Ensemble-based data assimilation for meshless simulations

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Introduction

- **Context**
  - **Meshless simulations**
    - **Lagrangian** representation of the solution
    - Adapted to **complex geometries** with **large deformations** and changes in the shape of a continuum (fragmentation, free-surface flow,. . .)
    - Applied to the resolution of flow problems (SPH, Vortex Method,. . .),or solid mechanics (MPM,. . .)
  - **Ensemble-based data assimilation**
    - Combining data and model solution to improve prediction
    - Correction of solution state with observations
    - Ensemble of states is used to approximate the solution pdf.
    - Ensemble Kalman Filter (EnKF), mainly used for this applicability to **high-order non-linear** models
- **Challenges**
  - Each member have a different state discretization $\neq$ common mesh discretization
  - Could not be directly used for meshless simulations
  - Given any analyzed field, the forward particle discretization may not support the solution
- **Goals**
  - **Propose** ensemble methods adapted to meshless simulations, avoiding as much as possible, remeshing process, or intermediate grid transfer
  - **Apply** those adapted method to a 1d transport case and a 2d vortex method simulation

Background

Meshless simulation

Particle approximation

$$u(\boldsymbol{z}) \approx \sum_{p=1}^{N_p} U_p \phi_\varepsilon(\boldsymbol{z} - \boldsymbol{z}_p),$$

- N_p the number of particles,
- $\boldsymbol{z}_p$ the position of the p-th particle,
- U_p its intensity,
- ϕ the *smoothing* kernel function,
- ε a smoothing length.

Operators

Some operators used to adapt the particle approximation (previously introduce to avoid high *distortion* in particle distributions [1, 3])

Interpolation operator

Change particle intensities, knowing particle positions $\boldsymbol{z}_q$, from field values $u(\boldsymbol{z}_q)$ through *interpolation*

$$\sum_{p=1}^{N_p} U_p \phi_\varepsilon(\boldsymbol{z}_q - \boldsymbol{z}_p) = u(\boldsymbol{z}_p) \quad ,1 \leq q \leq N_p, \tag{1}$$

e.g. : Beale's method/iterative methods, *radial basis function* interpolation (RBF).

Remeshing operator

Generate a *regular grid* of new particle locations $\boldsymbol{z}_q$

Obtain the new intensities U_q through a *redistribution* from previous particle discretization using redistribution kernel W_h with h the grid length

$$U_q = \sum_{p=1}^{N_p} U_p^{old} W_h(\boldsymbol{z}_p^{old} - \boldsymbol{z}_q) \quad ,1 \leq q \leq N_q' \tag{2}$$

Data assimilation - EnKF

Ensemble Kalman filter: combines a particle filter forward style and the analysis of the Kalman filter based on the approximation the first and second moment of the state or member predictions [4]

Stochastic Ensemble Kalman Filter:

- Initialisation/Previous step : $\{\boldsymbol{x}_i^f\}_{i=1}^N$,
- Analysis step :$\boldsymbol{x}_i^a = \boldsymbol{x}_i^f + \tilde{\boldsymbol{K}}(\boldsymbol{y} + \boldsymbol{\eta}_i - \mathcal{H}(\boldsymbol{x}_i^f)) = \boldsymbol{x}_i^f + \sum_{j=1}^N F_{ij}\boldsymbol{x}_j^f$,
- Forward step : $\boldsymbol{x}_i^f = \mathcal{M}(\boldsymbol{x}_i^a)$

- $\{\boldsymbol{x}_i^f\}_{i=1}^N$ the ensemble of states,
- $\tilde{\boldsymbol{K}}$ the approximated Kalman filter gain,
- $\boldsymbol{F}$ the correction matrix,
- $\mathcal{M}$, $\mathcal{H}$ the dynamic and observation operator,
- $\boldsymbol{\eta}_i$ a random drawings from the Gaussian observation error distribution $\mathcal{N}(\boldsymbol{0}, \boldsymbol{R})$
- $\boldsymbol{y}$ the observation.

$\boldsymbol{F}$ dependent *only* on the prediction of observations $\mathcal{H}(\boldsymbol{x}_i)$ [2]

EnKF with particle approximation

For **any particle discretization**, The functional representation of each member could be linearly updated such that

$$u_i^a(\boldsymbol{z}) = u_i^f(\boldsymbol{z}) + \sum_{j=1}^N F_{ij} u_j^f(\boldsymbol{z}) \quad ,\forall \boldsymbol{z} \in \Omega \tag{3}$$

For a **common particle discretization** (same $\boldsymbol{z}_p$ for all members), the correction can be apply to particle intensities U_p

$$U_{ip}^a = U_{ip}^f + \sum_{j=1}^N F_{ij} U_{jp}^f \quad ,1 \leq p \leq N_p \tag{4}$$

Method

Filters

- Compute the correction matrix $\boldsymbol{F}$ through the prediction of observations $\mathcal{H}(\boldsymbol{x}_i)$;
- Define different filters depending of the chose of particle discretization or remeshing method

Reference

- In the 1d case, a grid method is used to apply EnKF method on a fixed Eulerian mesh

Particles-Grid EnKF

- *Relocate* particles on the *same regular grid* using (2)
- Update directly new particules intensities with (4)

Particles-Particles EnKF

- Keep the same forward member's particle discretization
- Evaluate the analysis function u^a thanks to (3)
- Determine intensities U_p^a for each members using (1)

Applications

1D case problem

The first problem is the transport of a Gaussian distribution at a constant known velocity v on a 2π-periodic domain

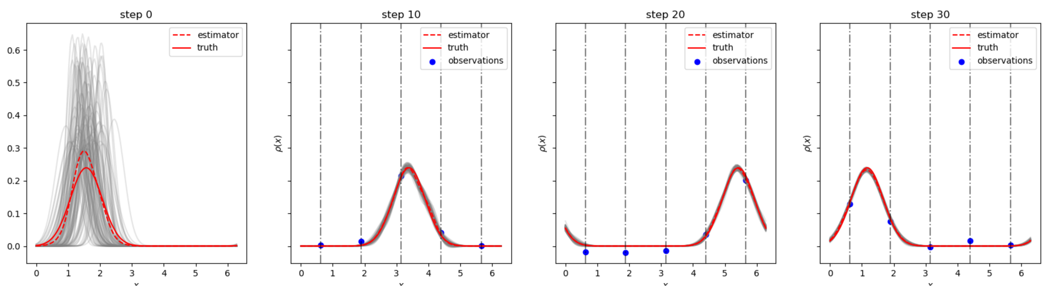
$$\frac{\partial u}{\partial t} + v\frac{\partial u}{\partial z} = 0 \quad \rightarrow \quad \frac{dU_p}{dt} = 0, \quad \frac{dz_p}{dt} = v$$

The analytic solution is simply $u(z, t) = u_0(z - vt \pmod{2\pi})$.

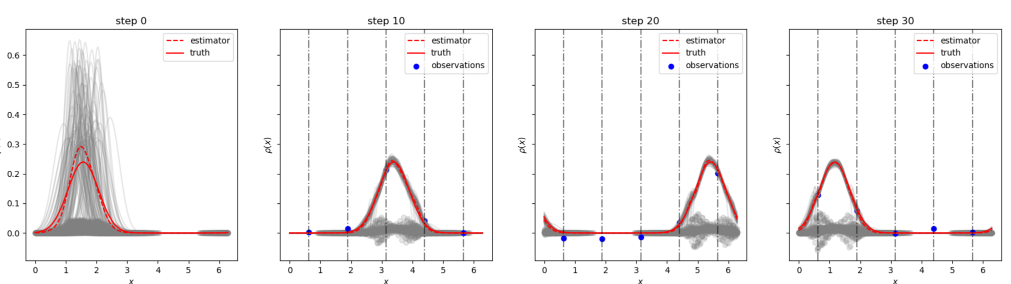
Solution : A Gaussian shape

Prior ensemble : $N = 100$ members, *shifted* and *scaled* Gaussian shapes. Particle locations are *shifted regular* grid. Intensity are fitted with interpolation process and low values are *thresholded*.

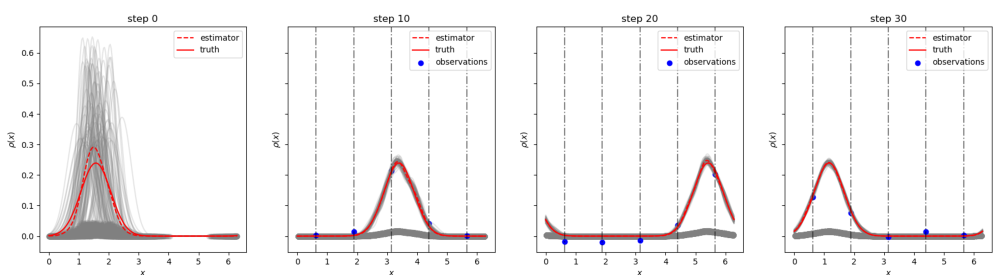
Assimilation parameters : $N_{assim} = 30$ steps, $t_{final} = \frac{2\pi}{v}$, $N_{obs.} = 5$ (regularly spaced).The observation errors follow a centered Gaussian independent distribution.



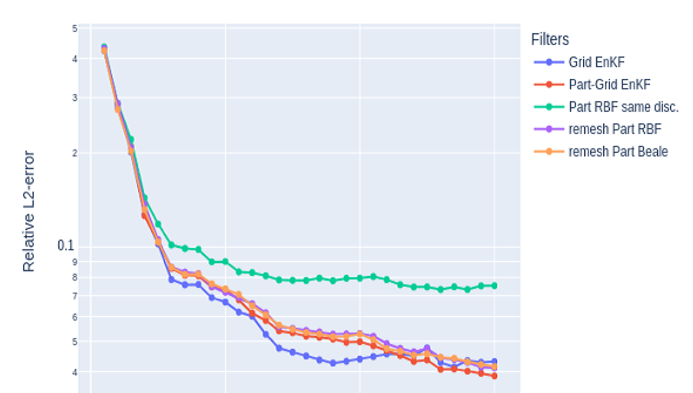
Assimilation snapshots of the reference filter.



Assimilation snapshots of the Particles-Particles EnKF filter.



Assimilation snapshots of the Particles-Grid EnKF filter.



Evolution of the normalized error with respect to number of assimilation for different filters.

2D case problem

Vortex Method:

- Solve the inviscid Navier-Stokes equations (Euler equations)

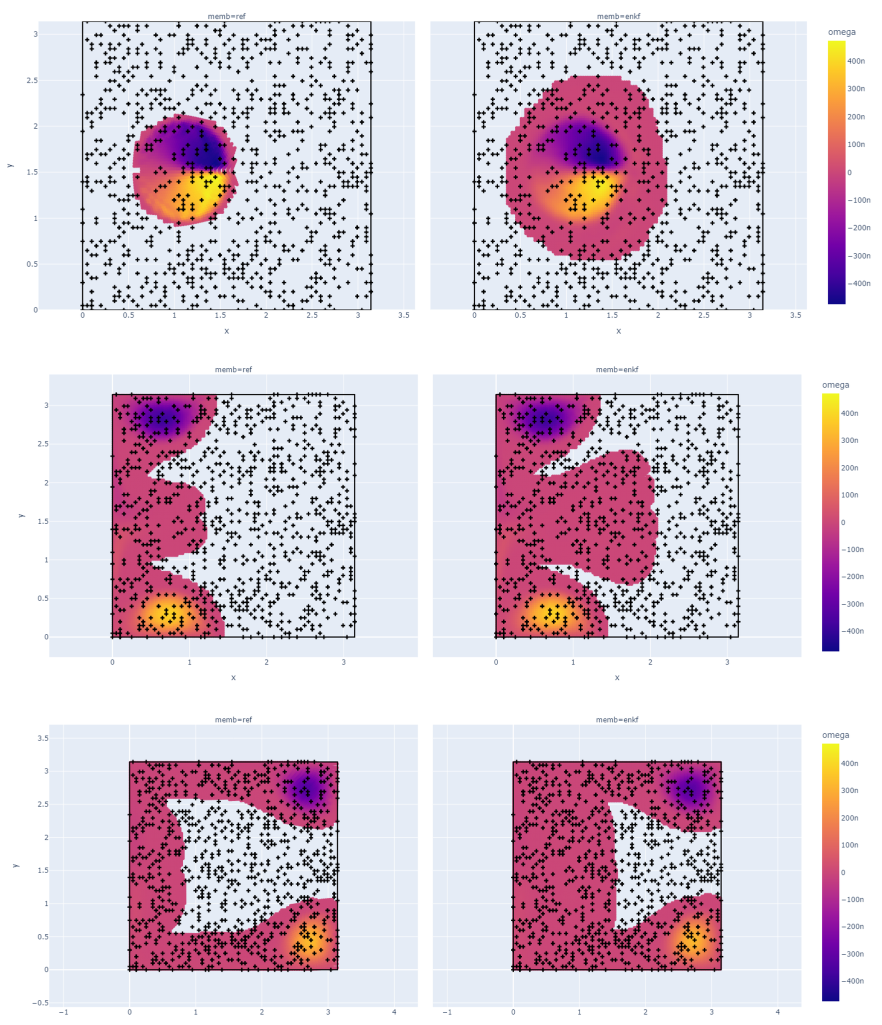
$$\begin{aligned} \frac{\partial \boldsymbol{u}}{\partial t} + (\mathbf{v} \cdot \nabla)\boldsymbol{u} &= 0 \\ \nabla \cdot \mathbf{v} &= 0 \end{aligned} \quad \rightarrow \quad \frac{d\boldsymbol{U}_p}{dt} = 0, \quad \frac{d\boldsymbol{z}_p}{dt} = \boldsymbol{v}$$

- Represent the vorticity field $\boldsymbol{u}$ as a series of discrete vortices $\boldsymbol{u}(\boldsymbol{z}, t) = \sum_{p=1}^m \boldsymbol{U}_p \phi_\varepsilon(\boldsymbol{z} - \boldsymbol{z}_p)$.
- Implement The Vortex In Cell (VIC) version for the computation of $\boldsymbol{v}$

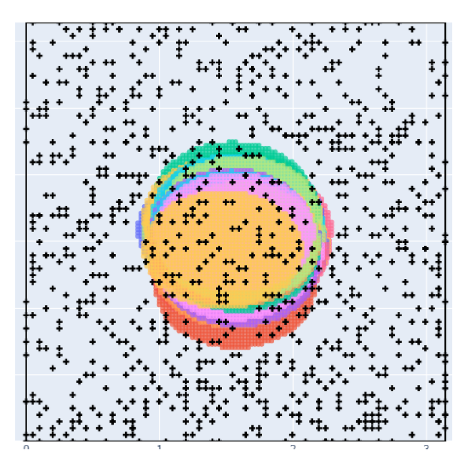
Solution : Initial elliptic dipole of vorticity in the center of a bounded box

Prior ensemble : An ensemble of elliptic dipoles of vorticity, shifted, rotated and scaled in intensity

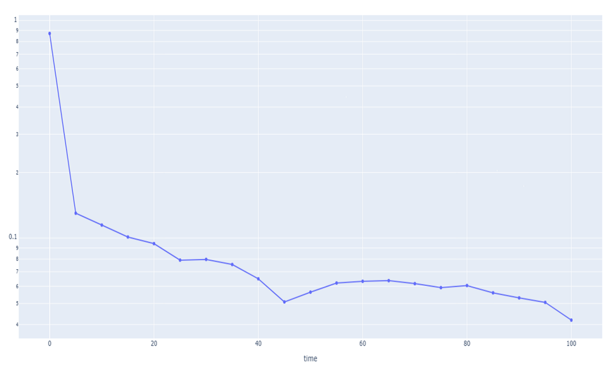
Assimilation parameters : $N_{assim} = 20$ steps, $t_f = 100s$ with $N_{obs} = 1000$ (randomly). The observation errors follow a centered Gaussian independent distribution.



Left: Target, Right : EnKF estimator. For time t=5s, t=50s, t=100s.



Overlapping of initial particle discretizations of members and observation locations in black dots.



Evolution of the normalized error with respect with time.

Conclusion and Perspectives

- EnKF algorithms adapted to meshless simulations are proposed
- The support of particle discrization must be adapted

- 2d flows: Test other filters and investigate the influence of filter parameters
- Computational efficiency: introduce algorithms to speed-up the update step
- Variational data assimilation: integrate constraints or optimize particles properties

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