdf’s

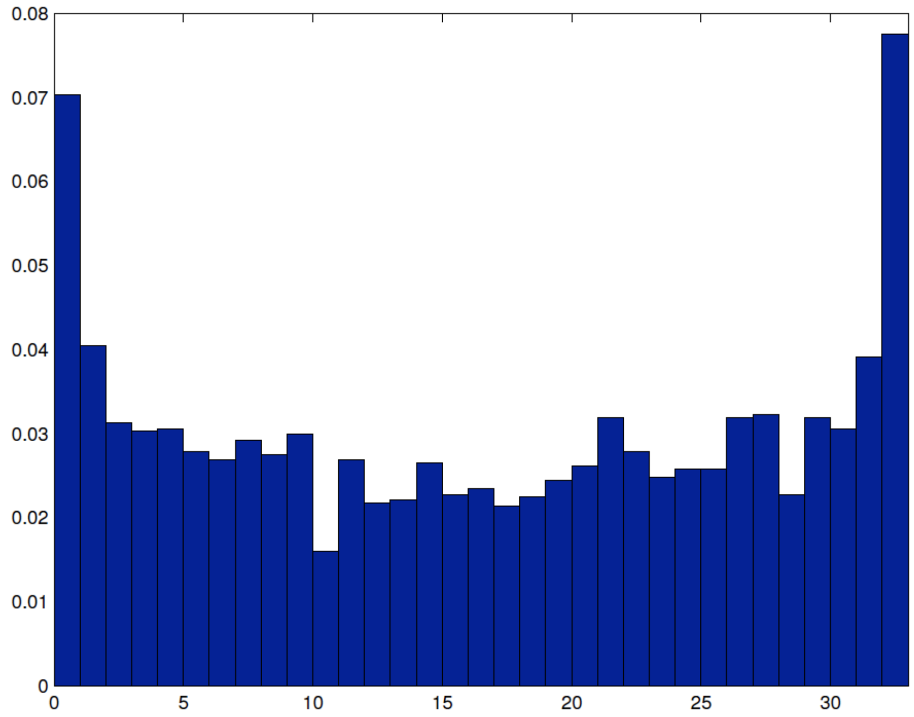


32 particles | 128 particles | 512 particles

Rank histograms

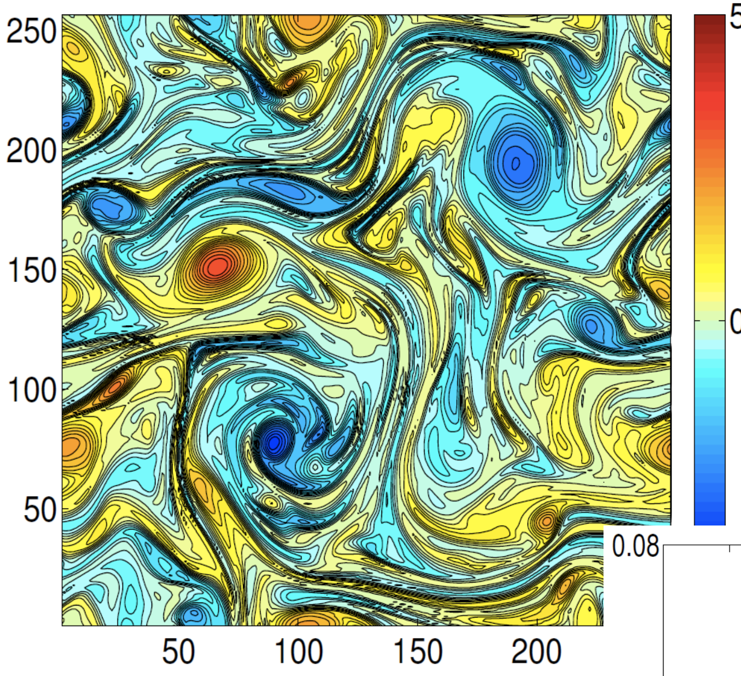


Full state observed

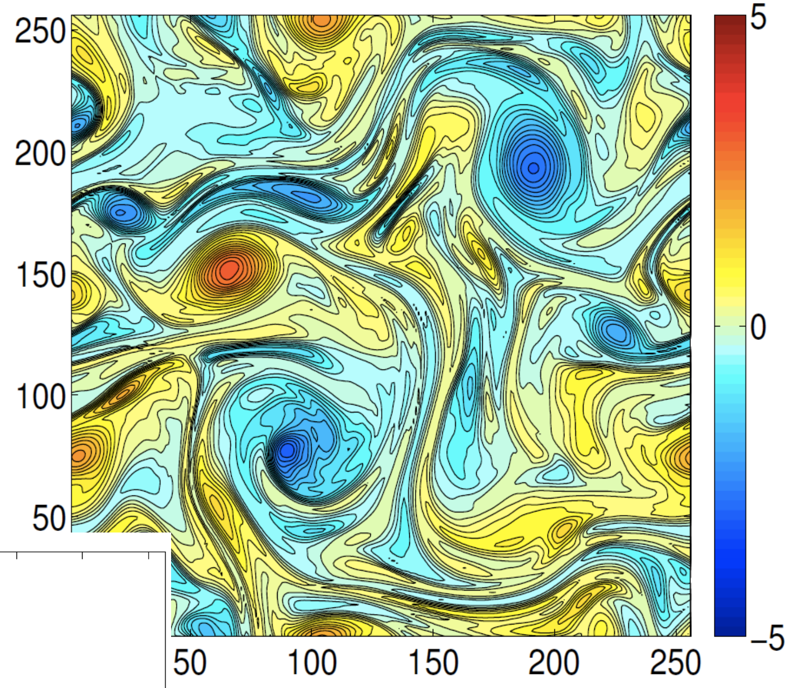


¼ of half state observed

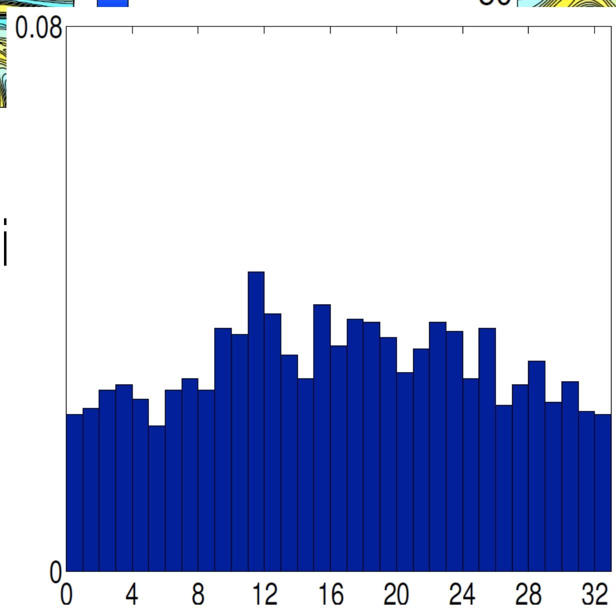
Miss-specification of process noise



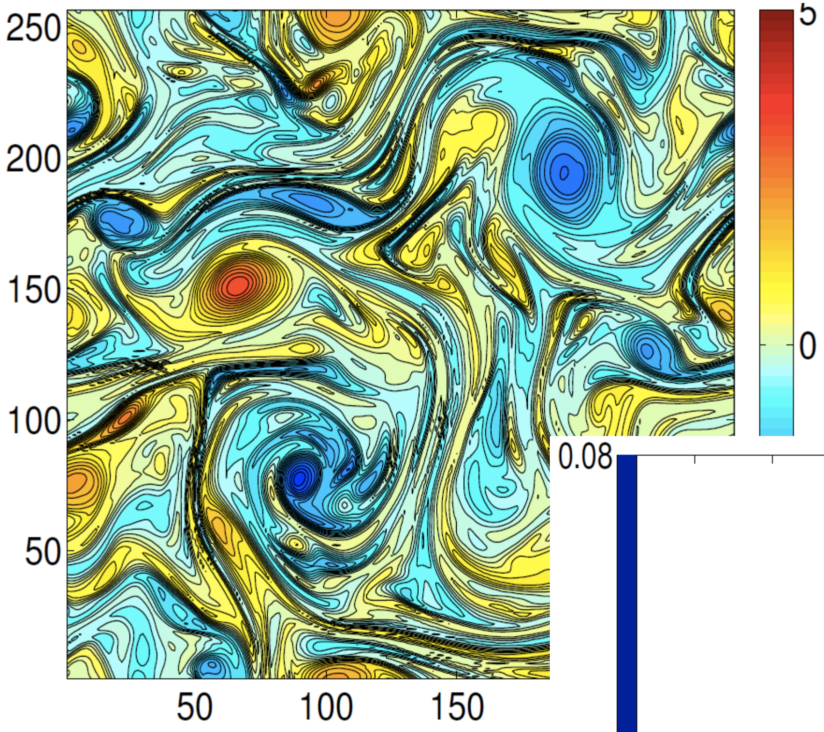
Truth: L_Q=5 gridpoi



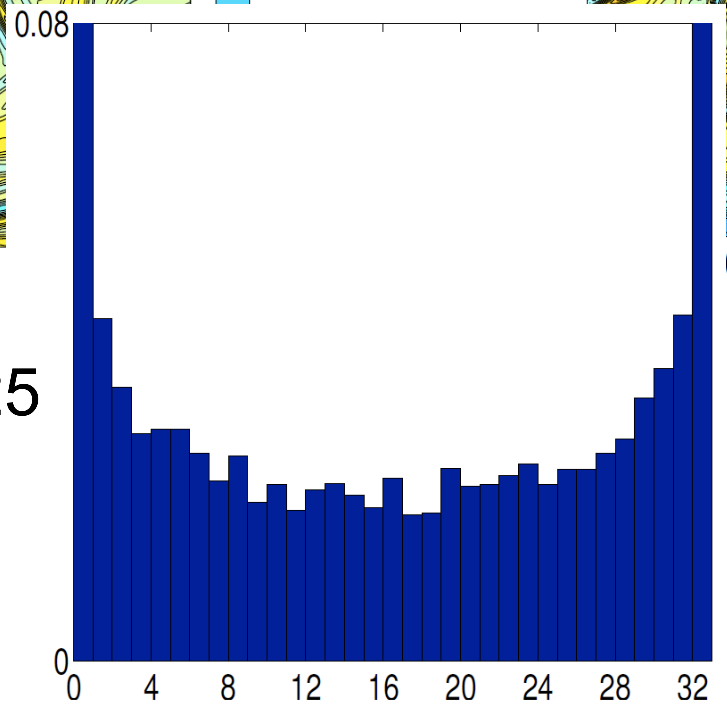
/-PF: L_Q=9 gridpoints

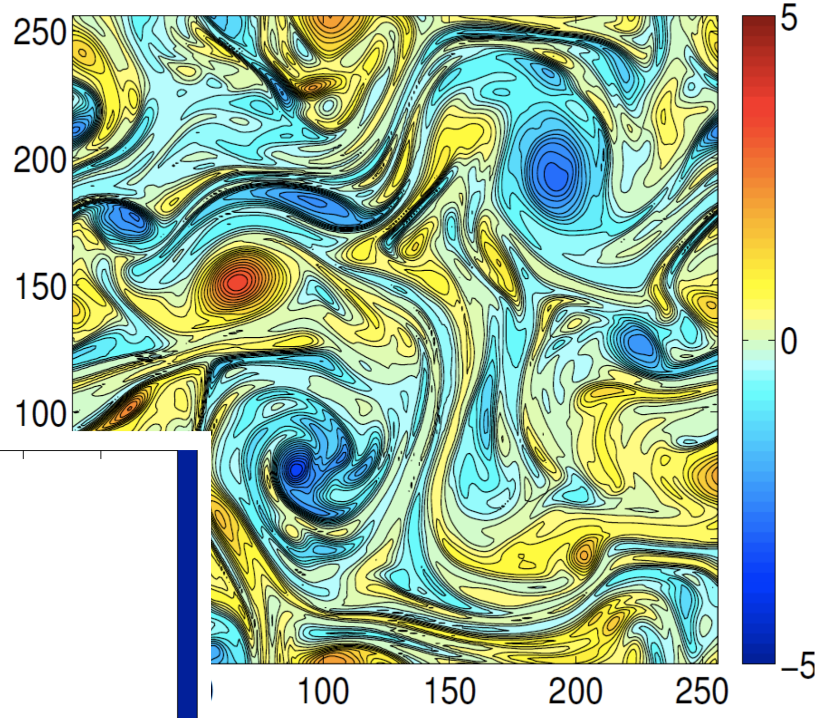


Miss-specification of process noise



Truth: Q=0.025





EW-PF: Q=0.1

Conclusions

- Particle filters do not need state covariances.
- Degeneracy is related to number of observations, not to size of the state space.
- Proposal density allows enormous freedom
- Equivalent-weights scheme solves dimensionality problem?
- Other efficient schemes are being derived.
- Future plans: numerical weather prediction, climate forecasting

References

All references can be found on my website
http://www.met.reading.ac.uk/~xv901096/research/publications.html

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