Study of Uncertainty Quantification Techniques for the NEPTUNE Project

Peter V. Coveney & Maxime Vassaux
Centre for Computational Science,
University College London,
UK

&

Institute for Informatics
University of Amsterdam,
Netherlands

Proposed 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**)
  - **Objective 2:** explicitly describe the architecture of UQ workflows for co-design purposes toward exascale (**June**)

- **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**)
  - **Objective 4:** hold a second meeting to present our shortlist of recommended UQ methods (**early July**)

January UQ workshop and hackathon

- **UQ NEPTUNE workshop on January 18**
  - Presentation of UQ and MOR capabilities
  - Presentation of application partners use cases

- **VECMA Hackathon from January 19 to 21**
  - assist adoption of EasyVVUQ and VECMAtk for multi-model coupling and HPC execution
  - provide hands-on tutorials and partners to present the structure of their codes and UQ requirements
  - detailed description and registration: https://www.vecma.eu/vecma-toolkit-hackathon-19-22-january-2021/

High-throughput UQ reporting

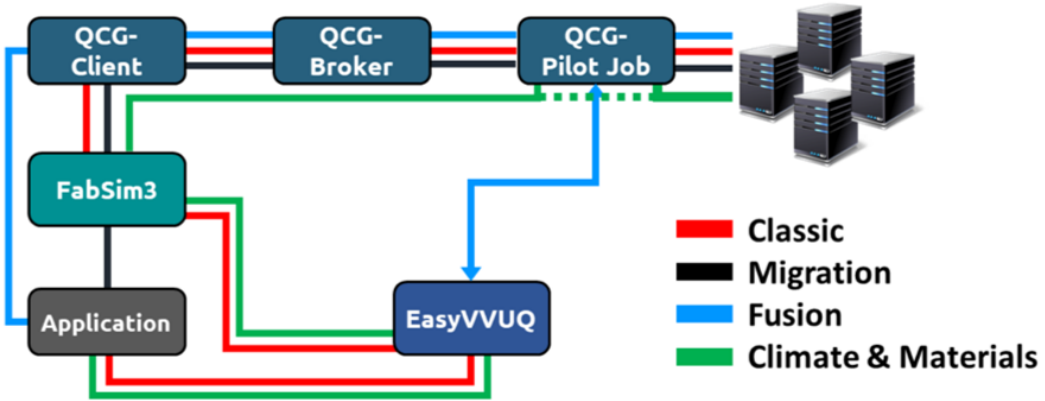
- **Concise set of recommendations as to which UQ methodologies to develop**
  - Establish standard use cases of Bout++ and Nektar++ simulations jointly with NEPTUNE partners
  - Perform UQ on the defined use cases using EasyVVUQ (VECMA) and MOGP (ATI) capabilities

- **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)

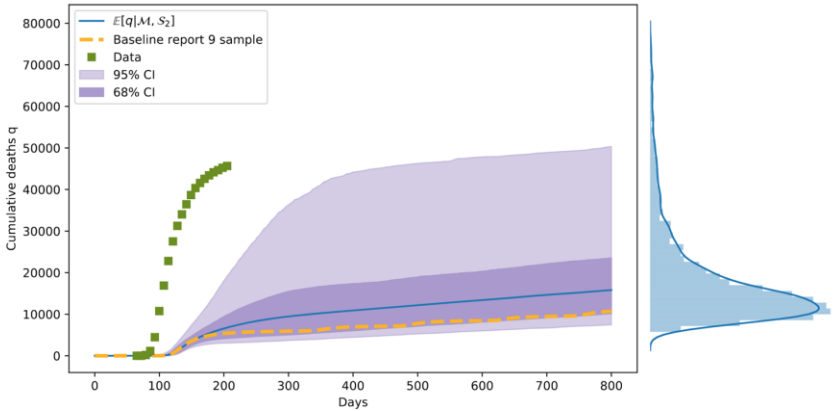
VECMAtk: a generic toolkit for (VV)UQ

- An actionable **VVUQ** toolkit for potential exascale **multiscale, multi-model** applications (VECMA)
  - identified UQ patterns
  - fully automated generation, management, and execution of UQ campaigns
- **EasyVVUQ**: library for creating application-specific UQ procedures, called Campaigns.
- **FabSIM**, **MUSCLE3** and **QCG-Client/PJM**: to ease data transfer and job submission onto multiple Tier-0/1 EU supercomputers

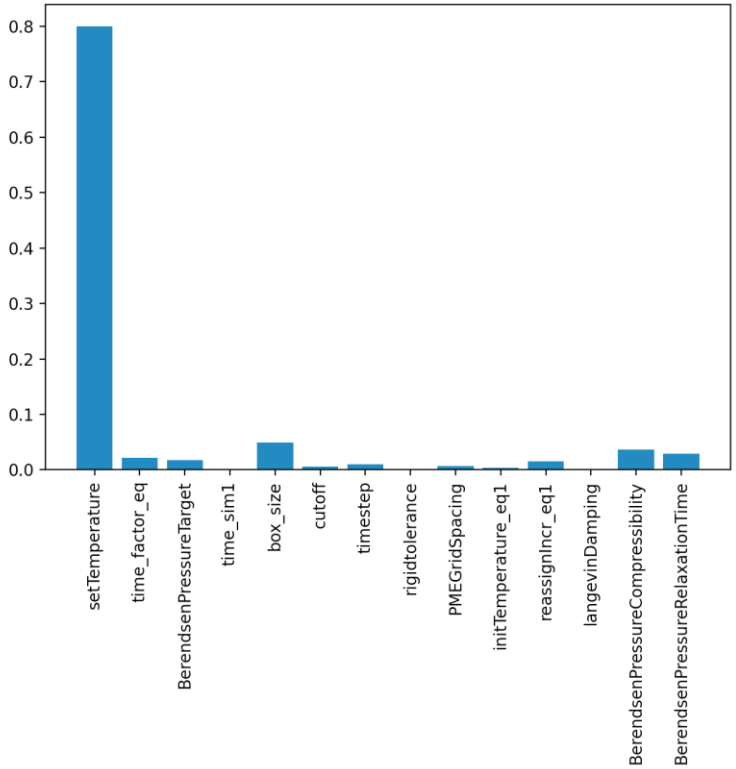


VECMAtk: a generic toolkit for (VV)UQ

- examples of application
  - large-scale SA and UQ campaign driven EasyVVUQ adaptive sampling capabilities
    - BAC using NAMD
    - CovidSim [1]



(a) Scenario S_1: $R_0 = 2.4$, ICU on/off triggers 60/15.



[1] Edeling, W., Coveney, P.V., et al. "Model uncertainty and decision making: Predicting the Impact of COVID-19 Using the CovidSim Epidemiological Code." (2020): https://www.researchsquare.com/article/rs-82122/v3

VECMAtk: a generic toolkit for (VV)UQ

- **Coupling FabSim with MOGP in collaboration with Eric Daub from ATI**
  - Uncertainty Quantification of Dynamic Earthquake Rupture Simulations
  - Tutorial: https://github.com/alan-turing-institute/fabmogp_paper