

Welcome

Prof. Peter V. Coveney
Principal Investigator



Following the first public release of our main deliverable, the VECMA Toolkit (VECMAtk), in Month 12 (M12) of the Project, June 2019, further technical developments have occurred. On September 13th, we announced the M15 release, further facilitating Verification, Validation and Uncertainty Quantification (VVUQ) for complex single- and multi-scale applications. You can read more about this release in the article below. Over the whole duration of the Project, three major annual releases have been planned.

We are establishing our presence in the scientific community through journal publications, contributions to international conferences, direct collaborations, and a growing network of Associate Partners. In July, we exhibited VECMA at the ECCOMAS Conference on Computational Methods in Multi-scale, Multi-Uncertainty and Multi-Physics Problems in Porto. In September we presented our work at the CompBioMed Conference in London in September,

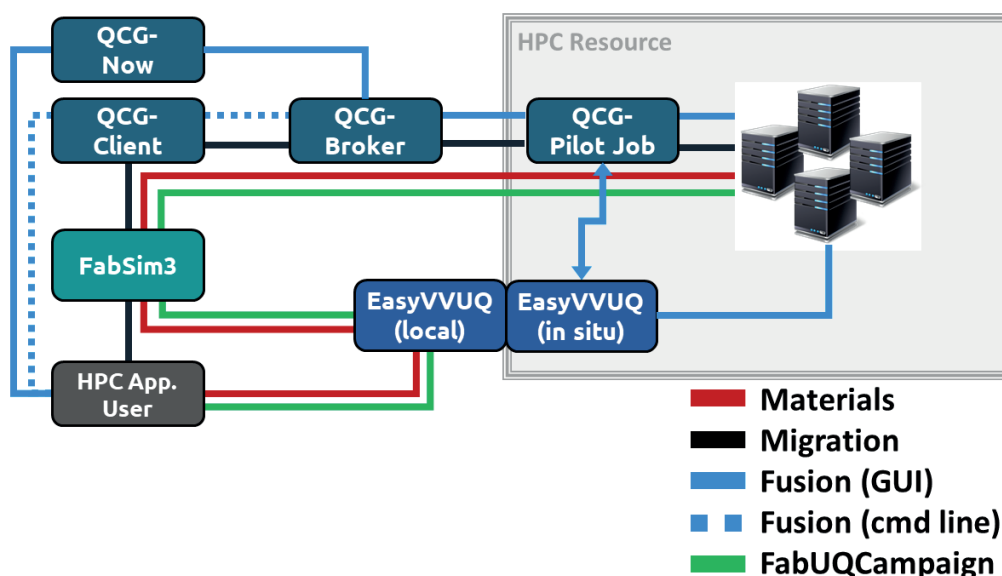
organized by the EC H2020 CompBioMed Centre of Excellence that we most closely collaborate with (www.compbiomed.eu). As this collaboration progresses, the application of Validation, Verification and Uncertainty Quantification will become increasingly important for the computational biomedicine codes developed by that Centre of Excellence.

We have also been involved in various events. Our second VECMA Hackathon took place at Brunel University London on September 23-24. The meeting focused on the Application perspective and how the VECMAtk can be used by other scientific applications. We are much looking forward to the 24th of January, when we join forces with the Alan Turing Institute for a "Reliability and Reproducibility in Computational Science" workshop, which we have been jointly organizing. You can read about these event in this Issue, while a full list of events in which we are involved can be found at www.vecma.eu/events/.

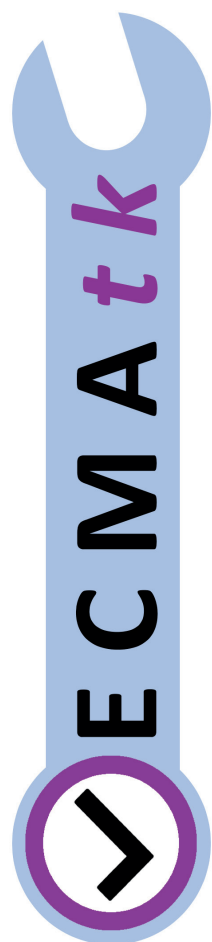
VECMA Toolkit (VECMAtk) Month-15 Release

In September 2019, VECMA announced the M15 release of VECMAtk. The Toolkit enables automated VVUQ for multiscale applications that can be deployed on emerging exascale platforms. The Toolkit provides support for software applications regardless of the domain of interest. The M15 release is made up of the following tools:

FabSim3 - EasyVVUQ - QCG Pilot Job - QCG-Now - QCG-Client - EasyVVUQ-QCGPilotJob - MUSCLE3.



The figure above shows how the different tools are combined when using each of the four application tutorials. VECMAtk components are given in boxes, while the application tutorials are indicated with colored lines. Note that EasyVVUQ can run either on a local desktop, for ease of use, or on a remote HPC resource, for improved performance.



FabSim3 v1.3:

- Extended documentation on how user/developers can create their own FabSim automations.
- First Python API for launching FabSim commands from Python scripts directly.
- Preliminary FabSim3 plugin for the MUSCLE toolkit – FabMUSCLE.
- Auto bash-completion for fabsim command.
- Bash aliasing functionality to shorten commands.
- Support for replica execution (multiple simulations with identical input data and input parameters).



EasyVVUQ v0.4:

- Parameter type and physical range checking (verification) implemented using Cerberus.
- Multisampler element, allowing arbitrary number of samplers to be chained together, but to behave as a single sampler.
- SweepSampler element, for parameter sweeps.
- Sparse grid functionality to the Stochastic Collocation sampler.
- "Worker" class (a stripped down version of the campaign) and associated tools (such as an external encoder script)



to allow non-linear workflows, such as when integrating with pilot job managers.

QCG-PilotJob v0.5:

- New launcher service that significantly reduces time needed to start tasks on nodes,
- Support for an allocation of dedicated core for a QCG PJ Manager instance,
- Automatic binding to free TCP ports (from port range),
- Support for Slurm CPU binding.

EasyVVUQ-QCGPJ:

- Updated to work with the recent releases of EasyVVUQ and QCG-PilotJob.

MUSCLE3 v0.2.0 (the second official release of MUSCLE 3, the MultiScale Coupling Library and Environment):

- Support for submodels (and other components) written in C++. MUSCLE 3 now offers a native C++ API, backed by a C++ implementation.
- The new C++ API also offers support for submodels that use MPI to communicate internally.
- Distributed running, i.e. running different submodels on different machines, has seen improvements and fixes.

VECMA Welcomes New Associate Partners



• Università
• degli Studi
• della Campania
Luigi Vanvitelli

in 12 EC projects and several national projects, including mOSAIC, Crystal, CoSSMIC, H2020 ICT-BIGDATA TOREADOR and H2020 SUV GREENCHARGE.

The University of Campania "Luigi Vanvitelli" (previously Second University of Naples - SUN), was established in 1991. Currently, there are thirty thousand students attending 16 Departments, and 1000+ tenured professors. The Dipartimento di Ingegneria (SUN-DI) performs research and educational activities in several scientific areas, including civil, mechanical and aerospace engineering, robotics, telecommunications and information systems. SUN-DI is participating

VECMA collaborates with Prof. Beniamino Di Martino, Scientific Responsible for the Information Systems Engineering Research Group. Over the last two years, his Group has authored over 300 publications in scientific journals and over 600 presentations to international conferences. The Group currently comprises 9 tenured positions, 2 PostDocs and 3 PhD students.



The Manufacturing Technology Centre (MTC) was established in 2010 as an independent Research & Technology Organisation (RTO) with the objective of bridging the gap between academia

and industry -often referred to as 'the valley of death'. MTC provides integrated manufacturing system solutions for customers large and small, across sectors as diverse as automotive, aerospace, rail, informatics, food & drink, construction & civil engineering, electronics, oil & gas and defence. With over 700 employees at present, MTC helps companies manufacture faster, at a consistently higher quality and lower cost, in an agile environment in partnership with industry and academia.

VECMA collaborates with Dr Anas Yaghi, Senior Research Engineer. His team performs numerical modelling of manufacturing processes for the support and promotion of high-value manufacturing in the UK, such as the simulation of mechanical, physical and metallurgical behaviour for the purpose of design, research and development as well as component integrity and product optimisation.



For more than 150 years, the Politecnico di Torino (POLITO) has been one of the most prestigious public institutions at both national and international education, research, technological transfer and services in the sectors of architecture and engineering. POLITO has over 33,000 students, and teaching is delivered according to a variety of methodologies, including frontal teaching, experiential learning and other educational methods. According to ARWU Ranking 2013, Politecnico Di Torino is 1st in Italy and 8th in Europe for Engineering.

VECMA collaborates with Prof. Pietro Asinay. His research activity deals with proposing mesoscopic descriptions of phenomena, designing new numerical schemes (mainly in the framework of Lattice Boltzmann Method), developing new numerical codes (including parallel codes on large cluster facilities) and finally applying the previous tools in order to investigate the microscopic fluidics of industrial devices.

News and Updates

The Problem With Digital Computers

The limitations of a computer are usually thought of in terms



of hardware, memory and calculations per second. However, a more fundamental complication arises because the numbers they rely on are a poor representation of reality, according to a new paper published by Professors Bruce M. Boghosian

(Tufts) and Peter V. Coveney (UCL), and Dr Hongyan Wang (Tufts).

The IEEE floating-point representation of real numbers has been standardized since the 1950s. While it is undoubtedly one of the great success stories of numerical computation, it also has known pathologies, such as roundoff error and loss of precision. In their article, the authors describe a new pathology that manifests itself when floating-point numbers are used to represent the statistical properties of chaotic dynamical systems. The authors show that, even for very simple chaotic systems, floating-point arithmetic can lead to errors that are

not obvious, are not small, and do not go away as the precision of the floating-point numbers is increased.

Professor Peter Coveney, said: “Our work shows that the behaviour of the chaotic dynamical systems is richer than any digital computer can capture. Chaos is more commonplace than many people may realise and even for very simple chaotic systems, numbers used by digital computers can lead to errors that are not obvious but can have a big impact. Ultimately, computers can’t simulate everything.”

This floating-point pathology is hitherto completely unknown and its ramifications are likely to be substantial. They may have an impact on climate modelling, other forms of fluid dynamics research (such as turbulence and fusion energy), astrophysics, as well as numerous areas of physics, chemistry, life / medical sciences, and machine learning/AI research. For the last named, where it has become quite fashionable to train “deep learning” networks on simulations of systems exhibiting chaotic dynamics, AI is liable to be learning behaviours which are not correct.

Establishing the detailed role of this pathology in everyday simulations using molecular dynamics and computational fluid dynamics will require examination of alternative representations of the real numbers and an investigation as to how far results produced by analogue computers differ from those of digital ones.

Cluster Review of FETHPC Projects

On Thursday 24th October, VECMA took part in this newly instated Cluster Review for FETHPC-02-2017 projects, in Luxembourg. The main objectives of this meeting is to assess the progress and the expected scientific and technological impact of the projects and to explore potential synergies between them. The Cluster Review meeting is not replacing the official mid-term Review (M18).

Inter alia, VECMA partners were called to present:

- The main objectives of the Project.
- Current state of implementation.

- Success stories and lessons learnt.
- How transition towards exascale is being addressed.
- Short- and medium-term R&I challenges.
- Synergies with FETHPC and other projects.
- Dissemination and impact on general public.

VECMA representatives met personnel from the Commission, representatives from all eleven funded FETHPC projects, a set of four experts appointed to assess progress within the projects, and key Commission Officers. The experts will be preparing a report for the Commission in due course.



Applications Hackathon at Brunel

Our second VECMA Hackathon took place at Brunel University London on September 23-24. The meeting focused on the Application perspective and how the VECMAtk can be used by other scientific applications. On day 1, we defined around 15 projects which focused on 1) supporting new applications with VECMAtk, 2) defining roadmaps detailing how external applications can be integrated/used with/by VECMAtk, and 3) prototyping new functionalities for the current tools in VECMAtk. Thanks to the diligent efforts put in during the Hackathon, we established several prototypes and even a few production-ready solutions. As an example, to support the external applications by VECMAtk, we had two application re-

quests from UCL to use FabSim3 tool as the software layer for creating, submission, and monitoring jobs on the supercomputers resources such as ARCHER. FabSim3 dev team developed, tested, and released the FabSMD plugin for the Steered Molecular Dynamics application. The second one is under progress. Also, EassyVVUQ and QCG dev team had several discussion and prototyping on EasyVVUQ and its integration with QCGPJ which will be used the roadmap for future development and release.

Additionally, we had a presentation about new feature/improvement on QCG tool by the team developer from Poznan Supercomputing and Networking Center (PSNC). Here they presented several improvements to QCG Pilot Job, as well as

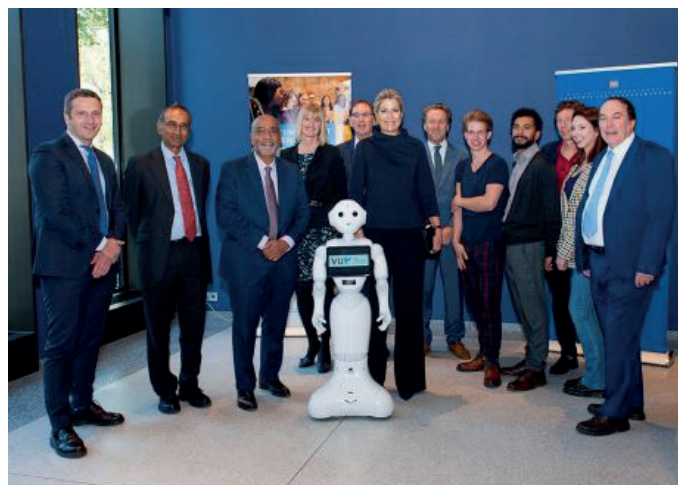
Flee workshop in Ethiopia

In mid July, we hosted the very first Flee workshop at the Adama Science and Technology University in Adama, Ethiopia. Here

we taught a cohort of 25 students and academics about the Flee code, how to prototype their own simulations, and how to use parts of VECMAtk to add robustness and automation to their solutions.

Queen Maxima at the Academy

On October 30th, Queen Maxima of the Netherlands visited the The Royal Netherlands Academy of Arts and Sciences to speak with scientists and students about the potential consequences of Brexit. Upon arrival at the Trippenhuis, where the Academy is housed, the Queen was received by Leolani, an interactive robot designed and programmed by students from the VU University in Amsterdam. The Queen then spoke with a number of students and scientists about the consequences of a Brexit on relations between universities, the position of science within Europe and the effect of a Brexit on euroscepticism. Professor Peter Coveney, who was among the participants, expressed his concerns, yet also hopes that continuing discussions between British and Dutch scientists would lead to initiatives mitigating the impact of Brexit.



Upcoming Events

Reliability and Reproducibility in Computational Science

Friday 24 January 2020

The Alan Turing Institute, British Library, London

VECMA Mid-Term Review

February 2020 (M20)

Luxembourg

The Alan Turing Institute

VECMA joins forces with The Alan Turing Institute to address the reliability and reproducibility of data produced by computer simulations in a number of research fields, including biomedicine, advanced functional materials, climate change, energy, and urban analytics.

The central objective of this meeting is to propose methods that enable computer simulation predictions to guide real decision-making. Theory, software, tools and services in support of these goals are being actively developed and will be showcased in a special interactive software session, featuring both VECMA and Alan Turing software.



The Mid-Term review will entail reporting to the EC on Period 1 (P1) and forecasting on Period 2 (P2). P1 runs from Month 1 to Month 18 (15th June 2018 – 14th December 2019). P2 runs from Month 19 to Month 36 (15th December 2019 – 14th June 2021).

A written Periodic Report will be submitted and will include a Technical and a Financial Report, both of which will require input from all partners. In preparation of the Periodic Report, an internal, pre-review meeting followed by two days' technical meetings will take place between 11-13 December 2019 at UCL, London.

Publications

- S. Wan, G. Tresadem, L. Perez-Benito, H. van Vlijmen, P. V. Coveney, "Accuracy and Precision of Alchemical Relative Free Energy Predictions With and Without Replica-Exchange", Advanced Theory and Simulations, In Press (2019).
- D. W. Wright, F. Hussein, S. Wan, C. Meyer, H. van Vlijmen, G. Tresadem, P. V. Coveney, "Application of the ESMACS binding free energy protocol to a multi-binding site lactate dehydrogenase A ligand dataset", Advanced Theory and Simulations, In Press (2019).
- M. Vassaux, R. C. Sinclair, R. A. Richardson, J. L. Suter, P. V. Coveney, "Toward high fidelity materials property prediction from multiscale modelling and simulation", Advanced Theory and Simulations, 1900122 (2019), DOI:10.1002/adts.201900122.
- B. M. Boghosian P. V. Coveney, H. Wang, "A New Pathology in the Simulation of Chaotic Dynamical Systems on Digital Computers", Advanced Theory and Simulations, 1900125 (2019), DOI:10.1002/adts.201900125.
- W. Edelin, D. Crommelin, "Reducing data-driven dynamical subgrid scale models by physical constraints", in a special data-driven issue of Computers & Fluids, In Press (2019), DOI:10.13140/RG.2.2.11045.86245.

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](https://twitter.com/VECMA4)). We are funded by the European Commission'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.

