Name of Bidding Organisation:	UKRI Science and Technology Facilities Council
Contract Title:	HT03467 NA084 Matrix-Preconditioning

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.

At the heart of the NEPTUNE Programme is the solution of coupled partial differential equations (PDEs) that exhibit challenging properties when trying to solve them. Following discretisation of the PDE, a large linear system ***Ax=b*** must be solved or a series of large linear systems: the size of the systems to be solved mean that iterative methods are preferable over direct factorisation methods but, without preconditioning to improve rate of convergence, the number of iterations needed to solve the system is too large and it is necessary to stop the iterative process before the required levels of accuracy are met. This loss in accuracy can have a detrimental effect on the convergence properties of any overarching iterative methods that are, for example, dealing with the non-linearity of the PDEs being solved. By using a preconditioner that is suitable for exascale computations, is relatively cheap to initialise and apply, and significantly speeds up the convergence towards the solution of ***Ax=b***, simulations should become faster to run and have improved accuracy. This allows the computational simulation of models that were previously infeasible to become feasible to run.

In the past couple of decades, a lot of research has been done with the aim of efficiently solving a range of individual partial differential equations (PDEs) for different discretisation methods. These preconditioners are often developed by considering the underlying mathematical problem being solved, for example, multigrid methods [1] [2]. The first part of our proposal involves **literature surveys** to identify the most appropriate existing preconditioners specifically designed for elliptical and hyperbolic PDEs identified within the NEPTUNE Programme. **We will collate information about their convergence properties, suitability for exascale and whether codes already exist that can be utilised within prototype tests. Consultation within the NEPTUNE collaboration will allow us to identify which PDEs to target and, following the literature survey, which of these PDE-based preconditioners are of most interest.**

There has also been a lot of development in more generalised preconditioning methods that only assume knowledge of the entries of the matrix A or the action of that matrix when multiplying the matrix with a series of vectors, for example, preconditioners based on sparse approximate inverses [8] [9] or incomplete factorisations [10] [11]. Of particular interest are Markov Chain Monte Carlo Matrix Inverse (MCMCMI) preconditioners, which are a class of sparse approximate inverse preconditioners. Alexandrov et al have shown that MCMCMI preconditioners very suitable for predicted exascale architectures and perform well [12] [13]. In particular, the MCMCMI preconditioner has been shown to be effective when reduced precision is used to form and apply the preconditioner via GPGPUs, which makes this preconditioner a cheap choice. Therefore, we will also **perform a literature and code survey on sparse approximate inverse preconditioners with a particular focus on MCMCMI preconditioners due to their expected suitability for exascale computing.**

The information from these literature and code surveys will be disseminated to other areas of the NEPTUNE Programme to help inform their decisions about numerical scheme choices, as required by this task.

When n PDEs are coupled together, as is required within the NEPTUNE Programme, the linear system will have a block-structure of the following form [3]:

$$\boldsymbol{A} = \begin{bmatrix} A_{1,1} & \cdots & A_{1,n} \\ \vdots & \ddots & \vdots \\ A_{n,1} & \cdots & A_{n,n} \end{bmatrix}, \tag{1}$$

where $A_{i,i}$ represents the discretisation of the *i*-th PDE and $A_{i,j}$ $(i \neq j)$ couple the *i*-th and *j*-th PDEs. As observed within the SD1D example, which uses BOUT++ [4], a simple yet effective preconditioner for a single PDE can be no longer effective when coupling is introduced and, hence, other tactics are required. Thorne (née Dollar) has extensive experience in designing, analysing and implementing preconditioners for block-structured systems, in particular, designing highly effective implicit-factorisation preconditioners [5] [6], which were very successfully used when some of the sub-blocks were discretisations of PDEs and the overall preconditioner incorporated known preconditioners for these PDEs [7]. **These implicit-factorisation preconditioners are related to the block-factorisation approach proposed by Ferronato *et al* [3] and, by combining these approaches, we will aim to form preconditioners that significantly improve the convergence of the iterative method being used to solve the system but are also relatively cheap to initialise. We will ensure that our implicit-factorisation preconditioning framework will allow us to precondition both close-coupled and loose-coupled problems.** It may also allow us to use reduced-subspace iterative methods based on iterative methods that are not immediately considered suitable for applying to (1) but have superior properties [5] [6]. **This approach will allow the Programme to solve the coupled systems in a manner suggested by the underlying physics and meets the associated task package objective.**

We will compare at least two classes of preconditioners for non-coupled problems: SPAI preconditioners and PDE-based preconditioners. For coupled problems, we will form MCMCMI preconditioners for the whole of $\boldsymbol{A}$, and also use produce a hybrid method where the MCMCMI preconditioners are used within the sub-blocks of our proposed implicit-factorisation preconditioners: these preconditioners will be compared with the implicit-factorisation preconditioners that feature PDE-based preconditioners. **Hence, we will be comparing at least three different preconditioning approaches for coupled problems and will compare the differences with regards whether the problem is close-coupled or weak-coupled.** Due to the complex nature of the coupled problems within the NEPTUNE Programme, this comparison will help us understand whether PDE-based preconditioners are required, which could require a different preconditioner for each PDE, or if a more generalised preconditioner can be used. If the latter is possible, then this will simplify the task of developing preconditioners for more complex coupled problems. **By drawing together the results from our literature and code surveys, implicit-factorisation preconditioner design (theoretical and exascale considerations), and numerical tests, we will be able to categorise the suitability of different approaches with regards to robustness, efficiency, suitability with respect to predicted exascale computing architectures, and how quickly they can be developed within the NEPTUNE Programme. This will then be used to provide our recommendations and, hence, the final outcome of this project will guide the Programme in its choice of preconditioner implementations within its proxyapp developments, which completes the overall objective for this NEPTUNE Task.**

References

[1] U. Trottenberg, C. W. Oosterlee and A. Schuller, Multigrid, Elsevier, 2000.

[2] Y. Shapira, “Matrix-Based Multigrid for Locally Refined Meshes,” in *Matrix-Based Multigrid*, Springer, 2003, pp. 133-166.

[3] M. Ferronato, A. Franceschini, C. Janna, N. Castelletto and H. A. Tchelepi, “A general preconditioning framework for coupled multiphysics problems with application to contact-and poro-mechanics,” *Journal of Computational Physics,* vol. 398, p. 108887, 2019.

[4] B. D. Dudson, M. V. Umansky, X. Q. Xu, P. B. Snyder and H. R. Wilson, “BOUT++: A framework for parallel plasma fluid simulations,” *Computer Physics Communications,* vol. 180, no. 9, pp. 1467-1480, 2009.

[5] H. S. Dollar, N. I. M. Gould, W. H. A. Schilders and A. J. Wathen, “Implicit-Factorization Preconditioning and Iterative Solvers for Regularized Saddle-Point Systems,” *SIAM Journal on Matrix Analysis and Applications,* vol. 28, no. 1, pp. 170-189, 2006.

[6] H. S. Dollar, N. I. Gould and A. J. Wathen, “On implicit-factorization constraint preconditioners,” *Large-scale nonlinear optimization,* pp. 61-82, 2006.

[7] T. Rees, H. S. Dollar and A. J. Wathen, “Optimal Solvers for PDE-Constrained Optimization,” *SIAM Journal on Scientific Computing,* vol. 32, no. 1, pp. 271-298, 2010.

[8] J. D. F. Cosgrove, J. C. Diaz and A. Griewank., “Approximate inverse preconditionings for sparse linear systems,” *International journal of computer mathematics,* vol. 44, no. 1-4, pp. 91-110, 1992.

[9] H. Anzt, T. K. Huckle, J. Bräckle and J. Dongarra, “Incomplete sparse approximate inverses for parallel preconditioning,” *Parallel Computing,* vol. 71, pp. 1-22, 2018.

[10] D. S. Kershaw, “The incomplete Cholesky—conjugate gradient method for the iterative solution of systems of linear equations,” *Journal of Computational Physics,* vol. 26, no. 1, pp. 43-65, 1978.

[11] J. D. Booth, K. Kim and S. Rajamanickam, “A comparison of high-level programming choices for incomplete sparse factorization across different architectures,” in *2016 IEEE International Parallel and Distributed Processing Symposium Workshops (IPDPSW)*, 2016.

[12] A. Lebedev and V. Alexandrov, “On Advanced Monte Carlo Methods for Linear Algebra on Advanced Accelerator Architectures,” in *2018 IEEE/ACM 9th Workshop on Latest Advances in Scalable Algorithms for Large-Scale Systems (scalA)*, 2018.

[13] M. E. Şahin, A. Lebedev and V. Alexandrov, “Empirical Analysis of Stochastic Methods of Linear Algebra,” in *nternational Conference on Computational Science*, 2020.

3 Scope

3.1 Key Deliverables and/or Desired Outcomes

A. Report: Literature survey of preconditioning approaches for elliptic problems, which are based on the underlying mathematical structure of the PDEs being solved and discretisation method. Information of gathered within the survey will include: theoretical convergence results for applicable iterative methods; cost of setting-up the preconditioner and executing the preconditioner; suitability of the preconditioner for Exascale computation; availability of existing codes.

B. Report: Literature survey of preconditioning approaches for hyperbolic problems, which are based on the underlying mathematical structure of the PDEs being solved and discretisation method. Information of gathered within the survey will include: theoretical convergence results for applicable iterative methods; cost of setting-up the preconditioner and executing the preconditioner; suitability of the preconditioner for Exascale computation; availability of existing codes.

C. Report: Literature survey of preconditioning approaches based on sparse approximate inverses, in particular, focussing on Markov Chain Monte Carlo approximate inverses. These are already being developed with exascale architecture consideration [12] [13] and use the entries of the matrix **A** to compute a preconditioner with no prior knowledge of the underlying mathematical problem. Information of gathered within the survey will include: theoretical convergence results for applicable iterative methods; cost of setting-up the preconditioner and executing the preconditioner; suitability of the preconditioner for Exascale computation; availability of existing codes.

D. Report: For both close-coupled problems and weak-coupled problems, the development of suitable implicit-factorisation preconditioners and reduced subspace iterative methods building on the work of Thorne [5] [6] [7] and Ferronato *et al* [3]. These implicit-factorisation preconditioners will be able to incorporate the preconditioners identified from our literature surveys. Theoretical convergence results will be developed.

E. Report and Prototype Code: Following consultation with the consortia, tests will be performed to solve selected close-coupled problems through the development of a prototype test code. Comparisons will be made between the use of block/implicit factorisation preconditioners and applying the Markov Chain Monte Carlo approximate inverse preconditioner to the whole system, as well as with weak-coupled versions of the problems. From this, recommendations will be made to allow deferred implementations to be facilitated within the next stage of the NEPTUNE Programme. *Note: the reports for D and E may be combined into 1 report*.

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)

- Development of proxyapp implementation of preconditioners that have been identified as promising. This is something that we would like to do but is out of scope due to the timescales.
- Comparison of all combinations of promising preconditioners from the literature surveys [ADD]

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.

- The available funding limits the amount time that can be devoted to this project, so it will be important to restrict the comparison to the higher priority coupled and non-coupled problems.

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.

Project Delivery Groups are responsible for developing and delivering the individual projects under each of the different programmes and funding streams. This includes identifying and mitigating potential risks; resolving issues within the remit of the project; developing detailed implementation plans and taking day-to-day responsibility for implementation of the project against the agreed scope once approved.
STFC project management is broadly based around the Association for Project Management, however the Hartree Centre's approach to project delivery additionally aims to combine the flexibility and responsiveness of AGILE with the governance of PRINCE2 when deemed appropriate for the type of project. The Hartree Centre is ISO 9001 accredited,

by demonstrating the ability to successfully complete projects and consistently meet customer and regulatory requirements. The key principles relating to the delivery of projects are:

- All individual projects complete internal management reviews and the 'Quality at Entry' (QaE) process before being submitted for Management Board approval.
- Projects that the Management Board feel warrant a more cautious approval process must include subsequent Decision Reviews at agreed points to assess the ongoing feasibility of the project with a Go/No-Go decision.
- Once approved, projects will be managed on a day to day basis by exception by an appropriate PMO representative and/or Programme Manager.
- Prioritisation and effort will be applied to ensuring the delivery of requirements, outputs, and acceptance criteria using the MoSCoW1 technique.
- Progress and success will usually be measured by completion of outputs rather than the completion of individual tasks.
- Each project must confirm the minimum acceptable outcomes (MUSTs) the project will deliver at the point of approval. These will form the minimum base line for project outcomes.
- Any change in 'Must have' requirements, timescales or budgets after a project has been approved will trigger an exception and must be approved by the Management Board via the Hartree Centre's Change Control process.
- The Operations board can approve changes to "Should have" requirements providing they are within the tolerance boundaries set for time and budget.
- The Project Manager can include or de-scope 'Could have' requirements as long as they are within the base lines set for time and budget.
- Any tolerances for budget, time and quality (Outcomes) will be defined and agreed for each project during the approval phase. Tolerances will be agreed at project approval stage and may only be changed by submission of a change request to the Management Board.
- Projects will review progress regularly and report progress or exceptions to the Operations Board at minimum on a monthly basis.

Customer updates and progress reports will be agreed as part of the project planning phase and will be completed as a minimum on a monthly basis.

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
Test matrices and right-hand sides to test preconditioners. This could be in the form of individual test matrices or codes that generate these matrices	UKAEA	Test matrices and right-hand sides for non-coupled and coupled problems
Interaction with project partners for prioritisation of PDEs	UKAEA	PDE prioritisation list

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.

<table>
<tr><td colspan="2" align="right">Activity No</td><td>1</td></tr>
<tr><td colspan="3"></td></tr>
<tr><td colspan="3"><u>Activity:</u>
Literature survey: preconditioners for elliptic PDEs from fusion modelling
<u>Assignee:</u> Sue Thorne</td></tr>
<tr><td colspan="3"><u>Objective 1:</u> Identify key elliptic PDEs for fusion modelling and proposed discretisation methods
<u>Objective 2:</u> Perform literature and code surveys to find preconditioners for the identified elliptic PDEs and their discretisations.
<u>Objective 3:</u> Catalogue each preconditioner in a report, recording theoretical convergence results for applicable iterative methods; cost of setting-up the preconditioner and executing the preconditioner; suitability of the preconditioner for Exascale computation; availability of existing codes.</td></tr>
<tr><td><u>Key Deliverables:</u>

D1.1) Report cataloguing preconditioners and codes for prioritised elliptic PDEs and associated discretisation methods</td><td><u>Start and Completion date:</u>

1) 04/01/2021-26/02/2021</td><td><u>Assignee:</u>

1) Sahin & Thorne</td></tr>
<tr><td><u>Milestones towards deliverables:</u>

M1.1) Prioritisation of elliptic PDEs and discretisation methods
M1.2) Complete literature and code survey for preconditioners applicable to prioritised elliptic PDEs and associated discretisation methods</td><td><u>Completion date:</u>

1) 20/01/2021
2) 19/02/2021</td><td><u>Assignee:</u>

1) Sahin & Thorne
2) Sahin</td></tr>
</table>

<table>
<tr><td align="right">Activity No</td><td>2</td></tr>
<tr><td colspan="2"></td></tr>
<tr><td colspan="2"><u>Activity:</u>
Literature survey: preconditioners for hyperbolic PDEs from fusion modelling
<u>Assignee:</u> Sue Thorne</td></tr>
<tr><td colspan="2"><u>Objective 1:</u> Identify key hyperbolic PDEs for fusion modelling and proposed discretisation methods
<u>Objective 2:</u> Perform literature search to find preconditioners for the identified hyperbolic PDEs and their discretisations.
<u>Objective 3:</u> Catalogue each preconditioner in a report, recording theoretical convergence results for</td></tr>
</table>

applicable iterative methods; cost of setting-up the preconditioner and executing the preconditioner; suitability of the preconditioner for Exascale computation; availability of existing codes.

Key Deliverables:	**Start and Completion date:**	**Assignee:**
D2.1) Report cataloguing preconditioners and codes for prioritised hyperbolic PDEs and associated discretisation methods	**1)** 04/01/2021-26/02/2021	**1)** Sahin & Thorne
Milestones towards deliverables:	**Completion date:**	**Assignee:**
M2.1) Prioritisation of hyperbolic PDEs and discretisation methods **M2.2)** Complete literature and code survey for preconditioners applicable to prioritised hyperbolic PDEs and associated discretisation methods	**1)** 20/01/2021 **2)** 19/02/2021	**1)** Sahin & Thorne **2)** Sahin

Activity No	3
Activity: Literature survey: sparse approximate inverse (SPAI) preconditioners **Assignee:** Sue Thorne	
Objective 1: Perform literature search to identify classes of sparse approximate inverses **Objective 2:** Catalogue each preconditioner in a report, recording theoretical convergence results for applicable iterative methods; cost of setting-up the preconditioner and executing the preconditioner; suitability of the preconditioner for Exascale computation; availability of existing codes. Particularly focus on MCMCMI Preconditioners.	

Key Deliverables:	**Start and Completion date:**	**Assignee:**
D3.1) Report cataloguing SPAI preconditioners and codes	**1)** 09/02/2021-05/03/2021	**1)** Alexandrov, Sahin & Thorne
Milestones towards deliverables:	**Completion date:**	**Assignee:**
M3.1) Complete literature and code survey for SPAI preconditioners	**1)** 26/02/2021	**1)** Sahin

Activity No	4
Activity: Theoretical development of implicit-factorisation preconditioners for coupled problems **Assignee:** Thorne	

Objective 1: Understand the differences, in general, between the problem set-up for loosely-coupled and strongly-coupled problems from NEPTUNE. This will be key to developing appropriate implicit-factorization/block-based preconditioners. **Objective 2:** Develop implicit-factorization preconditioners and any associated convergence properties for inclusion in Key Deliverable from Activity 5.

Key Deliverables:	**Start and Completion date:**	**Assignee:**
D4.1) Section on implicit-factorisation preconditioners for inclusion in Activity 6's report or separate report	**1)** 08/03/2021-31/03/2021	**1)** Sahin & Thorne
Milestones towards deliverables:	**Completion date:**	**Assignee:**
M4.1) Set of proposed implicit-factorisation preconditioners and initial theoretical results	**1)** 20/03/2021	**1)** Sahin &Thorne

	Activity No	**5**
Activity: Development of prototype code: implicit-factorisation preconditioners for coupled problems **Assignee:** Thorne		
Objective 1: Develop prototype code for proposed implicit-factorisation preconditioners including documentation for code		
Key Deliverables: **D5.1)** Prototype code **D5.2)** Documentation including readme file, installation documentation and simple user documentation	**Start and Completion date:** **1)** 01/04/2021-31/07/2021 **2)** 01/04/2021-31/07/2021	**Assignee:** **1)** Sahin **2)** Sahin
Milestones towards deliverables: **M5.1)** Prototype code for loosely & strongly coupled problems (Version 1) **M5.2)** Prototype code and documentation for loosely & strongly coupled problems (Final version)	**Completion date:** **1)** 07/05/2021 **2)** 31/07/2021	**Assignee:** **1)** Sahin & Thorne **2)** Sahin

	Activity No	6

Activity:
Comparison of preconditioners for fusion modelling
Assignee: Thorne

Objective 1: Comparison of preconditioners for non-coupled elliptic and hyperbolic problems from NEPTUNE Programme. Comparison will include scalability results for each preconditioner, preconditioner set-up times, preconditioner execution time for single application of preconditioner to vector, number of iterations for chosen iterative method and time to solution.
Objective 2: Comparison of preconditioners for coupled elliptic and/or hyperbolic problems from NEPTUNE Programme to understand effective of proposed approaches: SPAI-based preconditioner to be applied to whole system assuming no knowledge of block structure; implicit-factorization based preconditioner incorporating PDE-based preconditioner; implicit-factorization based preconditioner incorporating SPAI-based preconditioner. Comparison will include scalability results for each preconditioner, preconditioner set-up times, preconditioner execution time for single application of preconditioner to vector, number of iterations for chosen iterative method and time to solution.
Objective 3: Use comparison data to provide recommendations as to which preconditioners should be incorporated into the proxyapps being developed as part of the NEPTUNE programme.

Key Deliverables:	Start and Completion date:	Assignee:
D6.1) Test code(s) for preconditioner comparisons	**1)** 11/05/2021-31/07/2021	**1)** Sahin
D6.2) Data from preconditioner comparison tests for non-coupled problems	**2)** 11/05/2021-04/06/2021	**2)** Sahin & Thorne
D6.3) Data from preconditioner comparison tests for coupled problems	**3)** 24/05/2021-09/07/2021	**3)** Sahin & Thorne
D6.4) Report containing data analysis and recommendations	**4)** 11/05/2021-31/07/2021	**4)** Alexandrov, Sahin & Thorne

Milestones towards deliverables:	Completion date:	Assignee:
M6.1) Test code(s) & documentation for preconditioner comparison (Version 1) finished and added to repository	**1)** 21/05/2021	**1)** Sahin
M6.2) Creation of non-coupled test set and added to repository	**2)** 21/05/2021	**2)** Sahin & Thorne
M6.3) All data from non-coupled test runs added to repository	**3)** 04/06/2021	**3)** Sahin
M6.4) Creation of coupled test set and added to repository	**4)** 11/06/2021	**4)** Sahin & Thorne
M6.5) All data from coupled test runs added to repository	**5)** 09/07/2021	**5)** Sahin
M6.6) Test code(s) for preconditioner comparison (Final Version) finished and added to repository	**6)** 31/07/2021	**6)** Sahin