VECMA

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Welcome

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Now in Month 29, VECMA will soon enter its final phase of operations. The biggest part of 2020 has seen the project's activities take place on a remote-working, online basis. Nevertheless, we have gone through our most productive phase, both as far as internal and external operations are concerned.

The VECMA Toolkit, which has already seen two out of its three planned major releases and has further been upgraded last September to its Month-27 version. You can read about all the new features, below.

The coronavirus pandemic has led scientists and governments to redirect substantial research effort towards understanding this virus and how it spreads. VECMA has been contributing to this effort directly and also through its network of partners by providing validation and verification methods for various mathematical models. In our previous issue, you read about our collaboration with NHSX to model virus spread in an agent-based model into which open street maps are fed as input. In this issue, we are excited to tell you about our most recent contribution in quantifying the uncertainty of one of the most important models that the UK Government relied on to determine its policy in dealing with the rapid spread of the COVID-19 pandemic during March and April 2020 (page 2).

In addition to the above effort, we have launched a crowdfunder to support the creation of an interactive COVID-19 risk assessment map which will illustrate the spread risk in several UK universities. The risk map will be created by combining historical data with forecasts from our in-house Flu And Coronavirus Simulator (page 3).

We contiue to participate in virtual scientific meetings as well as to organize our own (page 3). Our network of Associate Partners is expanding and we are consolidating our relationships with other large European projects, such as ESiWACE, as well as with the private sector, such as Norton Straw consultants (page 4).

I hope that you will enjoy reading this issue of the VECMA Newsletter and I wish you to remain well and healthy.

VECMA Toolkit (VECMAtk) Month-27 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 September 2020, VECMA announced the M27 release of VECMAtk, which has been added on with a new component, EasySurrogate, and contains new features and updates for all other components as follows:

FabSim3:

- New features of added support for plugin machine-specific setting with updates for abbreviated form for PilotJob and virtualenv input args, fixed incompatibility with newer version of QCG-PilotJob, fixed reported bugs, and improved ensemble2campaign and campaign2ensemble functionalities. This version of FabSim3 has been used to enable five of the VECMA application tutorials on basic CFD models, molecular dynamics, migration modelling, Covid-19 simulation, and Multi-Output Gaussian Process Emulator.

EasyVVUQ:

- Added Kubernetes support via the ExecuteKubernetes action, which allows the user to execute their VVUQ workflows on a Kubernetes cluster with minimal set-up overhead, reworked the actions mechanism, in preparation of implementing it using the Futures mechanism which would allow for a more interactive use of the framework. It also added a CopyEncoder for easier handling of arbitrary configuration files, and a ReplicaSampler class for sampling simulations with different seed values. The updates include improvements to the Monte Carlo sampling and analysis classes, documentation restructuring and new tutorials, added a large interactive Jupyter notebook tutorial covering the major features of the software, and greatly expanded testing coverage. Most of the essential functionality is covered by high-quality tests that check for the correctness of the results.

QCG-PilotJob:

- New features for new execution models intelmpi, srunmpi, openmpi designed to launch MPI applications with different implementations and various HPC Slurm configurations. This version of the release provides initial support for hyper-threading nodes, discovering hyper-threading configurations and binding more than single CPU to process. The updates bug fix related to parsing slurm node list and bug fix related to freezing while launching MPI applications.

EasyVVUQ-QCGPJ v0.2:

- New features to support for campaigns consisting of multiple applications and added "model" parameter for tasks which allows to select the way of parallel execution of tasks by QCG-PilotJob. It has the updates for adjusted to run with EasyVVUQ v0.7 and QCG-PilotJob v0.9.0. It also has updated tutorials for the Cooling Cup and the Interactive Tutorial.

MUSCLE3 v0.3.0:

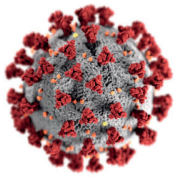
- New features of improved logging to aid in debugging Python submodels. The updates are fixes to sending and receiving lists, dictionaries and grids from C++, accessing settings from C++ is now more flexible, and compatibility improvements to the build system.

EasySurrogate:

- The first release of the EasySurrogate tool has the features of mimics the 'Campaign' structure of EasyVVUQ and quantized Softmax Networks available, which are stochastic, neural-network based surrogates used for conditional resampling of reference data. The release has available reduced surrogates, which are used to compress the size of training data by orders of magnitude while retaining accuracy for spatially-integrated quantities of interest. The release contains a general tutorial, and one for each type of available surrogate method.

News and Updates

VECMA and COVID-19



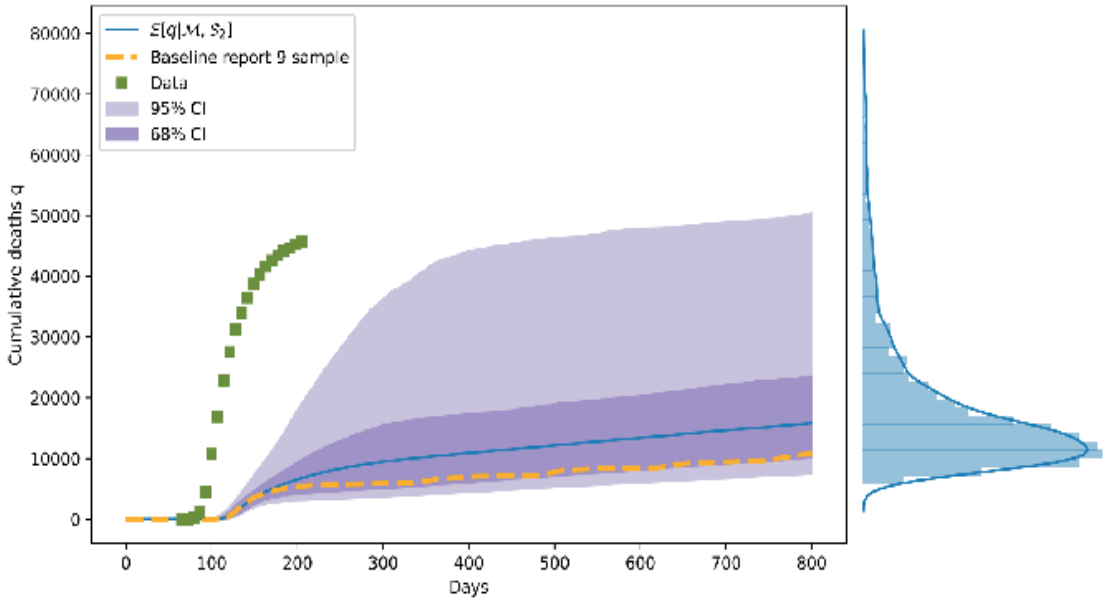
SARS-CoV2 has rapidly spread worldwide since December 2019, and early modelling work of this pandemic has assisted in identifying effective government interventions. The UK government relied in part on the CovidSim model developed by Professor Neil Ferguson's team at the MRC Centre for Global Infectious Disease Analysis at Imperial College London, to model various non-pharmaceutical intervention strategies, and guide its government policy in seeking to deal with the rapid spread of the COVID-19 pandemic during March and April 2020.

CovidSim, albeit a sophisticated model, contains a large degree of uncertainty in its predictions, due to its inherent nature. The model is subject to different sources of uncertainty, namely parametric uncertainty in the inputs, model structure uncertainty (i.e. missing epidemiological processes) and scenario uncertainty, which relates to uncertainty in the set of conditions under which the model is applied. A result of these different types of uncertainty combined was the serious underestimation of the first wave: predictions of COVID-19 deaths in the influential Report 9 issued in March were about half the number of deaths that actually occurred in the UK, when simulating the most comparable scenarios -albeit with some differences, such as lockdown occurring later than simulated.

Scientists from VECMA and CompBioMed analyzed CovidSim by undertaking an extensive parametric sensitivity analysis and uncertainty quantification of the publicly available code. The study concluded that the model can display significant bias with respect to observed data, such that the output variance does not capture this validation data with high probability. The large variance in the prediction of an outcome (coronavirus deaths, in this case) can be seen through the example in the accompanying figure, reported in the study, where it can be seen that the predicted cumulative deaths may vary by as much as 100% (i.e. double), while still remaining within one standard deviation in terms of confidence.

VECMA calls for a better public understanding of the inherent uncertainty of models predicting COVID-19 mortality rates, saying they should be regarded as "probabilistic" rather than being relied upon to produce a particular and specific outcome. VECMA principal investigator Professor Peter Coveney noted: "This is not a reason to disregard modelling. It is important that these simulations are understood in terms of providing a range of probabilities for different outcomes, rather than a single fixed prediction of COVID-19 mortality."

To learn more about the findings of this study and its implications, as well as to access the publication preprint, visit our news page, www.vecma.eu/news, and Nature Journal's news article www.nature.com/articles/d41586-020-03208-1.



VECMA Training Event: EasyVVUQ and FabSim3

On Thursday 12 November 2020, VECMA hosted its first Training Event open to the public on automated Verification, Validation and Uncertainty Quantification (VVUQ) to complex single- and multi-scale applications.

The event was well attended and participants were introduced to the various tools of VECMAtk and taken through interactive tutorials on the EasyVVUQ and FabSim3 tools specifically. The introductory hour of the training event was recorded and will be uploaded to our youtube channel, VECMA FET-HPC.

We thank our members Hamid Arabnejad, Derek Groen, Bartosz Bosak and Jalal Lakhlili for being in charge of training and the organizing team for making the event possible.

Participants in this training event will have the opportunity to register for a follow-up Hackathon in December 2020, where they can join VECMAtk experts to apply VECMAtk to their own codes. For more information on upcoming events, visit www.vecma.eu/events.

VECMA at ENES HPC Workshop

Fredrik Jansson of our Core Partner CWI in the Netherlands presented the EasyVVUQ framework for model validation, verification and uncertainty quantification at the 6th ENES HPC Workshop on High Performance Computing for Climate and Weather, which took place on on 25-26 and 28-29 May 2020 as a virtual event. The event was organized by the Centre of Excellence in Simulation of Weather and Climate in Europe (ESiWACE), which we have recently welcomed as a new Associate Partner to VECMA -see following section.

This workshop of the European Network for Earth System modelling (ENES) brought together experts on HPC in earth system modeling.

Fredrik discussed applying the EasyVVUQ framework to the atmospheric large eddy simulation model DALES and how uncertainty quantification can be valuable in different stages of model development. A traditional use of uncertainty quantification is to study the response of a model to uncertain physical parameters. In addition to this, Fredrik explored using uncertainty quantification tools on modeling choices, in this case the tolerance parameter of an iterative Poisson equation solver.

Fredrik's presentation was entitled "Uncertainty quantification of atmospheric models - applying the EasyVVUQ framework on the DALES model", with credits also to his collaborators Wouter Edeling, Jisk Attema, Daan Crommelin and Gijs van den Oord.

Crowdfunding to support the COVID-19 research project – an interactive risk assessment map

Our core Partner Brunel University London has launched this project to maximise the accessibility of research results in the fight against COVID-19.

Funds raised will be used to create an interactive COVID-19 risk assessment map which will illustrate the spread risk in several UK universities. The risk map will be created by combining historical data with forecasts from our in-house Flu And Coronavirus Simulator (https://facs.readthedocs.org), which predicts COVID-19 spread taking into account individual buildings and households.

The risk map allows people to:

- see forecasts of the expected number of infectious cases in the coming weeks,
- identify potential hot spots across universities,
- investigate how different lockdown measures may affect future spread,
- help give an idea of what could be expected, taking into account some key uncertainties.

The project is a first crowdfunding pilot, which will create this assessment map as a publicly available website, allowing students, families and other interested parties to interactively explore our main campus forecasts.

For more information on the background research, the team, how funds will be used, our motivation and goals in this project, and how to become a sponsor, please visit brunel.hubbub.net/p/covid-19-risk-map.

VECMA Welcomes New Associate Partners

Norton Straw is an independent consultancy working in engineering and technology. They provide specialist technical and management services to clients across a range of industries. Their technical teams combine first-principles engineering knowledge and applied mathematics to provide industry-leading services in numerical simulation, analysis and engineering design. Norton Straw combines technical expertise with commercial and industry experience, gained from leadership and senior management roles in engineering and technology.

Our contact at Norton Straw is Dr Bruce Kakimpa, Principal Engineer, with a wide experience in using High Performance Computing simulations of multi-scale fluid flow to address engineering challenges across a range of sectors.

The Poznan University of Medical Sciences (PUMS) is one of the best and largest medical universities in Poland, with 100 years of sound academic experience and a great growth momentum. PUMS is currently recognized as one of the largest educational, research, and clinical centers in Poland. PUMS maintains and develops various forms of cooperation with foreign research centers and universities worldwide.

Advanced research at PUMS is carried out in virtually every field of modern medicine and pharmacy including the stability of drugs, pharmacokinetics and biochemistry, the synthesis and analysis of new therapeutic agents, phytochemistry, toxicology and pharmacology.

Our contact for PUMS is Prof. Judyta Cielecka-Piontek, Head of Pharmacognosy Department.

ESiWACE is one of eight newly funded Centers of Excellence. Our goal is to improve efficiency and productivity of numerical weather and climate simulation on high-performance computing platforms by supporting the end-to-end workflow of global Earth system modelling in HPC environment. This will be obtained by improving and supporting: 1) Scalability of models, tools and data management on state-of-the-art supercomputer systems, 2) Usability of models and tools throughout the European HPC eco-system, and 3) Exploitability of the huge amount of resulting data.

ESiWACE will develop solutions for cross-cutting HPC challenges particular to the weather and climate domain ranging from the development of specific software products to the deployment of user-facing services for both, computing and storage. ESiWACE leverages two established European networks, namely the European Network for Earth System modelling (ENES) the European Centre for Medium-Range Weather Forecasts.

Our contact for ESiWACE is Dr Joachim Biercamp, Coordinator for the ESiWACE project.

Publications

- J. L. Suter, R. C. Sinclair and P. V. Coveney, “Principles Governing Control of Aggregation and Dispersion of Graphene and Graphene Oxide in Polymer Melts”, Adv. Mater. 2003213 (2020).
- W. Edeling, D. Crommelin, “Reducing data-driven dynamical subgrid scale models by physical constraints”, Journal of Computers & Fluids, 201, 104470 (2020).
- S. Wan, R. C. Sinclair and P. V. Coveney, "Uncertainty Quantification in Classical Molecular Dynamics", Phil. Trans. R. Soc. A, In Press (2020).

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-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.