

Welcome

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Having entered the second half of its time span, VECMA is now in a fully mature and productive phase. The end of the first half was marked by a successful Review by the European Commission on the progress of our Project hitherto and on the plans for its future. The Review was led by external experts who, following an examination meeting in Luxembourg, deemed the Project's implementation fully satisfactory, while providing recommendations for maximizing its impact over the second half and its legacy, beyond.

The pandemic caused by the SARS-CoV-2 coronavirus has disrupted scientific research over the last few months. Scientists and governments have been redirecting substantial research effort and funding towards understanding this virus and how it spreads. VECMA has been contributing in this effort directly and also through its network of partners by providing methods for validation and uncertainty quantification in mathematical models that aim to inform government policy about what social meas-

ures to take in order to contain the spread as well as in methods that aim to accelerate the development of antiviral drugs (page 2). The Centre of Excellence CompBioMed, with which VECMA most closely collaborates with, is active in a vast international consortium working on urgent coronavirus research across Europe and USA.

As far as the rest of our scientific activities are concerned, we have continued them on a remote-working, online basis. Our network of Associate Partners is growing still and we are consolidating our relationships with other large European projects, such as ESCAPE-2 and ChEESE (page 3). We are participating in virtual scientific meetings and workshops and we are organizing our first online all-hands meeting (page 4).

I hope that you will enjoy finding out about all our latest news and updates and I wish you to keep well and healthy.

VECMA Toolkit (VECMAtk) Month-21 Release

VECMAtk 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. In March 2020, VECMA announced the M21 release of VECMAtk, which contains the following updates:




FabSim3 v1.9:

- Added automated configuration of machines_user.yml file.
- Fixed Multi threading bug, allowing for much larger ensemble sizes.
- Disabled execution of run_prefix commands on the remote machine during the job submission.
- Defined additional functional tests for FabSim3 and plugins.



EasyVVUQ v0.5.1:

- Point Collocation method for PCE  sampling.
- GaussianProcessSurrogate class which will serve as a basis and testing ground for surrogate based workflows
- Added quasirandom sampling classes: LHCSampler and HaltonSampler.
- JSONDecoder class. It allows codes to use JSON as output format.
- Started measuring test coverage using coveralls.

QCG-PilotJob v0.7:

- Bugfix related to the 'job temporarily disabled' error.
- Bugfix related to the node launcher agent wait time.

EasyVVUQ-QCGPJ v0.2:

- Possibility to use `EXEC_ONLY` option for `SubmitOrder` that limits the application of the pilot job tasks just to the actual execution of model (with this option decoding is executed without PJ)
- Possibility to define a logging level of the QCG Pilot Job software directly from the API
- Internal tutorial material that can be helpful for new EasyVVUQ-QCGPJ users.

MUSCLE3 v0.3.0:

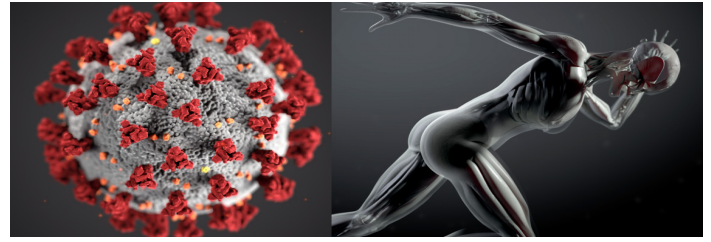
- Support for submodels (and other components) written in C++. MUSCLE 3 now offers a native C++ API, backed by a C++ implementation.
- Support for C++ submodels that use MPI to communicate internally.
- Improved handling of clusters with multiple networks.
- Improved error handling and shutdown.
- Support for Fortran, including MPI.

News and Updates

VECMA and COVID-19

VECMA is contributing to the efforts against the coronavirus directly and through its network of partners by providing methods for validation and uncertainty quantification in mathematical models that aim to inform government policy about what social measures to take in order to contain the spread as well in methods that aim to accelerate the development of antiviral drugs.

NHSX, a joint unit bringing together teams from the Department of Health and Social Care and NHS England and NHS Improvement to drive the digital transformation of care (<https://www.nhsx.nhs.uk/>), is collaborating with VECMA's Technical Director, Dr Derek Groen, and the Computer Science department at Brunel University to model virus spread in an agent-based model where open street maps are fed into it, providing the layout in which population movement may be modelled in towns, cities and boroughs. Various measures such as social distancing may be introduced to see the impact on the curves of infections and fatalities. These models have been able to reproduce the kinds of curves that have been seen



in the news. These models are currently using FabSim3 and EasyVVUQ, and expected to also implement PilotJob at the later stage of scaling up, for submitting a large number of simulation runs to HPC machines, for simulation progress monitoring, and large data management.

Through the EC Centre of Excellence CompBioMed, with which VECMA collaborates most closely, we contribute in the effort to accelerate the development of antiviral drugs by modelling proteins that play critical roles in the virus life cycle in order to identify promising drug targets. Machine learning (ML), deep learning (DL) and artificial intelligence (AI) techniques are used in that direction. More information can be found at <https://www.compbioed.eu/compbioed-and-coronavirus/>.

Success at European Commission Review

On Wednesday 26th February 2020, VECMA was summoned to take part in its mid-term Project Review by the European Commission (EC) in Luxembourg.

The goal of this meeting was to assess the progress of our project during the first half of its duration (15th June 2018 – 14th December 2019) and to assess our plans for the second half (15th December 2019 – 14th June 2021). In advance of the Review, VECMA had submitted a written Periodic Report including a Technical and a Financial part, while extensive presentations were given to cover activities across all Work Packages at the Review meeting.



The EC examined the following aspects, among others:

- The degree to which the work plan has been carried out and whether all deliver-

ables were completed.

- Whether the objectives are still relevant and provide scientific or industrial breakthrough potential.
- How resources were planned and used in relation to the achieved progress, and if their use respects the principles of economy, efficiency and effectiveness.
- The management procedures and methods of the project.
- The expected potential scientific, technological, economic, competitive and social impact, and plans for using and disseminating results.

The Review was led by external experts who, following the Luxembourg meeting, deemed the Project's implementation fully satisfactory, while providing recommendations for maximizing its impact over the second half and its legacy, beyond.

Reproducible Science

Following the successful workshop on *Reliability and Reproducibility in Computational Science* organized in collaboration with the Alan Turing Institute on the 24th of January 2020, VECMA is leading the preparation of a Theme Issue in the journal *Philosophical Transactions A* of the Royal Society under the title *Reliability and Reproducibility in Computational Science: Implementing Verification, Validation and Uncertainty Quantification in Silico*.

The collection of papers, which is soon due to be submitted for review, will contribute toward a unified set of methods that will increase confidence in computer-based simulation methods as trusted decision-making tools for those working in academia, industry and the third sector. The theme issue will look at how to achieve reliability and reproducibility in computational science, particularly by implementing verification, validation and

uncertainty quantification schemes. The following principal topics will be addressed:

- Fundamental aspects of reproducibility.
- Verification, validation, and uncertainty quantification (VVUQ).
- Reproducibility challenges for multiscale modelling and simulation.
- The limits of computation.
- Handling of data: best practices to ensure implementation of the scientific method.

We anticipate publication of this Theme Issue by the end of the year.



ESCAPE-2 VVUQ Workshop

A VVUQ workshop organized by our Associate Partner ESCAPE-2 (<http://www.hpc-escape2.eu/>) took place on 23-24 April in Saint-Rémy-les-Chevreuse, near CEA Saclay. The workshop aimed at formulating a common VVUQ (Verification Validation and Uncertainty Quantification) framework to be applied in Numerical Weather Prediction. Extensive descriptions of the VVUQ methodologies as performed on both the URANIE and NWP communities were presented, allowing the various members of the project to become more familiar with both approaches.

VECMA members Erwan Raffin, Wouter Edeling and Nicholas Monnier were present, consolidating the links between the two projects. Raffin and Edelin have also previously been pres-

ent at the 1st Dissemination Workshop of ESCAPE-2 on 21-22 October 2019, titled "Towards Energy-efficient Scalable Algorithms for weather and climate Prediction at Exascale - Status and Prospects", where they contributed with a talk on VVUQ for climate research. ECMWF, lead partner of ESCAPE-2, is also an Associate Partner of VECMA.



VECMA All-Hands Meeting (AHM): 11-12 May 2020, 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 second edition. In view of the Covid-19 pandemic 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, a meeting of the General Assembly to discuss and vote on matters pertinent to the project governance, and, finally, a roundtable discussion.



Day 2 comprised a full agenda of invited talks by external speakers who included new additions to our advisory boards as well as invited talks by Consortium members. A general discussion and closing remarks' session brought the two-day meeting to a close.

Our AHM attracted over 30 enthusiastic participants and an excellent collection of talks and short meetings. The meeting was also key in setting the direction for the third and final year of the Project as well as in preparing the ground for VECMA's legacy, beyond.

VECMA Welcomes New Associate Partners



ChEESE is the Center of Excellence (CoE) for Exascale in Solid Earth, a H2020-funded project with the aim of preparing flagship codes and enabling services for the upcoming exascale supercomputing era in the area of solid earth. VECMA also became a member of the Industry and Users Board (IUB) of ChEESE, which is comprised of representatives of industry, SMEs, academic networks, and public governance bodies with mutual interests in the project. Through its membership, VECMA will provide independent

feedback on the project's interim results and will participate in identifying and pursuing exploitation opportunities.

VECMA collaborates with Dr Arnau Folch Duran, ChEESE Project Coordinator and senior researcher in the Department of Computer Applications in Science and Engineering (CASE) at the Barcelona Supercomputing Center - Centro Nacional de Supercomputación (BSC-CNS) and also with Dr Erwan Raffin, senior HPC expert at Bull Atos, a Partner of ChEESE and a member of the Center for Excellence in Parallel Programming (CEPP).



The European Centre for Medium-Range Weather Forecasts (ECMWF) is an independent intergovernmental organisation supported by 34 states. ECMWF is both a research institute and a 24/7 operational service, producing and disseminating numerical weather predictions to its Member States. This data is fully available to the national meteorological services in the Member States. The Centre also offers a catalogue of forecast data that can be purchased by businesses worldwide and other commercial customers. The supercomputer facility (and associated data archive) at ECMWF is one of the

largest of its type in Europe and Member States can use 25% of its capacity for their own purposes.

ECMWF's core mission is to produce numerical weather forecasts and monitor the Earth system, carry out scientific and technical research to improve forecast skill, and maintain an archive of meteorological data. ECMWF also provides advanced training to scientific staff in our Member and Co-operating States and assists the WMO with its programmes. Our contact for ECMWF is Dr. John Hanley, Analyst, Forecast Department.



ALMA MATER STUDIORUM
UNIVERSITÀ DI BOLOGNA

The Alma Mater Studiorum, the oldest university in the Western world, paves the way for innovation through an increasingly rich programme catalogue, cutting-edge research and a constant and increasingly broad international perspective. Since its origins in 1088, Alma Mater has been student-centred hosting prominent figures from science and the arts. Based in five campuses (Bologna, Cesena, Forlì, Ravenna, Rimini), with a branch in Buenos Aires, it offers a teaching catalogue diversified and tailored to the needs of present-day society: over 200 degree-awarding programmes among its 32 Departments and 11 Schools are offered to over 81,000 students. 5,000 graduates are enrolled in PhDs and 3rd cycle programmes.

VECMA collaborates with Marco Viceconti, Professor of Industrial Bioengineering at the Department of Industrial Engineering of the University of Bologna, and Director of the

Medical Technology Lab, at the Istituto Ortopedico Rizzoli, the most prestigious orthopaedic hospital in Italy. Since 2005 his main focus has been the development and widespread adoption of modelling and simulation in healthcare. Co-author of the first white paper on the Virtual Physiological Human (VPH), coordinator of the STEP action and first author of the Europhysiome Research Roadmap, founder and first director of the VPH Institute, coordinator of the Avicenna action, and first Author of the Avicenna roadmap on in silico trials, founder and board member of the Avicenna Alliance.

In 2012, Professor Viceconti started the Insigneo Institute for in silico Medicine at the university of Sheffield (UK), the largest research institute in Europe entirely dedicated to in silico medicine. A fellow of the UK Royal Academy of Engineering, he is currently one of 25 members of the World Council of Biomechanics.

Upcoming Event

Multiscale Modelling, Uncertainty Quantification and the Reliability of Computer Simulations: 11-12 June 2020, online.

VECMA is holding a virtual workshop on 11-12 June 2020 on "Multiscale Modelling, Uncertainty Quantification and the Reliability of Computer Simulations". The virtual workshop is a combination of three workshops that were due to take place at the SIAM Conference on Uncertainty Quantification (UQ20) and the International Conference on Computational Science (ICCS) 2020, but were cancelled due to the global pandemic. The combined virtual workshop fulfils all three of these workshops in a two day online event, and is made freely available and accessible to all.

The three workshops are as follows:

1. A mini-symposium titled "Tools for enabling Verification, Validation and Uncertainty Quantification (VVUQ) in multi-scale simulations and workflows" as part of SIAM UQ20.
2. A workshop titled "Multiscale Modelling and Simulation Workshop (MMS), 17th edition", as part of ICCS2020.
3. A thematic track titled "Uncertainty Quantification for Computational Models (UNEQUIVOCAL)", also as part of ICCS2020.



Publications

- D. Groen, D. Bell, H. Arabnejad, D. Suleimenova, S. E. J. Taylor, and A. Anagnostou, "Towards modelling the effect of evolving violence on forced migration", In Proceedings of the 2019 Winter Simulation Conference, IEEE (2020)
- R. A. Richardson, D. W. Wright, W. Edeling, V. Jancauskas, J. Lakhilili and P. V. Coveney, "EasyVVUQ: A library for verification, validation and uncertainty quantification in high performance computing", Journal of Open Research Software, 8(1), 11 (2020) DOI:10.5334/jors.303
- P. V. Coveney and R. R. Highfield, "From Digital Hype to Analogue Reality: Universal Simulation Beyond the Quantum and Exascale Eras", Journal of Computational Science, available online: DOI:10.1016/j.jocs.2020.101093
- D. W. Wright, R. A. Richardson, W. Edeling, J. Lakhilili, R. C. Sinclair, V. Jancauskas, D. Suleimenova, B. Bosak, M. Kulczewski, T. Piontek, P. Kopta, I. Chirca, H. Arabnejad, O. O. Luk, O. Hoenen, J. Weglarz, D. Crommelin, D. Groen and P. V. Coveney, "Building confidence in simulation: Applications of EasyVVUQ", Advanced Theory and Simulations, In Press

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 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.

