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PROGRAMME DE RECHERCHE
NUMÉRIQUE POUR L'EXASCALE

ExaMA Work Package 6

Uncertainty Quantification

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ExaMA – Exa-scale Methodologies and Algorithms

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Overview

WP6 Objectives

- Objective 1: Adaptation of UQ algorithms to exascale numerical simulators (high-dimension output)
- Objective 2: Surrogate modeling of coupled/nested/chained of numerical simulators
- Objective 3: Adaptation of the software platform `Uranie` to exascale applications

WP6 Tasks

- T6.1 Kernel-based sensitivity analysis for high-dimensional data and integral computing
- T6.2 UQ in a PDE solving framework: CFD simulations
- T6.3 Surrogate modeling for UQ
- T6.4 Acceleration of the bricks of the UQ process steps by leveraging exascale calculations

Progress

Key Achievements (2024-2025)

- Achievement 1: Linear constrained prediction of high-dimensional physical fields
- Achievement 2: A new graph kernel to address Gaussian Process Regression with (large) graph inputs
- Achievement 3: Uncertainty propagation of parallelized `TRUST` simulations with `Uranie`

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Technical Highlights

Technical Highlight 1

Prediction of physical fields under linear constraints

Reliable prediction of spatial fields subjected to linear constraints governed by physical laws

- Mahamat Nassouradine's PhD work (2024 - 2027) between CEA Saclay & ENSAI
- Dimensionality reduction of high-dimensional data (i.e. spatial physical fields produced by CFD simulations)
- Preserve the physical constraints in the latent dimensions of the data $\Longrightarrow$ Multi-output Gaussian process regression with constraints-aware covariance kernel on the latent space
- First quarter of 2026 objective: submission to a scientific journal

Technical Highlight 1: Application to the Buice-Eaton diffuser

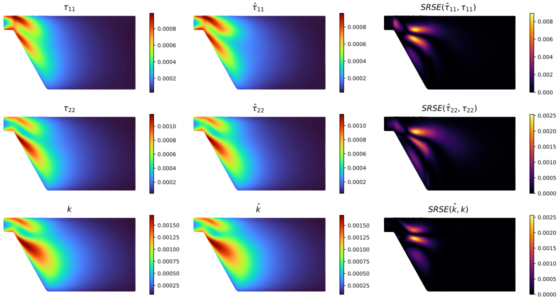


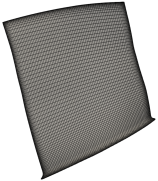
Figure 1: CFD test case. An exemple of fields predicted (left) in comparison to simulated fields (middle) and the Spatial Relative Squared Error (SRSE) (right). From top to bottom, the first and second component of Reynolds stress tensor (τ_{11}, τ_{22}) , and the turbulent kinetic energy k. The images have been horizontally compressed for display purposes.

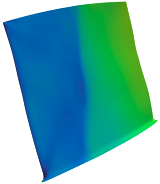
Technical Highlight 2: the Sliced Wasserstein Weisfeiler-Lehman kernel

A new graph kernel to address Gaussian Process Regression with graph inputs

- Raphael Carpintero Perez' PhD work between Polytechnique and SAFRAN
- Supervised learning for datasets consisting of inputs given as meshes (representing the problem geometry seen as graphs) and outputs obtained with a numerical solver.
- A Sliced Wasserstein distance to compare graph representations
- Can manage large graphs (10^5 nodes) with UQ
- Application: Gaussian process regression on high-dimensional simulation datasets from computational physics

3D-mesh corresponding to a turbine blade



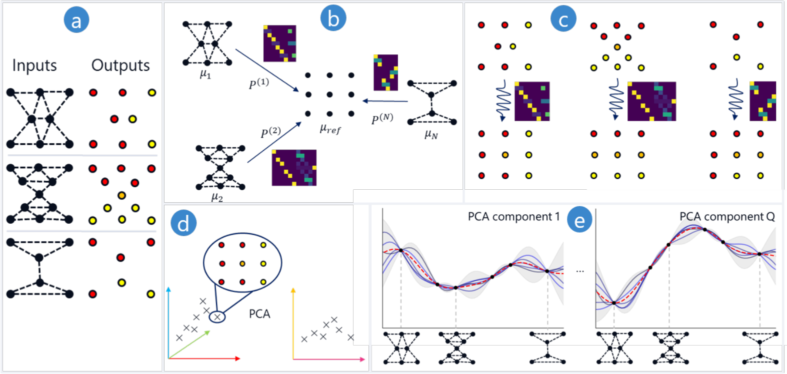


pressure field on the surface of the blade

Technical Highlight 2: the Sliced Wasserstein Weisfeiler-Lehman kernel

A new graph kernel to address Gaussian Process Regression with graph inputs

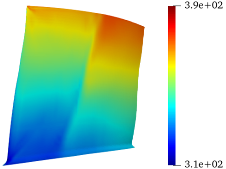
Training:



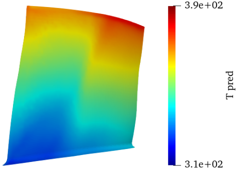
Technical Highlight 2: the Sliced Wasserstein Weisfeiler-Lehman kernel

A new graph kernel to address Gaussian Process Regression with graph inputs

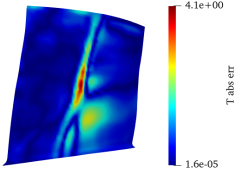
Results (predictions for a new mesh):



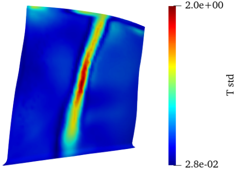
true field



predictive mean



absolute error



predictive standard deviation

Technical Highlight 3

Uncertainty propagation of parrallelized TRUST simulations with Uranie

Parrallel TRUST computation for different parameters values (e.g. Monte-Carlo sampling, ensemble runs)

- Technical tool: ICoCo coupling API between Uranie and TRUST
- Under the hood: Global communicator MPI_COMM_WORLD to organize the double parralelization (for the ensemble runs and the parralel TRUST calculation)

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Collaboration

Collaborations

- Collaboration with WP4:
  Uncertainty quantification of the NumPEx demonstrator `Ktirio Urban Building`.
  WP6 will help improve uncertainty propagation algorithm inside `feel++`
- Collaboration with industrial partners:
  Uncertainty quantification for several computationally intensive problems: design of turbine blade (SAFRAN); fuel assembly bow in pressurized water reactors - involves UQ for coupled, multi-physics codes - in progress (Framatome).
- Collaboration with other academic institutions:
  ICI project: The ICI project (INRIA – Collaboration – IGN) is an epidemic propagation simulator, particularly adapted to COVID-19, based on highly detailed modeling of an urban area and its corresponding population on an individual scale. Importance of UQ for decision making.

Next Steps

Plans for 2026

- Plan 1: Development of high-dimensional quantiles and/or confidence regions for physical fields
- Plan 2: Benchmarking of kernels for Gaussian process regression with mixed inputs (in particular, categorical inputs)
- Plan 3: Multifidelity surrogate modeling
- Plan 4: UQ for coupled, multi-physics codes

Challenges and Risks

- Challenge 1: High-dimensional quantiles: Find the good mathematical object tailored to WP6 objectives
- Challenge 2: Gaussian process regression with mixed inputs: Hyperparameter selection (high-dimensional non-convex optimization)
- Challenge 3: Multifidelity surrogate modeling: description of the relationship between different models (hierarchical, ...).

Conclusion

Summary

- WP6 is on track
- Key achievements on T6.2, T6.3, T6.4; not so much on T6.1 (kernel-based sensitivity analysis)
- Next priorities: high-dimensional quantiles and/or confidence regions for physical fields; Gaussian process regression with mixed inputs; multifidelity surrogate modeling

Questions?