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| **Name of Bidding Organisation:** | University College London |
| **Contract Title:** | **T/NA080/20** |

# Purpose of Document

This document provides a statement of how and when the Research Plan’s objectives would be achieved, by showing the major products, activities and resources required of the Research Plan.

# Benefits and alignment to Work Package objectives

Please evidence below how the submission aligns to the Work Package objectives outlined in Part 1 Section 2.3.

Our proposal features the following benefits:

* We have experience with developing and applying uncertainty quantification (UQ) methods applied to a wide range of domains including weather and climate forecasting, advanced materials, epidemiology, drug discovery, personalised medicine, human migration and, of most pertinence to the present proposal, fusion energy applications. The open source, open development software we have developed, called the VECMA Toolkit (VECMAtk) is freely available from the VECMA project ([www.vecma.eu](http://www.vecma.eu)) at [www.vecma-toolkit.eu](http://www.vecma-toolkit.eu). With such tools and experience at hand we are already able to assess the robustness of the codes that will be developed in FM-WP1.
* For the aforementioned applications, we have implemented within EasyVVUQ [1,2] a range of non-intrusive and semi-intrusive UQ methods featuring quasi-Monte Carlo, Polynomial Chaos Expansion and Stochastic Collocation, as well as dimension adaptive sampling, and surrogate models.
* We have established a taxonomy alongside a systematic and in-depth analysis of UQ workflows which we refer to as “UQ patterns”; analysing the pattern(s) of the NEPTUNE project workflow will immediately provide us with a refined idea of candidate UQ methods (already implemented with EasyVVUQ) which can then be applied very easily.
* We have decades of experience in developing scalable HPC methods for multiscale, multiphysics simulations. We have developed two very promising candidate exascale applications SCEMa (<https://github.com/UCL-CCS/SCEMa>) and HemeLB ([hemelb.org](http://hemelb.org/)). We have developed a third application, the Binding Affinity Calculator for ligand-protein binding free energy prediction, which at its core features large ensemble simulations, fully equipped with UQ capabilities [3] and runs at scale all over Europe and USA.
* Most interestingly we have developed scalable HPC methods specifically for VVUQ methods which run on several of Europe’s largest supercomputers (SuperMUC-NG, Eagle, Marconi). VECMAtk features two further pieces of software which are highly relevant and immediately applicable to the FM-WP1 objectives: MUSCLE3 enables the (exa)scalable execution of multi-model workflows (P7.a/b) while EasySurrogate is intended to perform dynamic training of surrogate models for UQ such as arise within multi-model simulations (P7.c).
* We have experience in developing standalone, versatile ProxyApps: EasyVVUQ, FabSim, MUSCLE3 and EasySurrogate (as part of the larger toolkit VECMAtk [4,5]). EasyVVUQ has been developed in order to be able to readily perform UQ on any model, a design feature which fits well the “separation of concerns” approach of the NEPTUNE project.
* We have experience with error propagation in chaotic dynamical systems, whether originating in fluid turbulence or particle based codes such as molecular dynamics; indeed, we have recently discovered a new floating point pathology in such systems when simulated on digital computers which will require investigation in the present context as well [6]. This pathology cannot be removed by increasing the precision of the floating-point numbers and requires further investigation.
* We will participate fully within the community built around the NEPTUNE project, providing training for our UQ tools, experience and know-how for organising (physical and virtual) workshops, and we can readily lead projects involving a large number of development teams.
* We have many years of scientific project management experience leading international multidisciplinary research projects involving ultra-high-end high performance computing.
* EasyVVUQ fits the requirements of the NEPTUNE charter as it is implemented in Python; the same applies to MUSCLE3, as it is implemented in C++. We are experienced at handling the standard HDF5 data format.

[1] Wright, D. W., Coveney, P.V., et al. "Building confidence in simulation: Applications of EasyVVUQ." *Advanced Theory and Simulations* (2020): 1900246.

[2] Richardson, R. A., Coveney, P.V., et al. "EasyVVUQ: A Library for Verification, Validation and Uncertainty Quantification in High Performance Computing." *Journal of Open Research Software* 8.1 (2020).

[3] Al Saadi, A., Coveney, P.V., et al. “IMPECCABLE: Integrated Modeling PipelinE for COVID Cure by Assessing Better LEads.” *arXiv preprint* (2020):2010.06574.

[4] Groen, D., Coveney, P.V., et al. "VECMAtk: A Scalable Verification, Validation and Uncertainty Quantification toolkit for Scientific Simulations." *arXiv preprint* (2020):2010.03923.

[5] Groen, D., Coveney, P.V., et al*.* "Introducing VECMAtk-Verification, validation and uncertainty quantification for multiscale and HPC simulations." International Conference on Computational Science. Springer, (2019).

[6] Boghosian, B. M., Coveney, P.V., Wang, H. "A New Pathology in the Simulation of Chaotic Dynamical Systems on Digital Computers", *Advanced Theory and Simulations* (2019): 1900125.

# Scope

## Key Deliverables and/or Desired Outcomes

We expect to produce the following three main outputs as deliverables from this project:

1. A clear and concise literature summary of VVUQ methods.
2. The organisation and running of two events, one at the start and one at the end of the project.
3. A concise summary of recommendations of methods to perform efficient and scalable uncertainty quantification (UQ) of the plasma edge multi-model code.

In more detail, we will:

* write a concise literature review of UQ methods suited for multi-model workflows and in particular simulating the physics of the plasma edge; the review will feature methods we already have experience with (advanced sampling, adaptive sampling, surrogate modelling) and also prospective methods among which some have been introduced during the Data Assimilation and UQ workshop organised by ExCALIBUR (https://excalibur-sle.github.io/workshop2.html); we will prioritise UQ methods that enable scalable computations on existing multipetascale and emerging exascale architectures for high-dimensional problems.
* exploit already implemented methods within EasyVVUQ and perform initial UQ and sensitivity analysis (SA) campaigns on available and the early-stage (or toy) models developed in FM-WP2 and FM-WP3 and on the existing European Boundary Code and B2-EIRENE.
* organise two event(s) to gather the community of NEPTUNE model developers, initially: (i) for them to explain the algorithmic structure of their models, what they would need to perform UQ on and for us to explain our capabilities and to demonstrate the use of EasyVVUQ by means of hands-on tutorials; (ii) we will present the methods we recommend at a final meeting and to confirm that the community is in collective agreement with our proposals.
* report on community-wide agreement as to what approach will be taken in terms of the use of VVUQ methods in the next phase of the NEPTUNE project; this outcome will be captured in our final report on recommendations concerning the optimal path to pursue.

## Exclusions

Activities/topic areas that are out of scope of the Bid and which will not be undertaken (may also include things that Bidder would like to do but are not currently in scope)

None.

## Constraints

Restrictions that affect proposals of the project by imposing limitations such costs, resources or project schedule, which may affect the execution of the Bid.

We will face four main constraints:

1. Limited time in which to implement and test the shortlisted methods;
2. Access to suitable compute resources, especially if we intend to test scalability;
3. Availability of the codes which will require instrumentation with UQ methods from various NEPTUNE partners;
4. The likelihood that we shall have to convene meetings online.

However, the present project is of limited duration (just six months) and is not intended to involve significant software development. Thanks to the usability and flexibility of the VECMAtk, we expect to be able to perform rapid prototyping to demonstrate feasibility by working in collaboration with code owners for around five codes in this period of time.

For demonstration purposes, we expect to have access to sufficient computing resources from our own end, in order to be able to accommodate some basic performance testing in this period.

# Approach

Describe how will the work be undertaken, including a definition of methodology that will be used in the project to deliver the work package and call objectives.

**Introduction**:

It is widely recognised that uncertainty quantification (UQ) is essential for any model simulation to be actionable, i.e. to have genuine predictive value. Ensemble-based methods lie at the heart of techniques enabling the evaluation of the uncertainty associated with a model parameter. A combinatorially large number of simulations of the model must be performed to probe the effects of the parameters comprising it. As a result, UQ is intrinsically expensive. Nevertheless, many methods can be used to accelerate UQ and reduce the computational costs in comparison to brute force quasi-Monte Carlo methods. Their efficiency depends on the model equations, the simulation workflow, and the number of parameters in play.

A distinction is made between intrusive UQ methods, where one substitutes the original model with a form of stochastic representation, and non-intrusive methods, where the original model is used as a black-box. Intrusive methods are efficient and relatively easy to apply to linear models. This, however, represents only a relatively small class of models. They can be applied to non-linear models as well, but the solution of the resulting equations may then become very demanding. Non-intrusive methods can be applied to any type of non-linear model. However, if a single model run requires large execution times, these UQ methods may be relatively ineffective, and at worst computationally intractable. In between, there exists a family of semi-intrusive UQ algorithms for multiscale models. These methods are called semi-intrusive since they are intrusive only on the level of the multiscale model workflow, that is, in the way the single scale components are coupled together. The single scale components themselves, however, are treated as black-boxes.

Non-intrusive methods rely primarily on advanced sampling methods such as Polynomial Chaos and Stochastic Collocation. Sampling efficiently the probabilistic distribution of the model’s parameters enables one to reduce the number of samples required to build trustworthy estimates of the uncertainty. Furthermore, dimension-adaptive sampling methods [1] enable one to refine the number of samples for parameters with higher sensitivity and thus evade the curse of dimensionality whereby the computational cost would scale exponentially in the number of dimensions of the parameter space.

Intrusive and semi-intrusive methods frequently depend on surrogate modelling. Expensive parts of a model are replaced by cheaper stochastic approximations. Gaussian processes and neural networks are key tools to build such models. In turn, such models can be simulated multiple times at far lower computational cost, while preserving the full model’s sensitivity to uncertain parameters.

There is forward propagation of uncertainty which originates in the uncertainty of model parameters, and the stochasticity in e.g. chaotic systems. When it comes to perform the inverse approach, to infer uncertainty from measured outputs, inverse Bayesian methods become relevant [2,3].

**Background**:

EasyVVUQ, the tool we intend to use to investigate different UQ methods, is designed for multiscale and multiphysics models, as well as single scale models. It is part of a larger toolkit, the VECMAtk, which also features tools for centralised execution on multiple petascale supercomputers (QCG), improved job array allocation management (PilotJob), efficient data management between geographically distributed e-infrastructure (FabSim) along with coordination of submodel execution and data transfer within complex workflows (MUSCLE3). Overall, investigations of methodologies to perform efficient UQ will benefit from the existing testbed we have available for this project (see table 1), which will ensure scalability and ease of implementation.

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| **Site** | **Architecture** | **Processors** | **Number of cores** |
| PSNC | AMD | AMD Opteron (Interlagos) | 5,500 |
| Intel Xeon | Intel Xeon E5 v3 | 36,650 |
| Intel Xeon | Intel Xeon E5 v4 | 1,760 |
| ARM | Toradex based on NVIDIA Tegra 3(Apalis T30), Samsung Exynos 5, and APM ARM 64bit | 400 |
| GPU | Nvidia Tesla M2050 | 150,000 |
| LRZ  page73image47120 | Intel Xeon | SandyBridge EP E5-2680 | 150,000 |
| Intel Xeon | Haswell E5 | 96,768 |
| Intel Xeon Phi | Knights Landing | 9,600 |

Table 1: Overview of established HPC resources available at PNSC (Poznan, Poland) and LRZ (Leibniz, Germany). These resources together comprise the VECMA VVUQ testbed.

EasyVVUQ already features the aforementioned non-intrusive UQ methods (PCE, SC, and adaptive sampling). We have applied those to a well-known epidemiological model featuring more than nine hundred parameters, which at first sight might be thought to suffer from the “curse of dimensionality”. By means of sensitivity analysis (SA) and adaptive sampling we have been able to reduce to a mere handful the parameters which dominate the variance in the code’s output data; in fact, over 60% of the variance in the model’s behaviour is attributable to a mere three parameters. It also serves as a very user-friendly environment for the aggregation and thorough analysis of data output from codes, including of course reporting on sensitivity analysis and UQ. We have also initiated the development of EasySurrogate to enable rapid substitution of expensive submodels with efficient, trained and verified surrogate models, as part of semi-intrusive UQ campaigns. It already features stochastic neural network surrogates. EasySurrogate is publicly available as an alpha version part of the latest VECMAtk release.

Outstanding applications of EasyVVUQ currently include enabling full *in silico* trials as part of the EU-funded INSIST project, as well as assessing a well-known epidemiological model featuring more than nine hundred parameters at the behest of RAMP [4]. The adoption of the individual VECMA tools (QCG-PJ, EasyVVUQ-QCGPJ, FabSim3, EasyVVUQ) has been increasing continuously in the research community for the last three months (see figure 1). Early adoption has been most significant for EasyVVUQ which has now been downloaded some three thousand times. Rapid increases in the number of views and downloads have followed the organisation of special events such as a workshop held at the Alan Turing Institute in January 2020 (https://www.turing.ac.uk/events/reliability-and-reproducibility-computational-science) and the VECMA-ICCS-SIAM Conference held online in June 2020 (<https://www.vecma.eu/siamuq20_iccs2020/>) which attracted over 300 attendees.

Figure 1: Cumulative number of individual downloads of the VECMAtk components (QCG-PJ, EasyVVUQ-QCGPJ, FabSim3, EasyVVUQ) since the initial release of the VECMAtk on the 23 August, 2019.

We have significant experience in designing ProxyApps which are compatible with various multiscale and multiphysics computational workflows. We have acquired proven expertise driving successive FET-HPC EU-funded projects over the last decade: MAPPER (http://mapper.pub.lab.nm.ifi.lmu.de/web/guest), ComPat (https://www.compatproject.eu/) and currently VECMA (http://https://www.vecma.eu). We have designed generic optimisation tools for the execution of multiscale simulations, as well as for the execution of large-scale UQ campaigns. One of the key aspects of these projects is their versatility; that is, we have designed tools that are efficient for a large spectrum of applications. Of most interest here is fusion, but these also include climate modelling, which suits the needs of the other major use case of ExCALIBUR. Indeed, the VECMAtk is being used to perform non-intrusive and intrusive UQ on the plasma simulation workflow developed at MPG-IPP [5] and the climate model developed at CWI [6].

In the current NEPTUNE project, the models and equations are already specified, so we can perform shortlisting for methods particularly suited for the plasma turbulence code. In particular, we are familiar with such codes either from personal experience with chaotic systems [7] and our longstanding collaboration with MPG-IPP.

The VECMAtk has been developed from the outset for use with large supercomputers. Therefore it has been designed to handle efficiently the following performance-critical aspects:

* the sampling of parameter values and creation of large numbers of simulation inputs;
* the submission, execution and retrieval of large ensembles of simulation jobs;
* the efficient movement of data between local and remote resources;
* the efficient movement of data between coupled models.

**Methodology**:

* We will investigate the prospective structure of the plasma edge code defined in the Science Plan and in the Equations for NEPTUNE Proxyapps document. We will compare the structure of the code with the UQ Patterns we have defined in our previous work in the context of the VECMA project. Based on the identified patterns, we will immediately be able to propose a selection of UQ methodologies suited for the plasma edge code. We anticipate that the structure of the plasma edge code will be similar to the MPG-IPP plasma turbulence code, which we already have substantial experience with and have performed non-intrusive UQ on using Marconi, the PRACE Tier-0 supercomputer at CINECA in Italy.
* We will complement this shortlist by means of a literature review and consultation with other partners funded within the NEPTUNE project. We have already initiated discussions at a DA and UQ workshop organised by the ExCALIBUR project held online the 24-25th of September, in which we were active participants (https://excalibur-sle.github.io/workshop2.html).
* We will organise a first workshop with representative partners from FM-WP1, FM-WP2, and FM-WP3 for them to explain the algorithmic structure of their models. We will also make sure that representatives from FM-WP4, WC-WP1 and XC-WP1&2 are able to attend for community building purposes. We will introduce and explain our existing UQ capabilities and demonstrate the use of EasyVVUQ by means of hands-on tutorials, which should be of interest to all attendees. Discussions should also help us to refine our shortlist of UQ methods based on expectations from model developers.
* According to the document FMS/0021, only the code to compute the Braginskii coefficients is already available. We expect to be able to rapidly gather toy models provided by partners involved in FM-WP2 and FM-WP3 during the first meeting. We would also hope to be able to use the existing European Boundary Code and B2-EIRENE which the future developments in FM-WP2 and FM-WP3 will rely on. In the same order of priority, we will immediately test the shortlisted UQ methods. Based on the similarity with the applications we have already instrumented with UQ, most of the shortlisted UQ methods will be already available within VECMAtk, and more precisely EasyVVUQ. These include the non-intrusive Polynomial Chaos Expansion and Stochastic Collocation sampling methods. We would expect to try adaptive SC sampling, as it is expected that the future plasma edge code will feature a large number of input parameters and therefore suffer from the curse of dimensionality. We will also investigate multi-level Monte Carlo methods (MLMC), computing the uncertainty at different level of accuracy. MLMC methods are currently not available within EasyVVUQ, but they can be implemented readily if required.
* In the meantime, we will perform SA of the available codes using the adaptive sampling method, which will enable us to determine the most influential input parameters of these plasma edge codes. We have designed template generation tools to automatically find and list parameters of a given code. This will enable us to perform an exhaustive SA of every single parameter from the codes we investigate. From the resulting SA, we will be able to establish a reduced list of parameters to perform UQ on, hindering the “curse of dimensionality” in future analysis. While performing SA, we will also test the scalability of our methodology. Such large-scale UQ campaigns, which we have performed in the context of applications in epidemiology and drug discovery, typically require scalable workflows that already push the limits of petascale infrastructures [8].
* Computations on toy models will be performed on local clusters at UCL, which do not have any resource usage restrictions. When it comes to perform UQ and SA of larger codes, we will access infrastructures on which we already have substantial allocations. Our allocations are largely sufficient for the execution of this project. The HPC resources we have access to are associated with the following supercomputers: ARCHER (EPCC), Eagle (PSNC), Marconi (HPC-Cineca, where MPG-IPP performs production runs) PizDaint (CSCS), and SuperMUC-NG (LRZ).
* We will convene a second workshop involving presumably many of the same partners from the initial meeting; our deeper connections established during the first meeting should also encourage us to update the list of partners involved in the community. We will report on our experience with our shortlist of UQ methods, the SA performed on available codes, and their computational efficiency in the context of emerging exascale UQ computing. We will also report on the structure of the established workflows to enable discussions on optimal computer architectures required to perform such computations. To that extent, we will consider the requirements of the submodel simulations, multi-model workflow execution as well as UQ workflows.
* The conclusions of our discussions and analysis of the most suitable UQ methods, preliminary SA of available codes and UQ workflows architectures will be disseminated in a final report as a set of recommendations for subsequent work within the NEPTUNE project.
* We expect to extend our UQ of the plasma edge code with verification and validation (VV). EasyVVUQ also provides a set of V and V patterns that enable *inter alia* automated verification of the accurate resolution of a model’s mathematical equations as well as comparison with experimental results. For the former, we will be able to determine automatically the level of refinement (e.g. discretisation in space and time) of the solution algorithms for convergence and accuracy of the code. For the latter purpose, we will be able to choose between several relevant metrics, such as the Hellinger distance [9], the Jensen–Shannon distance, which is a symmetrized and smoothed version of the Kullback–Leibler divergence [10], and the Wasserstein metrics for comparison of predicted and experimental data [11]**.**

[1] Gerstner, T. and Griebel, M. "Dimension–adaptive tensor–product quadrature." *Computing 71* (2003): 65–87.

[2] Edeling, W. N., et al. "Predictive RANS simulations via Bayesian Model-Scenario Averaging. " *Journal of Computational Physics*, 275 (2014): 65–91.

[3] Marzouk, Y. and Xiu, D. "A stochastic collocation approach to Bayesian inference in inverse problems." *Communications in Computational Physics*, 6 (2009): 826–847.

[4] Edeling, W., Coveney, P.V., et al. "Model uncertainty and decision making: Predicting the Impact of COVID-19 Using the CovidSim Epidemiological Code." (2020), *in review*.

[5] Lakhlili, J., et al. "Uncertainty Quantification for Multiscale Fusion Plasma Simulations with VECMA Toolkit*." International Conference on Computational Science*. Springer, Cham (2020).

[6] Edeling, W. N., and Crommelin, D. "Towards data-driven dynamic surrogate models for ocean flow." *Proceedings of the Platform for Advanced Scientific Computing Conference* (2019).

[7] Fazendeiro, L., Coveney, P. V., et al. "Unstable periodic orbits in weak turbulence." *Journal of Computational Science 1.1* (2010): 13-23.

[8] Al Saadi, A., Coveney, P.V., et al. “IMPECCABLE: Integrated Modeling PipelinE for COVID Cure by Assessing Better LEads.” *arXiv preprint* (2020):2010.06574.

[9] Nikulin, M. S. "Hellinger distance." *Encyclopedia of mathematics* 78 (2001).

[10] Kullback, S., and Leibler, R. A. "On information and sufficiency." *The annals of mathematical statistics* 22.1 (1951): 79-86.

[11] Villani, C. "*Optimal transport: old and new*." Vol. 338. Springer Science & Business Media (2008).

# External Dependencies

Information about potential dependencies on other activities/organisations involved eg. Data that would need to have access to as part of the research, what historical data would be available to run case studies, that the Bid would benefit from

| **Dependency Description** | **Responsible Owner** | **Required Data** |
| --- | --- | --- |
| Prototypes or toy models of the turbulence submodels code | PI of projects part of FM-WP2/3 | Executables of toy models and source codes |
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# Activity Plan

Identify activities plans for the Research Plan (please add and use as many activity templates as required into the document and complete Annex B with schedule). Please include any relevant planning assumptions.

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|  | | Activity No | | 1 |
| **Activity:**  Report the knowledge gathered during the initial literature review, the discussions during the two workshops as well as the execution of preliminary UQ and SA campaigns.  **Assignee:** Peter V. Coveney | | | | |
| **Objective 1:** write a concise set of recommendations as to which UQ methodologies to develop  **Objective 2:** explicitly describe the architecture of UQ workflows for co-design purposes toward exascale | | | | |
| **Key Deliverables:**  **1)** First report  **2)** Second final report | **Start and Completion date:**  **1)** 04/01/2021 to 31/01/2021  **2)** 01/07/2021 to 31/07/2021 | | **Assignee:**  **1)** Maxime Vassaux  **2)** Maxime Vassaux | |
| **Milestones towards deliverables:**  **1)** All codes for which UQ will be considered will be specified by the end of month 2  **2)** All (VV)UQ evaluations will be performed by the end of month 5 | **Completion date:**  **1)** 01/03/2021  **2)** 01/06/2021 | | **Assignee:**  **1)** Peter V. Coveney  **2)** Peter V. Coveney | |

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|  | | Activity No | | 2 |
| **Activity:**  Organisation of two meetings with the ExCALIBUR partners from FM-WP1, FM-WP2, and FM-WP3, and if possible WP4, WC-WP1 and XC-WP1&2  **Assignee:** Peter V. Coveney | | | | |
| **Objective 1:** hold the first meeting to introduce EasyVVUQ capabilities, provide hands-on tutorials and partners to present the structure of their codes and UQ requirements  **Objective 3:** hold the second meeting to present our shortlist of recommended UQ methods | | | | |
| **Key Deliverables:**  **1)** Initial workshop  **2)** Final workshop | **Start and Completion date:**  **1)** 14/01/2021  **2)** 01/07/2021 | | **Assignee:**  **1)** Peter V. Coveney  **2)** Peter V. Coveney | |
| **Milestones towards deliverables:**  **1)** confirmation of more than 15 attendees  **2)** confirmation of more than 15 attendees | **Completion date:**  **1)** 07/01/2021  **2)** 24/06/2021 | | **Assignee:**  **1)** Peter V. Coveney  **2)** Peter V. Coveney | |

Resource Plan

Research Plan Roles and Responsibilities

| **Name** | **Title** | **Organisation /institution** | **Required Role** | **Required Responsibility** | **Cost** | **Confirmation of payment source (Paid from the grant award / in kind/other funding)** |
| --- | --- | --- | --- | --- | --- | --- |
| Maxime Vassaux | Post Doctoral Research Associate | UCL | Researcher | Literature review, existing code UQ and SA |  |  |
| Peter V. Coveney | PI | UCL | Professor | Organisation of the two meetings and supervision |  | - |