FRANCE 2030

PROGRAMME
DE RECHERCHE

NUMÉRIQUE
POUR L'EXASCALE

ExaMA Work Package 6 -- Feedback Session

Uncertainty Quantification

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ExaMA – Exa-scale Methodologies and Algorithms

Key Takeaways

Key Takeaways from the GA

- Takeaway 1: Exascale applications are storage intensive: developments of online algorithms
- Takeaway 2: Need for good tools for visualization of uncertainties for exascale computations, in particular for high-dimensional outputs
- Takeaway 3: Fractal-based BayesOpt, adaptation for UQ ?

Discussions Summary

Main Discussion Points

- Discussion 1: HPC computation is storage intensive. Sometimes the storage of all ensemble runs is not possible. Online algorithms are dedicated to tackle this issue (i.e. only store a current simulation and delete it after aggregation into dedicated statistical information).

- Discussion 2: Questions about the visualization of uncertainties of (very) high dimensional data (physical fields). Definition and estimation of vector or functional quantiles.

- Discussion 3: Fractal-based Bayesian Optimization is exascale ready. Reflexion about the possibilities to adapt this algorithm for UQ.

Feedback from Other WPs

WP1 ∅

WP2 Interested by Global Sensitivity analysis tools (HSIC indices) from `URANIE`

WP3 ∅

WP4 Interested by multi output Gaussian process regression, visualization and online estimation of statistical quantities (quantiles, ...)

WP5 Explanation to WP6 about fractal-based Bayesian Optimization, interested by Global Sensitivity analysis (HSIC indices) tools from `URANIE`

New Collaborations

- Collaboration opportunity 1: `HiDALGO2` project for simulation using `feel++` of energetic consumption of buildings in a city (online estimation, visualization)
- Collaboration opportunity 2: `ICI` project between IGN & INRIA about epidemic propagation simulation at a individual scale (agent-based model)
- Collaboration opportunity 3: Improve the pruning of LLM using global sensitivity analysis tools developed in `URANIE` (in particular, HSIC sensitivity analysis, well adapted for arbitrary, independent samples)

Adjustments

Adjustments to WP6 Plans

- Adjustment 1: Take into account online learning algorithms (all tasks impacted)
- Adjustment 2: Help WP5 to use URANIE for their exascale app

Updated Priorities

1. Priority 1: multivariate quantiles with a peculiar focus on visualization:
   - quantization methods for vector or functional outputs (example: water level map for flooding visualization, by Jeremy Rohmer and Charlie Sire)
   - quantiles based on statistical depth functions (Monge-Kantorovich depth for instance)
   - nonparametric multiple-output quantile regression, measure-transportation-based quantile regression, quantile autoregression method, by Marc Hallin
   - desired properties : visualization (contour levels, bagplot, ...), guarantees for nested quantile domains, ...
2. Priority 2: Take into account online learning algorithms
   - define aggregation formulas for scalar, vector, functional quantiles (extension of Welford algorithm limited to moments)
3. Priority 3: HSIC sensitivity analysis
   - scalable method to be promoted towards other WPs
   - first version available in `Uranie`

Conclusion

Summary and Next Steps

- WP5 and WP4 are interested in `URANIE` and/or scientific developments in WP6 (e.g. visualization & online learning)
- Keep in touch with WP5 for helping them to install & run `URANIE` on their applications

Thank you!