RÉPUBLIQUE FRANÇAISE
Liberté Égalité Fraternité

PROGRAMME DE RECHERCHE
FRANCE 2030
NUMÉRIQUE POUR L'EXASCALE

ExaMA Work Package 4

Inverse Problems

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ExaMA – Exa-scale Methodologies and Algorithms

Overview

WP4 Objectives

- Objective 1: *Improve deterministic inversion methods*
- Objective 2: *Design new stochastic methods for inverse problems*
- Objective 3: *Improve observation strategies*
- Objective 4: *Implement multi-fidelity schedules at exascale*

WP4 Tasks

T4.1 Deterministic methods

T4.2 Stochastic methods

T4.3 Observations

T4.4 Multifidelity: modelling and inverse problems

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Progress

Task 4.1 : Variational data assimilation (Hélène Hénon's PhD)

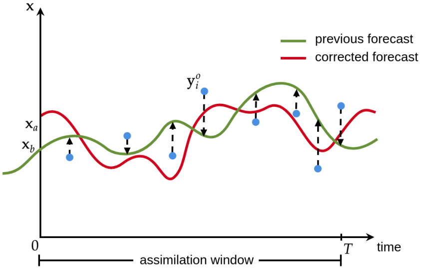
- Forecast the state of the system at the end of a time window by finding the initial condition on this interval
- Minimizing a **cost function** that measures the distance of the state to both the observations and the background :

$$J(\mathbf{x}_0) = \frac{1}{2}(\mathbf{x}_0 - \mathbf{x}^b)^T \mathbf{B}^{-1}(\mathbf{x}_0 - \mathbf{x}^b) + \frac{1}{2}\sum_{n=1}^{N}(\mathcal{G}_n(\mathbf{x}_0) - \mathbf{y}_n)^T \mathbf{R}_n^{-1}(\mathcal{G}_n(\mathbf{x}_0) - \mathbf{y}_n) \quad (1)$$

with $\mathcal{G}_n = \mathcal{H}_n \circ \mathcal{M}_{0,n}$, where :

- $\mathcal{H}_n$: observation operator
- $\mathcal{M}_{0,n}$: model propagating the state $\mathbf{x}_0$ to the state $\mathbf{x}_n$

Iterative minimisation,**sequential** in nature.



Limited Memory Preconditioner (LMP)

- Let $\mathbf{A}_B = \mathbf{B}^{1/2}\mathbf{A}\mathbf{B}^{1/2}$, $\quad \mathbf{b}_B = \mathbf{B}^{1/2}\mathbf{b}$ be the **symmetric** ***B*-preconditioned Hessian**

Truncated eigenvalues decomposition of $\mathbf{A}_B$ with the first l Eigen pairs

$$\mathbf{A}_B \approx \mathbf{S}_l \mathbf{\Lambda}_l \mathbf{S}_l^T \qquad (\lambda_1 \geq \cdots \geq \lambda_l)$$

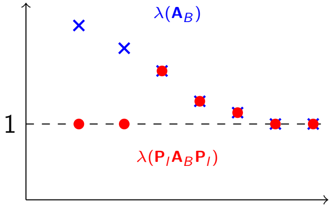
Limited Memory Preconditioner : $\mathbf{P}_l = \mathbf{I} + \mathbf{S}_l \left(\mathbf{\Lambda}_l^{-1} - \mathbf{I}_l\right) \mathbf{S}_l^T$

LMP preconditioned system (Tshimanga et al 2008):

$$\mathbf{P}_l \mathbf{A}^{BP} \mathbf{P}_l \widetilde{\mathbf{x}} = \mathbf{P}_l \mathbf{b}^{BP}$$

Spectral effect

$$\lambda_i(\mathbf{P}_l \mathbf{A}_B \mathbf{P}_l) = \begin{cases} 1, & i \leq l \\ \lambda_i(\mathbf{A}_B), & i > l \end{cases} \Rightarrow \kappa(\mathbf{P}_l \mathbf{A}_B \mathbf{P}_l) < \kappa(\mathbf{A}_B)$$



Less iterations, but still sequential

(Multifidelity) Stochastic Limited Memory Preconditioner

The truncated EVD $\mathbf{A}_B \approx \mathbf{S}_l \mathbf{\Lambda}_l \mathbf{S}_l^T$ is obtained using a **randomized low-rank approximation** (Daužickaitė et al 2021) in two steps:

1. **Range approximation**

   Approximate the range of $\mathbf{A}_B \in \mathbb{R}^{n \times n}$ using $l \ll n$ random vectors:

   $$\mathbf{Y} = \mathbf{A}_B \mathbf{\Omega}, \qquad \mathbf{\Omega} \in \mathbb{R}^{n \times l}$$

   $\Rightarrow$ **Strong parallelism**: l independent matrix–vector products.

2. **Reduced eigenvalue problem**

   Project $\mathbf{A}_B$ onto the approximated range and compute a small eigenvalue decomposition.

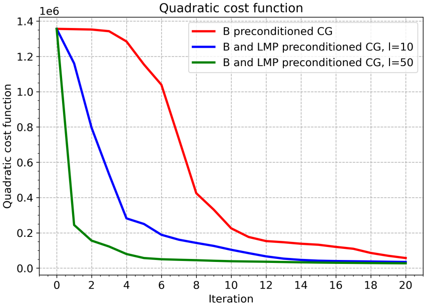
Multifidelity strategy

Use a low-fidelity Hessian to build the range $\mathbf{Y}$

Tests & Ongoing works

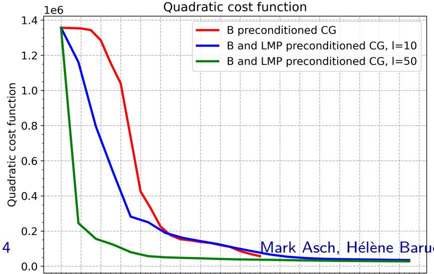
Test case

- 1 iteration of Gauss-Newton
- 2D Shallow-Water model
- Low-fidelity model : single precision
- Grid size : 120×120



Ongoing works

- Theory on a criteria for the low-fidelity model
- Broaden tests on different fidelities
- More demanding application



Task 4.3: Bayesian optimal sensor placement using model gradients (Mohamed Doumbouya's PhD)

Problem: find physically admissible observation operator $\mathbf{V}_s \in \mathcal{K}$ for observing data

$$\boxed{\mathbf{y}_s = \mathbf{V}_s^\top \mathbf{y}}$$

- Bayesian optimal sensor placement

$$\min_{\mathbf{V}_s \in \mathcal{K}} \mathbb{E}_Y \left[D_{\mathrm{KL}}(\underbrace{\pi(\mathbf{x}|\mathbf{y}_s)}_{\text{partial posterior}} \;||\; \underbrace{\pi(\mathbf{x}|\mathbf{y})}_{\text{full posterior}}) \right] \tag{2}$$

Three-issues: (1) $\min_{\mathbf{V}_s \in \mathcal{K}}$ (2) $\mathbb{E}_Y$ and (3) inverse-problems $\pi(\mathbf{x}|\mathbf{y})$

Task 4.3: Bayesian optimal sensor placement using model gradients

For **linear & Gaussian** problems $u(x) = Ax$, closed form expression:

$$\min_{\mathbf{V}_s \in \mathcal{K}} \frac{1}{2} \ln \det \left(I_d - \mathbf{G}^\top \mathbf{V}_s (\mathbf{V}_s \Sigma_Y \mathbf{V}_s^\top)^{-1} \mathbf{V}_s^\top \mathbf{G} \right) \tag{3}$$

For **nonlinear** or **nonGaussian** problems: nasty nested MonteCarlo estimate, super expensive...

Our objectif: find a gradient-based surrogate (upper-bound) for (2) with the same structure as (3)

- Employ functional inequalities to rigorously bound (2)
- Quasi-optimal solution for (2) with same complexity as (3)
- Randomize linear algebra to speed up computation of models gradients
- Compare (or precondition?) with 1.

Task 4.2: Stochastic Methods for Inverse Problems

- Web-book: Kalman Filters—from Bayes to Inverse Problems https://markasch.github.io/kfBIPq/
- Master-Class on Bayesian Inversion:
  - 3 days, ~20 participants (students, doctoral candidates, researchers)
  - Courseware (lectures and practicals) https://github.com/markasch/MAKUTU-BIP
- 3 month internship: Deterministic and Bayesian Inversion for the Helmholtz Equation (ongoing)

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Next Steps

Plans for 2026

- Plan 1: *Recrute candidate for PhD on Bayesian Inversion*

Challenges and Risks

- Challenge 1: *Find the good candidate...*

Conclusion

Summary

- WP4 is *on track and facing challenges*
- Key achievements: *2 PhDs ongoing, training material and session held*
- Next priorities: *Recrute last candidate*

Questions?