

Newsletter Issue No. 6 June 2021

Welcome

Prof. Peter V. Coveney Principal Investigator



New Now in month 35, VECMA is in its final phase of operations. While the original duration of the Project was 36 months, a 6-month extension has been granted by the European Commission on grounds of disruption caused by COVID, post-

poning the termination of VECMA in its current form to the end of 2021. Since the second quarter of 2020, VECMA devoted considerable human resources towards coronavirus research (you can read about this in Issue no. 5 of this Newsletter and on our website).

More than a third of the Project's lifetime thus far has taken place on a remote-working, online basis. Nevertheless, our efforts to remain connected and to adapt our mode of work have ensured that our productivity has remained around its peak.

A significant outcome of our research, pertaining to Reproducibility and Reliability in computational science, has seen publication in the Philosophical Transactions of the Royal Society A journal (page 2). This effort is an example of our desire to expand beyond the technical scope of verification, validation and uncertainty quantification (VVUQ), and to offer contributions to the wider computational domain. Further publications that came out over the last few months are reported in the relevant section on page 4, and you can find the full list, since the beginning of VECMA, on our webpages.

Our central deliverable, the VECMA Toolkit, which has

already seen two out of its three planned major releases and has further been upgraded last March to its Month-33 version (see below). The final and full release is on track and will be taking place as scheduled, in Month 36.

The past few months have also witnessed considerable activity in terms of (virtual) events (page 2). We recently held two hackathons and just hosted our largest, all-hands meeting (AHM). In addition, we will be taking part in two major conferences, the International Conference on Computational Science (ICCS) and ISC High Performance (page 3).

One of the central discussion topics at the AHM was the future of VECMA and the forms under which this effort may continue beyond our current timeline. A few different strategies were proposed and discussed, and we are particularly grateful to the members Scientific and Innovation Advisory Boards not only for their contributions in that respect, but for their guidance throughout the course of our activities. We are also grateful to all our readers, whom we would like to thank for their continued support and interest in our work.

As we near the end of VECMA, at least in its current form, we will focus on the opportunities that our Project has created for the future and will be providing updates via our website on our next steps.

VECMAtk M33 Release

The Toolkit enables automated VVUQ for multiscale applications that can be deployed on emerging exascale platforms and provides support for software applications for any domain of interest. It may be installed by component or as a package. On March 29th, VECMA released the M33 version of VECMAtk, with the following new features:



FabSim3 v2.8:

- Added new job submission workflow.
- Added QCG-PJ template files for ARCHER2
 Machine.
 FobSin
- Revamped FabMD plugin, and Added support EasyVVUQ.
- Setup new documentation website for FabMD plugin.
- Added support for 2-factor authentication.

EasyVVUQ v0.9:

- MCMC support for calibration prob- EasyVVUQ lems.
- Rework of the actions framework to allow a wider range of execution scenarios and to simplify the code base.
- CSV sampler for loading in data created with other software.

QCG-PilotJob v0.11:

• Support for gathering launched processes metrics.

EasySurrogate v0.15:

- Kernel mixture networks (with time-lagged features)
- Standard artificial neural networks (with time-lagged features)

EQI v0.5.2:

• Features stay the same as listed in the previous version, which is comprehensive.

MUSCLE3 v0.4.0:

• New yMMSL, compute_elements are now components.

VECMA and Reproducibility

We are delighted to announce the publication of a Theme Issue in the journal Philosophical Transactions of the Royal Society A. The issue is titled "Reliability and Reproducibility in Computational Science: Implementing Verification, Validation and Uncertainty Quantification in Silico" and a significant proportion of the papers contained therein stems from research led by UCL's Centre for Computational Science through VECMA. The theme issue also stems from an event hosted by The Alan Turing Institute in London in early 2020 under the same title, where several of the issue's contributors met to prepare for its production (see Newsletter Issue No. 3, November 2019).

The theme issue addresses the question whether the computational methods and models used today are sufficiently reliable to generate actionable results. The question is analyzed based on three notions of reliability. Verification (V): that the model correctly implements the intended theory. Validation (V): agreement between model and experiment. Uncertainty quantification (UQ): identification of the provenance and magnitude of errors within the model, in other words how accurately the model captures reality. VVUQ lies at the heart of VECMA's mission statement, "to enable trust in computer simulations as tools in the decision-making process for scientists as well as for policy makers in an era where science is afflicted by the 'reproducibility crisis' ".

Reproducibility, indeed, extends far beyond computational aspects of science. Experimental facts, observations and theories should not depend on who reports them but should be obtainable by anyone performing similar procedures. Indeed, the objectivity of science is its crowning and distinguishing feature. That, at least, is the aspiration. In practice, things are often less clear cut and, in a time where scientific data production is larger than ever, an increasing number of cases lacking reproducibility are reported. The authors hope to offer a contribution towards reproducible science by analyzing the problem and offering solutions within the computational domain.

Funding is gratefully acknowledged from the European Commission for VECMA and from the Alan Turing Institute towards the event in 2020. Nature Journal's news article can be found at www.nature.com/articles/d41586-020-03208-1.

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PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A

MATHEMATICAL, PHYSICAL AND ENGINEERING SCIENCES

Reliability and reproducibility in computational science: implementing verification, validation and uncertainty quantification *in silico*

Theme issue compiled and edited by P. V. Coveney, D. Groen and A. G. Hoekstra



VECMA 4th and 5th Hackathons - April and May

The fourth and fifth VECMA Hackathons took place on 21-23 April and 22-27 May, respectively. The two events, both taking place online, allowed participants to interact with VECMAtk experts, who guided the former to apply the right choice of VECMAtk tools on their codes. Sessions included team formation and preparatory background, social lunch, progress reports, and presentations of work. Hackathon participants also provided feedback on Toolkit usability and experience, which is crucial for VECMA's continuing improvement of service provision to its users.



VECMA All-Hands Meeting (AHM): 19-21 May, online.

The AHM is VECMA's largest meeting, to which all Members, Core and Associate Partners are invited. It occurs on an annual basis and this year we hosted its third edition. In view of the ongoing COV-ID-19 restrictions, and for the second time, we replaced the physical meeting with an online one.

The AHM took place over two days, following its usual format. Day 1 featured technical presentations across all Work Packages to update

the Consortium on recent developments, a discussion around technical developments of the Toolkit and its release plans, a meeting of the Scientific and Innovation Advisory Boards, and a meeting of the General Assembly to discuss matters pertinent to the project governance.

Day 2 comprised a full agenda of invited talks by external speakers and Consortium members. A general discussion on how to take VVUQ and VECMAtk forward after the end of VECMA brought the last AHM of the Project to a close.

VECMA at ICCS 2021 - 16 to 18 June

The International Conference on Computational Science (ICCS) is an annual conference that brings together researchers and scientists pioneering computational methods in sciences such as physics, chemistry, life sciences, engineering, as well as in arts and humanitarian fields.

ICCS 2021 will take place on 16-18 June. It will be the twenty-first in the series and the second where VECMA will have a presence through two *thematic tracks*, workshops which are intended to provide a forum for the discussion of one or more specific topics in the field of computational science among an international group of researchers:

- 1. Multiscale Modelling and Simulation (MMS): This thematic track aims to provide a forum for multiscale application modellers, framework developers and experts from the distributed infrastructure communities to identify and discuss challenges in and possible solutions for modelling and simulating multiscale systems, as well as their execution on advanced computational resources and their validation against experimental data. Key topics will include:
- Challenging applications in science, industry or society;
- Verification, validation and uncertainty quantification;
- New approaches for coupling and scale bridging;

VECMA at ISC 2021 - 24 June to 2 July

For the second consecutive year, VECMA will be joining one of the most prestigious supercomputing conferences. Running



ISC HIGH PERFORMANCE 2021 DIGITAL

JUNE 24 - JULY 2, 2021 ISC-HPC.COM

yearly since 1986, it stands as the oldest supercomputing conference in the world, with a community devoted to the relentless improvement of technologies and products that aim to drive the future of computing. As a Future and Emerging Technologies (FET) project addressing the imminent exascale era of supercomputing, VECMA is well-placed within that community.

- Advanced numerical methods;
- Executing multiscale models on advanced computational infrastructures (distributed, HPC, cloud, etc.);
- Performance analysis;

MMS is organized by VECMA Technical Director, Derek Groen. More information: https://mms.computationalscience.nl/

- 2. Uncertainty Quantification for Computational Model (UNEQUIV-OCAL): This thematic track aims to attract research that focuses on new methods, which outperform existing techniques, as well as uncertainty quantification applications to complex problems.
- Forward and inverse UQ;
- Model inadequancy;
- Dimension reduction;
- Surrogate modelling -including machine-learning techniques and reduced-order modelling;
- Software for uncertainty quantification;

UNEQUIVOCAL is organized by VECMA member Wouter Edeling. More information: https://unequivocal.computationalscience.nl/

This year, ISC High Performance will address current developments critical to high performance computing, machine learning and data analytics, as well as the future advances that will shape these technologies, through the following topics: System Architecture, Applications/Algorithms, Emerging Technologies, Parallel Programming Models & Performance Modelling, and Machine Learning Day.



VECMA will be presenting two posters, on workflow automation with FabSim3 and on large-scale computations with

QCG-PilotJob. For abstracts and more information on our participation, visit vecma.eu/vecma-at-isc-2021.

VECMAtk Online Training Event - 23 July

Learn to apply automated Verification, Validation and Uncertainty Quantification (VVUQ) to complex single- and multi-scale applications!

We are pleased to announce a free online training event on **EasySurrogate**, **QCG-PilotJob**, and **FabSim3**. Participants will receive a general introduction to the Toolkit before focusing on those three tools through interactive tutorials.

EasySurrogate is a tool designed to facilitate the creation of surrogate models for multiscale simulations by replacing the expensive (small-scale) components of multiscale simulations by a surrogate model. The overall design is similar to EasyVVUQ, our forward uncertainty propagation tool.

QCG PilotJob is a lightweight implementation of the Pilot Job mechanism. It can be easily incorporated into scientific workflows to provide efficient and reliable execution of a large number of computational jobs.

FabSim3 is an automation toolkit for performing complex, remote tasks from a local command line and for automatically organising data and environment variables during those tasks. FabSim3 supports single jobs, ensembles of multiple jobs, and dynamic workflows through schedulers such as Slurm, PBSPro, LoadLeveller and QCG.

Please register before 21 July 2021. More information and registration: https://www.vecma.eu/vecma-training-event-easysurrogate-qcg-pilotjob-and-fabsim3/



Latest Associate Partners

ESCAPE-2 stands for Energy-ef-

ficient SCalable Algorithms for

weather and climate Prediction

at Exascale and is the follow-on



initiative of the ESCAPE project.

ESCAPE-2 will develop world-class, extreme-scale computing capabilities for European operational numerical weather and climate prediction systems. It continues the pioneering work of the ESCAPE project.

HPC and Big Data Technologies for Global Systems (HiDALGO) is a European project funded by the Horizon 2020 Framework Programme, comprising 13 partner institutions from seven countries.

Understanding major global challenges as well as their underlying parameters is a vital issue in our modern world. Various examples, such as health care, the transition of green technologies or the evolution of the global climate up to hazards and stress tests for the financial sector demonstrate the complexity of the involved simulation systems. This high level of complexity becomes even more evident in the case of coupled systems: the problem statements

netherlands



The Netherlands eScience Center is the Dutch national centre of excellence for the

development and application of research software to advance academic research. The eScience Research Engineers at the center work together with researchers in academia, enabling them to address compute-intensive and data-driven problems within their research. The eScience Center is involved in more than 90 collaborative re-

The project aims to attack all three sources of enhanced computational performance at once, namely (i) developing and testing bespoke numerical methods that optimally trade off accuracy, resilience and performance, (ii) developing generic programming approaches that ensure code portability and performance portability, (iii) testing performance on HPC platforms offering different processor technologies.

Our contacts for ESCAPE-2 are Dr. Daniel Thiemert and Dr. Peter Bauer, Coordinator for the ESCAPE-2 project.

and their corresponding parameters depend on each other, which results in very involved and interconnected simulations.



HiDALGO's mission is to develop novel methods, algorithms and software for HPC and HPDA to accurately model and simulate the complex processes which arise in connection with major global challenges.

search projects, spanning many different research disciplines and application domains. Many of the projects are related to HPC and multiscale applications.

Our contacts for the eScience Centre are Dr Robin Richardson and Mr Lourens Veen. Robin has previously led development on the EasyVVUQ Python framework in the VECMA project on behalf of UCL. Lourens is leading the development of the MUSCLE 3 multiscale coupling toolkit.

New Publications

- P. V. Coveney, D. Groen and A. G. Hoekstra, "Reliability and reproducibility in computational science: implementing validation, verification and uncertainty quantification in silico", Phil. Trans. R. Soc. A. 379, 20200409 (2021), DOI:10.1098/rsta.2020.0409 [and further articles in the homonymous Theme Issue]
- D. Groen, H. Arabnejad, V. Jancauskas, W. N. Edeling, F. Jansson, R. A. Richardson, J. Lakhlili, L. Veen, B. Bosak, P. Kopta, D. W. Wright, N. Monnier, P. Karlshoefer, D. Suleimenova, R. Sinclair, M. Vassaux, A. Nikishova, M. Bieniek, Onnie O. Luk, M. Kulczewski, E. Raffin, D. Crommelin, O. Hoenen, D. P. Coster, T. Piontek and P. V. Coveney, "VECMAtk: a scalable verification, validation and uncertainty quantification toolkit for scientific simulations", Phil. Trans. R. Soc. A. 379, 20200221 (2021), DOI:10.1098/rsta.2020.0221
- D. Ye, A. Nikishova, L. Veen, P. Zun and A. G. Hoekstra, "Non-intrusive and semi-intrusive uncertainty quantification of a multiscale in-. stent restenosis model," Reliability Engineering and System Safety 214 (2021) 107734. doi.org/10.1016/j.ress.2021.107734
- A. Gheorghiu, P. V. Coveney and A. A. Arabi, "The influence of external electric fields on proton transfer tautomerism in the guanine-cytosine base pair", Phys. Chem. Chem. Phys. 23, 6252-6265 (2021), DOI:10.1039/D0CP06218A
- W. Edeling, H. Arabnejad, R. Sinclair, D. Suleimenova, K. Gopalakrishnan, B. Bosak, D. Groen, I. Mahmood, D. Crommelin, P. Coveney, "Model uncertainty and decision making: Predicting the Impact of COVID-19 Using the CovidSim Epidemiological Code", Nat Comput Sci 1, 128-135 (2021), DOI:10.1038/s43588-021-00028-9
- M. Bieniek, A. Bhati, S. Wan and P. V. Coveney, "TIES 20: Relative Binding Free Energy with a Flexible Superimposition Algorithm and Partial Ring Morphing", J. Chem. Theory Comput., 17, 2, 1250–1265 (2021), DOI:10.1021/acs.jctc.0c01179

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) and YouTube (VECMA FET-HPC). 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-emergingtechnologies) 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.

