

Name of Bidding Organisation:	University College London (UCL)
Contract Title:	Steps towards Accurate Fusion modelling at the Exascale: Model Order Reduction (SAFE-MOR)

1 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.

2 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.

- We will review and investigate concretely methods and codes for Model Order Reduction (MOR) in the context of complex UQ of multi-physics and multi-fidelity codes at the Exascale for fusion. This effort benefits from our ongoing Alan Turing Institute (2018-2021) project “Uncertainty quantification of multi-scale and multi-physics computer models” and our EPSRC ExCALIBUR software working group “Exascale Computing for System-Level Engineering” (EP/V001396/1 & EP/V001531/1) in which S. Guillas is the UQ lead coinvestigators, as Professor of Statistics, specialist in Uncertainty Quantification of complex computer models, Group Leader in the Data-Centric Engineering programme at the Alan Turing Institute and founder of the Turing UQ interest group. This aligns with the main objective of building a UQ strategy within the overarching project of fusion at the exascale.
- PI Serge Guillas is also the Met Office Joint Chair in Data Sciences for Weather and Climate, which allows synergies in defining the strategies for Reduced Order Modelling of complex fusion and weather/climate models, therefore providing robustness in the developed infrastructure for UQ at the exascale. The PI S. Guillas was the lead organiser for the ExCALIBUR Software Workshop on “Data Assimilation and Uncertainty Quantification at the exascale”, 24-25 September 2020 (<https://excalibur-sle.github.io/workshop2.html>), with STFC, Met Office, UKAEA and international leaders in the field from Japan and the USA invited in talks and panels to discuss and establish pathways towards actionable UQ at the exascale, in which models of high dimensions and complexity need to be reduced.
- We will quantify shortcomings and benefits of Reduced Order Modelling approaches, some already implemented, including making use of reduced dimensions and complexities to design computer experiments of small sizes at high fidelity (for some or all the components). This aligns with the objective of reduction of sizes of the ensembles, and the objective that the eventual platform is actionable.
- We will provide tangible pathways to solutions for the Bayesian calibration of reduced order models against disparate and sparse measurements. It aligns with the objectives that the eventual platform is actionable, and the accuracy/robustness of the developed infrastructure becomes fully established.
- We have made use of the HDF5 data formats in other contexts for data compression (e.g. earthquake-generated tsunamis, climate models), to facilitate data exchanges as required in NEPTUNE.

3 Scope

3.1 Key Deliverables and/or Desired Outcomes Our

key deliverables are:

1. A summary of benefits and shortcomings of three different families of approaches to ROM, Proper Orthogonal Decomposition (POD), Proper Generalised Decomposition (PGD), Reduced Basis Methods (RB) in the specific context of promise of suitability for HPC/Exascale implementation particularly for a spectral element code.
2. Small development tasks to test candidate methods for accuracy, stability and HPC scalability potential, in the specific context of promise of suitability for HPC/Exascale implementation particularly for a spectral element code. Key outcomes would be suitability to reduced designs of computer experiments for multi-physics and multi-scale exascale computing. We will also assess the suitability of ROM calibration against data, one of NEPTUNE overarching goal, when the model (or some sub-parts) are reduced.
3. A joint strategy for ROMs as part of the overarching project, through interactions with the community (the other NEPTUNE projects, UKAEA, Met Office). The emphasis will be on developing both coherent and bespoke strategies across ROM and UQ NEPTUNE projects.

These investigations will be carried out by means of literature and code surveys and consultation with experts, especially the ones funded by the other NEPTUNE calls.

Implementations and suitability will be examined through co-design with NEPTUNE project partners and initial implementation only in a restricted class of machine architectures.

3.2 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.

3.3 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.

None.

4 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

Reduced Order Models (ROM) lessen the computational and mathematical complexity of challenging codes. For instance, inputs can be reduced to a smaller set, either by ruling out parameters or in terms of dimensionality, see e.g. Morris (1991) or Liu & Guillas (2017). Similarly, outputs can be shrunk to a more

manageable representation in terms of basis expansion of either time series of outputs or spatial representations.

Our experience in ROM for UQ exactly targets the kind of complex, multi-physics, multi-scale codes that UKAEA will employ at the exascale. Our key ingredient is to use Gaussian Processes (GPs) as surrogates (also known as emulators) of the computer models. These are comparable to Polynomial Chaos (PC) approaches in terms of accuracy (Owen et al., 2017). GPs can be nowadays parallelised for large input/output spaces, as we are doing in the released Alan Turing Institute Package for fitting Gaussian Process Emulators to multiple output computer simulation results. It is named the *Multi-Output Gaussian Process Emulator (MOGP)* and relies on Research Software Engineering to manage, organise, and accelerate/parallelise some computations. For instance, in 2020, two postdocs in the group of S. Guillas have created up to 500,000 emulators in parallel representing each grid cell in an unstructured mesh output of a Finite Volume code ran on the GPU cluster Wilkes-2 on CSD3 at Cambridge.

The Turing platform MOGP and its few existing tools for ROM can interoperate with other UQ platforms such as the now mainstream EasyVVUQ: both are Python libraries with a similar philosophy but complement each other in terms of workflows (actually much more elaborate in EasyVVUQ), sampling (more elaborate in MOGP), surrogates (PC for EasyVVUQ, GP for MOGP) which are now well understood and interchangeable in workflows.

Our approach

We will first explore the various possible methods (or more precisely families of approaches and their extensions that include active subspace approaches) that can lead to a reduced order model. A literature review of the various strands will summarise the strengths and weaknesses of these approaches for the multiple types of models that may emerge in FM-WP1, FM-WP2, FM-WP3 and FM-WP4. We will describe these carefully to help the various communities of users.

We will work then together with the modellers of these Proxyapps in order to investigate potential strategies and methods to the early stages. This will enable feedbacks on the kind and size of inputs and outputs that can be reduced, with a quantification of the trade-offs in terms of losses in approximation, gains in computational burden and/or surrogate building complexity. It will also offer space for discussions of the critical leaps towards exascale which will have the most influence on the next methodological and computational research required to provide ROM for fusion modelling.

Key questions will be model-dependent, but always aim at addressing the trade-off between computational burden, accuracy of the model and input-output dependencies across the whole system. We endeavour to embed the concern of ROM into the initial development of approaches in FM-WP1, FM-WP2, FM-WP3 such as:

- **spectral/hp element methods:** integration of the choices of polynomial order (p-adaptivity), mesh refinement (h-adaptivity), etc into the ROM
- **Particle methods:** in one study, Nicolini et al. (2019) developed a proper orthogonal decomposition technique, applied to a finite-element time-domain particle-in-cell (PIC) algorithm for the simulation of kinetic plasmas. However, it can also lead to spurious results if proper care is not taken when assembling the reduced-order system. Hence, we will focus on exploring prospective strategies in terms of quantification of uncertainties for ROM that can likely mitigate these issues.
- **5D gyrokinetic models:** the computational burden is the main obstacle and thus ROM ought to give preference to this aspect while ensuring validity and stability. Truncations of spherical harmonics (as we did in Chang & Guillas 2019) are one option, among others to be explored.

FM-WP4 is devoted to **Code structure & coordination** and will have a specific status as the integrator of the various sub-models. We will investigate how our ROM approaches can be tailored to the computational implementation to further reduce data flows, as well as frequencies and latencies of I/O exchanges across

sub-models. We developed the first surrogate models of feed-forward suites of models (Ming & Guillas 2020), which have analytical expressions, and will thus be able to illustrate the promise of ROM in this context. Key questions will be around the ability to identify the valuable coupling strategies that reduce dimensionality of data exchanges across the sub-models or the value of information propagated from an additional experiment at the sub-model level to further enhance the overall ROM of the system. We anticipate cooperating with the Met Office work package WC-WP1, as concerns are shared.

Finally, the testing against data is essential to validate models for e.g. the critical high fidelity modelling the edge region of the tokamak plasma. The aim is mainly to tune unknown parameterisations or e.g. boundary conditions. With two decades of research since the seminal paper of Kennedy & O'Hagan (2001), the calibration against observations of complex models with ROM has made progress: for instance Chang & Guillas (2019) made use of reduced spatial representations over the globe for a high exascale code by targeting the principal modes of variability of the field (dominant spherical harmonics) and incorporated the key non-stationary behaviour (e.g. local regimes), in terms of spatial variations of both variance and correlations, in the Bayesian calibration, the technique that provides the best uncertainties in the tuning, albeit at some cost of running MCMC. We will illustrate potential for these and other approaches, especially for the calibration of multi-physics and multi-scale models against complex/missing/sparse/multivariate/high dimensional/asynchronous measurements. This effort will be co-designed with the modellers and experimentalists in FM-WP1, FM-WP2, FM-WP3. Other real-time alternatives of adjustment of the model using Data Assimilation will also be explored (e.g. Maldi & Poux 2017 for Kalman filtering, and others for particle filtering).

References:

Chang, K. L., & Guillas, S. (2019). Computer model calibration with large non-stationary spatial outputs: application to the calibration of a climate model. *Journal of the Royal Statistical Society: Series C (Applied Statistics)*, 68(1), 51-78

Kennedy, M. C., & O'Hagan, A. (2001). Bayesian calibration of computer models. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 63(3), 425-464

Liu, X., & Guillas, S. (2017). Dimension reduction for Gaussian process emulation: An application to the influence of bathymetry on tsunami heights. *SIAM/ASA Journal on Uncertainty Quantification*, 5(1), 787-812.

Maldi, M., & Poux, A. (2017). A reduced order model based on Kalman filtering for sequential data assimilation of turbulent flows. *Journal of Computational Physics*, 347, 207-234.

Ming, D., & Guillas, S. (2020). Integrated Emulators for Systems of Computer Models. arXiv preprint, under review at *SIAM/ASA Journal on Uncertainty Quantification*

Morris, M. D. (1991). Factorial sampling plans for preliminary computational experiments. *Technometrics*, 33(2), 161-174.

J. L. Nicolini, D. Na and F. L. Teixeira, "Model Order Reduction of Electromagnetic Particle-in-Cell Kinetic Plasma Simulations via Proper Orthogonal Decomposition," in *IEEE Transactions on Plasma Science*, vol. 47, no. 12, pp. 5239-5250, Dec. 2019, doi: 10.1109/TPS.2019.2950377.

Owen, N. E., Challenor, P., Menon, P. P., & Bennani, S. (2017). Comparison of surrogate-based uncertainty quantification methods for computationally expensive simulators. *SIAM/ASA Journal on Uncertainty Quantification*, 5(1), 403-435.)

5 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	Required Data
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	Owner	
Edge plasma simplified Proxyapp models	UKAEA & partners	Inputs, codes for each sub-component to be run by UCL for design and surrogate modelling
Pseudo or real observations	UKAEA	Data and attributes (nature, time, space) in HDM5 format or equivalent with readme files and explanation, feedback if questions arise. To be used by UCL for calibration of the model against data

6 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.

Duplicate this table for each Activity		Activity No	1
Activity: Report on suitability and potential of ROM to fusion models			
Assignee: Prof. Serge Guillas			
<p>Objective 1: Summary of strengths and weaknesses of three families of existing ROM approaches (POD, PGD, RB) and their current and ongoing extensions (e.g., active subspace).</p> <p>Objective 2: Description of ROM potential for the reduction of size of inputs, size of design, size of outputs, and computational benefits for multi-physics fusion modelling at multiple scales for toy models and ProxyApps in discussions with FM-WP1, FM-WP2, FM-WP3 and FMWP4</p>			
Key Deliverables:	Start and Completion date:	Assignee:	
1) deliver a progress report with preliminary findings 2) Final report	1) 4 January-20 March 2021 2) 20 March-31 July 2021	1) D. Ming 2) D. Ming	
Milestones towards deliverables:	Completion date:	Assignee:	
1) literature and codes identified 2) ROM benefits on toy model	1) 1 March 2021 2) 15 May 2021	1) S. Guillas 2) S. Guillas	

Duplicate this table for each Activity		Activity No	2
Activity: Exploration of ROM for individual codes and their UQ			
Assignee: Prof. Serge Guillas			
Objective 1: co-organisation of two workshops with the T/NA080/20 activity for UQ, and FM-WP1, FM-WP2, FM-WP3 and FM-WP4 to integrate ROM within the overarching UQ framework. Scope:			

(workshop 1) gather evidence of needs and potential; (workshop 2) display possible methods and implementations.

Objective 2: direct interaction with researchers in FM-WP1, FM-WP2, FM-WP3 and FM-WP4 to scope the reduction of the number of spatial dimensions across models of different complexities and other ROM topics such as bespoke sensitivity analysis, data compression, reduced basis representations across fidelities and scales.

<u>Key Deliverables:</u> 1) workshop 1 2) workshop 2 3) potential quantified cost/benefit for a few key codes through scientific interactions	<u>Start and Completion date:</u> 1) 4 January-15 February 2021 2) 1 July-15 July 2021 3) 15 February -15 July 2021	<u>Assignee:</u> 1) S. Guillas 2) S. Guillas 3) D. Ming
<u>Milestones towards deliverables:</u> 1) 10 participants secured in workshop 1 2) 1 set of codes and developers engaged amongst one of: FM-WP1, FM-WP2, FM-WP3	<u>Completion date:</u> 1) 15 January 2021 2) 1 May 2021	<u>Assignee:</u> 1) S. Guillas 2) S. Guillas

7 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)
Serge Guillas	Prof	UCL	PI	Direction of research, reporting and meetings		
Deyu Ming	Dr	UCL	Postdoc	Researcher		