D1.4: Business Plan

Due Date	14 June 2021
Delivery	04 June 2021
Submission of updated version	N/A
Lead Partner	BULL
Dissemination Level	Public
Status	Final
Approved	Executive Board
Version	V1.0

This project has received funding from the *European Union's Horizon 2020 research and innovation programme* under grant agreement No 800925.

DOCUMENT INFO

Date and version number	Author	Comments
11.09.2020 v0.1	Erwan Raffin	Initial Draft
22.04.2021 v0.2	Erwan Raffin	Update with more input from project partners
03.05.2021 v0.3	Erwan Raffin	Update with more input from project partners
06.05.2021 v0.4	Erwan Raffin	Add users' feedback
07.05.2021 v0.5	Apostolos Evangelopoulos	Addition of information on external applications of VECMAtk; minor corrections elsewhere.
10.05.2021 v0.6	Erwan Raffin	Add contribution from Paul Best and Hugh Martin
11.05.2021 v0.6	Xuanye Gu	Addition of section "Applying VECMA as a Provider to EOSC portal"
14.05.2021 v0.7	Apostolos Evangelopoulos	Miscellaneous comments / proposed additions
18.05.2021 v0.8	Erwan Raffin	Address comments and add more text in future business and sources of finance section
26.05.2021 v0.9	Erwan Raffin	Update thanks to reviewer's feedback
04.06.2021 v1	Erwan Raffin	Final version

CONTRIBUTORS

- Erwan Raffin – Main Author, Editor
- Paul Best – Advisor
- Hugh Martin - Author
- Apostolos Evangelopoulos – Author
- Xuanye Gu – Author
- Derek Groen - Author
- David Coster – Reviewer
- Bartosz Bosak – Reviewer
- Tomasa Piontek – Reviewer
- Peter Coveney – Approver, Editor

Disclaimer

TABLE OF CONTENTS

LIST OF FIGURES

1 Executive summary

This deliverable reports on achievements from Task 1.5, which developed a business plan for the VECMA project continuance. This task aimed at capturing the project outcomes that support future revenues in collaboration with the innovation management task (T6.7). In addition, T1.5 assessed the potential for future business and revenue streams that can ensure the continuity of the innovation developments toward a long-term exploitation. The main project outcome supporting continuation of the VECMA project work, the VECMA Toolkit [1], and its current licence are presented in the first part of the report. Then, an estimation of the required funding level is presented. Finally, future business and the different sources of finance identified are detailed.

2 Introduction

The fundamental mission for VECMA is to generate a widely available toolkit for VVUQ in the domain of multiscale simulation using high performance computers, as these begin to enter the exascale. The core strategy then for the VECMA toolkit is to be fully open source in its nature to ensure barrier-less take up and use by the widest community possible. In order to perpetuate this toolkit and the expertise that develops and supports, funding will be required.

Therefore, both to survive and to support the European exascale computing initiative, VECMA will need to secure sources of funding after the project end to:

- Promote and extend the application of the toolkit across all actors in the European exascale computing initiative – exascale machine development, application co-design, user community engagement *et al.*
- Provide expert toolkit support to encourage and assist the user community
- Training in toolkit use and VVUQ
- Continue to develop the toolkit as its use is widened and more user feedback occurs
- Software as a service
- Maintain and continue coordination of core and associated partners, manage the grants

3 Project results toward VECMA Toolkit continuation

3.1 VECMA Toolkit (VECMAtk)

The last major release of the VECMA Toolkit[1] (tagged M36, i.e. June 2021) is briefly described in this section, a minor release is planned for M42 (i.e. December 2021) thanks to the 6 months project extension.

3.1.1 Description of the final Toolkit

The VECMA Toolkit is a set of open source tools that enables automated Verification, Validation and Uncertainty Quantification (VVUQ) for complex single- and multi-scale applications for any domain of interest. It allows to verify key aspects of simulations, compare and validate their outputs against observational or benchmark data, and run simulations conveniently on any platform from the desktop to current multi-petascale computers toward exascale platforms.

Figure 1. VECMA Toolkit logo

The VECMA Toolkit M36 release components are the following:

- FabSim3
- EasyVVUQ
- EasySurrogate
- QCG-PJ
- QCG-Now
- QCG-Client
- MUSCLE3

Users can pick up and combined the tools they want according to their needs as shown in the following figure.

[1] Release history can be found at https://www.vecma-toolkit.eu/tools

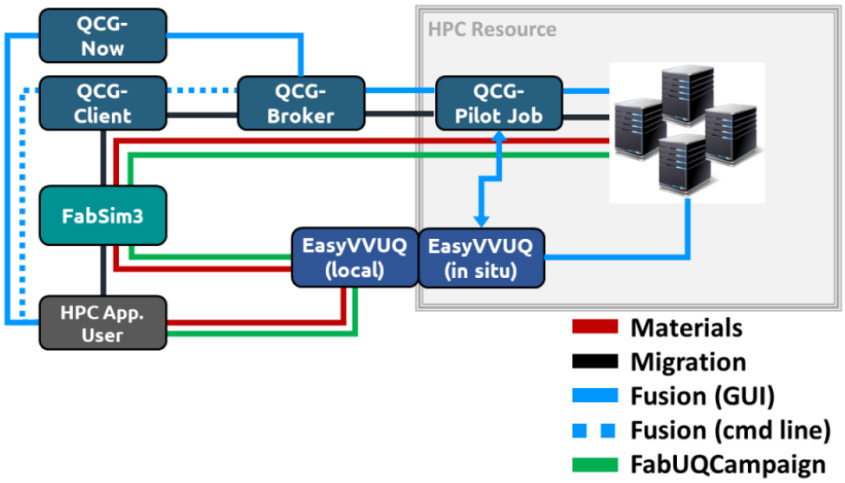


Figure 2. Example of a VECMA tools combination

3.1.2 Current licence and IP Rights

The VECMA Toolkit components, and its training material, are fully open source with their own licence (GNU LGPL, Apache v2, BSD-3), thus anyone wanting to use it, develop it, or derive any other development from it, can do this without any charge. It has been decided by all the consortium members to facilitate its adoption and expand its user community, mainly composed by scientific researchers doing VVUQ on their own simulation models. This approach leads to easy exploitation beyond the project while keeping possible future revenue from licencing and commercializing dedicated training, advisory services, or features. Section 5 addresses this point.

It should be noticed that the Foreground IP generated by VECMA is registered by WP6 and will be updated until the end of the project.

3.2 VECMA Toolkit applications and users' needs

The VECMA Toolkit has been successfully used for the applications shown in Figure 3 which also present the components used. In addition to the applications planned in the project, other ones from internal and external partners have used the VECMA Toolkit, this is the case for BAC/NAMD (UCL), UrbanAir (PSNC), MDDT w/Alya (BSC/ELEM), BOUT++/Nektar++ (UKAEA, University of York) and Fabmogp (Alan Turing Institute).

	EasyVVUQ	QCG-PJ	FabSim3	EasySurrogate	MUSCLE3
CovidSim	x			x	
Migration	x	x	x		
FACS			x		
Dutch-Covid	x	x	x		
Climate	x		x	x	
Fusion	x	x		(x)	x
ISR2D					
ISR3D		x			x
Materials	x			(x)	(x)
BAC /NAMD	x	x			
UrbanAir	x	x			
MDDT w/ Alya	x		x		
BOUT++/Nektar++	x				
Fabmogp		x	x		

Figure 3. VECMA Toolkit components used per application

External applications are particularly significant in that they promote VECMA beyond its own network of partners and in that they constitute an endorsement or seal of approval of the Toolkit's usefulness. Some users have provided a valuable feedback on the benefits of using the VECMA Toolkit which is presented in Annexes: Examples of VECMA Toolkit benefits for users.

Following the two first hackathons organized by the project (first on in January 2021 and second one in April 2021), participants were invited to fill a questionnaire in which a question regarding the future of their use and potential collaborations was asked:

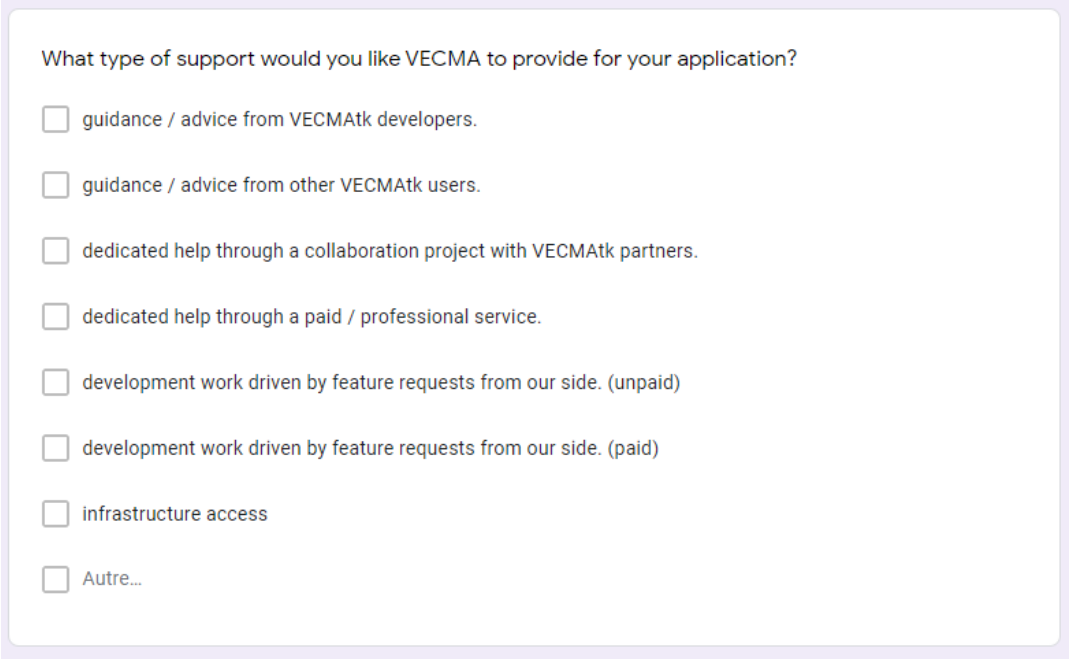


Figure 4. Question from the hackathon questionnaire

Here are the results:

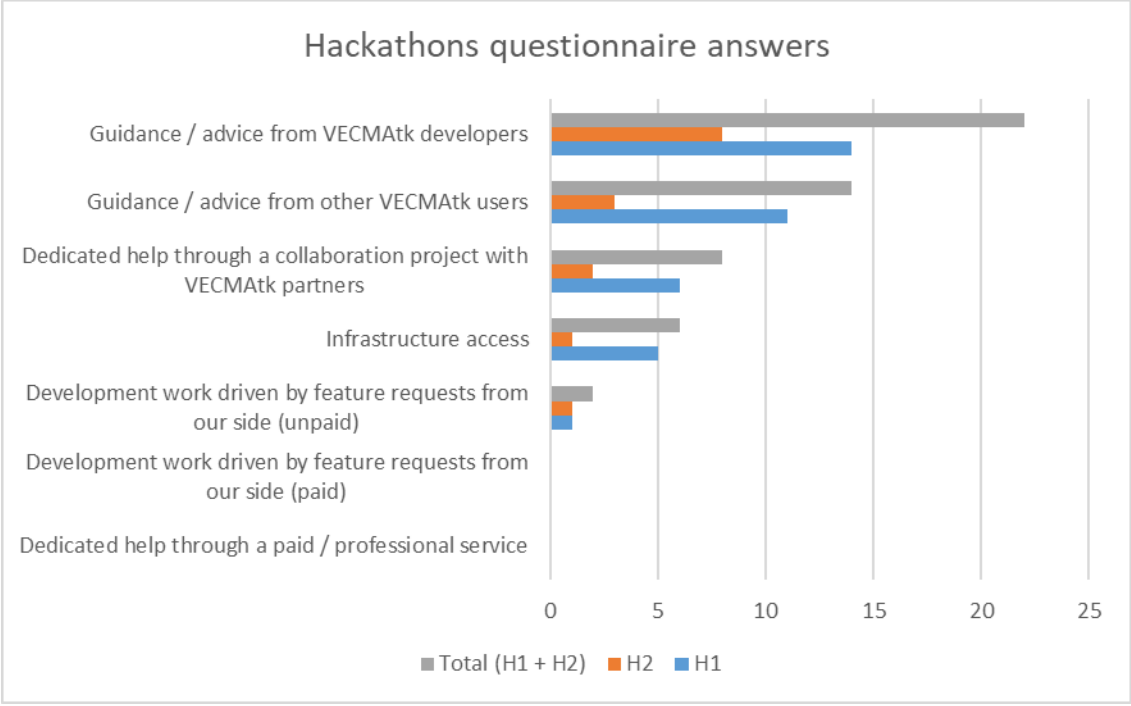


Figure 5. Detailed results from the hackathons' questionnaire for the support question (H1 refers to the January 2021 Hackathon and H2 to the April 2021 one)

As one can see, the most asked type of support expressed by the questionnaire answers is “guidance and advice from the VECMAtk developers” while the paid and professional service is the least popular one.

Last but not least, as is mentioned in the first line of the VECMA website; “The purpose of the VECMA project is to enable a diverse set of multiscale, multiphysics applications to run on current multi-petascale computers and emerging exascale environments with high fidelity such that their output is “actionable”. Indeed, even if the main users are the scientists, the ultimate end users are decision maker, policy makers and in a sense too the general public when decisions affect their way of life. The most recent example is the COVID-19 crisis which has a lot of implications in our daily life and for which many simulations and forecast have been done to simulate the potential drugs but also the virus spread.

4 Required funding levels

We have made an assessment of the realistic cost for continuance of core functions based on an analysis of the outputs and the relevant costs incurred during the execution of VECMA. Much of the early set-up and infrastructure is relevant to the longer term existence of VECMA and therefore these costs do not need to be incurred again. We have assumed that there are low start-up costs (i.e. that the project continues in a significant form before the established team disperses) and that much of the infrastructure remains intact during the gestation period associated with putative future funding.

The cost of VECMA is approximately €4m over 3 years of operation, which includes a significant element of start-up and initial development costs. We anticipate, according to the experience of developing and maintaining the toolkit, that the effort required of VECMA in providing the continued core functions at an effective level would cost approximately at least 3 full time equivalents (FTE). Indeed, for the next two years we estimate this effort to be necessary in order to keep the core VECMA Toolkit running, updated and enhanced. In addition, we estimate a requirement of around 0.5 FTE for each application to keep that up and running.

At the time of writing, and thanks to the effort invested by us in creating a VECMA Toolkit user community, some projects plan to continue to use the VECMA Toolkit as CompBioMed2, STAMINA, and ITFLOWS which represent an already living community for the next year. This community requires and will require some support.

5 Future business and sources of finance

There is growing interest and investment in the reliability of scientific output, and specifically so on the subject of VVUQ in HPC. This provides funding opportunities that can be leveraged in order to maintain and develop the VVUQ toolkit after the termination of VECMA. The project coordinator and team will continue to be in active dialogue with public funding organizations in order to maintain the gains made in the successful execution of VECMA. This discussion is aimed at determining the optimum route towards core funding that will prevent the sudden ending of the project and dispersal of the team.

Alongside this, the team has established an active search activity to identify upcoming candidate calls and actions relevant to the use of the toolkit, both within and beyond the application domains so far addressed.

5.1 Funding opportunities

At the time of publishing this business plan (June 2021), the following opportunities have been identified with the aim of securing funding to meet the required functions:

- Within the UK, the wider ExCALIBUR project funding the path to exascale is expected to have a series of calls within which VVUQ may play a key role. We plan to bid for any such relevant opportunities. For instance, the United Kingdom Atomic Energy Authority held a call for proposals in late 2020 on "Numerical Representation: Study of Uncertainty Quantification Techniques" for the ExCALIBUR Fusion Modelling System. This call resulted in the new NEPTUNE project, which currently collaborates with VECMA in order to use the VECMA toolkit in the NEPTUNE project and will contribute somehow to its continuity.

- The European Commission has recently launched the Multi Annual Financial Framework (MFF) 2021-2027. As part of MFF 2021-2027 “European Strategic Investments” a new Digital Europe programme will be implemented in order to “reinforce EU critical digital capacities”. The “Accelerating best use of technologies” target of this program has the goal to address crucial societal challenges including fighting climate change and protecting the environment and to support the European Green Deal policy. Specific developments in this programme in relation to Destination Earth Initiative (DestinE) represent a clear chance

for VECMA project results. Indeed, it appeared as a great opportunity to deploy the VECMA Toolkit for such projects in which the reliability of the results is particularly important as the end users are both the decision makers and the EU citizens. To illustrate, Atos has participated to several workshops on Destination Earth in which quality mapping was one of the topics addressed[2]. The quality mapping, according to the EU Commission, is to:

- Provide a comprehensive (single) quality index to assess digital twin validity
- Allow the selection of possible results based on quality/validity model maturity
- Automatically exclude more speculative/early results for policy and decision making to prevent confusion
- Guarantee transparency and traceability independent of digital twin inputs
- Help policy makers identify areas in need of further research to increase quality
- Ensure public trust in digital twin validity by using a quality system not just aimed at scientists

We believe that the VECMA Toolkit can help in addressing this kind of quality mapping.

- The Software Sustainability Institute (https://www.software.ac.uk/) may provide assistance as it can help in the funding of research software development.

- The experience gained when trying to register VECMA an EOSC provider is given in Annexe 9 “Applying VECMA as a Provider to EOSC Portal”.

5.2 Crowd funding campaign

Because conventional commercialization and monetisation routes have not been proven to be effective for the majority of EU software research projects, we chose to dedicate some effort to exploring alternative routes. As an initial experiment, we launched a crowdfunding campaign centred on the VECMA toolkit, highlighting one application in particular (The Flu And Coronavirus Simulator, FACS). We have no prior crowdfunding experience, and did not expect the attempt to succeed in advance, but chose to pursue it nevertheless because we believe it could provide us with valuable knowledge on how to sustain projects in this way.

Our main purpose within the crowdfunding campaign was to finance something that was obviously not funded by VECMA, namely the development of a user-friendly web interface for FACS which would

[2] Workshops reports on Elements of Digital Twins on “Weather-induced and Geophysical Extremes” and “Climate Change Adaptation”

allow people to investigate the robustness of the underlying assumptions in the code, visualize the uncertainty of different forecasts, given a scenario of their choice, and allowed them to explore the simulation results, and their associated uncertainty and validation information, more broadly. The main campaign was launched in November using the Brunel University hubbub.net platform, with support from Brunel's crowdfunding team. We also created satellite pages on Facebook, Instagram and LinkedIn and made a set of videos to provide the backers with periodic updates. Our minimum target was set at £5,000, with a stretch target set at £100,000.

In terms of funding, the campaign was unsuccessful, largely as we expected, having raised just £540 by the end of January 2021. However, we did get a clear indication of what worked well, and what worked less well. First of all, we found that we engaged people more effectively when we provided more frequent updates, particularly when using Twitter. Many of our external backers joined when we were doing near-daily updates, and when we shared other outputs that were related to the crowdfunding campaign. For instance, we attracted ~£150 of external investments when we made an update video that discussed a companion article that we released in *The Conversation*[3]. In addition, word of mouth to family and friends did lead to additional donations by them, and sometimes by people that they knew in turn.

We also attempted to attract views by funding a *Facebook* advertising campaign using personal funds ($30), but this led to virtually no exposure and could be considered wasted money. In addition, we noticed that the update videos themselves received relatively few views, leading us to think (contrary to our previous intuition) that posts and infographics ("memes") may be more effective than sound-enabled videos. In addition, we realized halfway in the campaign that our core narrative was ambiguous, and that it was not sufficiently clear whether our campaign was targeted to students, COVID-19 research enthusiasts, businesspeople or the general public. On future occasions, we will therefore tailor smaller campaigns to more specific audiences, rather than stick to one overarching narrative.

After this experiment, we chose not to follow up on this path during the VECMA project. Although we do think we could make a crowdfunding campaign work on a subsequent occasion, raising at least a few thousand pounds, we learned that a lot of repetitive daily press release effort would be required,

[3] "Coronavirus: how school closures affect infection numbers"

and we felt that the current resources allocated in the project would not be sufficient to support such a major effort.

5.3 VECMA club

Another interesting possible funding model has been identified following a suggestion by our MPG partner and advice from the Innovation Advisory Board members: namely, the creation of a VECMA club. This club, as a non-profit organisation, would propose to its members, in exchange for paid membership, different services as dedicated training, advisory services, or access to dedicated software feature/pre-release and also shared data. It can also serve as a bridge with academia to promote the VECMA Toolkit as a reference platform to experiment with state-of-the-art VVUQ methods. An annual meeting could foster interactions between members and disseminate advances in VVUQ using the toolkit.

One example of such club is the ADAS "Atomic Data and Analysis Structure" (ADAS) project (https://www.adas.ac.uk). The ADAS funding model is based on the premise that providing, maintaining and improving the atomic data used in a specific domain (magnetic confined fusion) needs dedicated resources. The data is used across the community in many organizations so there is a benefit of this being a shared activity. It is also important that there are many stakeholders. An equally significant reason for a diffuse funding model is to ensure longevity of the project since there is a continuing need for atomic data for models and diagnostic analysis.

Therefore, a modest funding level, equivalent to 1-2 FTE provides a baseline for continuity. However, it is crucial that the project does not become moribund so new developments, improved calculations and advancing science rely on more typical research funding streams such as national research programmes. Here, one of the deliverables would be that new codes or data will become part of ADAS, which are then available to all in the ADAS consortium. The shared nature of the project leads to smaller scale collaborations between subsets of its members, again with the goal that the results are distributed to all. ADAS has developed a standing within the community so including data in OPEN-ADAS is a recognised dissemination pathway. This is particularly significant for fundamental atomic data producers, usually university based and funded by research grants.

6 Conclusions

The VECMA project has succeeded among its core aims to develop and use the toolkit, with a substantial set of application users that have actively used the toolkit and helped provide feedback in its development. That feedback has also confirmed that the emerging exascale community is very much operating in a pre-commercial environment and with the development of fully exascale computers in the European HPC ecosystem still some years away, this pre-commercial environment will continue for the foreseeable future after the end of VECMA. We believe that while some modest contributions in-kind or via user group membership may be possible prior to our user community securing revenue in the exascale world, these contributions will not support any continuance of VECMA in any meaningful way.

For these reasons we conclude there is little opportunity for any significant private sector funding on a timeframe relevant to this business plan.

The core strategy for continuing VECMA's key functions, i.e. a core team for VECMA Toolkit maintenance is to secure:

- European grant funding
- Complementary national grant support
- Repurposing of existing programmes of research

Alongside these main sources of funding, we anticipate continuing to explore possible contributions from our user community or dedicated "club" including:

- Expert user support
- Generation of bespoke adaptation software
- Specialist training

We expect that as the emerging European exascale computing community grows and matures, these sources of funding may well increase.

7 References

[1] 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 et P. V. Coveney, VECMAtk: a scalable verification, validation and uncertainty quantification toolkit for scientific simulations, Phil. Trans. R. Soc. A., 2021.

8 Annexes: Examples of VECMA Toolkit benefits for users

8.1 Fusion application

The fusion application uses various tools within the VECMAtk, including 1. EasyVVUQ, 2. QCG Pilot Job (QCG-PJ), 3. EasyVVUQ-QCGPilotJob (EQI), 4. EasySurrogate, and 5. MUSCLE3.

From the application developers' perspective, these tools are very useful because they ease the process of uncertainty quantification (UQ), validation, and verification (VV) of the multiscale simulation model.

We use the python-based EasyVVUQ library to perform VV and UQ of the workflow. We can specify parameters, such as range of expected values of uncertain inputs, method of interest (polynomial chaos expansion and quasi Monte Carlo) and related inputs (e.g. polynomial order).
EasyVVUQ then generates samples and, with a large amount of samples, QCG-PJ becomes especially handy in managing job executions. The EasyVVUQ library can then collate and analyze all the job outputs to provide distributions to quantities of interest (QOI) and Sobol indices. We also use the validation option to quantitatively compare QoI from simulations with experiment measurements. In this case, we would use the integration of both tools provided by the EQI library.

The EasySurrogate guides us through the process of building a surrogate model for the most expensive single-scale model within the workflow, which is the turbulence model. It provides a set of surrogate models implementations based on Artificial Neural Networks and Gaussian Processes, as well as common tools to operate on simulation data results from EasyVVUQ, train machine learning models

on them and analyse the performance of the resulting models for the sake of uncertainty quantification, including obtaining probability density functions and sensitivity indices for simulation quantities of interest.

We are in the process of coupling the single-scale models in Multiscale Fusion Workflow with MUSCLE3. This allows us to easily describe the structure of the workflow, number of instances, and how we want to couple the single-scale models in a YAML file. MUSCLE3 then manages the communication amongst compute elements. Other potential benefit in using MUSCLE3 is that it aims to scale towards exascale and integrate QCG-PJ to handle the execution of a large number of jobs (for UQ) within a cluster allocation.

8.2 3D In-Stent Restenosis Model

The 3D In-Stent Restenosis Model (ISR3D) is a cyclic multiscale simulation with multiple submodels, including smooth muscle cell (SMC) model, blood flow (BF) model, and three helper modules (referred as mapper in MUSCLE3) in between the SMC model and BF model assisting the transmission of data. They are voxelizer, distributor and collector. Figure 6 shows the communication diagram between submodels and mappers. To implement such a multiscale model in software, some kind of subsystem is required that is responsible for coupling the submodels. MUSCLE3 provides a solution for this coupling. The main advantages of applying MUSCLE3 as a communication tool between the models are the following:

- Building a structured and unified communication scheme between the submodels. The data sending and receiving are implemented in a unified way, which also allows switching different implementations of the same submodel, as long as they implement the same communications scheme.
- It also supports communications between the models coded in different programming languages (C++/Python/Fortran).
- Using a standard input file (ymmsl file) to manage the model settings, including model components (submodels, conduits between submodels and model configurations. Multiple ymmsl files can be used to separate model structure and implementation from the simulation parameters.
- The communications between submodels are automatically recorded during execution and can be easily supervised through MUSCLE3 log files.

- Easy swapping of submodels also provides a straightforward way to implement semi-intrusive uncertainty quantification methods. The original submodel model can be replaced with a surrogate model with a minor modification.
- MUSCLE3 supports the execution of models in HPC environments using Slurm.

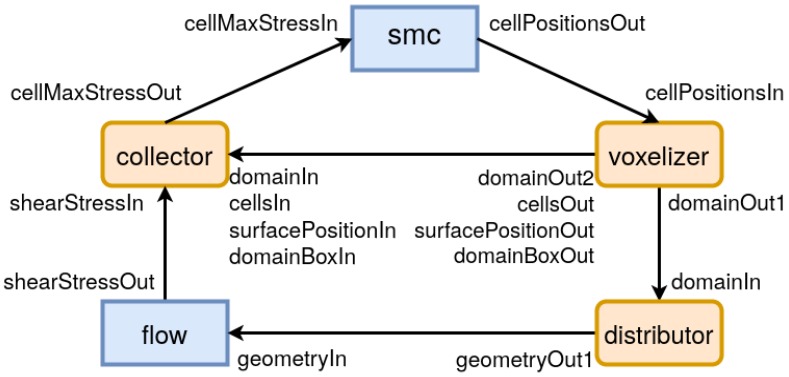


Figure 6. Communication scheme of the ISR3D model

8.3 Cardiac modelling and Medical Device Development with Alya

VECMA has been collaborating with Alya Red, a project of the Barcelona Supercomputing Centre (BSC) for simulating a human heart. The uptake of VECMAtk in BSC's cardiac model has been in terms of two of its components:

a. FabSim3: A FabSim3 plugin called FabAlya has been created for automating the Alya simulation code in terms of workflow management and remote submission capabilities. FabAlya has been tested and is fully functional. Technical details about this plugin can be found here.

b. EasyVVUQ: The Alya Red cardiac model comprises aspects of electrical propagation, mechanical deformation and blood flow. These aspects introduce great complexity in terms of the physical processes taking place, giving rise to a large number of modelling parameters in terms of anatomical description, electromechanical properties and fluid mechanics across considerable length and time scales. To create the best possible cardiac simulator in terms of realism and detail, sensitivity analysis performed by VECMAtk will identify those parameters that have the biggest impact in the cardiac model's predictions and quantify the uncertainty (UQ) that they introduce. EasyVVUQ's implementation is currently calibrated against existing SA and UQ frameworks used at BSC.

There are further perspectives following the above applications of VECMAtk on Alya which are expected to give VECMA even greater visibility in the biomedical domain and allow the toolkit to have direct impact on medical device development: The Alya team are validating various aspects of cardiac

function of their model using experimental data from San Diego State University (http://www.maynewman.us/) and against the V V 40 – 2018 verification and validation standard of the American Society of Mechanical Engineers with the aim to help design a left ventricular assist device (LVAD), a mechanical pump that is implanted inside a person's chest to help a weakened heart pump blood. Ultimately, the model will be included in the FDA's Medical Device Development Tools (MDDT) program, which is a way for the FDA to qualify tools that medical device sponsors can use in the development and evaluation of medical devices. This qualification would be a considerable achievement for VECMA, giving direct access to commercial applications with potential for revenue streams.

9 Applying VECMA as a Provider to EOSC portal

In February 2021, we applied for VECMA to be registered as a new EOSC Provider and for VVUQ Toolkit as a new Resource to the EOSC Portal through this portal: https://eosc-portal.eu/for-providers. This allows to be more visible and get a free access to an online service platform. Indeed, by becoming a provider, according to EOSC, you can:

- *Choose to advertise them on the EOSC Portal and promote their adoption outside your traditional user groups, reaching a wider user base.*
- *Get statistics about access requests and customer feedback*
- *Get a free online platform where you can manage service requests, interact with users and provide support to them, and agree the most suitable service levels.*
- *Allow users to authenticate with their own credentials to access your services and resources and get support to enable this.*
- *Contribute to the definition and maintenance of EOSC service provisioning policies and the portfolio roadmap.*
- *Join the group of providers that meet EOSC quality standards.*

The application was divided into two steps:

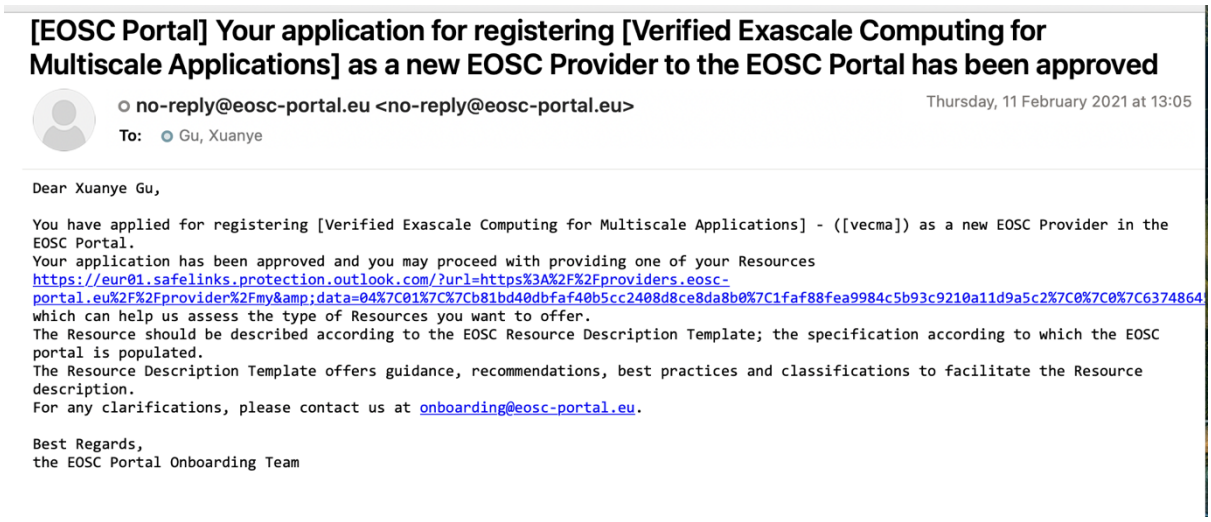
- Apply VECMA to be registered as a new EOSC Provider, where we were successful
- Apply VVUQ Toolkit as a new Resource to the EOSC Portal

We were asked to create first an entry reporting information about the provider; once approved, VECMA would then be able to add information about the service, the so-called "resource" that will be associated to the "provider" entry.

We applied through the link: https://eosc-portal.eu/for-providers to become a EOSC provider using the following marketing information as requested by them:

> *VECMA enables a diverse set of multiscale, multiphysics applications to run on current multi-petascale computers and emerging exascale environments with high fidelity such that their output is "actionable". The aim is to establish a toolkit for verification, validation and uncertainty quantification for multiscale applications that require large scale supercomputers. The central deliverable is an open source toolkit for multiscale VVUQ based on generic multiscale VV and UQ primitives known as VVUQ Toolkit (VECMAtk), to be released in stages over the lifetime of this project, fully tested and evaluated in emerging exascale environments, actively promoted over the lifetime of this project, and made widely available in European HPC centres and public, which is the service we provide to public via the EOSC portal.*

We were accepted as a new EOSC provider.



[EOSC Portal] Your application for registering [Verified Exascale Computing for Multiscale Applications] as a new EOSC Provider to the EOSC Portal has been approved

no-reply@eosc-portal.eu <no-reply@eosc-portal.eu> Thursday, 11 February 2021 at 13:05

To: Gu, Xuanye

Dear Xuanye Gu,

You have applied for registering [Verified Exascale Computing for Multiscale Applications] - ([vecma]) as a new EOSC Provider in the EOSC Portal.
Your application has been approved and you may proceed with providing one of your Resources
https://eur01.safelinks.protection.outlook.com/?url=https%3A%2F%2Fproviders.eosc-portal.eu%2F%2Fprovider%2Fmy&data=04%7C01%7C%7Cb81bd40dbfaf40b5cc2408d8ce8da8b0%7C1faf88fea9984c5b93c9210a11d9a5c2%7C0%7C0%7C6374864
which can help us assess the type of Resources you want to offer.
The Resource should be described according to the EOSC Resource Description Template; the specification according to which the EOSC portal is populated.
The Resource Description Template offers guidance, recommendations, best practices and classifications to facilitate the Resource description.
For any clarifications, please contact us at onboarding@eosc-portal.eu.

Best Regards,
the EOSC Portal Onboarding Team

We then moved further into the second stage to register the VECMA VVUQ Toolkit (VECMAtk) as a new Resource to the EOSC Portal.

The marketing information for our is described below.

> *The VECMA VVUQ Toolkit (VECMAtk) enables automated Verification, Validation and Uncertainty Quantification (VVUQ) for complex single- and multi-scale applications that can be deployed on emerging exascale platforms and provides support for software applications for any domain of interest. VECMAtk contains a suite of components, providing tools to:*

- *create VVUQ procedures (EasyVVUQ),*
- *to facilitate the creation of surrogate models for multiscale simulations (EasySurrogate)*
- *to automate the complex workflows emerging from these procedures (FabSim3),*
- *to enable the efficient execution of large numbers of jobs on computational resources (QCG Pilot Job Manager),*
- *to provide convenient means to use HPC facilities for users (QCG-Now) and user-developers (FabSim3 and QCG-Client),*
- *and to make creating coupled multiscale simulations easy, and to then enable efficient Uncertainty Quantification of such models using advanced semi-intrusive algorithms (MUSCLE3).*

However, our application for registering the VECMA VVUQ Toolkit (VECMAtk) as a new Resource in the EOSC Portal was not accepted. The reason EOSC gave was that VECMAtk was classified as “software” and not an actual “service” (either IT or human) offered ‘live’ to customers. EOSC subsequently responded to say that even though at the moment EOSC cannot include our software in the EOSC Portal, this should become possible in the near future. EOSC proposes to hold our request and get back to us when this kind of service can be published in the EOSC Portal.