vecma.eu @VECMA4 VECMA FET-HPC

VECMA

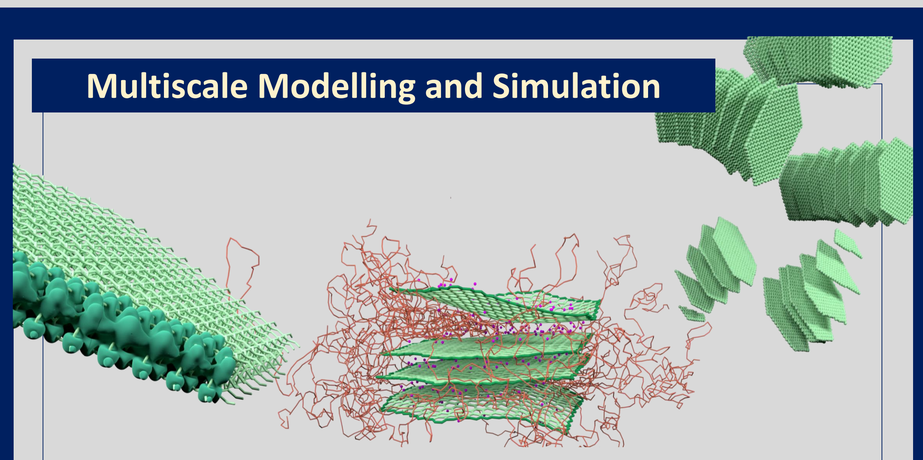
Verified Exascale Computing for Multiscale Applications

VECMA's central objective is, for a diverse set of multiscale computing applications, to automate the stages of VVUQ by developing generic algorithms and approaches into an open source toolkit, exploiting the computational power offered by existing petascale and emerging exascale computing environments.

High-Performance Computing (HPC)

- High-performance computing has unlocked a new dimension in scientific research and simulation-based decision making.
- With this ever-growing forefront of computational power, we can simulate increasingly complex systems of interest.
- Exascale computing systems can perform > 1 exaFLOPS, or a quintillion calculations per second.
- We currently sit on the brink of the exascale.

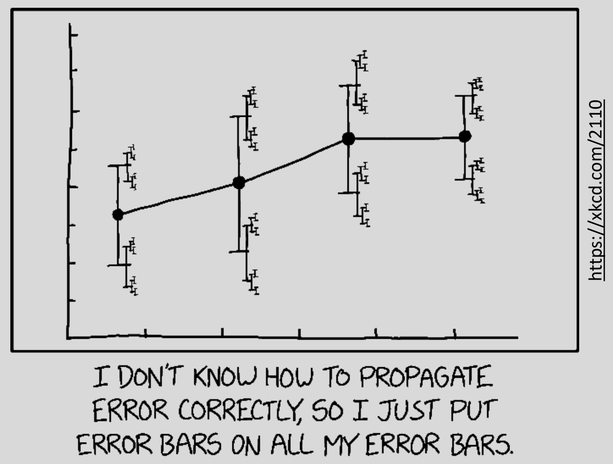
Multiscale Modelling and Simulation



- Systems of interest can be examined at a wide range of physical and temporal scales using high performance computing
- Multiscale modelling and simulation combines different scales in order to make new discoveries and inform critical decisions.
- It is widely applied in fields ranging from the physical sciences, engineering, and the life science domain.

VVUQ

- **VVUQ** - Validation, Verification, and Uncertainty Quantification
- **Verification -** Determines if the computational model fits the mathematical description.
- **Validation -** Determine if the model accurately represents the real-world application.
- **Uncertainty Quantification** - Determine how variations in the numerical and physical parameters affect simulation outcomes.



VECMA VVUQ Software Toolkit

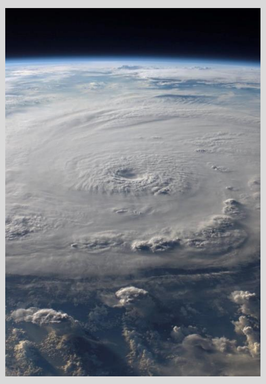
VECMAtk: An open-source Toolkit for multiscale VVUQ based on generic multiscale VV and UQ patterns (software solutions to reoccurring problems)

D. Groen, et al., "Introducing VECMAtk – verification, validation and uncertainty quantification for multiscale and HPC simulations", Lecture Notes in Computer Science, 1153, 479-492 (2019), DOI:10.1007/978-3-030-22747-0_36

VECMAtk

- EasyVVUQ for VVUQ definitions
- MUSCLE3 for model coupling
- FabSim3 for automation and tool integrations
- Quality in Cloud and Grids (QCG)/Radical for pilot jobs
- Alpha users testing

Climate Modelling

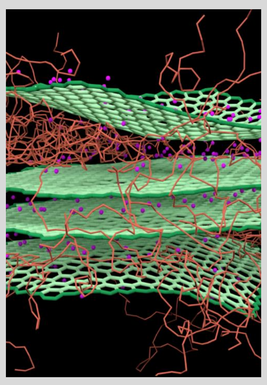


We use stochastic methods, which can be used to represent uncertainties due to the small unresolved scales, taking into account that these uncertainties are dynamic, owing to the underlying chaotic / turbulent behaviour.

Migration Prediction

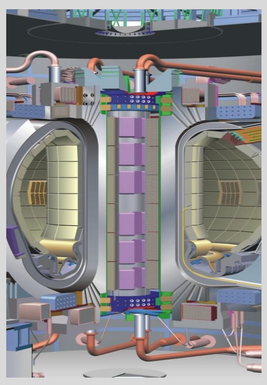
We have created a new simulation approach that allows us to forecast movements of refugees and Internally Displaced People (IDPs) in conflicts.

Material Science



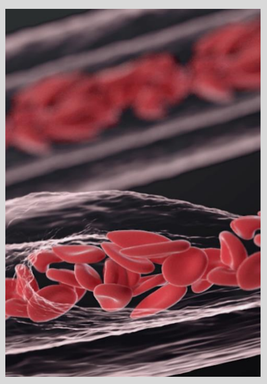
We use computational modelling and simulation in materials research, assisting experimental work via quantitative predictions, economizing time and resources by steering the design of new materials.

Fusion Energy



We build and develop models to study nuclear fusion that potentially provides a carbon free solution to the provision of base load electricity, without geo-political complications.

Biomedicine

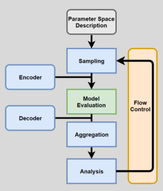


The computational biomedicine community is adopting VVUQ procedures now defined by the FDA. Our research shows great potential in advancing biomedicine, particularly in personalised medicine.

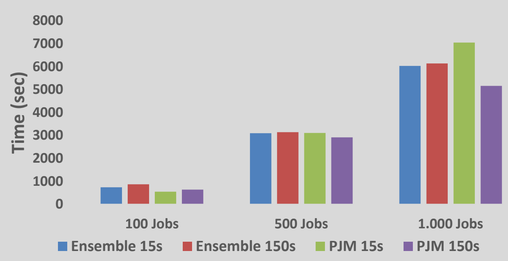
VECMAtk Early Scalability Study

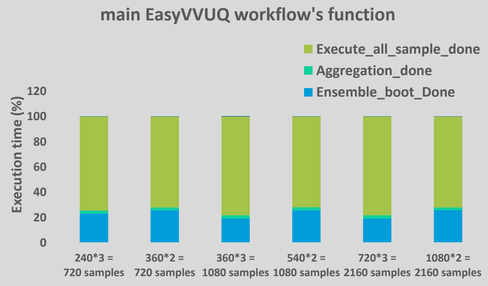
FabSim3:
Help users to perform complex remote tasks from a local command-line, and to automatically organize their data environment variables when they perform task.

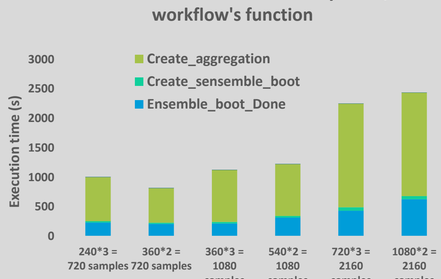
EasyVVUQ:
Make it as easy as possible to implement advanced techniques for uncertainty quantification for existing application codes (or workflows).

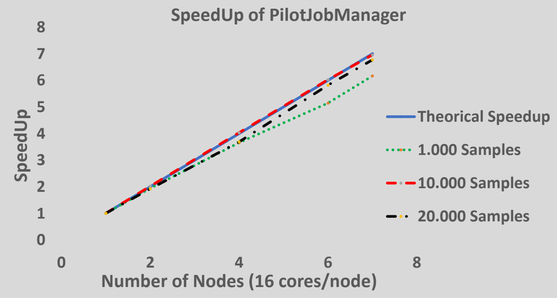


QCG Pilot Job Manager:
Lightweight implementation of the Pilot Job mechanism. It can be easily incorporated into scientific workflows to provide efficient and reliable execution of large number of computational jobs.









The VECMA Consortium

RUTGERS (International Partner)

Join us as an Associate Partner

Authors: Erwan Raffin, Atos Bull CEPP, erwan.raffin@atos.net
Nicolas Monnier, Atos Bull CEPP

Coordinator: Prof. Peter Coveney, UCL, p.v.coveney@ucl.ac.uk
Project manager: Xuanye Gu, UCL, xuanye.gu@ucl.ac.uk

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