

T/NA086/20

Code structure and coordination

Benefits and alignment to Work Package objectives

- **Alignment with other work packages:** This submission represents the core work in the Fusion Modelling System's fourth work package, *Code structure and coordination*. In particular this project is well aligned with the proxy applications being developed in the second and third work packages. Close coordination between these three groups will therefore be vital to the success of this project. Additionally, the output from the first work package, *numerical representation*, will feed into this project by influencing the design of data structures that remain performant at scale.
- **Benefits to other work packages:** The *code structure and coordination* work package will directly benefit the other NEPTUNE groups by highlighting approaches to software development that are appropriate for Exascale systems.
- **Interdisciplinary team with broad experience:** The researchers involved in this bid have a wide range of backgrounds in high performance computing and research towards exascale computing, in collaboration with industry, national and international universities, UK and US national labs: The lead (Dr Steven Wright) and Warwick Co-I (Dr Gihan Mudalige) have extensive experience of DSL development for modern scientific libraries, and application to HPC for performance portability. The team also includes the lead maintainers of BOUT++, a world-leading framework for plasma simulations which makes extensive use of performant abstractions to combine a DSL for easy implementation of equations, with high performance. By including domain experts in both fluid and kinetic plasma systems, research software engineers with experience of software sustainability, and performance portability experts, we can ensure that the recommendations arising from this work are suitable for NEPTUNE applications and go beyond the current state-of-the-art.
- **Close links to broader ExCALIBUR effort:** Through the Warwick Co-I (Dr Gihan Mudalige) this proposed work package will have direct links to ExCALIBUR working groups on code generation and high-level abstractions for exascale applications. This will ensure that the work here is aligned and complementary to the broader ExCALIBUR programme, benefiting from those working groups while focussing more specifically on NEPTUNE applications to tokamak plasma physics.

Scope

Key Deliverables and/or Desired Outcomes

The deliverables of the work package will be:

- **Survey of available technologies:** The first task will be to survey available and upcoming hardware that are likely to be present in exascale systems, and identify appropriate programming models that will allow full exploitation of these systems. Particular focus will be paid to performance portable programming models, such that NEPTUNE does not become limited to particular systems.

- **Identification of Representative Applications:** To evaluate the portability of the identified software approaches, representative algorithms and datasets will be identified for evaluation. In particular, proxy apps that implement the equations described in FMS0021 (Equations for NEPTUNE Proxyapps) will be identified or developed using the software frameworks described above such that the performance portability of the approaches can be evaluated. An example of such a representative application is system 2-5, to be implemented by the successful bidders to work package T/NA083/20.
- **Evaluation of Approaches to Performance Portability:** The applications identified previously, and/or those developed by the successful bidders of T/NA078/20 and T/NA083/20, will be evaluated on a range of hardware (e.g., Bede [V100+Power9], Viking [x86], Isambard [Arm], Archer2 [AMD]) to identify key performance indicators and to assess the performance portability of the above identified approaches.
- **Identification and Dissemination of Best Practices:** Key to this work package is working with the developers of the two proxyapps being developed by the related projects, T/NA078/20 and T/NA083/20, but also with other NEPTUNE work packages and ExCALIBUR groups to ensure any software developed for NEPTUNE is fit for purpose and resilient to shifts in hardware. Therefore this work package will involve analysis of performance evaluations using appropriate metrics to identify a set of best practices, and will focus on the dissemination of these best practices through documentation and training resources.

The specific tasks identified to achieve these deliverables are:

- **Task 1:** Survey of available technologies
 - o **Activity 1.1:** Survey of available and upcoming hardware that is or is likely to be present in pre- and post-Exascale HPC systems.
 - o **Activity 1.2:** Survey of domain specific languages, performance portable programming models and accelerated scientific libraries.
 - o **Activity 1.3:** Survey of parallel file systems, I/O libraries and approaches to in-memory data management.
 - o **Deliverable:** A report summarising the findings of activities 1.1-1.3, outlining the opportunities and potential risks of these technologies to NEPTUNE. The report will include specific details on achieved performance, as reported in the latest literature for the above identified programming models, DSLs and libraries. Wherever available, the measure of achieved performance and/or performance portability with these technologies will be detailed.
- **Task 2:** Identification of testbed platforms and applications
 - o **Activity 2.1:** Identification of a broad range of proxy applications that have computationally similar algorithms to those in FMS0021 (Equations for NEPTUNE Proxyapps).
 - o **Activity 2.2:** Identification of testbed platforms, seeking systems that cover the range of alternative technologies that are likely in exascale systems.
 - o **Activity 2.3:** Acquire data sets that will give a representative view of application performance at scale on a variety of systems.
 - o **Deliverable:** A repository of benchmarks (with a number of alternative implementations using various DSLs, performance portable programming models, etc) and data sets for assessing the various technologies identified in Task 1.

- **Task 3:** Evaluation of approaches to future-proofed applications
 - o **Activity 3.1:** Set up testbed system environment, build dependencies, configure build systems etc.
 - o **Activity 3.2:** Evaluate the performance of the previously identified proxy applications in a range of configurations and using a broad range of approaches to portability at scale.
 - o **Activity 3.3:** Analyse the performance portability of the selected applications using appropriate metrics, [e.g. Pennycook et al. <https://doi.org/10.1016/j.future.2017.08.007>].
 - o **Deliverable:** Report on the approaches analysed providing recommendations on best approaches for Exascale software development.
- **Task 4:** Dissemination of Best Practices
 - o **Activity 4.1:** Coordination with other groups, in particular successful bidders of T/NA078/20 and T/NA083/20 to gather requirements, and relevant proxy applications.
 - o **Activity 4.2:** Coordination throughout project with NEPTUNE groups to facilitate performance portable implementation of proxy applications.
 - o **Deliverable:** Final report on best approaches to scientific software development for portable performance on post-exascale HPC systems.

Exclusions

- **Performance assessment of parallel file systems:** While this project seeks to evaluate a small number of parallel file systems and I/O libraries, access to test bed systems with alternative file systems is likely to be limited. While the assessment of parallel file systems will form some part of this project, it is likely to be limited in scope.
- **Performance of programmable hardware:** A number of the programming models and DSLs being investigated in this project can target programmable devices (i.e., FPGAs). However, again there is likely to be limited availability of these systems on which to evaluate performance. A best-effort approach will be taken to evaluate as many alternative platforms as possible.

Constraints

- This project would benefit directly from the outputs from other successful bidders. In particular, the outputs of T/NA078/20 [Performance of spectral elements], T/NA079/20 [Optimal use of particles], and T/NA083/20 [Plasma fluid referent model] will provide much better proxies of performance than other open-source alternatives. We will engage with these groups to encourage performance portable development, and also to ensure our own evaluations are as representative as possible, by using their developed applications where possible.
- During the project, we should have access to a range of HPC platforms, allowing a wide range of hardware options to be assessed. However, full coverage of likely post-Exascale systems may not be possible -- to mitigate this, we will leverage access to systems at Warwick, York, the N8 and EPCC (if available) to ensure as broad a spectrum of systems as possible are evaluated.

Approach

The key determinant in understanding the limitations and opportunities of the current UKAEA/NEPTUNE codebase when targeting exascale systems is through the identification of algorithms of interest within this workload and ascertaining their performance on current and emerging HPC architectures. As such the project will use a repository of proxy applications, developed as part of NEPTUNE or taken from publicly available benchmark suites, to evaluate approaches to performance portable software development. These evaluations will be conducted on the HPC systems available at the University of York (Viking), University of Warwick (Avon, Orac) and within the N8 (Bede), as well as through collaborations with the ExCALIBUR groups at EPCC (Archer2) and the University of Bristol (Isambard).

Our performance evaluations will be based on a series of “ground rules” for assessing performance portability in a fair way. This will take the form of the metrics outlined by Pennycook et al. [<https://doi.org/10.1016/j.future.2017.08.007>].

To ensure the evaluation is relevant to the NEPTUNE project, we will use our domain knowledge of the plasma physics systems for NEPTUNE as outlined in the call document, and work with other successful bidders to use the proxy applications that they are developing (or have been developed) as the basis of our evaluation. If these proxy applications are not yet ready for performance portable evaluation, we will identify key kernels in existing open source applications which are representative of NEPTUNE systems of equations.

Each task outlined above builds incrementally on the previous tasks and activities, and where applications are not available, open source alternatives will be found such that we can evaluate as many options of post-exascale software development as possible. While each task culminates in a deliverable report, these will be living documents -- continually being updated throughout the project as new hardware emerges and as support for software evolves.

The work in this proposal will take direction from and inform the direction of several of the NEPTUNE work packages, and so coordination between projects will be vitally important to its success and is included as Task 4 (Dissemination of Best Practices) which will run throughout the project.

As travel may be restricted throughout the project, due to the COVID-19 pandemic, many of the coordination activities will necessarily have to take place virtually. However, should travel restrictions be lifted, we would hope to attend relevant conferences, such as ISC High Performance 2021. To support this, we request a travel and subsistence budget of [redacted]. Additionally, should in-person meetings become possible during the project, we request an additional [redacted] for UK travel and subsistence.

Relevant Experience

A brief summary of the relevant expertise and track record of the people involved in this bid is given below. Further information can be found in the CVs submitted with this bid.

- **Dr Ben Dudson** is a Reader in the Department of Physics at the University of York, specialising in tokamak boundary plasma physics. Lead designer and author of BOUT++ (2007-present), a high performance, object-oriented C++ framework used

worldwide as a basis for plasma simulations. 72 publications in experimental, theoretical and computational plasma physics, with an h-index of 29 (Google Scholar). Chair of the EPSRC Software Outlook Working Group, and deputy director of the York Plasma Institute, with extensive experience of mentoring students, postdocs and junior staff. Funding application and project management lead, as PI and Co-I, with a record of sustained funding income from a range of funding agencies, in particular UK EPSRC and EU EuroFusion (Horizon 2020). He leads a team at the University of York working on plasma edge and divertor modelling for STEP, under contract with UKAEA.

- **Dr Steven Wright** is a Lecturer in Computer Science at the University of York. He has worked in High Performance Computing (HPC) for 10 years, particularly in the areas of performance analysis, benchmarking and optimisation of HPC systems. His Ph.D. was completed at the University of Warwick in collaboration with collaborators at Lawrence Livermore National Laboratory and Los Alamos National Laboratory, analysing and optimising the performance of parallel file systems and I/O in HPC applications. Before joining the University of York, he was a postdoctoral research fellow at the University of Warwick working with UK AWE on the Computational Collaborative Project in Plasma Physics [EP/M011534/1], assessing the sustainability and adaptability of the Odin Arbitrary Lagrangian-Eulerian (ALE) code. Following a secondment as a visiting research fellow at Sandia National Laboratories (NM), he has been collaborating on the ElectroMagnetic Plasma in Realistic Environments (EMPIRE) project, focussed on the development of a performance portable unstructured FEM-PIC code.
- **Dr Peter Hill** is a research software engineer (RSE) in plasma physics and currently provides support to several computational projects at the York Plasma Institute (YPI) totalling more than £6M, including as Researcher Co-I on the Turbulent Dynamics of Tokamak Plasmas (TDoTP) EPSRC Programme grant (EP/R034737/1). His current interests are in software sustainability and reproducible research, both of which are vital to maintaining trust in research. Peter is a lead maintainer on two world-class plasma codes, BOUT++ and GS2, and regularly contributes to many other software projects, including external open-source projects such as PETSc, netCDF and CMake, collectively used in millions of projects.
- **Dr David Dickinson** is a Lecturer in the Department of Physics at the University of York with a primary physics interest in core plasma turbulence and associated instabilities. He has a research focus of first-principles computational analysis of gyrokinetic/gyrofluid instabilities and brings experience with using and developing world-class tools for core, pedestal and SOL gyrokinetic/gyrofluid simulation. He has been a leading developer and maintainer for the gyrokinetic code GS2 since 2012 and has also made substantial contributions to BOUT++ since 2016. He is Co-I on the Turbulent Dynamics of Tokamak Plasmas (TDoTP) EPSRC Programme grant (EP/R034737/1) and leads work at the University of York for core turbulence modelling for STEP, under contract with UKAEA.
- **Dr Gihan Mudalige** is an Associate Professor in the Department of Computer Science at the University of Warwick. His research focuses on the development of next-generation High Performance Computing numerical simulation software libraries through the utilization of domain-specific high-level abstraction frameworks. In 2018, he was awarded a four-year Royal Society Industry Fellowship with Rolls-Royce (INF/R1/180012), focusing on developing future-ready massively-parallel CFD simulations for Exascale HPC systems. He is also a co-investigator in the £6.8M EPSRC Prosperity Partnership (EP/S005072/1) for Advanced Simulation and Modelling of Virtual Systems (ASiMoV) aiming to realise new simulation technologies at ultrahigh resolution and extreme scales. Dr. Mudalige is a Co-I on two of the recently awarded ExCALIBUR working groups, both on applying code-generation

and high-level abstractions for exascale software. The research software developed by Dr. Mudalige and his team is now utilized in projects carried out by a range of academic and commercial organizations, including EPSRC (EP/V00140X/1), Rolls-Royce plc., STFC, AWE plc., the Numerical Algorithms Group (NAG), UCL, ATI London, ETH Zurich and the Universities of Nottingham and Southampton.