Data assimilation analysis for a stochastic one-layer rotating shallow water system driven by transport noise

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1. Stochasticity and Data Assimilation Data-Driven Stochastic Lie Transport Models (SALT)

Stochasticity & Data Assimilation

Motivation

- atmospheric data assimilation: challenges generated by
  - the multi-scale regime
  - the nonlinear aspect

  of the atmosphere
- resolved and unresolved scales of motion $\rightarrow$ certain small/sub-grid scale geophysical processes and their influence are still under-represented[10] $\rightarrow$ introduce stochasticity $\Rightarrow$ improved representation of the missing physics.

Challenges

- physical properties of the original system are preserved[4]
- analytical properties $\rightarrow$ as good as those of the deterministic model[3][1].

Approach: Stochastic Advection by Lie Transport (**SALT**)

Small-scale processes

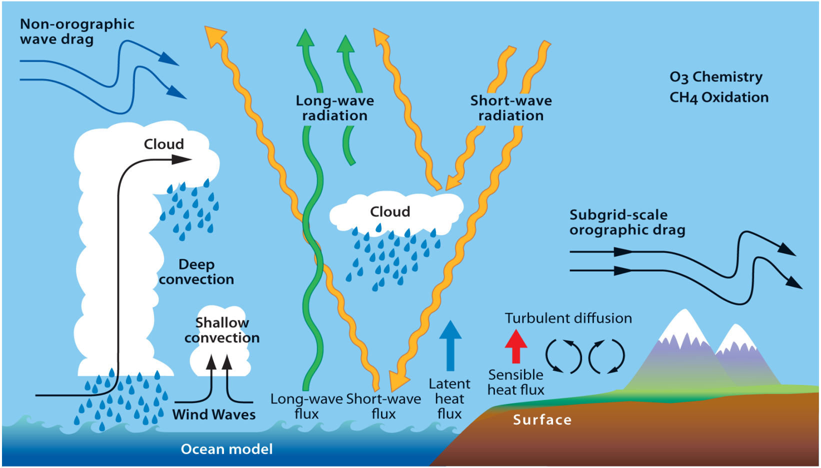


Figure : Physical processes which influence the large-scale phenomena but are usually active at scales smaller than those represented within the model grid.

Source: www.ecmwf.int/en/research/modelling-and-prediction/atmospheric-physics

Data-Driven Stochastic Lie Transport Models (SALT)

- deterministic transport: the Lie form of the vorticity equation contains a Lie derivative which expresses the change of vorticity along the flow generated by the velocity vector field:

$$\partial_t \omega_t + \mathcal{L}_{u_t} \omega_t = 0 \quad \Leftrightarrow \quad d\omega_t + u_t \cdot \nabla \omega_t dt = 0$$

- vorticity: $\omega_t = curl\ u_t = \nabla \times u_t$

- stochastic transport: perturb the velocity vector field and investigate the case where vorticity is transported along the newly perturbed trajectory[3][4]:

$$dy_t =: u_t dt + \sum_i \xi_i \circ dW_t^i.$$

$$d\omega_t + u_t \cdot \nabla \omega_t dt + \sum_i \xi_i \cdot \nabla \omega_t \circ dW_t^i = 0$$

- from fine-grid PDE $\rightarrow$ coarse-grid SPDE $\Rightarrow$ reduced computational cost $\Leftrightarrow$ model reduction, rigorously justified in nonlinear filtering through the continuity of the conditional distribution of the signal.

Data-Driven Stochastic Lie Transport Models (SALT)

The ξ_i vector fields:

- divergence-free, time-independent, derived from the underlying physics
- play 2 roles:
  - improved representation of the missing physics
  - induce variability in the particle filter ensemble (for DA)
- can be derived by comparing the fine grid and the coarse grid Lagrangian trajectories $\Rightarrow$ correspond to spatial correlations defined by a velocity-velocity correlation matrix
- for an incompressible fluid this spatial structure can be estimated from data in such a way that an ensemble of this type of stochastic paths will successfully track the large-scale behaviour of the original deterministic system: Cotter, C. et. al., *Numerically Modelling Stochastic Lie Transport in Fluid Dynamics*, 2018.

SGLE: Between Euler and the Rotating Shallow Water Model

Euler	Lake	Great Lake	SRSW
$\omega = curl\ u$	$\omega = b^{-1} curl\ u$	$\omega = b^{-1} curl\ v$	$\omega = z \cdot curl\ v$
		$v = u + \frac{1}{6}\delta^2 b^2 \nabla(\nabla \cdot u)$	$v = \epsilon u + R$
		$=: \mathcal{L}u$	time-evolution for $(h+b)$
$u = \nabla^\perp \psi$	$u = b^{-1}\nabla^\perp \psi$	$u = b^{-1}\nabla^\perp \psi$	
$u = K\omega$	$u = K\omega$	$u = K\omega$	...
$K = curl^{-1}$	$K = curl^{-1} b$	$K = (curl \mathcal{L})^{-1} b$	
$\nabla \cdot u = 0$	$\nabla \cdot (bu) = 0$	$\nabla \cdot (bu) = 0$	time-evolution for $\nabla \cdot u$

$$\mathcal{L}u = u + \delta^2 b^{-1}\Big[-\frac{1}{3}\nabla(b^3 \nabla \cdot u) - \frac{1}{2}\nabla(b^2 u \cdot \nabla b) + \frac{1}{2} b^2 (\nabla \cdot u)\nabla b + b(u \cdot \nabla b)\nabla b \Big]$$

- $\mathcal{L}$ is self-adjoint, positive-definite $\Rightarrow$ invertible $\Rightarrow$ K is continuous
- we need smoothing properties for K i.e a generalization of the Biot-Savart law

$$\|K\omega\|_{k,2} \leq C\|\omega\|_{k-1,2}.$$

2D Stochastic Euler Equation with Transport Noise

Theorem (Crisan, L., 2019)

If $\omega_0 \in \mathcal{W}^{k,2}(\mathbb{T}^2)$ is a divergence-free function then the two-dimensional stochastic Euler vorticity equation

$$d\omega_t + u_t \cdot \nabla \omega_t dt + \sum_{i=1}^{\infty} (\xi_i \cdot \nabla \omega_t) \circ dW_t^i = 0$$

admits a global, pathwise unique, $\mathcal{F}_t$-adapted solution $\omega = \{\omega_t, t \in [0, \infty)\}$ in $C\left([0, \infty); \mathcal{W}^{k,2}(\mathbb{T}^2)\right)$. In particular, if $k \geq 4$ the solution is classical. Moreover, if $\tilde{\omega} = \{\tilde{\omega}_t, t \in [0, \infty)\}$ is another solution of this equation, then, for all $T \in [0, \infty)$ there exists a positive constant C independent of the two solutions such that

$$\mathbb{E}\left[e^{-CA_t} ||\omega_t - \tilde{\omega}_t||_{k,2}^2\right] \leq ||\omega_0 - \tilde{\omega}_0||_{k,2}^2.$$

The process A is defined as $A_t := \int_0^t \|\omega_s\|_{k,2} ds$, for any $t \geq 0$.

- The result holds for the more general class of SPDEs

$$dx_t = F(x_t)dt + \sum_{i=1}^{\infty} \mathcal{L}_i x_t \circ dW_t^i$$

where F is a nonlinear operator satisfying specific conditions and $\mathcal{L}_i x_t := \xi_i \cdot \nabla x_t$.

Stochastic Great Lake Equations with Transport Noise

Theorem (Crisan, L., in preparation)

Under certain conditions on the vector fields $(\xi_i)_i$ the two-dimensional stochastic great lake equation system

$$\begin{aligned} &\partial_t \omega_t + u_t \cdot \nabla \omega_t dt + \sum_i (\xi_i \cdot \nabla \omega_t) \circ dW_t^i = 0 \\ &\nabla \cdot (bu) = 0 \\ &\omega = b^{-1} curl\ v \\ &v = u + \frac{1}{6} \delta^2 b^2 \nabla (\nabla \cdot u) \end{aligned} \tag{1}$$

admits a unique global (in time) solution in the *weighted Sobolev space* $\mathcal{W}^{b,k,2}(\mathbb{T}^2)$. In particular, if $k \geq 4$ the solution is classical. Moreover, if $\tilde{\omega} = \{\tilde{\omega}_t, t \in [0, \infty)\}$ is another solution of this equation, then, for all $T \in [0, \infty)$ there exists a positive constant C independent of the two solutions such that

$$\mathbb{E}[e^{-CB_t} ||\omega_t - \tilde{\omega}_t||^2_{b,k,2}] \leq ||\omega_0 - \tilde{\omega}_0||^2_{b,k,2}.$$

The process B is defined as $B_t := \int_0^t \|\omega_s\|_{b,k,2} ds$, for any $t \geq 0$.

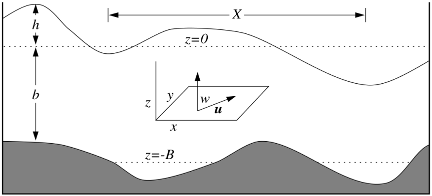
2. The Stochastic Rotating Shallow Water Model (SRSW)

A Viscous Stochastic Rotating Shallow Water System
- Overview -

$$dv_t + \left[u_t \cdot \nabla v_t + f\hat{z} \times u_t + \nabla p_t\right] dt + \sum_{i=1}^{\infty} \left[\xi_i \cdot \nabla v_t + (v_t)_j \nabla \xi_i^j\right] \circ dW_t^i = \nu \Delta v_t$$

$$d\eta_t + \nabla \cdot (\eta_t u_t) dt + \sum_{i=1}^{\infty} \left[\nabla \cdot (\xi_i \eta_t)\right] \circ dW_t^i = \delta \Delta \eta_t \qquad \nabla \cdot v_t \neq 0$$

$v := \epsilon u + \mathcal{R}$, *curl* $\mathcal{R} = f\hat{z}$, $p = \frac{\eta - b}{\epsilon \mathcal{F}}$, η = total depth, b = bottom topography.



Picture source: Levermore, Oliver, Titi, *Global Well-posedness for the Lake Equations* (1996).

The Viscous Stochastic Rotating Shallow Water System

- Main result -

Theorem (Crisan, L., in preparation)

Given $(u_0, \eta_0) \in \mathcal{W}^{1,2}(\mathbb{T}^2) \times \mathcal{W}^{1,2}(\mathbb{T}^2)$ and a fixed stochastic basis $\mathcal{S} = (\Omega, \mathcal{F}, (\mathcal{F}_t)_t, \mathbb{P}, W^i)$, there exists a unique local pathwise solution of the stochastic rotating shallow water system

$$dv_t + \left[\mathcal{L}_{u_t} v_t + f\hat{z} \times u_t + \nabla p_t\right] dt + \sum_{i=1}^{\infty} \left[(\mathcal{L}_i + \mathcal{A}_i) v_t\right] \circ dW_t^i = \nu \Delta v_t dt$$

$$d\eta_t + \nabla \cdot (\eta_t u_t) dt + \sum_{i=1}^{\infty} \mathcal{L}_i h_t \circ dW_t^i = \delta \Delta \eta_t dt$$

with values in the space $\mathcal{W}^{1,2}(\mathbb{T}^2) \times \mathcal{W}^{1,2}(\mathbb{T}^2)$.

- $\mathcal{L}_i v_t := \xi_i \cdot \nabla v_t$
- $\mathcal{A}_i v_t := (v_t)_j \nabla \xi_i^j = (v_t)_1 \nabla \xi_i^1 + (v_t)_2 \nabla \xi_i^2$
- $\nabla \cdot \xi_i = 0$, $\nabla \cdot u \neq 0$

The Viscous Stochastic Rotating Shallow Water System

- Strategy & Key facts -

- Consider the truncated linearised system (Itô form):

$$dv_t^n = \nu\Delta v_t^n dt + P_t^{n-1,n}(v_t^n)dt - \sum_{i=1}^{\infty}\left[(\mathcal{L}_i + \mathcal{A}_i)v_t^n\right]dW_t^i$$

$$d\eta_t^n = \delta\Delta\eta_t^n dt + Q_t^{n-1,n}(\eta_t^n)dt - \sum_{i=1}^{\infty}\mathcal{L}_i\eta_t^n dW_t^i$$

$$P_t^{n-1,n}(v_t^n) := -f_R(u_t^{n-1})\mathcal{L}_{u_t^{n-1}}v_t^n - f\hat{z}\times u_t^n - f_R(\eta_t^{n-1})\nabla p_t^{n-1} + \frac{1}{2}\sum_{i=1}^{\infty}\left[(\mathcal{L}_i + \mathcal{A}_i)^2 v_t^n\right]dt$$

$$Q_t^{n-1,n}(\eta_t^n) := -f_R(u_t^{n-1})\nabla\cdot(\eta_t^n u_t^{n-1}) + \frac{1}{2}\sum_{i=1}^{\infty}\mathcal{L}_i^2\eta_t^n dt$$

- $\mathbb{E}\left[\sup_{t\in[0,T]}\|v_t^n\|_{1,2}^2 + \sup_{t\in[0,T]}\|\eta_t^n\|_{1,2}^2\right] \leq \mathcal{C}_1$
- $\mathbb{E}\left(\int_0^T\|\Delta v_t^n\|_2^2 dt + \int_0^T\|\Delta\eta_t^n\|_2^2 dt\right) \leq \mathcal{C}_2$

$\Big\}$ a priori estimates

The Viscous Stochastic Rotating Shallow Water System

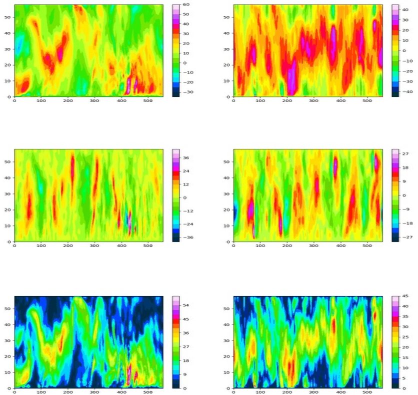
- Strategy & Key facts -

- The truncated linear system admits a global pathwise solution in $C^\infty(\mathbb{T}^2) \times C^\infty(\mathbb{T}^2)$ (Rozovskii)
- The family of solutions $(v_t^n, \eta_t^n)_n$ is relatively compact in the space of càdlàg functions $\mathcal{D}([0,T], \mathbb{L}^2(\mathbb{T}^2))$; Kurtz's criterion: find a family of random variables $(\gamma_\alpha^n)_\alpha$ s.t. $\mathbb{E}\left[\|Y_{t+l}^n - Y_t^n\|_2^2 | \mathcal{F}_t\right] \leq \mathbb{E}\left[\gamma_\alpha^n | \mathcal{F}_t\right]$ and $\lim_{\alpha\to 0} \limsup_n \mathbb{E}[\gamma_\alpha^n] = 0$ for $t \in [0,T] \leftarrow$ we use the mild form to show this.
- $(v_t^n, \eta_t^n)_n$ converges in distribution to a truncated form of the original system $\overset{\text{Skorohod}}{\Longrightarrow}$ weak (probabilistic) solution
- Stochastic Gronwall lemma $\Rightarrow$ pathwise uniqueness $\overset{\text{Yamada-Watanabe}}{\Longrightarrow}$ strong solution for the truncated form of the original system
- Remove the truncation up to a positive stopping time

$\Rightarrow$ strong local solution for the stochastic rotating shallow water system.

Numerical implementation of the SRSW model

- In the first phase we use an ideal simulation of the *truth*, when the model is run at fine resolution for 1000 and 10 000 time steps respectively, with initial data (pressure) from a DWD numerical weather prediction analysis field.
- The velocity solution (zonal velocity, meridional velocity), and the magnitude of the velocity vector (given by the L_2 -norm)
- The scale of the fields decreases during the integrations due to developing instabilities within the flow.



Code by P.J. van Leeuwen

Nonlinear Stochastic Filtering

- Overview -

Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a probability space.

Signal process/model $\quad dX_t = f_t(X_t)dt + \sigma(X_t)dW_t \quad$ (X is unknown)

Observation process $\quad Y_t = h_t(X_t) + V_t \quad$ (Y is known)

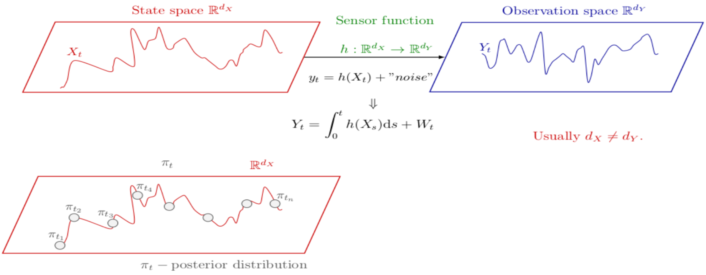
where $f_t, h_t, \sigma_t : \mathbb{R}^d \to \mathbb{R}^d$ are measurable functions and $(W_t)_t, (V_t)_t$ are normal, independent and identically distributed random variables.

Goal

Find the best estimate of X_t given the σ - algebra $\mathcal{Y}_t = \sigma(Y_s, s \in [0, t])$ generated by observations i.e. find the probability measure valued process $(\pi_t)_t$ such that for any $A \in \mathcal{F}$

$$\pi_t(A) = \mathbb{P}(X_t \in A | Y_1, \ldots, Y_t).$$

Stochastic Filtering/Data Assimilation



- intractable for nonlinear problems $\Rightarrow$ approximation methods required:
  - variational and ensemble methods: 3dVar, 4dVar, EnKF, LETKF, ...
  - particle filters

A Data Assimilation Problem using the SRSW model

$$\pi^a_{t-1} \xrightarrow[\text{forecast prediction}]{K_t = model} K_t(\pi^a_{t-1}) = \pi^b_{t-1} \xrightarrow[\text{assimilation analysis}]{\text{tempering},\ g_t\star} g_t \star \pi^b_{t-1} = \pi^a_t$$

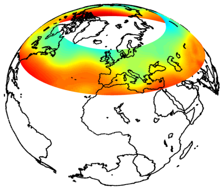
Model (signal process):

$$dq + (u \cdot \nabla q)dt + \sum_i (\xi_i \cdot \nabla q) \circ dW^i_t = 0, \qquad q = \frac{\omega}{\eta},\ \omega = \hat{z} \cdot curl(\epsilon u + \mathcal{R})$$

$$d\eta_t + \nabla \cdot (\eta_t u_t)dt + \sum_{i=1}^{\infty} [\nabla \cdot (\xi_i \eta_t)] \circ dW^i_t = 0, \qquad \nabla \cdot v_t \neq 0$$

$$dv_t + \left[u_t \cdot \nabla v_t + f\hat{z} \times u_t + \nabla p_t\right]dt + \sum_{i=1}^{\infty} [\xi_i \cdot \nabla v_t + (v_t)_j \nabla \xi^j_i] \circ dW^i_t = 0$$

Data (observation process): pointwise measurements for the pressure field between 20 and 70 degrees north latitude, collected using commercial aircraft (Deutscher Wetterdienst).



Methodology: Particle Methods.

3. Adaptive Tempering Particle Filter Algorithms

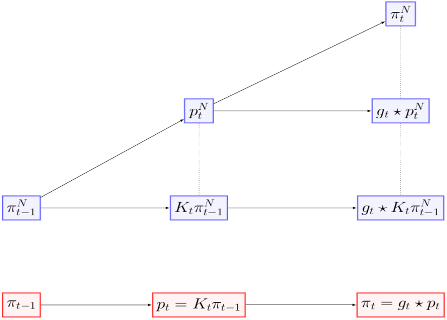
Particle Filters - Overview

$$\pi_{t-1}^{a,y_{0:t-1}} \xrightarrow[\substack{\textit{model}\\ \textit{forecast}\\ \textit{prediction}}]{K_t} K_t \pi_{t-1}^{a,y_{0:t-1}} =: \pi_{t-1}^{b} =: p_t \xrightarrow[\substack{\textit{assimilation}\\ \textit{analysis}}]{\textit{update using data, } g_t^{y_t} \star} g_t^{y_t} \star \pi_{t-1}^{b} = \pi_t^{a,y_{0:t}}$$

$$K_t : \mathbb{R}^{d_s} \times \mathcal{B}(\mathbb{R}^{d_s}) \to [0,1],\ \ K_t(X_{t-1}, A) = \mathbb{P}(X_t \in A | X_{t-1})$$

$$g_t^{y_t} : \mathbb{R}^{d_X} \to [0,1],\ \ g_t^{y_t}(x) = g_t(y_t - h(t,x)) = \mathbb{P}(Y_t \in dy_t | X_t = x_t)$$

- $\pi_t \approx \pi_t^N = \sum_{l=1}^{N} \bar{w}_t^l \delta(x_t^l), x_{t_2}^l = K(x_{t_1}^l, \omega^l, t_2), \pi_{t_2}^a = \sum_{l=1}^{N} \bar{w}_{t_2}^l \delta(K(x_{t_1}^l, \omega^l, t_2)) = \sum_{l=1}^{N} \bar{w}_{t_2}^l \delta(x_{t_2}^l)$



Particle Filters - Overview

- too informative observations $\Rightarrow \pi_{t_2}^N$ and π_t become singular with respect to each other exponentially fast $\Rightarrow$ resampling: particles with low weights are discarded and replaced with higher weighted particles $\Rightarrow$ new ensemble $(\tilde{x}_{t_2}^l)_l$ with equal weights

$$\pi_{t_2}^N = \frac{1}{N} \sum_{l=1}^{N} \delta(\tilde{x}_{t_2}^l)$$

- resampling $\leftrightarrow$ duplicates $\Rightarrow$ degenerate distribution $\Rightarrow$ jittering (MCMC) $\rightarrow$ evaluation of the solution map $K \longleftrightarrow$ computationally expensive $\Rightarrow$ quantify the non-uniformity/variance of the weights using the *effective sample size (ess)* statistic:

$$ess(\bar{w}) = \frac{1}{\sum_{l=1}^{N} (\bar{w}^l)^2}$$

- π_t^N can become degenerate exponentially fast in high dimensions $\longleftrightarrow$ low ess $\Rightarrow$ tempering $\Rightarrow$ smoother transitions between posterior distributions
- standard particle filters do not work in high-dimensional systems

Particle Filters - Algorithm[6]

- Draw independent samples $x_0^l \sim \pi_0, l = 1, 2, \ldots, N$ and assign equal normalised weights $\bar{w}_0^l = 1/N$
- For $i = 1, 2, \ldots$ do
  - Compute $x_{t_i}^l = K(x_{t_{i-1}}^l, \omega^l, t_i) l = 1, 2, \ldots, N$
  - Collect observation y_i and compute the weights $\bar{w}_i^l \propto \bar{w}_{i-1}^l g_i^{y_i}(x_i^l), l = 1, 2, \ldots, N$
  - If $ess < N_{threshold}$ then
    - Sample $\tilde{x}_i^l, l = 1, 2, \ldots, N$ according to the weights $\bar{w}_i^l$
    - Assign equal weights $\bar{w}_i^l = 1/N$
    - If there are duplicates then do jittering and obtain the jittered set $\tilde{\tilde{x}}_i^l$
    - Set $x_i^l = \tilde{x}_i^l = \tilde{\tilde{x}}_i^l$
  - end If
- Move on to the next For loop cycle.

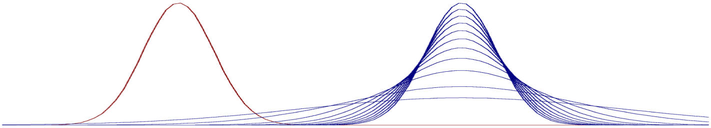
Tempering[6]

- Sometimes the *ess* is smaller than a representative threshold $N_{threshold} \leftrightarrow$ equal-weighted particles concentrate in a 'wrong' direction
- Tempering: increase gradually the variance of the distribution so that $N_{threshold}$ is attained, then resample $\Rightarrow$ a more diverse ensemble of particles which are samples corresponding to a sequence of *altered* distributions $\rightarrow$ repeat until the original distribution is recovered
- Sequence of *temperatures* $0 = \phi_0 < \phi_1 < \dots \phi_R = 1 \Rightarrow$ sequence of tempered posteriors with corresponding normalised tempered weights $(\phi \in (0, 1])$

$$\bar{w}_i^l(\phi, \mathbf{x}) := \frac{exp(-\phi \lambda_i^l)}{\sum_j exp(-\phi \lambda_i^j)}$$

and the corresponding ess

$$ess_i(\phi, \mathbf{x}) := \|\bar{w}_i(\phi, \mathbf{x})\|_{l^2}^{-1}$$

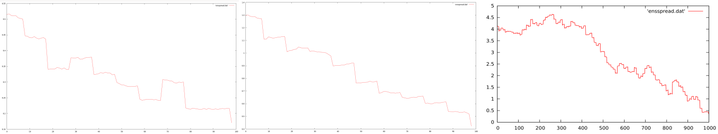


Tempering[6]

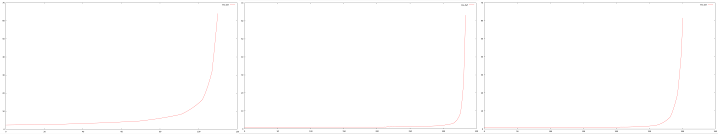
- $t = 0$: Sample N particles from the prior distribution.
- $(t_{i-1}, t_i]$: we have an ensemble $\mathbf{x}$ of particles with positions $(x^l_{t_{i-1}})_l$ and we want to assimilate observational data y_{t_i} in order to obtain a new ensemble $(x^l_{t_i})_l$ that defines $\pi^N_{t_i}$:
  - Evolve $x_{t^l_{i-1}} \xrightarrow[SRSW, Lorenz63]{SPDE} x^l_{t_i}$.
  - Set temperature $\phi = 1$.
  - While $ess_i(\phi, \mathbf{x}) < N_{threshold}$ do
    - Find $\phi' \in (1-\phi, 1)$ such that $ess_i(\phi' - (1-\phi), \mathbf{x}) \approx N_{threshold}$. Resample according to $\bar{w}^l_i(\phi' - (1-\phi), \mathbf{x})$ and apply MCMC with jittering if required (i.e. if there are duplicates) $\Rightarrow$ a new ensemble $\mathbf{x}(\phi')$.
    - Set $\phi = 1 - \phi'$ and $\mathbf{x} = \mathbf{x}(\phi)$.
  - If $ess_i \geq N_{threshold}$ then Stop and go to the $(i+1)^{th}$ filtering step with $(x^l_{t_i}, \bar{w}^l_i)_l$.

Application for Lorenz 63

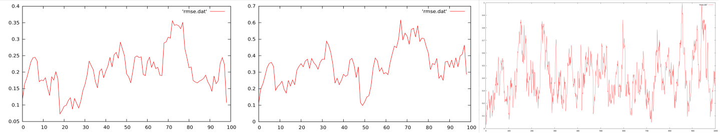
- Ensemble spread



- Effective sample size



- RMSE



Summary

- **Storyline**: Change a classical model in such a way that the missing physics is better represented and therefore we are able to produce a better approximation of the real geophysical processes which characterise the dynamics of the atmosphere (SALT). Show that the new model makes sense from a mathematical point of view (the solution does not blow-up in finite time), and it can eventually be used operationally (it can assimilate real data).

Remarks:

- The atmosphere is more turbulent and faster than the ocean $\Rightarrow$ increased complexity when we go to finer grid scales.
- When the ξ_i parameters are chosen such that they induce enough variability in the particle filter ensemble $\Rightarrow$ the missing physics is also modelled properly.

Results:

- The SRSW model is well-posed in $\mathcal{W}^{1,2}(\mathbb{T}^2) \times \mathcal{W}^{1,2}(\mathbb{T}^2)$.
- An adaptive tempering particle filter has been implemented for both Lorenz63 and SRSW. It produces good results in the first case. Optimal ξ_i parameters are still being tested in the second case. No extra approximations required.

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Thank you!