Data assimilation method for particle-based simulations: EnKF adaptations and optimal transport perpectives

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PhD expected duration: Oct. 2021 – Sep. 2024

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Abstract

Meshless methods are simulation approaches relying on Lagrangian representations that can accommodate complex geometries with large deformations and changes in the shape of a continuum (fragmentation, free-surface flow,...). These methods discretize the continuous fields and operator using an ensemble of particles (computational elements) that move according to a velocity field.The Vortex Method (VM) is one of these methods dedicate to solve the incompressible fluid dynamic [2]. A typical particle approximation $\hat{\omega}$ of a field $\omega(z)$ writes as

$$\omega(z) \approx \hat{\omega}(z) = \sum_{p=1}^{m} \Gamma_p \phi(z - z_p),$$

with m the number of particles, z_p the position of the p-th particle, Γ_i its weight, and ϕ the kernel of the approximation.

This work aims to propose new data assimilation methods adapted for meshless simulations. Data assimilation concerns the update of the model state using sequential observations [4]. Generally, the assimilation problem is formulated either with a variational approach (minimization of a cost function), a Bayesian approach (estimation of the model state's posterior distribution), or a hybridization of the two previous approaches.

Variational methods define the best possible estimate of the state by a weighted least squares problem (3DVar, 4DVar methods). Bayesian approaches approximate distributions usually through a sequential scheme based on the assumption of linear equations and Gaussian noises (Kalman Filter) or a Monte-Carlo approximation (Particle filter). Hybrid approaches combine the benefits of variational analyses with the flexibility of ensemble methods for posterior estimation.

Ensemble approximations of the Kalman filter are called Ensemble Kalman Filters (EnKF) [3]. EnKF methods propagate an ensemble of states to estimate the covariance of the Gaussian forecast distribution (before assimilation) and compute the associated Kalman gain. EnKF methods are applied to high-dimensional non-linear systems without suffering from the curse of dimensionality (thanks to low-rank approximations of the covariance matrices), in contrast to Particle Filters.

Standard EnKF methods use an identical discretization (computational grid) for all members, enabling simple linear combinations of members to define the corrections. This restriction has led our work to introduce two adaptations of this filter that have been previously presented. They are based either on the remeshing of each particle discretization on a common one or by a projection of the analyzed solution on each particle discretization. The two filters have been evaluated on a two-dimensional vortex problem.

Although the two filters offer a way to apply data assimilation techniques, they still face two main issues. On the one hand, they need a remeshing process, which is not in the spirit of Lagrangian methods. On the other hand, the interpolation method requires having particle discretization conform to the analysis one. Usually, this is not the case if the location error is too significant.

This last error is commonly observed in the field of geoscience data assimilation, leading to what is called to the double penalization error, referring to an over-penalization of the model and observation error. To address this issue, new metrics need to be introduced to account for the non-locality error. Various metrics have been introduced for this purpose, based on a step that measures a translation error on the prior and observations [5] or calculates a deformation field that transform the domain [6, 7]. These filter are then based on two-stage scheme, leading to convenient adaptation with classical filter. Nevertheless, others consider to solve this issue in a one-shot scheme using recent advance in Optimal Transport (OT). It consist to use a variational approaches that will use a Wasserstein distance to construct the cost fonction to reduce. This option have been first introduce by Feyel for the assimilation of image. Other improvement are still in work particularly in order to use unbalance OT [1].

Based on these recent advances, we propose in this presentation a data assimilation method that improve our previous filter and overcome the issue linked to non-conforming particle support. Futhermore, it will reduce the non-locality error. The method will be illustrate with two dimensional vortex simulation and compare with previous filters.

Short biography (PhD student)

I'm a PhD student in the CEA center of Cadarache and the Platon team at the Inria Saclay Center (CMAP). I'm currently working on the development of assimilation methods that would be adapted to a grinding mill facilities involved in the fuel manufacturing process.

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