Name of Bidding Organisation:	University of York
Contract Title:	**T/NA083/20 - Fluid Referent Models**

1 Purpose of Document

2 Benefits and alignment to Work Package objectives

- **Holistic, collaborative design:** Our approach will be to develop a series of proxyapps, with associated tests and documentation, structured around the 5 tasks specified in the call document. These will be made available to the community, and used to undertake studies of issues such as preconditioning, UQ, and DSL design, in collaboration with the successful bidders to the relevant calls, UKAEA and the NEPTUNE community. Lessons learned from these studies will be written up (see deliverables below), and used to inform the following tasks.
- **Task delivery**: The Work Package objectives set out five tasks, involving increasingly complex models, and integration with other work packages. To address these tasks with limited resources, we have designed a set of ambitious but realistic activities and deliverables. Where there is insufficient knowledge to enable a reliable resource estimate to be carried out, a pathway to obtaining the required knowledge has been identified, and the deliverable includes a suggested roadmap to achieving the objective.
- **Performance portability**: Researchers involved in this bid will have access to a range of workstations and high performance computing facilities at York and Exeter universities. This includes for example the York Viking cluster (Intel Xeon x86, NVIDIA TESLA v100 GPUs) and the new N8 Bede (IBM Power 9 CPUs and NVIDIA Volta GPUs). This will enable proxyapps to be developed and tested on a range of architectures. Access to these facilities is an in-kind contribution to the project.
- This submission aligns with the Excalibur pillars**:**
  - **Separation of Concerns:** The most complete proxyapp in this call is Task 5, which must integrate a number of different aspects of the project (e.g. DSLs, UQ), including outputs from bidders to other calls. To do this we will explore and develop capabilities in simpler proxyapps, and then use these to test integration with other aspects of the project. We will use both BOUT++ and Nektar++ to develop these proxyapps, to ensure that our solutions are not tightly coupled to a single framework.
  - **Co-design:** This proposal directly involves domain experts in plasma physics, computer scientists, Research Software Engineers with expertise of coordinating large-scale open source scientific research code development (e.g. BOUT++, GS2), and experts in the Nektar++ spectral/hp library. We have also identified that close coordination with other NEPTUNE and Excalibur work packages will be essential at an early stage, and will be an iterative process of improvement. Specific activities, deliverables and resources are described below, in order to carry out the coordination and training required.
  - **Data Science:** By providing functioning code which solves the referent systems of equations at an early stage of the project, we will enable other researchers to develop new work flows to analyse the data in-situ and in post-processing. Part of our coordination efforts will be in teaching other groups to use the codes and data we produce.
  - **Investing in People:** To deliver the goals of the NEPTUNE project, it is our aim to build a team of researchers and software engineers who understand holistically the issues involved, from plasma physics, algorithms, sustainable software engineering, to the hardware likely to be used at exascale. We have brought together a collaboration including engineers, physicists and computer scientists, who between them have the required expertise. During the course of this project the RSEs and researchers involved will work together, to spread and exchange their domain knowledge. To help build careers in this interdisciplinary work, we request funds to support attendance at high profile international conferences. We recognise that collaboration between successful bidders on the various NEPTUNE projects will also be essential, so have requested travel funding to support these collaborations.

3 Scope

3.1 Key Deliverables and/or Desired Outcomes

The deliverables of this work package will consist of the following types:

- **Test cases :** A report describing the test cases to be used to compare the accuracy, efficiency and scalability of implementations. This to be accompanied by data and scripts (written in python) to enable testing of new implementations. Where possible these will include analytic solutions, or manufactured solutions (MMS) for convergence testing in realistic complex cases.
- **Reference implementations**, implemented using BOUT++, to provide a baseline for comparison with other implementations, and a platform which can be used for initial exploration of preconditioning, intrusive UQ, and the development of DSLs. Our vision is to replace these BOUT++ implementations with Spectral/hp or other high-order implementations, but while those are being developed we will make use of the capabilities which already exist in BOUT++ to accelerate progress in other areas.
- **Spectral/hp implementations,** implemented using Nektar++. These will be tested using the same test cases as the reference implementations (in addition to implementation-specific unit tests). The accuracy and efficiency of the codes will be compared using the methodology to be established during the first three months of the call (deliverable 0.1).
- **Exploratory mini-apps**, which implement an algorithm in a higher-level language, for example Python or Julia. These would be used to investigate the accuracy and robustness of algorithm choices, for example phase space representation, time stepping methods and preconditioning. We see Task 3 (system 2-4) in particular as a suitable system with which to explore some of these design decisions which will inform the full 5D gyrokinetic implementation.

This work package brings together and interfaces with multiple other work packages, in particular calls T/N/A078/20 [Performance of spectral elements], T/NA084/20 [preconditioners], T/NA080/20 [Study of Uncertainty Quantification Techniques] and T/NA086/20 [DSL techniques]. We therefore propose an activity, Task 0, to carry out the required coordination and project management.

Task 0 : Coordination and management

- **Deliverable 0.1** : Set up environment e.g version control, continuous development/integration, automated testing and documentation services, coding standards. Set up testing framework for evaluating parallel scaling on e.g. Archer2 / Viking / Bede
- **Deliverable 0.2** : A report on coordination with UKAEA and other work groups, including any training activities carries out, during FY 2021/22
- **Deliverable 0.3** : A report on coordination with UKAEA and other work groups, including any training activities carries out, during FY 2022/23

The remaining deliverables are organised under the tasks specified in section 1.3 of the call document:

- **Task 1** : System 2-2, 2D elliptic solver in complex geometry
    - **Deliverable 1.1:** Test cases for system 2-2.
    - **Deliverable 1.2:** Reference implementation in BOUT++, using PETSc and Hypre. This early implementation will allow testing of the performance of Hypre, including on GPU systems (Bede), making use of ongoing collaborations with LLNL.
    - **Deliverable 1.3:** Spectral/hp implementation in Nektar++, to be developed in collaboration with the winning bidders of call T/N/A078/20 [Performance of spectral elements].
    - **Deliverable 1.4:** A report on progress in preconditioning of this system, developed in collaboration with the winning bidder of call T/NA084/20 [preconditioners]. Initial work may

make use of the BOUT++ implementation, but will switch to the Spectral/hp implementation when that becomes available.

- **Task 2** : System 2-3, 1D fluid solver with UQ and realistic boundary conditions
  - o **Deliverable 2.1:** Test cases for system 2-3
  - o **Deliverable 2.2:** Reference BOUT++ implementation. This will build on existing models which have been used in production (SD1D).
  - o **Deliverable 2.3:** Nektar++ implementation of the 1D system of fluid equations, including the sonic outflow (plasma sheath) boundary condition and sources. This will be used to assess numerical accuracy and stability at this boundary.
  - o **Deliverable 2.4:** Report on intrusive UQ, in collaboration with the winning bidder of project T/NA080/20 [Study of Uncertainty Quantification Techniques]. We expect that this initial work will be based on the BOUT++ implementation, and will include a roadmap for its extension to higher order implementations and eventually the full NEPTUNE system.
  - o **Deliverable 2.5**: A report on intrusive UQ, including an assessment of its likely impact on performance, and the number of moments/polynomials needed to represent the error due to boundary conditions.
- **Task 3** : System 2-4, 1D plasma model with velocity space effects
  This task is a 1D kinetic system, and serves as a useful test-bed for exploring algorithms which will be required to build the full gyrokinetic NEPTUNE system.
  - o **Deliverable 3.1**: Test cases for system 2-4
  - o **Deliverable 3.2**: Report on phase space representation through exploratory mini-apps. This will draw on previous work on kinetic (Vlasov) solvers [e.g. Arber&Vann, https://doi.org/10.1006/jcph.2002.7098] and more recent work on the Gkeyll gyrokinetic code, in particular basis function choice, and positivity preserving reconstructions [Hakim et al. https://doi.org/10.1063/1.5141157]. System 2-4 will be implemented, likely in a high-level language such as Python or Julia, to explore these approaches.
  - o **Deliverable 3.3:** Report on time-stepping methods for kinetic systems, using implementations in high-level languages such as Python or Julia: Compare the accuracy and robustness of time integration, with an assessment of the impact of this choice on parallel scaling to Exascale. The baseline comparison will be between an explicit SSP-RK scheme, and a fully implicit Jacobian-free method such as LSODE or CVODE. If time permits, we would explore Semi-Lagrangian methods, which have potential stability advantages. A further extension would be to explore asynchronous or local time-stepping methods, which have the potential to reduce or eliminate global communications, and so may scale more favourably to Exascale hardware.
- **Task 4 :** System 2-5, Spatially 1D multispecies plasma model
  - o **Deliverable 4.1** : Test cases for system 2-5
  - o **Deliverable 4.2** : Reference BOUT++ implementation. During the last 2-3 years we have developed and implemented methods to modularise and generalise simulations codes to multiple species. We will build on this as-yet unpublished work on multifluid versions of the SD1D and the Hermes-3 BOUT++ models.
  - o **Deliverable 4.3** : Report on DSL adoption, and approaches to code design which are flexible in the number of equations/species solved. This will be done in collaboration with the successful bidder to T/NA086/20 [DSL and code generation], to test the methods developed under that call in a complex setting. We will work with the successful bidders of T/N/A078/20

[Spectral Elements] to explore how this same DSL could drive both BOUT++ and Nektar++ solvers.

- **Task 5 :** System 2-6, 2D plasma model with velocity space effects
  This referent model will be important for further development, and is an ambitious undertaking: It must incorporate research and development carried out during the course of previous tasks within this project, and also work carried out by other projects. In particular the outputs of the T/N/A078/20 [Spectral Elements], T/NA086/20 [DSL and code generation techniques] and T/NA084/20 [preconditioners].
  - **Deliverable 5.1 :** Test cases for system 2-6
  - **Deliverable 5.2:** A report on progress in FY 2021/22, detailed assessment and roadmap for completion of this proxyapp. At the current time the resources required to carry out this task are uncertain. Work on deliverables 1.3 and 2.3, and coordination with the other NEPTUNE groups, will enable an assessment of the steps required to implement system 2-6 in a Spectral/hp framework, and any obstacles to be overcome.
  - **Deliverable 5.3:** A report on progress in FY 2022/23 towards implementation in Nektar++ or other Spectral/hp framework, all source code and documentation produced, and an updated roadmap leading to the full NEPTUNE code.

3.2 Exclusions

3.3 Constraints

- A number of deliverables are dependent on, or would benefit significantly from, the outputs from other successful bidders. These are highlighted in the description of deliverables above, and include the outputs of T/N/A078/20 [Performance of spectral elements], T/NA084/20 [preconditioners], T/NA080/20 [Study of Uncertainty Quantification Techniques] and T/NA086/20 [DSL techniques]. We will actively engage with these groups, and have allocated time and resources to coordination activities. To mitigate the risk that this implies, we have identified fall-back activities within each deliverable, so that we can ensure that progress is made towards the project goals.

4 Approach

This work package links together the work of several work packages, and so activities and associated resources to form and coordinate a community around the NEPTUNE project is included as deliverables 0.1-0.3. The proposed approach is based on our experience in building and maintaining large open-source plasma physics simulation codes, and coordination of communities around them. Most relevant to this call is our expertise and experience with BOUT++ and GS2: In the first FY (deliverable 0.1) we will use online meetings with the other successful bidding groups and UKAEA, to establish contacts and create a community. The outcome of these meetings will be to establish agreed community guidelines and software development practices to be used in developing our proxyapps, building on the NEPTUNE charter. Our expectation at this stage is that proxyapps will be made available under a BSD 3-clause licence; development will be carried out in public Github repositories, using a system of pull requests and code review, with automated tests using a continuous integration/development service, an approach successfully used in BOUT++ development. In addition to these processes which increase the development efficiency, speed and reliability, we will also establish a performance testing methodology, in discussion with UKAEA, so that performance regressions can be identified and quickly addressed. To do this we have access to HPC clusters at both York and Exeter, including GPU nodes, x86 and Power 9 processors, to ensure performance portability and scalability of the software algorithms.

Once the development environment and connections are established, it will be necessary to continue coordination between work packages, so that we can make use of the outputs of these other groups, and ensure that they benefit from our work. During FY 2021/22 and 2022/23 we have therefore included coordination activities across groups (deliverables 0.2 and 0.3). These will be used to ensure that development across the groups converges on common standards, APIs, libraries, build systems, and vocabularies/ontologies, all of which will be vital for the overall success and sustainability of NEPTUNE. COVID-related restrictions on travel and gathering are likely to be in place for a significant fraction of this project, and so the majority of seminars and meetings will be held online.

Management, oversight and reporting of the project activities will be led by the PI Ben Dudson, working closely with the other researchers involved. The initial work on Nektar++ implementations will be led by Dr David Moxey at the University of Exeter, supervising a PDRA to do this work. Some University of York staff time is also included in the Nektar++ implementation development: This will be used initially to enable Dr Peter Hill to participate in deliverables 1.3 and 2.3, before widening the number of researchers involved as focus shifts to Spectral/hp implementations. This will transfer plasma physics knowledge to the University of Exeter staff, in particular the PDRA involved, and enable the University of York RSEs and staff to gain experience of applying Nektar++ to plasma physics applications. Work on DSLs, performance portability and UQ aspects of the deliverables will be led by Dr Steven Wright, who will coordinate with the successful bidders to call T/NA086/20 [DSL techniques]. This methodology will enable us to build a team with the capability to work collaboratively across disciplines, in order to deliver the ambitious objectives of NEPTUNE and ExCALIBUR projects.

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 Owner	Required Data
Deliverable 1.4 depends on work carried out under work package reference T/NA084/20, where preconditioners will be developed, and applied to the systems implemented in this project. The required activity is scheduled to run in the second half of FY 2021/22. If T/NA084/20 is able to provide input then we will build on that work; if not then we have experience with physics-based preconditioning which we would employ to perform initial exploration of preconditioning.	Successful bidder to work package T/NA084/20	
Deliverable 2.4 depends on work package reference T/NA080/20 [Study of Uncertainty Quantification Techniques]. This activity is scheduled to start in April 2022, and will benefit from work carried out under that project. If for some reason such input is not available, we will draw on literature, and discussions with UKAEA and the ExCALIBUR/NEPTUNE community to guide our efforts.		
Deliverable 4.3 depends on work package T/NA086/20 [DSL and code generation techniques]		

Deliverable 5.3 brings together much of the previous work under this work package, together with work under other work packages.	NEPTUNE team	

6 Activity Plan

In all following activity descriptions the deliverables constitute milestones towards the overall task objective. Within each financial year, progress towards deliverables will be reported according to the schedule specified in Part 1 of the call document: Monthly and quarterly reports will summarise status against our expectations, and annual reports will report deliverables due to be completed in the corresponding financial year.

Task 0: NEPTUNE community coordination	**Activity No**	0
Activity: To set up and maintain the software repository, testing, documentation, and performance evaluation environment for proxyapp development; Organise meetings with NEPTUNE partners to exchange knowledge and build a community; Coordinate activities and training; disseminate results and engage collaborators through conference & workshop attendance. **Assignee:** Dr Peter Hill		
Objective 1: To establish community standards and strong links between NEPTUNE groups **Objective 2:** Set up and maintain the software development environment, coordinating with other NEPTUNE groups. **Objective 3:** Disseminate findings of other activities, within and outside the NEPTUNE project partners.		
Key Deliverables: **1)** Deliverable 0.1 **2)** Deliverable 0.2 **3)** Deliverable 0.3	**Start and Completion date:** 1) 4/1/2021 - 31/3/2021 2) 1/4/2021 - 20/3/2022 3) 1/4/2022 - 20/6/2023	**Assignee:** 1) Peter Hill 2) Peter Hill 3) Peter Hill

Task 1 : System 2-2, 2D elliptic solver in complex geometry	**Activity No**	1
Activity: To define a set of test cases and performance metrics; implement the system in both BOUT++ and Nektar++ frameworks and test; apply and evaluate preconditioning methods developed in other work packages, or if not available carry out development work. **Assignee:** Dr Ben Dudson		
Objective 1: Assess the performance of a Nektar++ implementation in simplified tokamak geometry against a reference BOUT++ case **Objective 2:** Assess the additional numerical cost of realistic tokamak geometry solves with detailed geometry (Nektar++ only)		

Objective 3: Evaluate preconditioning strategies, building on work performed under work package T/NA084/20 or developed under this work package.		
Key Deliverables: 1) Deliverable 1.1 2) Deliverable 1.2 3) Deliverable 1.3 4) Deliverable 1.4	**Start and Completion date:** **1)** 4/1/2021 - 20/3/2021 2) 4/1/2021 - 20/3/2021 3) 1/4/2021 - 20/3/2022 4) 1/4/2021 - 20/3/2022	**Assignee:** 1) Ben Dudson 2) Ben Dudson 3) David Moxey 4) Ben Dudson

Task 2 : System 2-3, 1D fluid solver with UQ and realistic boundary conditions		**Activity No**	2
Activity: Define a set of tests and performance measures; implement the system in BOUT++ and Nektar++ frameworks; use these implementations to explore intrusive UQ techniques. **Assignee:** Dr Ben Dudson			
Objective 1: Evaluate the performance and stability of Spectral/hp methods with sheath boundary conditions **Objective 2:** Compare the performance of finite difference and spectral/hp implementations **Objective 3:** Explore the implementation and implications of intrusive UQ			
Key Deliverables: 1) Deliverable 2.1 2) Deliverable 2.2 3) Deliverable 2.3 4) Deliverable 2.4 5) Deliverable 2.5	**Start and Completion date:** 1) 4/1/2021 - 20/3/2021 **2)** 1/4/2021 - 20/3/2022 **3)** 1/4/2021 - 20/3/2022 **4)** 1/4/2021 - 20/3/2022 5) 1/4/2022 - 20/6/2023	**Assignee:** 1) Ben Dudson 2) Ben Dudson 3) David Moxey 4) Steven Wright 5) Steven Wright	

Task 3 : System 2-4, 1D plasma model with velocity space effects		**Activity No**	3
Activity: Define tests to exercise physics of 1D kinetic model of the tokamak SOL; compare phase space representations in terms of accuracy and scaling; compare time stepping approaches, with a view to their scaling to large problems and exascale hardware. **Assignee:** Dr David Dickinson			
Objective 1: Create a set of test cases against which implementations can be compared for accuracy, performance and scaling **Objective 2:** Provide guidance on the choice of phase space representation for kinetic systems, in collaboration with other work packages **Objective 3:** Provide guidance on choice of time stepping method for kinetic systems, to inform the design of future NEPTUNE models.			
Key Deliverables: 1) Deliverable 3.1 2) Deliverable 3.2 3) Deliverable 3.3	**Start and Completion date:** 1) 1/4/2021 - 20/3/2022 2) 1/4/2021 - 20/3/2022 3) 1/4/2021 - 20/3/2022	**Assignee:** 1) David Dickinson 2) David Dickinson 3) David Dickinson	

Task 4 : System 2-5, Spatially 1D multispecies plasma model		**Activity No**	4
Activity: To define correctness tests and performance metrics; implement system 2-5 in BOUT++, building on and extending design patterns for modular code reuse; apply and evaluate DSL techniques in collaboration with the NEPTUNE DSL and code generation work package. **Assignee:** Dr Steven Wright			
Objective 1: Define a set of tests and performance metrics against which implementations can be compared **Objective 2:** Implement a reference BOUT++ implementation **Objective 3:** Guide the choice DSL and code design pattern for NEPTUNE, through implementation in a plasma model and exploration of the performance and code maintenance trade-offs.			
Key Deliverables: 1) Deliverable 4.1 2) Deliverable 4.2 3) Deliverable 4.3	**Start and Completion date:** 1) 1/4/2021 - 20/3/2022 2) 1/4/2021 - 20/3/2022 3) 1/4/2021 - 20/3/2022	**Assignee:** 1) Ben Dudson 2) Ben Dudson 3) Steven Wright	

Task 5 : System 2-6, 2D plasma model with velocity space effects	Activity No	5
Activity: Define tests and performance metrics; evaluate the steps required to implement system 2-6, integrating the outputs of earlier tasks and other NEPTUNE work packages; begin implementation of the code base and documentation; design and refine the roadmap to completion of the implementation. **Assignee:** Dr David Moxey		
Objective 1: Define tests and performance metrics for system 2-6 **Objective 2:** Begin implementation in Nektar++, with a design taking into account earlier results and other work package outputs **Objective 3:** Plan a recommended roadmap to completion of the implementation		
Key Deliverables: **1)** Deliverable 4.1 **2)** Deliverable 4.1 **3)** Deliverable 4.1	**Start and Completion date:** **1)** 1/4/2021 - 20/3/2022 **2)** 1/4/2021 - 20/3/2022 **3)** 1/4/2022 - 20/6/2023	**Assignee:** **1)** David Moxey **2)** David Moxey **3)** David Moxey