Study of Uncertainty Quantification Techniques for the NEPTUNE Project

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Recap of proposed and completed activities

- **Activity 1: Knowledge report on high-throughput VVUQ capabilities for the NEPTUNE software**
  - **Objective 1:** write a concise set of recommendations as to which UQ methodologies to develop (**March**)
    - **Completed**, submitted on 02/02/2021; review on UQ for fusion submitted on 18/02/2021
  - **Objective 2:** explicitly describe the architecture of UQ workflows for co-design purposes toward exascale (**June**)
    - M33 VECMA Toolkit code release is 29 March; starting initial work on active subspaces and semi-intrusive UQ for a chaotic code (molecular dynamics)

- **Activity 2: Workshops on UQ for ExCALIBUR partners**
  - **Objective 3:** hold a first meeting to introduce EasyVVUQ capabilities, provide hands-on tutorials and partners to present the structure of their codes and UQ requirements (**mid-January**)
    - **Completed**, UQ workshop held on 18/01 and Hackathon organised on 19-22/01 with participation of BOUT++ team
  - **Objective 4:** hold a second meeting to present our shortlist of recommended UQ methods (**early July**)
    - next Hackathon will take place 21-23 April.

Outline of report on high-throughput UQ

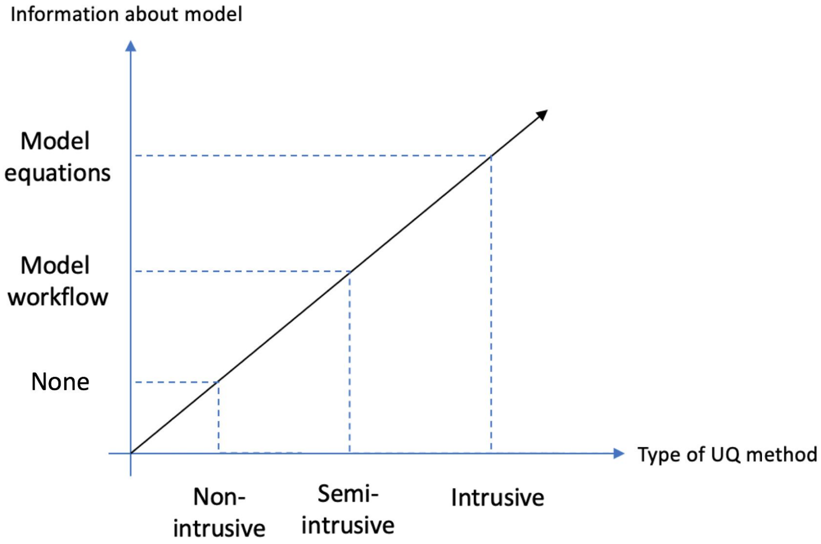
- **Concise set of recommendations as to which UQ methodologies to develop**
  - Establish standard use cases of Bout++ and Nektar++ simulations jointly with NEPTUNE partners
  - Perform UQ on the defined use cases using EasyVVUQ (VECMA) and MOGP (ATI) capabilities

- **Draw on VECMA expertise**
  - open source and open development software
  - D2.2: Report on advanced multiscale UQ algorithms, including intrusive approaches, and mapping thereof in UQPs and first results on V&V.
  - D2.1: Report on multiscale UQ algorithms based on non-intrusive MC and semi-intrusive MC and mapping thereof in UQPs

- **Involvement of David Coster and Jalal Lakhlili (Fusion, MPG-IPP), Wouter Edeling (UQ, CWI) and Eric Daub (MOR, ATI)**
  - in particular during NEPTUNE UQ workshop (18/01) and VECMA hackathon (19-21/01)

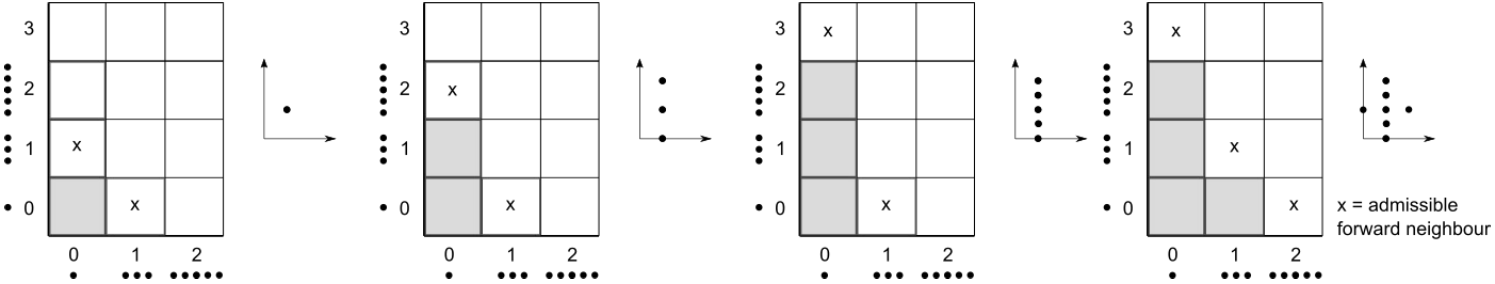
High-throughput UQ reporting

- short overview of approaches to uncertainty quantification most relevant to the Neptune project
- draws upon the experience gathered during the past three years in the VECMA project (www.vecma.eu)
    - facilitate the use of VVUQ techniques in multiscale, multi-physics applications
- classification of UQ methods based on their level of intrusiveness
    - focus on **non-intrusive** and **semi-intrusive** methods
    - intrusive methods are much cheaper but hardly automated
        - no generic solver
        - solver must be reimplemented for every different UQ
        - comparison with non-intrusive PCE on the basis of 2^{nd}-order exp. and 10 parameters:
            - non-intrusive PCE: 59049 samples
            - intrusive (stoch. Galerkin): 66 couples PDEs



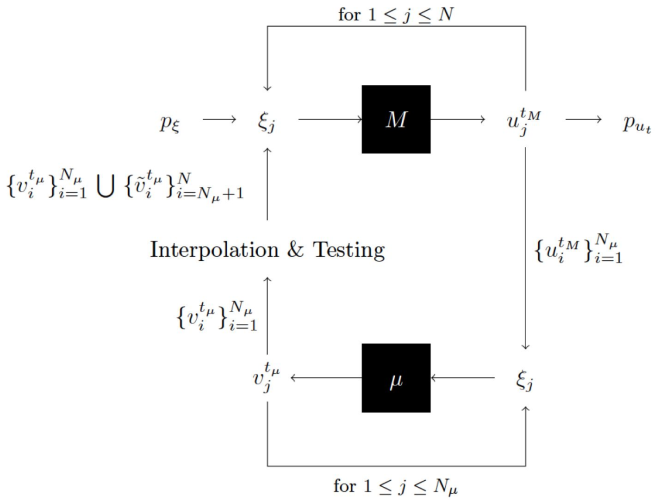
Non-intrusive methods: enhanced sampling

- Monte Carlo sampling: systematic convergence, but slow convergence rate
- Stochastic or point collocation (Spectral UQ): faster convergence (exponentially) in the most favourable cases
- Computational costs increases exponentially with the number of considered input parameters
- Fighting off the curse of dimensionality:
  - **delaying the curse**: adaptive sampling of the stochastic dimensions
  - **circumventing the curse**:
    - High-Dimensional Model Representation: never sample a high-dimensional space, break problem up into a series of low-dimensional subproblems.
    - Active subspaces: project inputs to a rotated (low-dimensional) coordinate system aligned with direction of strongest variability
- Dealing with irregular outputs (e.g. discontinuities or high gradients in stochastic space)
  - Use localised basis in stochastic space (Adaptive sparse grid / Simplex Stochastic Collocation methods)

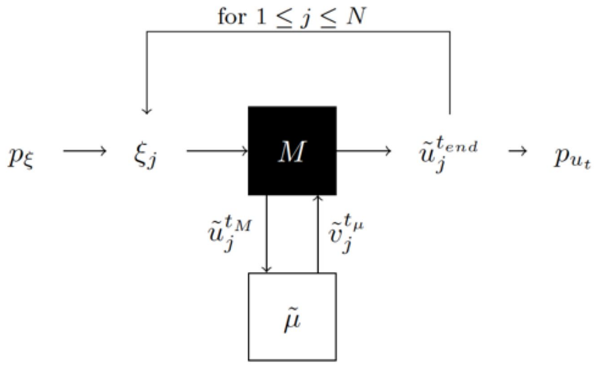


Semi-intrusive methods

- suited for coupled models applications
- individual models are treated as black-boxes, but the workflow is modified to accelerate UQ
- maintains “separation of concerns” for complex workflows



A smaller number of samples of the expensive submodel are simulated using advanced sampling.



The expensive submodel is replace by a cheaper surrogate model when computing ensembles of simulation to perform UQ.

Nikishova, Hoekstra. "Semi-intrusive uncertainty propagation for multiscale models." *Journal of Computational Science* 35 (2019): 80-90.

Surrogate modelling for multiscale models: stochastic surrogates

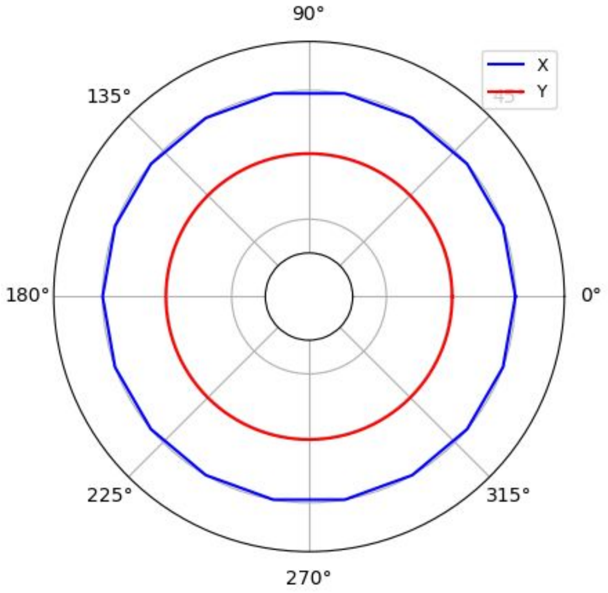
Example L96 multiscale problem:

- Toy model for the atmosphere at constant latitude.
- Full system: N x L couples ODEs (e.g. N=18, L = 20)

$$\frac{dX_n}{dt} = X_{n-1}\left(X_{n+1} - X_{n-2}\right) - X_n - F + r_n$$

$$r_n := \frac{h_x}{L}\sum_{l=1}^{L} Y_{l,n}$$

$$\frac{dY_{l,n}}{dt} = \frac{1}{\epsilon}\left[Y_{l+1,n}\left(Y_{l-1,n} - Y_{l+2,n}\right) - Y_{l,n} + h_y X_n\right].$$



Surrogate modelling for multiscale models: stochastic surrogates

- Works well for this problem, more complex problems might require **online** training. Ongoing research.
- More complex codes will also require coupling library.
  - VECMA option: Multiscale Coupling Library and Environment (MUSCLE 3, https://muscle3.readthedocs.io/)
- Thus far we only tested this on 2D, spectral codes

Edeling, Wouter, and Daan Crommelin. "Reducing data-driven dynamical subgrid scale models by physical constraints." *Computers & Fluids* 201 (2020): 104470.

January UQ workshop and hackathon

- **UQ NEPTUNE workshop held on January 18**
- **VECMA Hackathon held from January 19 to 21**
    - Participation of teams using BOUT++
    - Teams managed to perform basic UQ using either PCE or SC sampling methods
    - Respondents are so far satisfied with the UQ capabilities of VECMAtk and its ease of use
        - Use of EasyVVUQ and Dask
        - Interest in the PilotJob mechanism and FabSim3 to coordinate large ensembles
        - Interest in **adaptive sampling methods** available
        - More sophisticated model may be required for Neptune applications, questions remain:
            - will ever feature such large number of parameters (in the final coupled model)?
            - will there ever be a need to investigate all uncertainties at the same time?
            - each individual application developer might be able to significantly narrow down the number of uncertainties.
        - Both respondents indicate that they foresee **surrogates as being useful** but highlight the challenges in creating them. The main question remains **training**, as usual… That's where recent developments from CWI, when it comes to **online learning/training** could become interesting.
    - Hackathon participants **gained insight in what entails performing UQ** of their application
        - more precise idea of the inputs and outputs of their application (needed to couple single models, could be done with MUSCLE3)
        - distribution of inputs stochasticity

January UQ workshop and hackathon

- **Questionnaires to applications developers on UQ needs**
  - Applications type
    - Single Models (6 respondents)
    - Coupled Models (1 respondent)
  - Typical simulations will have between 2 and 100 uncertainty parameters
    - recommend **expert or sensitivity analysis based dimension reduction**
  - Interest in both **intrusive and non-intrusive** UQ methods
    - the first not compatible at first with "separation of concerns" paradigm
  - A desire for UQ codes which integrate easily with theirs and the availability of suitable surrogates.
    - **stochastic surrogates for turbulent flow** model simulation (see MUSCLE3/EasySurrogate tutorial for coupled stochastic surrogate)
    - concern about challenges in creating surrogate, in particular **training**
      - recent developments from CWI when it comes to **online learning/training** could become interesting