VECMA

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Welcome

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Principal Investigator

In the months that have elapsed since the publication of our first issue, many developments have occurred. The most important milestone has been the first public release of the VECMA Toolkit (VECMAtk), which aims to facilitate Verification, Validation and Uncertainty Quantification (VVUQ) for complex single- and multi-scale applications. This is the first of three annual releases planned over the duration of the VECMA project and you can read more about it in the article below.

Our All-Hands Meeting (AHM) in May attracted over 40 participants and comprised presentations from all Work Packages, contributing talks on multiscale modelling, the VECMA Toolkit, Algorithms, and HPC infrastructure, as well as invited talks from our new Associate Partners. There were also sessions dedicated to VECMA's management and the Science and Innovation Advisory Boards.

Our presence in the scientific community is growing through journal publications, contributions to international conferences, participation in other events, and also through direct collaborations. We exhibited VECMA at the EOSC-hub week in Prague in April, at the EuroHPC Summit Week 2019 in Poznan in May, at the International Conference on Computational Science (ICCS) in Faro in June, and at the ISC 2019 in Frankfurt. Upcoming events include the ECCOMAS Conference on Computational Methods in Multi-scale, Multi-Uncertainty and Multi-Physics Problems in Porto in July and the CompBioMed Conference in London in September, organized by the EC H2020 Centre of Excellence that we most closely collaborate with (www.compbiomed.eu). A full list of events in which we are taking part can be found at www.vecma.eu/events/.

VECMA Toolkit (VECMAtk) Month 12 Release: FabSim3, EasyVVUQ, QCG and Application Tutorials

VECMAtk

The VECMA project announces its Month 12 (M12) Validation, Verification, Uncertainty Quantification (VVUQ) Software Toolkit release, available as of June 13th. This is the first major release of three which are planned over the three years of the VECMA project. The Toolkit release contains documentation and tutorials in addition to the software.

The software Toolkit has been developed to enable automated VVUQ, providing support for software applications regardless of the domain of interest. We have established a collection of readily working non-intrusive UQ algorithms within existing multiscale computing tools (such as MUSCLE2 and FabSim). The Toolkit release is also linked to some applications which are provided in the application tutorials. All codes and documentation, component releases, training material, and other technical information may be found at the Toolkit website: www.vecma-toolkit.eu/

The components of the toolkit are as follows:

- FabSim3 is an automation toolkit for complex simulation tasks. FabSim3 helps users to perform complex remote tasks from a local command-line, and to automatically organise their data and environment variables when they perform these tasks.
- EasyVVUQ is a Python library designed to facilitate verification, validation and uncertainty quantification (VVUQ) for a wide variety of simulations.
- QCG Pilot Job is a 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.
- QCG-Now is a portable desktop program that allows to prepare and run computational jobs on the HPC machines.
- QCG-Client a command-line interface to the QCG middleware. QCG-Client provides support for variosity of computing jobs, from simple ones to complex distributed workflows.
- EasyVVUQ-QCGPilotJob is a lightweight integration code that simplifies usage of EasyVVUQ with a QCG Pilot Job execution engine.

VECMAtk will be fully tested and evaluated in emerging exascale environments, actively promoted over the lifetime of this project, and made widely available in European HPC centres.

VECMA Welcomes New Associate Partners

UK Atomic Energy Authority

Nuclear fusion, the process that powers the Sun and the stars, can play a big part in our carbon-free energy future. At the UK Atomic Energy Authority (UKAEA) scientists and engineers are working with partners around the globe, in Universities, in National Laboratories and in industry to develop fusion as a new source of cleaner energy for tomorrow's power stations. UKAEA owns and operates the Culham Centre for Fusion Energy (CCFE), the world's leading laboratory for fusion research. CCFE is based at Culham Science Centre in Oxfordshire.

VECMA collaborates with Dr Robert Akers, Head of Scientific Computing at CCFE.

UNIVERSITY OF EXETER

The University of Exeter combines world class research with excellent student satisfaction at its campuses in Exeter and Cornwall. It is a member of the Russell Group of leading research-intensive universities. Formed in 1955, the University has 22,085 students from more than 130 different countries. Its success is built on a strong partnership with its students and a clear focus on high performance.

VECMA collaborates with Prof. Peter Challenor at the Department of Mathematics, whose interests are primarily in uncertainty in the natural world. These range from the statistical analysis of complex numerical models (such as those used to simulate climate) to the interpolation of noisy data and the estimation of the amount of renewable energy in the ocean.

BSC Barcelona Supercomputing Center Centro Nacional de Supercomputación

Located in Barcelona, the BSC is the national supercomputing centre in Spain. BSC specialises in high-performance computing (HPC) at all levels: hardware architecture, programming models, code optimization or basic and applied computational mechanics. BSC manages MareNostrum, one of the most powerful supercomputers in Europe, located in the Torre Girona chapel.

VECMA collaborates with Dr Mariano Vazquez, Research Team Leader at BSC. Dr Vazquez's main research lines fall within computational science, such as computational bio-mechanics (particularly solid mechanics of organic tissue and electrophysiology) at organ and system level. Following these lines, his team develops a simulation tool to study the cardiovascular and respiratory systems targeted to biomedical researchers in academia, the medical devices sector and the pharmaceutical industry. Infarction, ageing, aneurism rupture risk, arrhythmias, stent design and drug delivery are among the topics where such a tool can become a decisive help. Since 2005, Dr Vazquez has co-led the Alya Project, which has produced a simulation code for high performance computational mechanics. Alya solves coupled multiphysics problems using high performance computing techniques for distributed and shared memory supercomputers, together with vectorization and optimization at the node level. The multiphysics problems solved by Alya are in areas including incompressible/compressible flows, non-linear solid mechanics, chemistry, particle transport, heat transfer, turbulence modeling, electrical propagation, etc.

ELEM THE VIRTUAL HUMANS FACTORY

ELEM Biotech is a biomedical software company which creates software products for the medical industry to optimize and test medical treatments. The company is a spin-off from Barcelona Supercomputing Centre (BSC), BarcelonaTech (UPC) and the Spanish Scientific Council (CSIC). It has offices in Barcelona and Bristol. ELEM's Virtual Humans Factory provides digital avatars to perform complex simulations at organ level (now focused on cardiovascular and respiratory systems). ELEM Biotech has rights to commercialise Alya Red, a project of BSC for simulating a human heart and part of the Alya Project (see previous).

Dr Mariano Vazquez (see above) is president and CTO of ELEM Biotech and our main collaborator.

News and Updates

Special Appointments

Professor Peter V. Coveney has been appointed professor by special appointment of Applied High Performance Computing at the Faculty of Science of the University of Amsterdam (UvA). The chair was established on behalf of the Bèta Plus Foundation and will run concurrently with his position as Professor of Physical Chemistry at University College London (UCL). As professor by special appointment, Coveney will carry out research to develop codes which run efficiently on the largest petascale architectures today as well as the exascale architectures which are expected to emerge in the near future. His research is also aimed at building complex problem-solving environments, including ones for clinical decision support.

In addition to his professorial appointment, Peter Coveney has been elected to membership of the Academia Europaea, based on his outstanding achievements as a scientist. The object of Academia Europaea is the advancement and propagation of excellence in scholarship in the humanities, law, the economic, social, and political sciences, mathematics, medicine, and all branches of natural and technological sciences anywhere in the world for the public benefit and for the advancement of the education of the public of all ages. The Academy aims to promote European research, advise governments and international organisations in scientific matters, and further interdisciplinary and international research.

All-Hands Meeting (AHM) 2019

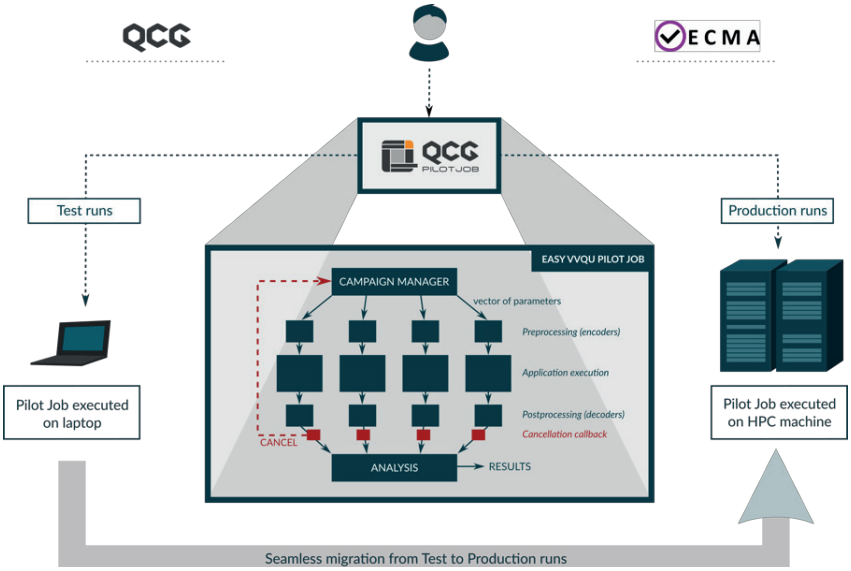
Our first AHM took place at the University of Amsterdam on the 9th and 10th of May attracted over 40 participants with an excellent collection of speakers and short meetings. On day 1, presentations from all Work Packages took place to update the Consortium on the developments within each, followed by a discussion on the VECMAtk release plans and invited talks from Core and Associate Partners. The end of day 1 saw General Assembly meeting to discuss and vote on matters pertinent to the project governance and a concurrent Science and Innovation Advisory Board meeting. We look forward to receiving the minutes from this meeting to put into action the ideas that resulted from this. On day 2, we had a full agenda of speakers from Core and Associate Partners explaining their latest work in Multiscale Modelling, VVUQ, Algorithms and Analysis, and HPC Infrastructure. We will be able to share some of this work on the website shortly. The AHM came to a close with a sessions dedicated to VECMA's WP1 - Management.

New VECMAtk Website

As of June 2019, the VECMA Toolkit has its own designated website: www.vecma-toolkit.eu. All codes and documentation, component releases, training material, and other technical information may be found there. The codes and documentation for these components can be accessed at www.vecma-toolkit.eu/toolkit/. A detailed release history for all packages leading up to the above components can be found at www.vecma-toolkit.eu/tools/. Tutorials for installing and using the Toolkit components may be found at www.vecma-toolkit.eu/tutorials/.

QCG PilotJob - EasyVVUQ Integration

The target runtime environment for the VECMA's applications is in the future exascale systems. At present, only large-scale HPC machines of PRACE TIER-0 and TIER-1 offer sufficient amount of computing power necessary for analysis of uncertainty quantification. For this reason, all VECMA's software is intended and constructed for either multi-peta or exascale environments. However, in comparison to local systems, the access to remote HPC installations is usually less convenient and burdened with unavoidable time overheads. These delays, particularly related to queueing time, are unacceptable for the period of intense developments and tests of the software. Taking the above conditions into account and meeting the expectations of VECMA developers, Work Package 5 has recently adjusted the QCG Pilot Job mechanism, so it can be seamlessly used also on the personal computers emulating HPC environment. What is worth emphasizing is the fact that the same code without any changes can be executed both locally and also on an HPC machine managed by a queueing system. This new feature contributes significantly to the reduction of time and effort needed for the transition to the target system. Independently to the provided local execution of QCG Pilot Jobs, there is work underway to integrate EasyVVUQ with QCG Pilot Job Manager. It is believed that thanks to this integration, the tasks defining EasyVVUQ campaigns will be executed in the HPC environment in effective and flexible manner.



Brexit

As the UK becomes increasingly mired in the question of whether or not it will exit the European Union and, if so, how, it has become clear to many that if there is to be any certainty about the future of Britain and British institutions in a European context, individuals are going to have to act. Coordinator of the project, Prof. Peter Coveney, has ensured that funding for VECMA can and will continue via his professorship at the University of Amsterdam (UvA). In an article that he wrote for the *Times Higher Education* (https://www.timeshighereducation.com/opinion/uk-academics-should-not-rely-their-universities-save-them-brexit-fallout) he explains the current funding landscape and ways of mitigating Brexit repercussions.

Domestic funding for HPC-related research in the UK has significantly decreased in recent years, whereas, funding from the European Union has steadily increased. The multidisciplinary teams that have been established from this funding have progressed their research and established collaborations that would otherwise have been impossible. The UK has benefited from this as much as any other European country.

While the UK government has promised to underwrite funding for UK co-investigators, there has been no explicit statement about those in the UK leading EU projects. If, as would be the case in a no-deal Brexit, the UK became a third country, there is no legal certainty about the status of coordinators. Some UK universities are looking to affiliate themselves with EU universities to aid in the continued participation in EU funded projects; however, there is no certainty that this course of action will be successful, and it behoves those in a suitable position of responsibility to make their own decision.

Deliverables

Month 9 (March 2019) public releases:

- **D3.1 Report on the fast-track implementation of the VECMA Toolkit:** Three internal releases have already been made (M1, M3 and M6) and two components have been successfully applied (FabSim3 and EasyVVUQ) to multiple diverse HPC applications. Both components are now in open development.
- **D4.1 Report on Application Software Readiness:** Preparing and studying VECMA applications to drive the developments and requirements of the technical work-packages (WP2, WP3, WP5).
- **D5.1 Architecture of the VECMA system:** Architecture of the infrastructure and tools developed within VECMA.

Month 12 (June 2019) public releases:

- **D2.1 Report on multiscale UQ algorithms based on non-intrusive MC and semi-intrusive MC and mapping thereof in UQPs:** A family of semi-intrusive multiscale UQ algorithms is proposed and tested and a family of UQPs is designed.
- **D3.2 Fast-track release of the WP3 VECMA toolkit:** A software deliverable -contents available on the VECMA Toolkit website, www.vecma-toolkit.eu.

All deliverables at public dissemination level are available at www.vecma.eu/about/deliverables/.

Upcoming Events

Conference on Computational Methods in Multi-scale, Multi-Uncertainty and Multi-Physics Problems

15-17 July 2019

Porto, Portugal

We are presenting VECMA at this ECCOMAS conference, which targets the latest advances in the modelling of multi-scale, multi-uncertainty and multi-physics problems, and welcomes research topics such as computational homogenization and multi-scale modelling, stochastic modelling, probabilistic engineering, reliability and risk assessment, computational coupling strategies, HPC, etc.

CompBioMed Conference

25-27 September 2019

Institute of Engineering & Technology, Savoy Place, London, United Kingdom

The conference of our closest collaborating EC H2020 Centre of Excellence will address all aspects of the rapidly burgeoning domain of computational biomedicine, from genome through organ to whole human and population levels, embracing data driven, mechanistic modelling and simulation, machine learning and combinations thereof. We welcome contributions from academic, clinical and industrial participants alike.

VECMA Technical and Pre-Review Meeting

11-13 December 2019

London, United Kingdom

The three days will comprise on the one hand technical meetings and on the other hand a meeting for the overall assessment of the project at mid-term (M18). This will serve as preparatory work for the production of Periodic Report I, which will be submitted to the EC and will contain technical and financial reporting.

Publications

- A. Nikishova, A. G. Hoekstra, "Semi-intrusive Uncertainty Propagation for multiscale models", *Journal of Computational Science*, Available Online (2019), DOI:10.1016/j.jocs.2019.06.007
- W. N. Edeling, D. Crommelin, "Reduced model-error source terms for fluid flow", UNCECOMP19 Conference, Preprint (2019), DOI:10.13140/RG.2.2.36773.35048
- R. C. Sinclair, P. V. Coveney, "Modeling Nanostructure in Graphene Oxide: Inhomogeneity and the Percolation Threshold", *J. Chem. Inf. Model.*, Article ASAP (2019), DOI:10.1021/acs.jcim.9b00114
- D. Groen, R. A. Richardson, D. W. Wright, V. Jancauskas, R. Sinclair, P. Karlshoefer, M. Vassaux, H. Arabnejad, T. Piontek, P. Kopta, B. Bosak, J. Lakhlili, O. Hoenen, D. Suleimenova, W. Edeling, D. Crommelin, A. Nikishova, P. V. Coveney, "Introducing VECMAtk – verification, validation and uncertainty quantification for multiscale and HPC simulations", *ICCS*, In Press (2019)
- David W. Wright, Shunzhou Wan, Christophe Meyer, Herman van Vlijmen, Gary Tresadern, Peter V. Coveney, "Application of ESMACS binding free energy protocols to diverse datasets:Bromodomain-containing protein 4", *Scientific Reports* 9, 6017, (2019), DOI:10.26434/chemrxiv.7327019
- A. Potterton, F. Husseini, M. Southey, M. Bodkin, A. Heifetz, P. V. Coveney, A. Townsend-Nicholson, "Ensemble-Based Steered Molecular Dynamics Predicts Relative Residence Time of A2A Receptor Binders", *J. Chem. Theory Comput.*, 15 (5), 3316–3330 (2019), DOI:10.1021/acs.jctc.8b01270

Find VECMA Online: Our main website (www.vecma.eu) contains all the latest news and information about VECMA, its Partners, events, publications, and more. Our Toolkit website (www.vecma-toolkit.eu) is specifically dedicated to the VECMA Toolkit and contains software releases, training material and other technical information. We have an active presence and growing following on Twitter (@VECMA4). We are funded by the European Commision's (EC) Future and Emerging Technologies (FET) programme (ec.europa.eu/programmes/horizon2020/en/h2020-section/future-and-emerging-technologies) under grant no. 800925.

VECMA aims to create a unified European Verification, Validation, and Uncertainty Quantification (VVUQ) Toolkit for exascale computing which will facilitate the adoption of numerical simulations as trusted tools of decision-making.