Ensemble Kalman Filter Adapted to Particle Simulations

Marius Duvillard[1,2], Loïc Giraldi[1], Olivier Le Maître[2]

[1]CEA, DES, IRESNE, DEC, SESC, LMCP, Cadarache, F-13108 Saint-Paul-Lez-Durance, France

[2]Centre de Mathématiques Appliquées, Ecole Polytechnique, IPP, Route de Saclay, 91128, Palaiseau Cedex, France

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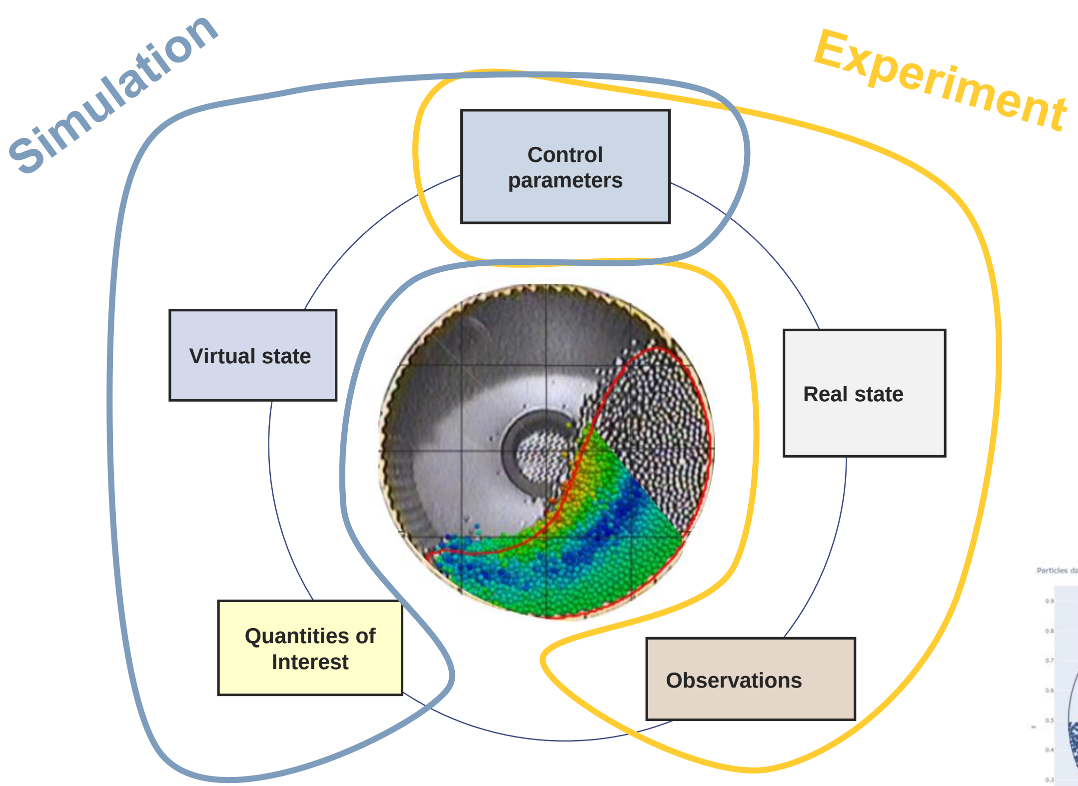
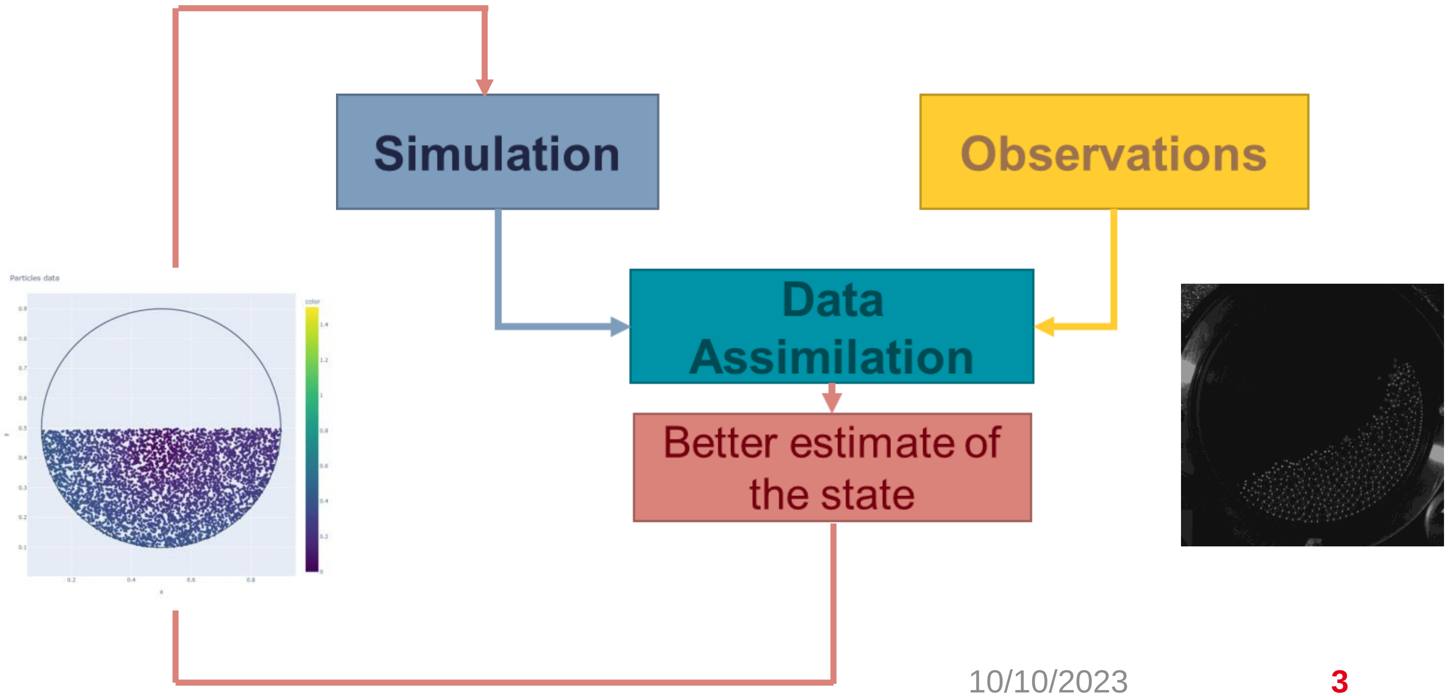
Context - Digital twin of a rotating drum

Définition [Digital twin consortium] : “*A **digital twin** is a **virtual representation** of **real-world entities** and processes, **synchronized** at a specified frequency and fidelity.*”



Goal: Approximate the true state of the system using a dynamic model and observations in an optimal way

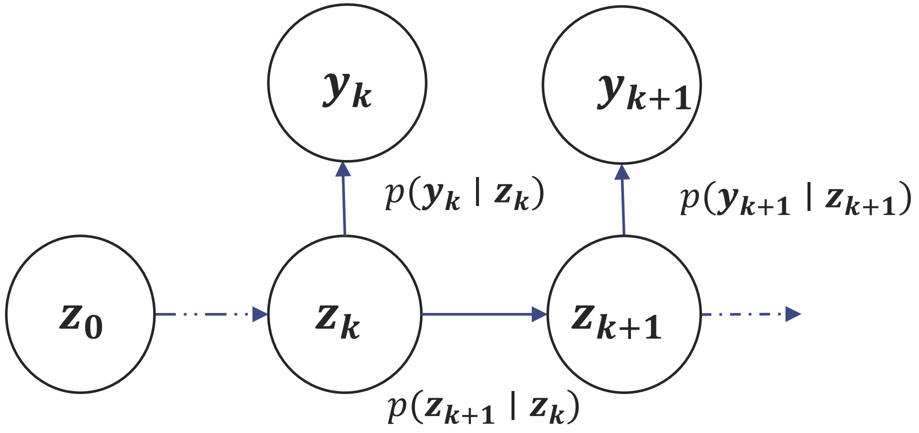
→ Data Assimilation



Ensemble Kalman Filter

- **Data Assimilation:** Is an approximation of the true state $\boldsymbol{X_t}$ by combining, in some optimal fashion, the time-distributed observations $[\boldsymbol{Y_1}, \ldots, \boldsymbol{Y_t}]$ with the dynamic model $\boldsymbol{M}$, taking into account the background (prior) $\boldsymbol{X_0}$ information. (see Asch et al., 2016)

- **Hidden Markov Chain Model**:
  - State and initial conditions: $\boldsymbol{X_0} \in \mathbb{R}^n, \boldsymbol{X_0} \sim \mathcal{N}\left(\boldsymbol{x_0^f}, \boldsymbol{P_0^f}\right)$
  - Forecast equation: $\boldsymbol{X_{t+1}} = \boldsymbol{M_t}(\boldsymbol{X_t}) + \boldsymbol{\eta_t}, \quad \boldsymbol{\eta_t} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{Q_t})$
  - Observation equation: $\boldsymbol{Y_{t+1}} = \boldsymbol{H_{t+1}}(\boldsymbol{X_{t+1}}) + \boldsymbol{\epsilon_{t+1}}, \quad \boldsymbol{\epsilon_{t+1}} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{R_{t+1}})$
  - $\boldsymbol{X_0} \perp \{\boldsymbol{\eta_n}\} \perp \{\boldsymbol{\epsilon_n}\}$: mutually independant



Markov Chain (unobserved)

- **Sequential Filter:** Update the state $\boldsymbol{x_t}$ given the previous updated state $\boldsymbol{x_{t-1}^a}$

and the current observation $\boldsymbol{y_t}$ based on Bayesian estimation

$$\boxed{p(X_t | Y_t, \ldots, Y_1) \propto p(Y_t \mid X_t)\, p(X_t)}$$

- **Kalman Filter (Kalman 1960):** linear models, normal distributions
- **Ensemble Kalman Filter (EnKF, Evensen 1994)**
  - ☺ Non-linear model, High-dimensional, Uncertainty Quantification of the state
  - ☹ Sampling issue → Localisation and Inflation

Asch, Mark, Marc Bocquet, et Maëlle Nodet. *Data Assimilation: Methods, Algorithms, and Applications*. Fundamentals of Algorithms 11. Philadelphia: Society for Industrial and Applied Mathematics, 2016.

Kalman, R. E. « A New Approach to Linear Filtering and Prediction Problems ». *Journal of Basic Engineering* 82, nº 1 (1 mars 1960): 35-45.

Evensen, Geir. « Sequential Data Assimilation with a Nonlinear Quasi-Geostrophic Model Using Monte Carlo Methods to Forecast Error Statistics ». *Journal of Geophysical Research: Oceans* 99, nº C5 (1994): 10143-62.

Ensemble Kalman Filter

Equivalent formulation to the usual EnKF, see Siripatana et al., 2019 for details

Initialisation: Create an ensemble of $\boldsymbol{N}$ virtual states

$\{\boldsymbol{x}_{0,i}^{f}\}_{i=1}^{N}$ with $\boldsymbol{x}_{0,i}^{f}$ $\boldsymbol{i.i.d.}$

Forecast: Forecast sample with the model $\boldsymbol{M}$ and predict the observation with $\boldsymbol{H}$

$$\boldsymbol{x}_i^f = \boldsymbol{M}(\boldsymbol{x}_i^a),$$

$$\boldsymbol{h}_i^f = \boldsymbol{H}\left(\boldsymbol{x}_i^f\right), \bar{\boldsymbol{h}} = \frac{1}{N}\sum_{k=1}^{N}\boldsymbol{h}_k^f \quad , \boldsymbol{C}_h = \frac{1}{N-1}\sum_{k=1}^{N}(\boldsymbol{h}_k^f - \bar{\boldsymbol{h}})(\boldsymbol{h}_k^f - \bar{\boldsymbol{h}})^T$$

Analysis: Linear combination of the prediction with $\boldsymbol{F}$ depending only on the prediction of observation $\boldsymbol{h}_i$ and observation $\boldsymbol{y}$

$$\boldsymbol{x}_i^a = \boldsymbol{x}_i^f + \sum_{j=1}^{N}\boldsymbol{F}_{ij}(\boldsymbol{y}, \boldsymbol{h}_1, \dots \boldsymbol{h}_N)\boldsymbol{x}_j^f$$

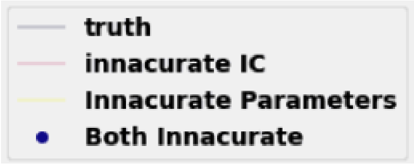
With $\boldsymbol{F}_{ij}(\boldsymbol{y}, \boldsymbol{h}_1, \dots \boldsymbol{h}_N) = \frac{1}{N-1}\left(\boldsymbol{h}_j - \bar{\boldsymbol{h}}\right)^T(\boldsymbol{C}_h + \boldsymbol{R})^{-1}(\boldsymbol{y} + \boldsymbol{\epsilon}_i - \boldsymbol{h}_i)$, and $\boldsymbol{\epsilon}_i \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{R})$

Siripatana, A., L. Giraldi, O. P. Le Maître, O. M. Knio, et I. Hoteit. « Combining Ensemble Kalman Filter and Multiresolution Analysis for Efficient Assimilation into Adaptive Mesh Models ». *Computational Geosciences* 23, nº 6 (décembre 2019): 1259-76.

Example: Lorenz63

Chaotic system: trajectory sensitive to initial conditions and difficult to predict

- **Non-linear model**
- **Uncertainties sources**:
  - Initial conditions
  - Model parameters (σ, ρ, β)
  - Observation errors

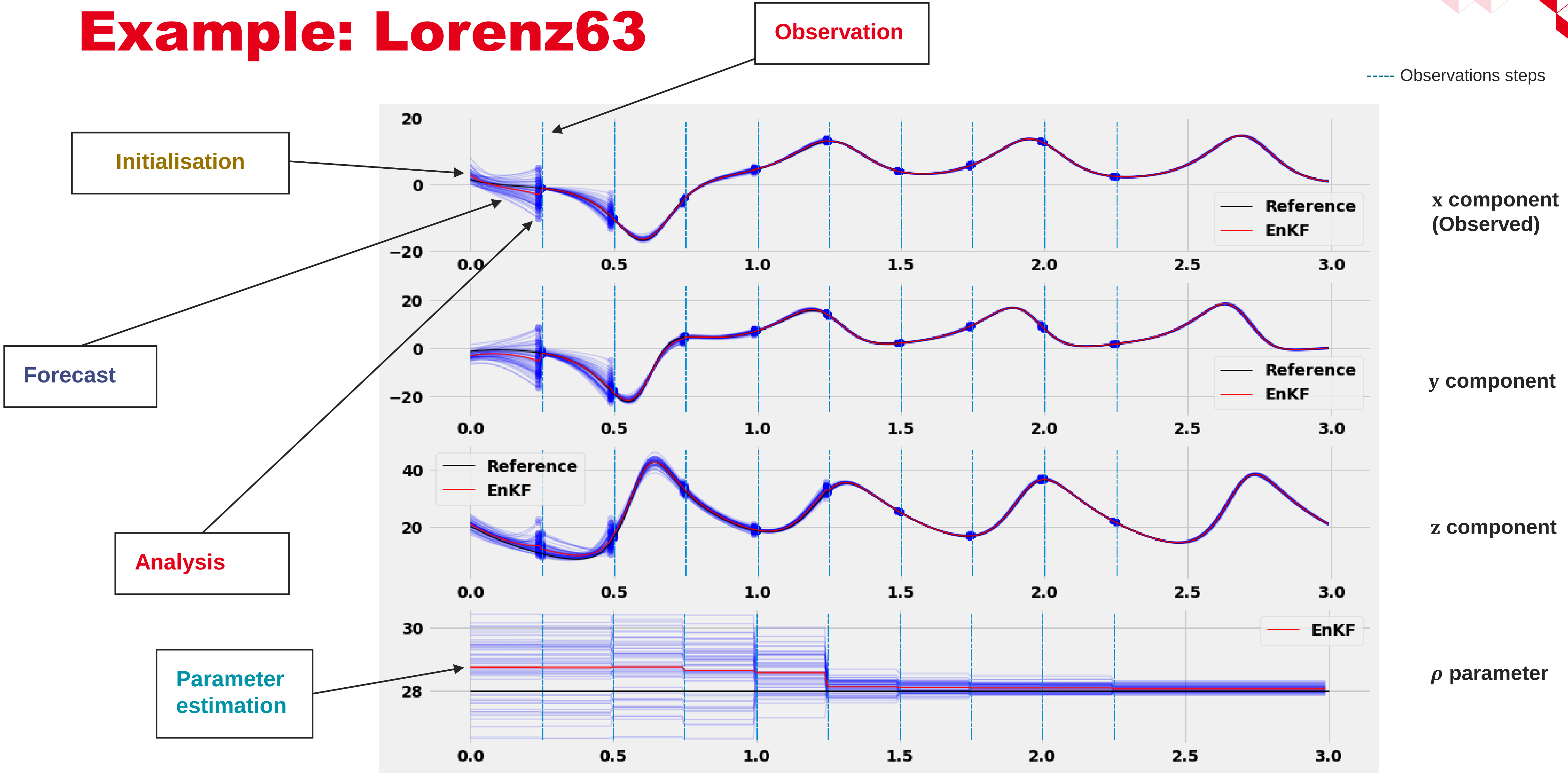


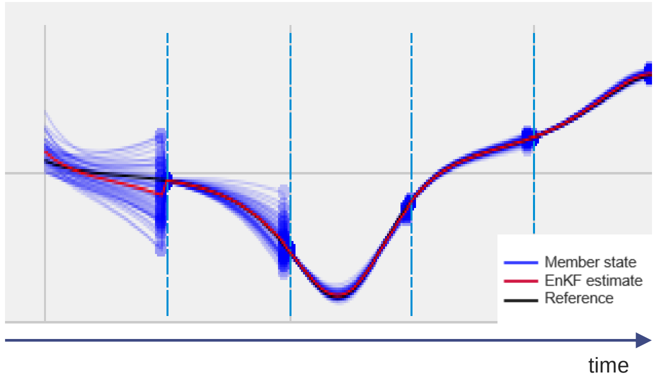
$$X = (x, y, z) \in \mathbb{R}^3$$

$$\begin{cases} \dfrac{\mathrm{d}x}{\mathrm{d}t} = \sigma\,[y(t) - x(t)] \\ \dfrac{\mathrm{d}y}{\mathrm{d}t} = \rho\, x(t) - y(t) - x(t)\, z(t) \\ \dfrac{\mathrm{d}z}{\mathrm{d}t} = x(t)\, y(t) - \beta\, z(t) \end{cases}$$

Observation : $h(X) = x$

Example: Lorenz63





Member state
EnKF estimate
Reference

Reference
EnKF

Modelisation

Continuum methods

Discrete methods

Well developped

My Focus

Costly

Mesh-based methods

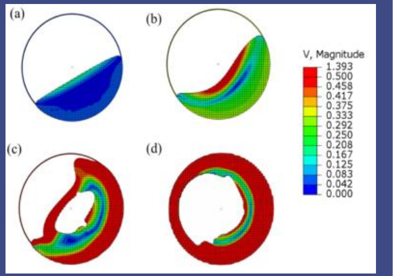
Particle-based methods

N-Body Equilibrium

Euler **Finite Element Method** (EFEM)

[Q.J. Zheng, 2015]

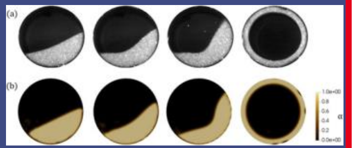
Loi de Druker-Prager



Computational Fuid Dynamics, Finite **Volume Method** (FVM)

[Arseni et al. 2020].

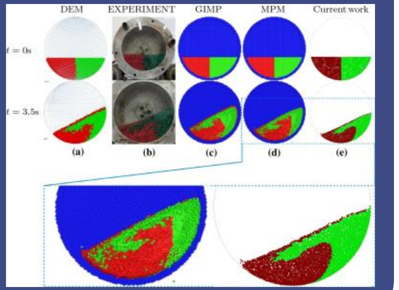
Loi rhéologique $\mu(I)$



Material Point Method (MPM)

[Zuo et al. 2020, Chandra et al. 2021]

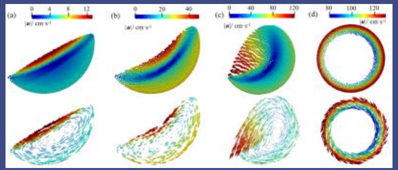
Loi de Druker-Prager / Loi rhéologique $\mu(I)$



Smoothed Particle Hydro-dynamics (SPH)

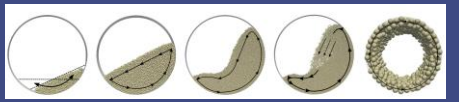
[Zhu et al. 2022]

Loi rhéologique $\mu(I)$



Discret Element Method (DEM)

[Condall 1972],[Mishra and Rajamani 1991],[Orozco 2020]



Limitations and issues with particles simulation

How to define the state?

***Eulerian method**: Node values*

***Lagrangian discretization:** Particle positions and intensities? Different numbers of particles?*

- Darakananda et al. 2018 apply EnKF for Vortex Method directly on quantities of particles in a case of constant number of particles

How to update the state?

***Eulerian method**:*

***- Single mesh for all members**: Linear combination of node values on a common mesh*

- Otherwise: Projection over different meshes (Multi Resolution Analysis, Siripatana et al. 2019, Moving mesh simulation Bonan et al. 2018)

Lagrangian discretization:

- Each member has its own particle representation: Linear combination of all members is prohibitive → **exponential growth** of the total number of particles

Darakananda, Darwin, Andre Fernando De Castro da Silva, Tim Colonius, et Jeff Eldredge. « Data-assimilated low-order vortex modeling of separated flows ». Physical Review Fluids, 2018.

Siripatana, A., L. Giraldi, O. P. Le Maître, O. M. Knio, et I. Hoteit. « Combining Ensemble Kalman Filter and Multiresolution Analysis for Efficient Assimilation into Adaptive Mesh Models ». *Computational Geosciences* 23, nº 6 (décembre 2019): 1259-76.

Bonan, Bertrand, Nancy Nichols, Michael Baines, et Dale Partridge. « Data assimilation for moving mesh methods with an application to ice sheet modelling ». *Nonlinear Processes in Geophysics* 24 (2017)

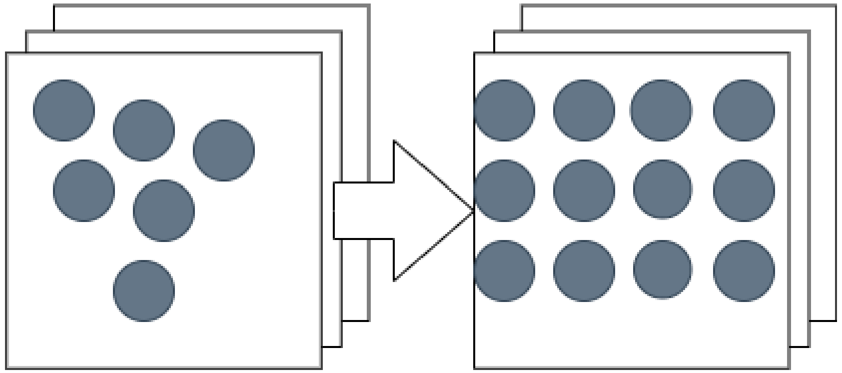
New approaches

Remesh-EnKF

Idea: Define a common particle space by *remeshing* the particle distribution

- Single particle distribution for all members

→ Require a remeshing operator



N_p configurations

One common discretization

Part-EnKF

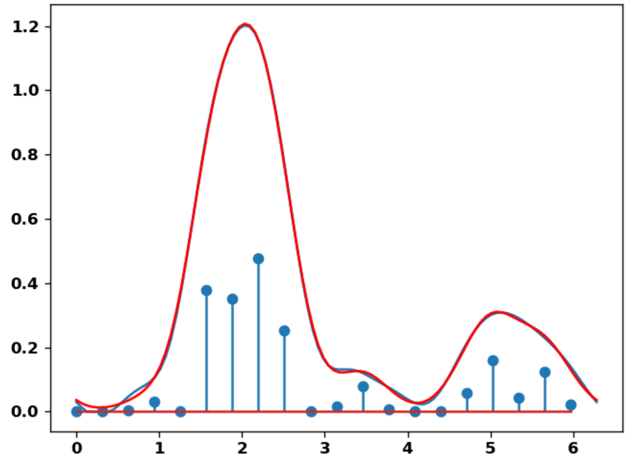
Idea: Update the intensity of the particles of each members

- The particle discretization do not change

→ Require an approximation operator

→ Interpolation

→ Regression

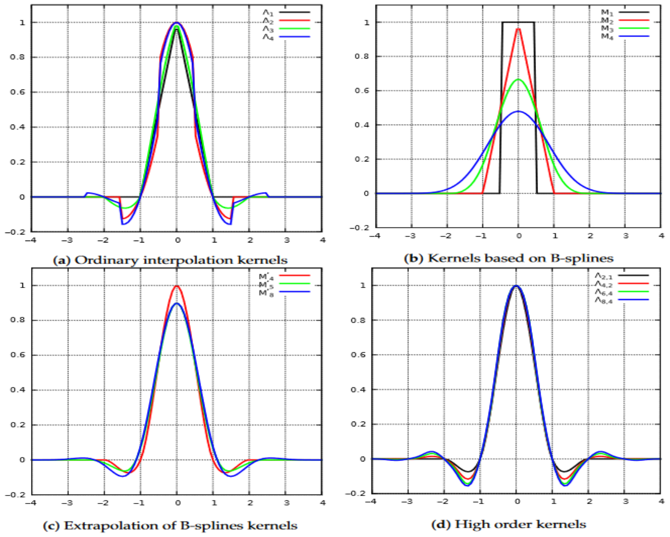


Update particle intensity to fit the analysed field u^a

Remesh-EnKF

Assumption: All members have the same particle discretization

Principle: Remesh each member on a common particle discretization



Different 1D remeshing kernel $\boldsymbol{W}$ from (Mimeau et Mortazavi, 2021)

Remeshing (see Cottet, G., & Koumoutsakos, P., 2000, chap. 7-8).

- Generate a **regular grid** of particles at the position $\boldsymbol{z_q}$
- **Intensities of particles** $\boldsymbol{U_q}$ are obtained by redistributing the previous $\boldsymbol{U_p^{old}}$ using a remeshing kernel $\boldsymbol{W}$

$$\boldsymbol{U_q = \sum_{p=1}^{N_p} U_p^{old} W\left(\frac{z_p^{old} - z_q}{h}\right), 1 \leq q \leq N'}$$

- W is chosen to conserve particle distribution moments:

$$\boldsymbol{\sum_q U_q\, z_q^{\alpha} = \sum_p U_p^{old} z_p^{old,\alpha}, 0 \leq \alpha \leq r,}$$

Compute the correction matrix F
- From observation and predictions

Remesh
- Generate a new commun particle discretization

Update
- Update new particles intensities

Update

- The Analysis is directly applied on the new intensities

$$\boldsymbol{U_{i,t}^{a} = U_{i,t}^{f} + \sum_{j=1}^{N} F_{ij} U_{j,t}^{f}}$$

Cottet, G., & Koumoutsakos, P. (2000). Lagrangian Grid Distortions: Problems and Solutions. In Vortex Methods: Theory and Practice (pp. 206-236). Cambridge: Cambridge University Press. doi:10.1017/CBO9780511526442.008

Mimeau, Chloé, et Iraj Mortazavi. « A Review of Vortex Methods and Their Applications: From Creation to Recent Advances ». Fluids 6, nº 2 (2021): 68.

Part-EnKF

Assumption: The fields can be evaluated at any point of the space.

Principle: Update only the intensities of particles (same positions).

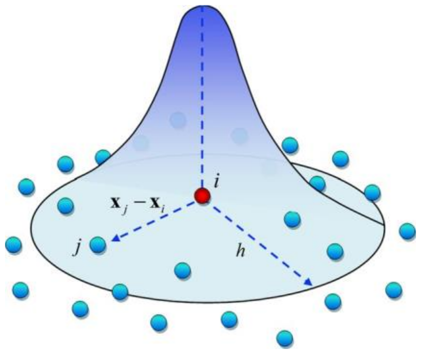
The prediction solution could be evaluate over the spatial domain, for $z \in \Omega$

$$u(z) = \sum_p U_p \, \phi_h(z - z_p)$$

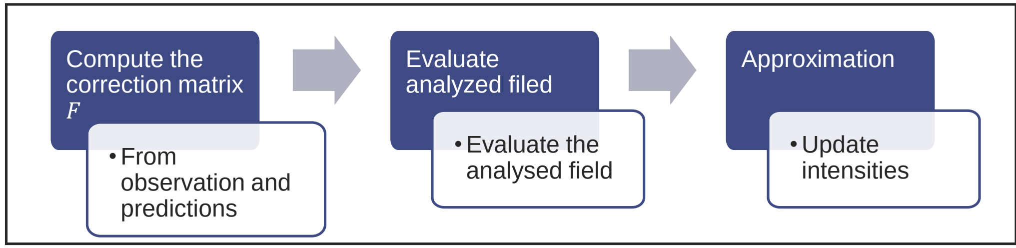
The analysed field u^a is evaluated by a linear combinaison of the forecast fields

$$u_i^a(z) = u_i^f(z) + \sum_{j=1}^{N} F_{ij} u_j^f(z)$$

Update the particle intensities U_p based on an approximation of u_i^a



[from Mohd Atif et al., 2019]



Mean value approximation

$$U_p^a = u^a(z_p)\, V_p, \quad 1 \leq p \leq N_p$$

Kernel Regression

$$\sum_{p=1}^{N_p} U_p^a \phi_h(z_q - z_p) \approx u_i^a(z_p), \quad 1 \leq q \leq N_p$$

Minimise the **Least Square Error,**

$$\mathcal{L}_q(\boldsymbol{U}) = \sum_p \left[u_q^a(z_p) - \sum_{p=1}^{N_p} \boldsymbol{U}_p \phi_h(z_q - z_p) \right]^2 = \left\| \boldsymbol{u}_q - \boldsymbol{\Phi}\mathbf{U} \right\|_2^2$$

Ill-conditioning problem → Relocate particles & regularization (Ridge, Lasso, Thikonov and see *Nocedal, Jorge, et Stephen J. Wright. Numerical Optimization. 2nd ed. Springer Series in Operations Research. New York: Springer, 2006.*

2D Vortex Method

Vortex Method: Used to solve uncompressible flow (Cottet and Koumoutsakos, 2000, Mimeau and Mortazavi, 2021)

- Each particle in position $\boldsymbol{x}_p$ transport a quantity of circulation Γ_p

$$\omega(\boldsymbol{x}, t) = \sum_{p=1}^{m} \Gamma_p \phi_h(\boldsymbol{x} - \boldsymbol{x}_p)$$

- Euler equation for inviscid flows. The vorticity $\omega = \nabla \times \boldsymbol{v}$ satisfies

$$\frac{\partial \omega}{\partial t} + (\boldsymbol{v} \cdot \nabla)\omega = 0\,, \nabla \cdot \boldsymbol{v} = 0 \Rightarrow \frac{d\Gamma_p}{dt} = 0, \frac{d\boldsymbol{x}_p}{dt} = \boldsymbol{v}(\boldsymbol{x}_p)$$

- Non-linear dynamic model
- Non-uniform particle distribution
- 2d velocity field only modeled through a scalar field

Reference: A Lamb–Chaplygin dipole → propagates at a translation velocity U

Orlandi, Paolo (August 1990). "Vortex dipole rebound from a wall". *Physics of Fluids A: Fluid Dynamics*. **2** (8): 1429–1436

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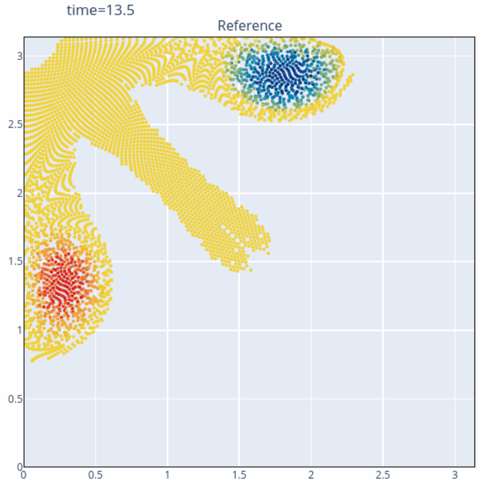
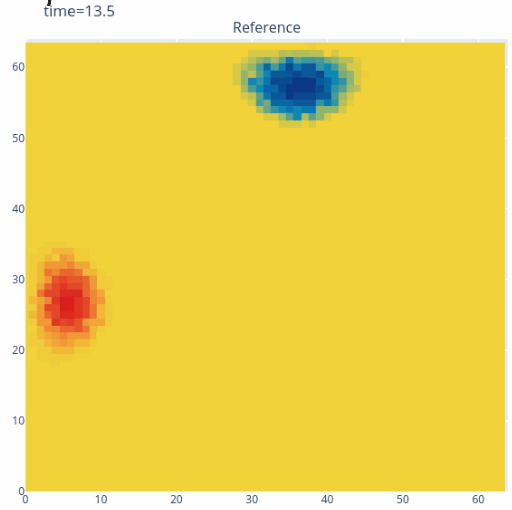


Particle discretization with particles circulations

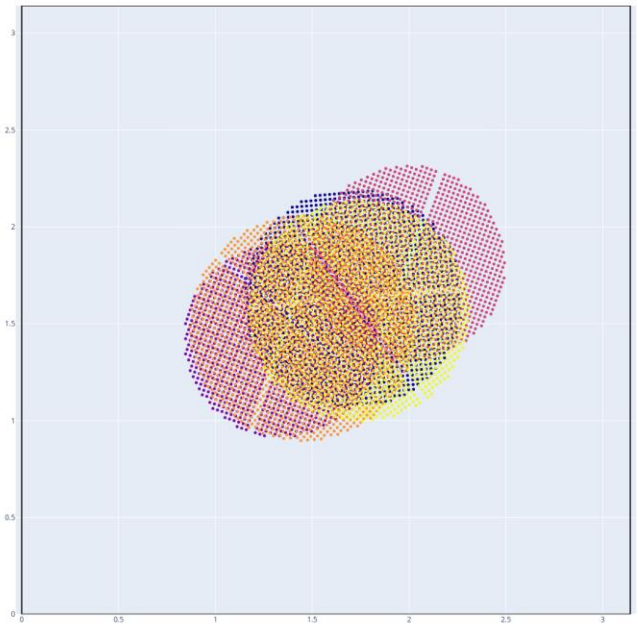


Vorticity field on a regular grid

Generation of the ensemble

Ensemble :

- Sample 50 members from a distribution of dipole with uncertainty on the **orientation**, The **translation velocity,** the **mean position,** the **radius** of the dipole



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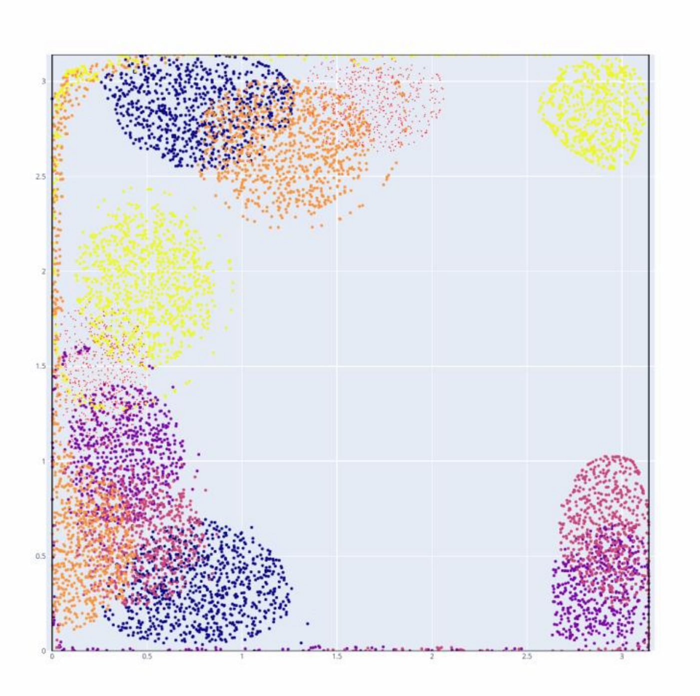
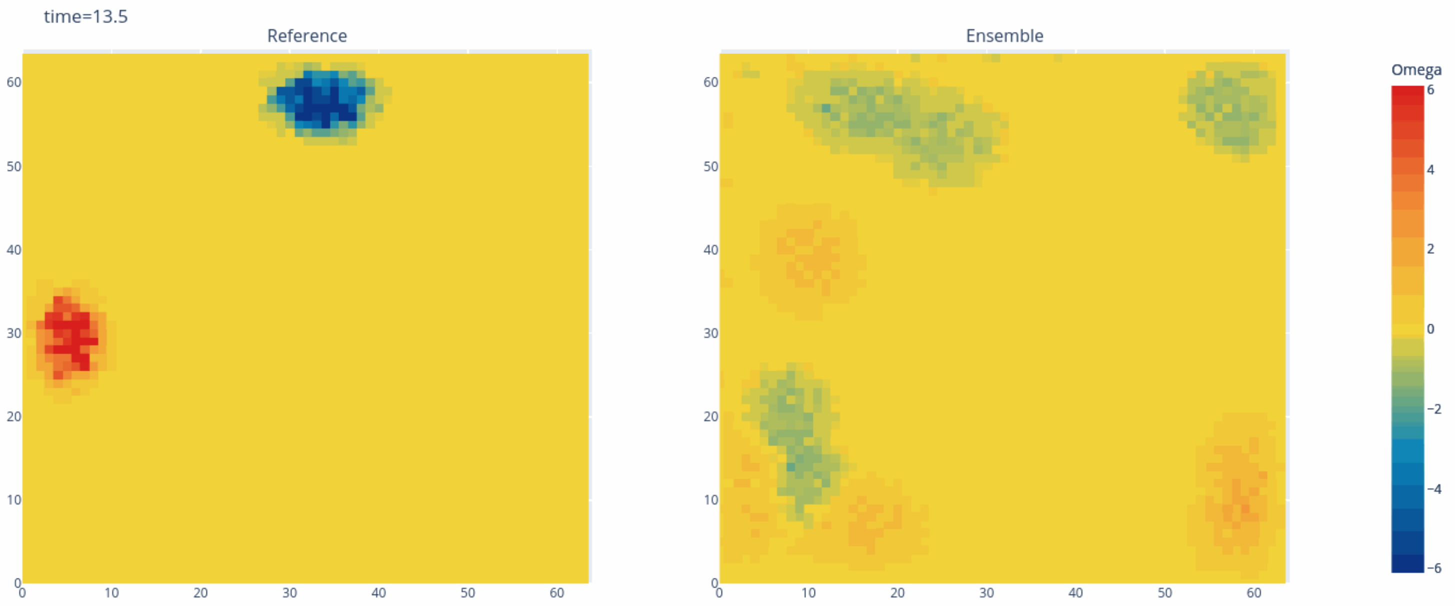
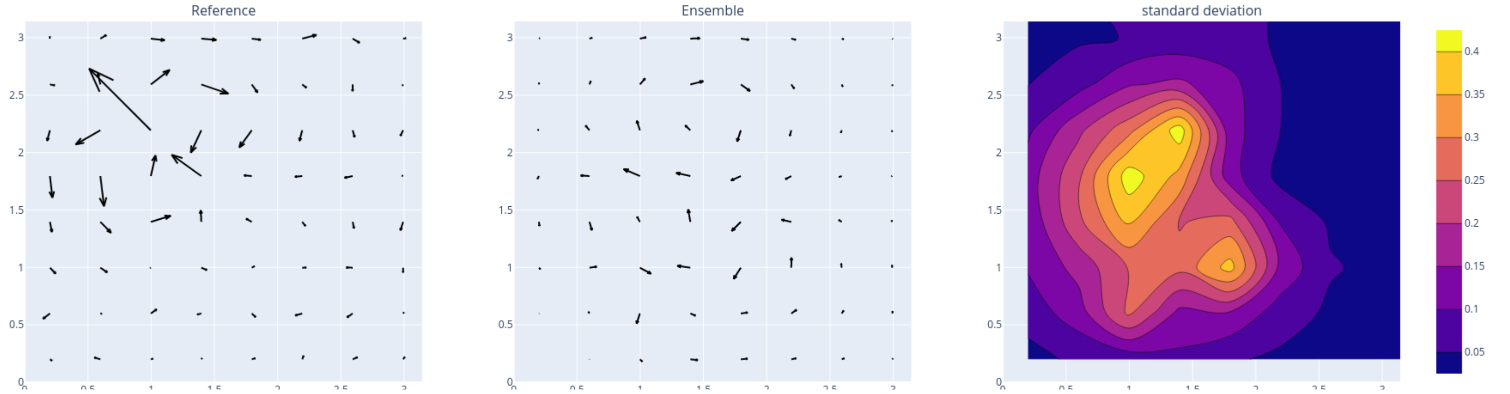


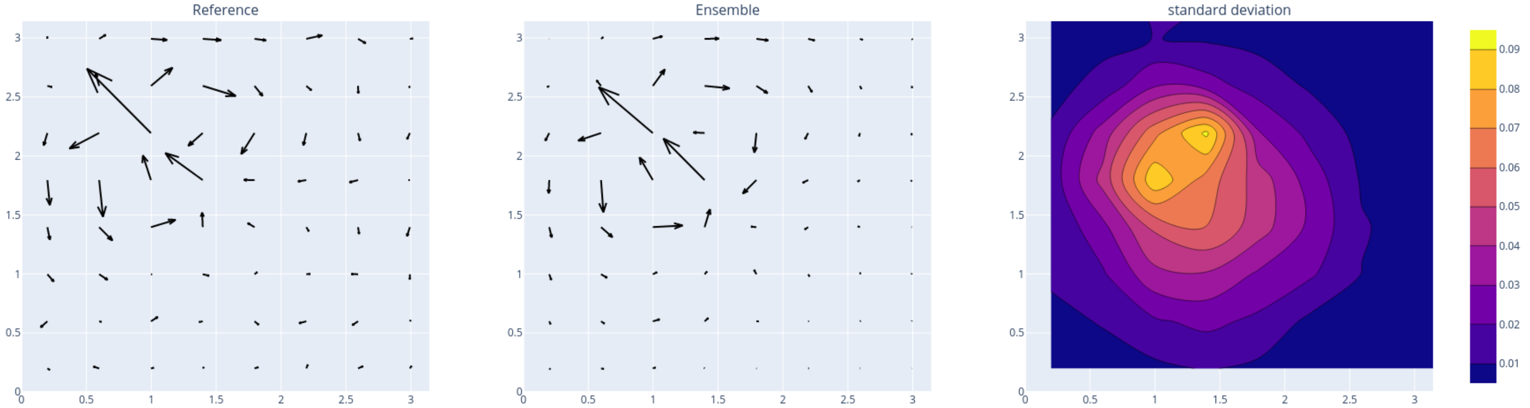


Observation and analysis

Observe the velocity on a coarse regular grid (8x8) with observation noise

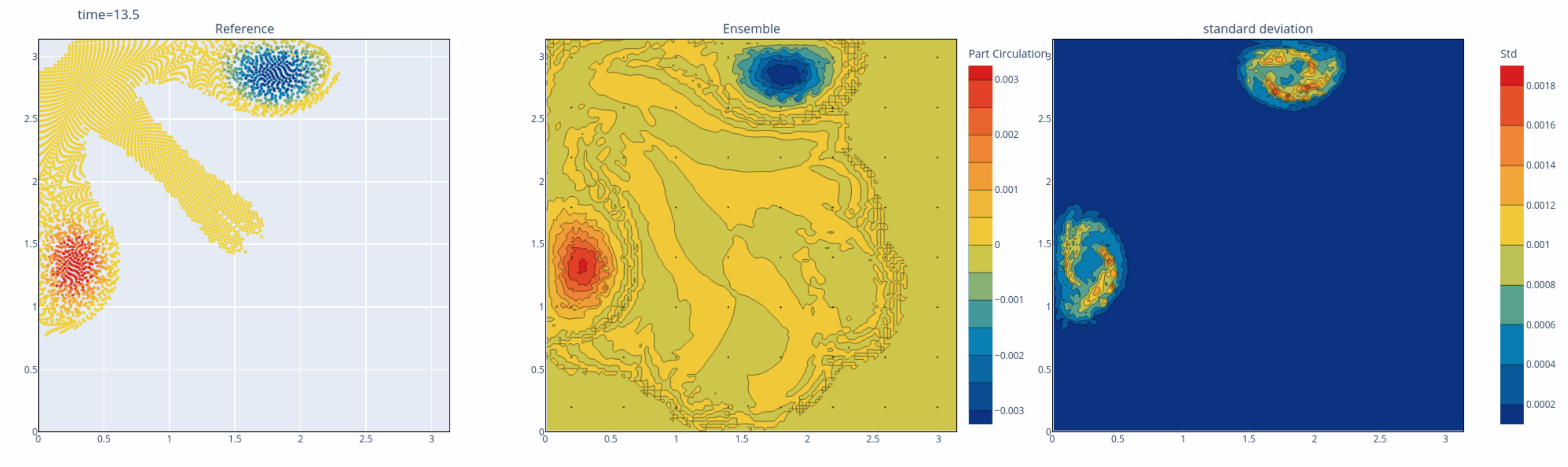


Predicted observations



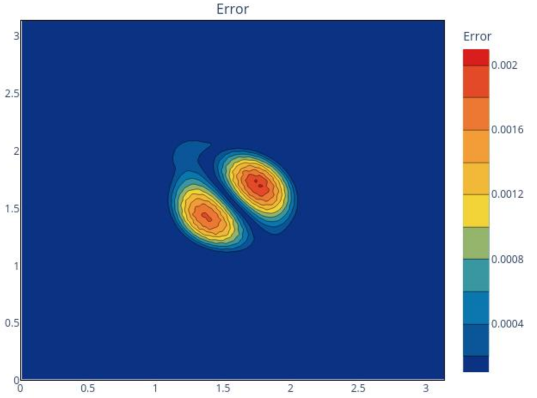
Observation prediction afiter analysis

Filtering

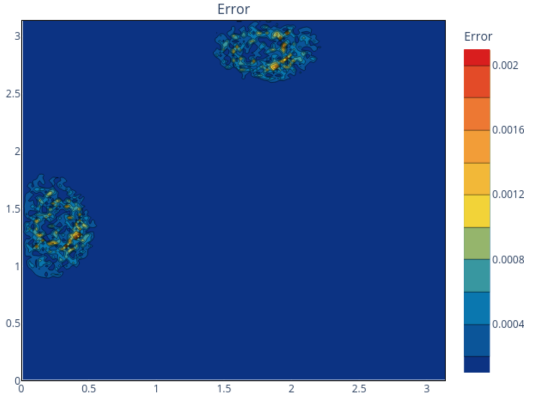


Reference, Ensemble contour-plot, Standard deviation through space

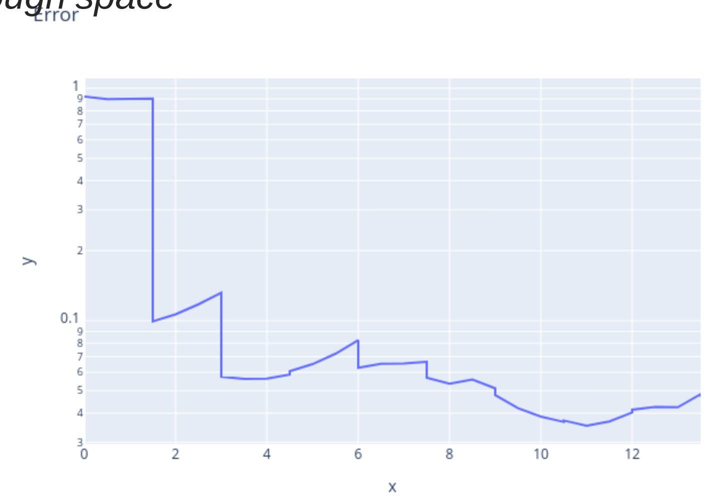
Remesh-EnKF Filtering



Error at $t = 0s$



Error at $t = t_f$



Evolution of the normalized error with respect to time

Comparison

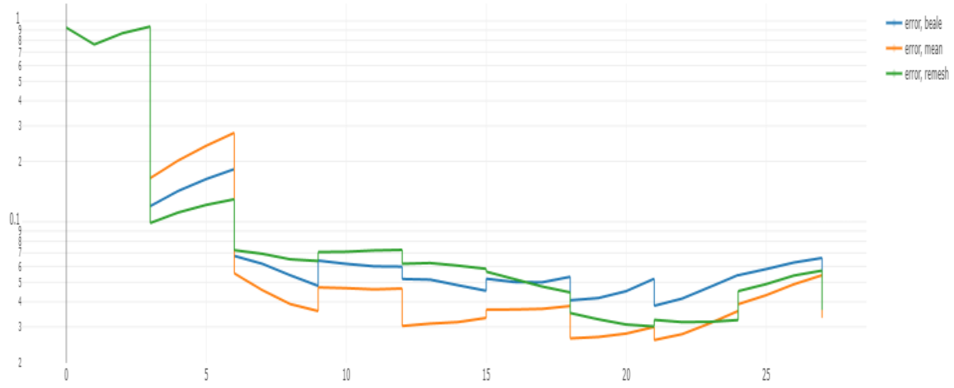
Good agreement with reference state ($\sim 4\%$ error)

Remesh-EnKF

- The regridding process introduced dissipation

Part-EnKF

- Keep a complete Lagrangian discretization with an update at the particle level
- Need to deal with different particle domain discretization
- Ill-condition regression problem needing particle relocation at the member border & regularization



Evolution of the normalized error with respect to time for different filters

Conclusions and Perspectives

Conclusions

1 – Ensemble Data Assimilation for some Lagrangian methods

2 - Two ways

2.1 By projection on a new common grid of particles

2.2 Directly treating the forecast particle configuration

Perspectives

A publication in progress on those methods

Extension for Material Point Method (MPM)