Name of Bidding Organisation:	University of Exeter
Contract Title:	Examining the performance of Nektar++ for fusion applications

1   Purpose of Document

2   Benefits and alignment to Work Package objectives

We propose a schedule of work to develop proxyapps to investigate and quantify the performance of spectral element methods in the context of modelling anisotropic heat transport in the tokamak plasma edge in close proximity to a complex, 3D first wall, part of the NEPTUNE fusion modelling system. Specifically, we will target the computational and algorithmic developments required to construct a proxyapp for a sample 2D model of anisotropic heat transport (output 2.1.5), by combining efforts on two separate fronts:

- The development of bespoke high-order mesh generation techniques that are capable of faithfully representing the physics found in tokamak plasma edge, both in terms of handling X-point geometries (output 2.1.1) and highly accurate surface meshing (output 2.1.2).
- Extending the capability of the *Nektar++* spectral/*hp* element framework (www.nektar.info, [1, 2]), in collaboration with UKAEA, the successful bidder of call T/NA083/20, and other stakeholders of the NEPTUNE and ExCALIBUR projects, to enable the development of proxyapps for related problems in edge plasma physics, taking into account factors such as performance portability, separation of concerns and sustainable code development (outputs 2.1.3 and 2.1.4).

To enable these developments, the investigatory team will draw on unique expertise with *Nektar++* and the high-order mesh generator *NekMesh*. In the following sections, we outline how the objectives of this work package (and broader goals of the NEPTUNE project) can be met through the development of high-order methods, and how the goals and background of the investigatory team map onto those objectives.

Background. High-order methods are increasingly being viewed as an enabling technology for bespoke high-fidelity modelling of challenging physical systems. The use of high-order polynomials within elements, when compared to classical linear and second-order methods, offers advantages from both a numerical analysis and implementation perspective. The 'resolution power' of high-order discretisations is far greater than at lower orders, with favourable dispersion and diffusion characteristics meaning that complex spatial structures and phenomena spanning multiple length scales can be accurately resolved and tracked across long timescales. This accuracy is critical in highly sensitive and complex systems, such as fluid dynamics, where energetic and inherently unsteady phenomena such as vortex interactions require accurate resolution. From an implementation perspective, the modern many-core hardware architectures that will power upcoming exascale platforms are increasingly reliant on algorithms and methods that are *arithmetically intense*: that is, they perform a sufficiently large number of floating-point operations (FLOPS) per byte of data transferred from memory in order to realise the full potential of the available hardware. This trend towards arithmetic intensity holds on any of the traditional CPU (Intel Skylake or AMD Threadripper), energy-efficient architectures (e.g. ARM ThunderX2) or GPU based platforms (e.g. Nvidia Tesla) and, to date, lower order methods have struggled to realise the full potential of these platforms. Since the resolution power of high-order methods comes at the cost of additional FLOPS, this makes high-order methods ideally placed as an enabling technology for exascale simulations.

Enabling high-order methods within NEPTUNE. The primary goal of the work we propose in this project is to develop the necessary algorithmic and software improvements required to enable high-order simulations to be performed for the problems of interest to the NEPTUNE community, and demonstrate that high-order

methods meet a significant number of the requirements **P1** through **P8** that have been identified in the call document. We highlight that high-order methods meet some of these requirements already, for example:

- the accurate solution of the compressible Navier-Stokes simulations as a hyperbolic system **(P1)** for direct numerical simulation of high-Reynolds number flows, as shown in [3];
- more broadly, high-order discontinuous Galerkin formulations are used to ensure e.g. conservation of mass in the above **(P6)**;
- the accurate solution of elliptic problems **(P2)** such as the pressure Poisson equation are routinely solved in complex geometries as part of e.g. velocity or pressure correction schemes for the incompressible Navier-Stokes equations, which feature highly anisotropic dynamics **(P3)** in boundary layer regions and in modelling vortex interactions [4].

The focus of this project will therefore be to demonstrate that these properties are not restricted to e.g. only the fluid dynamics community, but can be observed in the plasma-edge specific systems, by considering the overriding problem at the heart of this call: developing a proxyapp, based on high-order spectral/*hp* element methods, that can work towards the goal of anisotropic heat transport in the tokamak plasma edge, accounting for a complex 3D wall geometry. To meet this objective, we separate the goals of this project into two tasks which will be required to meet the identified outputs from this work package.

Task 1: Curvilinear mesh generation. One of the significant bottlenecks in developing and running a high-order simulation is the ability to generate high-quality, boundary conforming meshes. Unlike linear meshes, high-order meshes must be curved and deformed so that they align with the boundary, which makes the generation of slender anisotropic grids (such as in a boundary layer) a significant challenge. Creating a valid and accurate mesh for the simulation of, for example, a full car or aircraft configuration, therefore remains an unresolved challenge, posing a significant hurdle to the uptake of these methods. To work towards addressing this, the *Nektar++* team has invested significant academic development of the *NekMesh* mesh generator [5, 6], in order to establish a set of pre-processing modules for the generation of high-quality curvilinear meshes for *Nektar++*. This is an area where both commercial and academic codes are scarce. In this task, the *NekMesh* generator will be augmented to support the geometries that are critical in the modelling of tokamak edge regions:

- **Task 1.1: Generation of tokamak edge region meshes:** To support the clustering of elements around X-point configurations and other divertor configurations (output 2.1.1), we will leverage and significantly extend the variational framework outlined in [5], in order to produce refined anisotropic grids that can accurately model the X-point configuration. This will extend and strengthen existing efforts in this area for *rp*-adapted grids [7] which leverage this approach in order to refine grids for shock capturing purposes. **Deliverable 1.1**: A set of mesh generation routines, embedded in NekMesh, for modelling the tokamak edge region.
- **Task 1.2: Quad-based mesh generation for 2D configurations:** One of the main themes in the use of high-order methods in exascale applications is the use of *matrix-free methods*. In this approach, the generation of either large, sparse global matrices (for the whole grid), or smaller, locally-dense matrices (for each element) is avoided by recasting the action of the matrix as a summation and reduction operation. This therefore reduces the memory bandwidth requirements and allows high-order methods to attain 50-70% of the peak performance of modern CPU and GPU platforms [8, 9]. This is most effective when combined with a tensor contraction technique called sum-factorisation alongside a mesh of quadrilateral or hexahedral elements [10], which readily admit such a decomposition. In this deliverable we will leverage a proof-of-concept 2D quadrilateral generation technique, developed in NekMesh [11]. Although this method shows great potential, it requires a concerted software development effort to increase its robustness. This task will support this development and integrate the changes of D1.1 to generate high-quality, adapted grids suitable for the tokamak edge region. **Deliverable 1.2:** Augmentation of the NekMesh generator to provide quad-based meshes for 2D configurations.

- **Task 1.3: Accurate surface mesh generation:** In this task, we will first validate surface quality for representative meshes supplied by UKAEA, by generating meshes using the existing NekMesh high-order generation techniques and investigating important metrics such as surface normal accuracy. Where necessary, we will improve the surface mesh generation technology contained with *NekMesh* to ensure that sufficiently accurate grids by, for example, examining whether the metrics used to optimise node positions for the high-order mesh can be improved, or if change within the CAD system will improve vertex placement. We will ensure that the requirements outlined in output 2.1.2 are met for representative geometries. As well as those supplied by UKAEA, we will also validate meshes from other related calls, such as the successful bidders for call T/NA083/20, and other bidders who require high-order meshes as part of their tasks where required. **Deliverable 1.3:** Report outlining validation process for accurate surface meshes, and/or required improvements to NekMesh to deliver this.
- **Task 1.4: End-user interfaces and workflow integration:** A key theme within this call is the requirement for software that is not only exascale-capable (or in the case of mesh generation, that supports an exascale-capable end-goal), but can align with user requirements and is easy to deploy, use and develop. Although *NekMesh* and *Nektar++* already strive for excellence in this area through the provision of high-quality documentation, continual integration and code review, in this deliverable, we will ensure that these themes are translated across to these mesh generation developments through the provision of documentation, tutorials and training sessions. Working with UKAEA and other call partners, we will ensure that these can be embedded within workflows as required with the overall NEPTUNE project. To this end we will extend and solidify a Python interface to enable advanced scripted usage of *NekMesh* in a variety of pre-processing environments, as well as to embed this within existing and future workflows. **Deliverable 1.4:** Python interface, documentation and continual integration for the NekMesh generator for the developments undertaken in task 1.

Task 2: Developing flexible and performance portable proxyapps. The primary objective will be to construct a proxyapp for 2D anisotropic heat transport, as required in output 2.1.5. As part of this, we will extend the existing x86 algorithmic kernels with kernels for ARM and GPU architectures to demonstrate the code will be performant on a range of potential exascale platforms. This task is therefore broken down into the following stages:

- **Task 2.1: Implementation and validation of baseline x86 proxy-app for anisotropic 2D heat transport.** This will be built within the *Nektar++* framework, leveraging high-order spectral elements and using the existing matrix-based local elemental operators. This initial proxy-app will be used to verify correctness of the initial algorithmic implementation and used as a baseline case for performance optimisations undertaken in the later part of this task. **Deliverable 2.1:** Baseline proxy-app, built on Nektar++, for solving the anisotropic heat transport equation for x86 architectures.
- **Task 2.2: Matrix-free anisotropic Laplacian kernel.** Matrix-free kernels enable high-order methods to achieve high arithmetic intensity. We will develop matrix-free kernels for the Laplacian kernel which minimise data movement and can exploit the vectorisation capabilities of modern x86 processors. In particular, we will focus on how best to incorporate the second-order coefficient tensor into this operator which allows for the representation of anisotropic media. Benchmarking will be performed to measure performance gain over baseline case, percentage of peak FLOPS, with results characterised using roofline plots. **Deliverable 2.2**: Matrix-free kernel for the anisotropic Laplacian operator for x86 architectures.
- **Task 2.3: Matrix-free kernels for ARM and GPU.** Spectral/hp element kernels will be developed for the ARM architecture to allow performant vectorised execution of the proxy-app on the power-efficient ARM architecture. We will also develop corresponding kernels for NVidia GPU architectures, enabling use of a range of potential exascale platforms. Our previous work [12, 13] have demonstrated we can achieve performance portability on GPUs with this approach, but a more considered approach to e.g. memory layout and thread distribution & scheduling must be employed to achieve peak performance. The performance of these kernels will be benchmarked against the baseline case on a flops-per-watt basis. **Deliverable 2.3:** Collection of matrix-free kernels for ARM and GPU architectures.

- **Task 2.4: Preconditioning for highly anisotropic systems.** The 2D heat transport test case is strongly ill-conditioned due to the strong anisotropy required. Iterative solvers, used for large scalable parallel runs, will consequently converge slowly. We will identify the best choice of preconditioners for use with this problem, with input from the preconditioning work undertaken by the winning bidders of task T/NA084/20. **Deliverable 2.4**: Report summarising benchmarking and preconditioner assessment undertaken in Task 2.

Task 3: Engagement with NEPTUNE partners and the broader proxyapp ecosystem. A critical part of this call is to ensure engagement with the wider NEPTUNE and ExCALIBUR community, particularly around the development of the proposed proxyapp within this call, the work undertaken within closely related calls T/NA083/20 (development of plasma fluid referent model) and T/NA084/20 (preconditioning), as well as to align with the overriding goals of enabling performant, sustainable and easily usable software. In this task, we lay out a series of deliverables to deliver coordination of our efforts with those of other calls and the wider NEPTUNE and ExCALIBUR projects.

- **Task 3.1: Coupling with other proxyapps.** To enable the connection of the proxyapps being developed in Task 2 with those being developed in other work package partners, we will leverage the coupling technology (CWIPI) already in Nektar++ to enable the coupling of different proxyapps. A proof-of-concept approach has been demonstrated in [14] for the integration of an aeroacoustic model together with a combustion LES code. In this task we will undertake software development work to solidify this interface and provide a documented example case to highlight its usage. **Deliverable 3.1:** Proof-of-concept coupling example that demonstrates the use of the proxyapp with another CWIPI-compatible solver.
- **Task 3.2: Training materials.** As a fundamental issue in the coordination of work package efforts will be to communicate progress on the various objectives throughout this project. Furthermore, ensuring the usability and longevity of the software requires a concerted effort to thoroughly document the resulting proxyapps and developments. To tackle this challenge, the focus of this continuing task is to document progress in an evolving manner throughout the project. **Deliverable 3.2:** training materials for the developments undertaken in tasks 1 and 2.
- **Task 3.3: Coordination efforts.** To engage with UKAEA and other work package partners, we propose to hold community engagement events, through e.g. workshops/training days, tutorials, etc. We will aim to align this with other projects, such as PRISM and ELEMENT (noted above) to highlight broader engagement with ExCALIBUR as well as other codes in development. To support these efforts, we have requested a small travel budget for coordination purposes. Although we anticipate that in-person travel will suffer from restrictions due to Covid-19 in the short-term, these funds will be used wherever possible and appropriate to encourage collaboration between ourselves and other work package partners. The PRISM project will also supplement the travel budget should further travel or conference attendance become possible. **Deliverable 3.3:** activity such as an end-of-project workshop to highlight the developments in all tasks.

Alignment with ExCALIBUR goals. The work we propose in this project closely aligns with the goals and pillars of the ExCALIBUR project, as well as other ExCALIBUR-funded and EPSRC-funded projects. The work we propose under task 1 on mesh generation relates directly to the *ELEMENT* project (EP/V001345/1), funded as a priority use case under the phase 1 EPSRC calls for ExCALIBUR. Additionally, our team are also investigators of the closely aligned *Platform for Research in Simulation Methods (PRISM)* project. In terms of ExCALIBUR's pillars, we closely align with:

- **Co-design:** The investigators form a highly interdisciplinary team, who sit at the interface of applied mathematics, scientific computing and applications in engineering and physics. Through projects such as ELEMENT and PRISM, as well as e.g. Sherwin's role as Director of Research Computing Service (RCS) at Imperial College London, the team has a wide range of experience in coordinating large-scale scientific computing projects, such as the project we propose here.

- **Investing in people:** The mesh generation and proxyapp development we outline here relies on the investment in scientific computing researchers, in order to develop their RSE skillset and coordinate with other work package leaders. The investigatory team is committed to supporting work in this area, as evidenced by Sherwin's position as RCS director, as well as the PRISM project, which for several years has underpinned RSE activities within a wide range of codes, including Nektar++, and allowed researchers to develop interdisciplinary careers in research software engineering. As a concrete example, the project's recent continual integration upgrade to a modern container-based environment, which will benefit the testing and quality this project significantly, was supported through the RSE team at Imperial College.
- **Data Science:** A significant part of Task 3 is to ensure that the proxyapp developed in Task 2 is rigorously documented and, moreover, can align with the workflows of other work packages in this call. Moreover, we will invest effort in Task 3 into ensuring our solvers can be integrated with other codes using coupling frameworks, allowing data science and other researchers to use these tools in the broader context of NEPTUNE.
- **Separation of concerns:** The implementation of the high-order kernels in Task 2 will be implemented in Nektar++ in a manner so that the performance portability aspects between architectures can be preserved, but at a higher level, modellers can still interface with these routines in the same manner without concern of specific performance considerations.

Sustainability and usability of software. All codes will be developed within, or upon, the Nektar++ framework and NekMesh tools and therefore adhere to good programming practices already applied within these software packages. Consequently, this will lead to sustainable software which can be easily accessed, extended and integrated into new workflows. Codes will leverage the build system and packaging tools used within the Nektar++ project and therefore the developed proxyapp will be easily built and deployed. Performance portability is addressed through platform-specific kernels and support for multiple compiler toolchains in the build system.

References

[1] C. D. Cantwell *et al.*, 'Nektar++: An open-source spectral/hp element framework', *Comput. Phys. Commun.*, vol. 192, pp. 205–219, 2015, doi: 10.1016/j.cpc.2015.02.008.

[2] D. Moxey *et al.*, 'Nektar++: Enhancing the capability and application of high-fidelity spectral/hp element methods', *Comput. Phys. Commun.*, vol. 249, p. 107110, Apr. 2020, doi: 10.1016/j.cpc.2019.107110.

[3] D. de Grazia, D. Moxey, S. J. Sherwin, M. A. Kravtsova, and A. I. Ruban, 'DNS of a compressible boundary layer flow past an isolated three-dimensional hump in a high-speed subsonic regime', *Phys. Rev. Fluids*, vol. 3, p. 024101, 2018, doi: 10.1103/PhysRevFluids.3.024101.

[4] J.-E. W. Lombard, D. Moxey, S. J. Sherwin, J. F. A. Hoessler, S. Dhandapani, and M. J. Taylor, 'Implicit large-eddy simulation of a wingtip vortex', *AIAA J.*, vol. 54, no. 2, pp. 506–518, 2016, doi: 10.2514/1.J054181.

[5] M. Turner, J. Peiró, and D. Moxey, 'Curvilinear mesh generation using a variational framework', *Comput.-Aided Des.*, vol. 103, pp. 73–91, 2018, doi: 10.1016/j.cad.2017.10.004.

[6] D. Moxey, M. D. Green, S. J. Sherwin, and J. Peiró, 'An isoparametric approach to high-order curvilinear boundary-layer meshing', *Comput. Methods Appl. Mech. Eng.*, vol. 283, pp. 636–650, 2015, doi: 10.1016/j.cma.2014.09.019.

[7] J. Marcon, G. Castiglioni, D. Moxey, S. J. Sherwin, and J. Peiró, 'rp-adaptation for compressible flows', *Int. J. Numer. Methods Eng.*, vol. n/a, no. n/a, 2020, doi: 10.1002/nme.6529.

[8] M. Kronbichler and K. Kormann, 'Fast matrix-free evaluation of discontinuous Galerkin finite element operators', *ACM Trans. Math. Softw. TOMS*, vol. 45, no. 3, pp. 1–40, 2019.

[9] M. Kronbichler and W. A. Wall, 'A performance comparison of continuous and discontinuous Galerkin methods with fast multigrid solvers', *ArXiv Prepr. ArXiv161103029*, 2016.

[10] D. Moxey, R. Amici, and M. Kirby, 'Efficient matrix-free high-order finite element evaluation for simplicial elements', *SIAM J. Sci. Comput.*, vol. 42, no. 3, pp. C97–C123, 2020.

[11] J. Marcon, D. A. Kopriva, S. J. Sherwin, and J. Peiró, 'A high resolution PDE approach to quadrilateral mesh generation', *J. Comput. Phys.*, vol. 399, p. 108918, Dec. 2019, doi: 10.1016/j.jcp.2019.108918.

[12] J. Eichstädt, M. Green, M. Turner, J. Peiró, and D. Moxey, 'Accelerating high-order mesh generation with an architecture-independent programming model', *Comput. Phys. Commun.*, vol. 229, pp. 36–53, 2018, doi: 10.1016/j.cpc.2018.03.025.

[13] J. Eichstädt, M. Vymazal, D. Moxey, and J. Peiró, 'A comparison of the shared-memory parallel programming models OpenMP, OpenACC and Kokkos in the context of implicit solvers for high-order FEM', *Comput. Phys. Commun.*, vol. 255, p. 107245, Oct. 2020, doi: 10.1016/j.cpc.2020.107245.

[14] K. Lackhove, A. Sadiki, and J. Janicka, 'Efficient Three Dimensional Time-Domain Combustion Noise Simulation of a Premixed Flame Using Acoustic Perturbation Equations and Incompressible LES', presented at the ASME Turbo Expo 2017: Turbomachinery Technical Conference and Exposition, Aug. 2017, doi: 10.1115/GT2017-63050.

3   Scope

3.1   Key Deliverables and/or Desired Outcomes

The objectives and deliverables for this work plan are listed as follows. Please refer to the description of tasks in section 2 for further details of each deliverable.

- **Task 1:**
    - o **Deliverable 1.1**: A set of mesh generation routines, embedded in NekMesh, for modelling the tokamak edge region.
    - o **Deliverable 1.2:** Augmentation of the NekMesh generator to provide quad-based meshes for 2D configurations.
    - o **Deliverable 1.3:** Report outlining validation process for accurate surface meshes, and/or required improvements to NekMesh to deliver this.
    - o **Deliverable 1.4:** Python interface, documentation and continual integration for the NekMesh generator for the developments undertaken in task 1.
- **Task 2:**
    - o **Deliverable 2.1:** Baseline proxy-app, built on Nektar++, for solving the anisotropic heat transport equation for x86 architectures.
    - o **Deliverable 2.2**: Matrix-free kernel for the anisotropic Laplacian operator for x86 architectures.
    - o **Deliverable 2.3:** Collection of matrix-free kernels for ARM and GPU architectures.
    - o **Deliverable 2.4**: Report summarising benchmarking and preconditioner assessment in Task 2.
- **Task 3:**
    - o **Deliverable 3.1:** Proof-of-concept coupling example that demonstrates the use of the proxyapp with another CWIPI-compatible solver.
    - o **Deliverable 3.2:** Training materials for the developments undertaken in tasks 1 and 2.
    - o **Deliverable 3.3:** Activity such as an end-of-project workshop to highlight the developments in all tasks.

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

Asides from any potential restrictions/risks (and the corresponding mitigations) noted elsewhere in the document (the most notable due to Covid-19), there are no constraints that we are aware of.

4 Approach

Software development process. As set out in section 2, the work to be undertaken in this project will be implemented within the Nektar++ spectral/hp element framework and its constituent mesh generation software, NekMesh. To achieve this work package's objectives, we will rely on the extensive background and experience of the investigatory team in leading the numerical and computational development of spectral element methods.

Since software developments form the central deliverables of the project, we will leverage the extensive work and existing processes undertaken within Nektar++ to ensure sustainable software is delivered. To be specific, the resulting software will:

- use the Nektar++ build system, based on CMake, in order to be both cross-platform and offer a user-friendly and easy to build environment;
- leverage our existing continual integration platform, utilising Docker images and GitLab CI to ensure the rigorous testing of the developed software;
- similarly, leverage the continuous delivery mechanism of Nektar++ to support automatic generation of Docker containers of latest developments;
- maintain performance portability is addressed through platform-specific kernels and support for multiple compiler toolchains in the build system.

Project structure. Organisation of the project's deliverables, which we set out in the following chart, have been timed to ensure a linear progression of the project from mesh generation through to. Consideration has also been given to the requirements of other calls; for example, the generation of meshes under D1.1 has been timed to be completed by the half-way stage of the project, to enable their potential usage in e.g. call T/NA083/20.

		20/21			21/22												22/23		
	Deliverable	J	F	M	A	M	J	J	A	S	O	N	D	J	F	M	A	M	J
Task 1 (Lead: UoE)	D1.1				█	█	█	█	█	█									
	D1.2										█	█	█	█	█	█			
	D1.3	█	█	█															
	D1.4																█	█	
Task 2 (Lead: ICL)	D2.1							█	█	█									
	D2.2								█	█	█								
	D2.3										█	█	█	█	█	█			
	D2.4																█	█	█
Task 3 (UoE/ICL)	D3.1												█	█	█				
	D3.2						█	█	█	█	█	█	█	█	█				
	D3.3																█		

Personnel. The work to be undertaken in this project will be supported through two PDRAs: PDRA1 will be based in the Department of Engineering at the University of Exeter, employed from 02/20 (to allow sufficient time for recruitment) until the end of the project. They will be supervised by Dr. David Moxey, who will also coordinate the project as PI. Primarily, PDRA1 will focus on the development of mesh generation (task 1). They will also coordinate with PDRA2 on solver aspects under task 2 as required. PDRA2 will be based in the Department of Aeronautics at Imperial College London. They will be supervised by Dr. Chris Cantwell and Prof. Spencer Sherwin, where they will focus on developing the flexible proxyapp/kernels under task 2, in collaboration with PDRA1 as appropriate. PDRA1 and PDRA2 will both assist in coordination efforts under task 3.

Coordination efforts and travel. In light of the ongoing coronavirus pandemic, the initial stages of the project will be coordinated via regular online meetings, both for internal project meetings between the investigators/PDRAs, as well as with UKAEA and other winning bidders of related calls where appropriate. Although the restrictions to travel imposed by Covid-19 are likely to endure for some time into the project, we hope for (and anticipate) the ability to conduct some in-person collaboration in FY 21/22.

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
Task/deliverable 2.4 will leverage developments from the winners of call T/NA084/20 on preconditioning. Should this input not be possible or should the task be delayed, we will leverage our previous experience on the development of preconditioning approaches for fluid dynamics systems.	T/NA084/20	Preconditioning
Tasks/deliverables 3.1 & 3.3 will rely on input from other work packages; primarily we believe from the winners of call T/NA083/20 on fluid-referent models. Should input from these bidders not be possible, we will aim to demonstrate the potential of our developments using the proxyapp developed in task 2.	T/NA083/20	Other proxyapp development

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.

	Activity No	1
Activity: Task 1: Curvilinear mesh generation **Assignee:** PDRA1 / David Moxey (DM)		
Objective 1: Enable the generation of 2D tokamak edge geometries with quadrilateral meshes.		

Objective 2: Ensure that surface mesh generation is accurate for required simulations. Objective 3: Software development to enable workflow integration & widespread usage of NekMesh.		
Key Deliverables: **Deliverables D1.1, D1.2, D1.3 and D1.4.**	**Start and Completion date:** **D1.1: 01/04/21 - 30/09/21** **D1.2: 01/10/21 - 31/03/22** **D1.3: 04/01/21 - 31/03/21** **D1.4: 01/04/22 - 30/06/22**	**Assignee:** **PDRA1 will lead with support from DM.**
Milestones towards deliverables: Reporting via call requirements.	**Completion date:** As above.	**Assignee:** As above.

	Activity No	2
Activity: Task 2: Developing flexible and performance portable proxyapps **Assignee: PDRA2 / Chris Cantwell (CC) & Spencer Sherwin (SJS)**		
Objective 1: Implementation and validation of baseline x86 proxy-app for anisotropic 2D heat transport **Objective 2:** Matrix-free anisotropic Laplacian kernel for ARM/GPU **Objective 3:** Consideration of preconditioning for highly anisotropic systems		
Key Deliverables: **Deliverables D2.1, D2.2, D2.3 and D2.4.**	**Start and Completion date:** **D2.1: 01/07/21 - 31/08/21** **D2.2: 01/08/21 - 31/10/21** **D2.3: 01/10/21 - 31/03/22** **D2.4: 01/04/22 - 30/06/22**	**Assignee:** **PDRA2 will lead with support from CC & SJS.**
Milestones towards deliverables: Reporting via call requirements.	**Completion date:** As above.	**Assignee:** As above.

	Activity No	3
Activity: Task 3: Engagement with NEPTUNE partners and the broader proxyapp ecosystem **Assignee: PDRAs & investigators (DM, CC, SJS)**		
Objective 1: Coupling with other proxyapps. **Objective 2:** Production of training materials for tasks 1 and 2. **Objective 3:** Coordination efforts (e.g. workshop or seminar) to engage with other work package coordinators and UKAEA.		
Key Deliverables: **Deliverables D3.1, D3.2 and D3.3.**	**Start and Completion date:** **D3.1: 01/01/22 - 31/03/22** **D3.2: 01/08/21 - 31/01/22** **D3.3: 01/05/22 - 30/06/22**	**Assignee:** **PDRA1 will lead D3.2 and D3.3 with support from DM. PDRA2 will lead D3.1 with support from CC/SJS.**
Milestones towards deliverables: Reporting via call requirements.	**Completion date:** As above.	**Assignee:** As above.

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)
David Moxey	Dr	University of Exeter	PI	Overall project coordination, supervision of PDRA1 under tasks 1/2		
Chris Cantwell	Dr	Imperial College London	Co-I	Supervision of PDRA2 under tasks 2/3		
Spencer Sherwin	Prof	Imperial College London	Co-I	Supervision of PDRA2 under tasks 2/3		
PDRA1	-	University of Exeter	PDRA	Task 1 + 3		
PDRA2	-	Imperial College London	PDRA	Task 2 + 3		