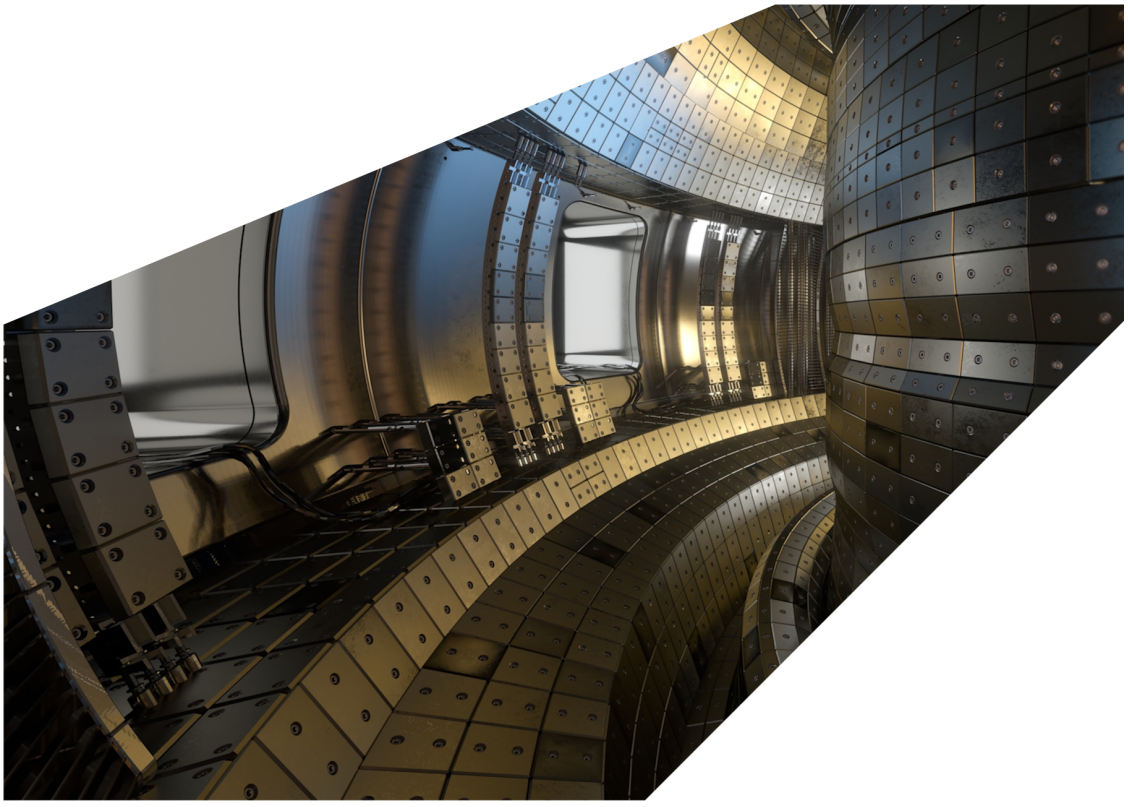
UK Atomic Energy Authority

ExCALIBUR

Identification of suitable preconditioner techniques

M2.7.1

Abstract
The report describes work for ExCALIBUR project NEPTUNE at Milestone 2.7.1. Minutes of meeting to form report on technical progress.



UKAEA REFERENCE AND APPROVAL SHEET

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Project Name: ExCALIBUR Fusion Modelling System		

	Name and Department	Signature	Date
Prepared By:	Ed Threlfall Wayne Arter BD	N/A N/A	April 27, 2021 April 27, 2021
Reviewed By:	Rob Akers Advanced Computing Dept. Manager		April 27, 2021
Approved By:	Rob Akers Advanced Computing Dept. Manager		April 27, 2021

1 NEPTUNE Meeting: 22 April 2021 10.15-10.45am BST

Present

- Chair: Wayne Arter, UKAEA
- Ed Threlfall, UKAEA
- Vassil Alexandrov, STFC
- Sue Thorne, STFC

2 Minutes

WA presented the agenda: to go through the most recent report received from STFC, to discuss STFC's work since the submission of that report, and to conclude with a general discussion about proposed work going forward. The '01' report [1] was not discussed.

WA thanked ST and VA for their most recent '02' report [2], noting that this meeting included only two of the four authors named on the report. WA praised the report as a useful introduction, then noted that it was useful to have received also the LaTeX source which allows UKAEA to make minor notational corrections. WA had a slight issue with some of the syntax in the report, taken from a textbook to which he had no access (something like $diag(\mathcal{L}_x(\phi))$, with the confusion being that the diagonal of the matrix would be zero for a centred-difference scheme. However, WA requested no changes to the report. Another question WA had concerned S.3.4, which mentioned other libraries of interest but which did not include direct sparse solvers. ST answered that this section was concerned only with preconditioners and iterative methods - not direct solvers. WA said he was not very familiar with direct solver libraries and asked whether ST was proposing to use them as part of a preconditioner; ST replied that she was not, but noted that direct solvers could be applied to preconditioner sub-blocks (note Jack Dongarra list *does* include direct solvers); though indicated that the sub-blocks are probably too large for direct methods to be useful. WA concurred - he had expected this to the the case - though noted that there was historically a commercial direct-solver electromagnetism code (and cited the then-lack of understanding of preconditioners for the high-frequency Helmholtz problem). ST noted that MUMPS can be used directly or for preconditioning (incomplete factorization). WA concluded this discussion by again commending the report.

WA moved on to a discussion of work performed since the submission of the report; ST confirmed that work had continued. WA asked whether STFC planned to consider stochastic/Monte Carlo methods; ST and VA replied in the affirmative. ST described current work as having two phases:

1. Examining integration of preconditioners with BOUT++ and NEKTAR++ (Emre Sahin has been in contact with David Moxey re. the latter code, though this work has been delayed by unavoidable circumstance); the aim is to interface a MCMCMI (Markov Chain Monte Carlo Matrix Inversion) preconditioner acting on the entire matrix; and

2. work on blocking, for which ST has developed new theory for a class of 'non-symmetric constraint preconditioners' (her term) aimed at clustering eigenvalues, also trying different families of block factorizations for efficient generation of preconditioners. ST is currently working on narrowing down the factorizations to the most useful ones.

WA acknowledged the challenge of the problem including hyperbolics, than agreed that the direction of current work was promising.

WA asked whether there was anything else to discuss - ST and VA explained that their co-workers Anton Lebedev and Emre Sahin were stuck on other projects, so they intend to onboard a new person formerly of Manchester and prior to that Jack Dongarra's group (and who has worked with Anton/Emre in the past). WA acknowledged that the shortness of this project was a potential issue and also that the Manchester group was very strong (and that UKAEA had tried to entice them onto NEPTUNE , though there will be future opportunity to do so). ST noted the advantage of having a flexible team of people at the Hartree Centre.

WA steered the discussion to work going forward. ST is working on interfaces for BOUT++ and NEKTAR++ and implementing preconditioning for the core test problems supplied by Ben Dudson. ST plans also to test multigrid methods against stochastic / Monte Carlo. WA confirmed that it was acceptable for STFC to abandon any directions they judged to be of less promise (eg. direct solvers). ST confirmed this, noting that the future direction toward matrix-free implementations was likely to favour hybrid stochastic methods and not direct solvers. WA asked what experience STFC had in domain decomposition methods; ST replied that she personally had more of a background in nested linear algebra techniques, citing her work with Jennifer Scott in the computational mathematics group. Others at STFC have implemented a domain decomposition load balancing for OPENFOAM with new domain decomposition algorithms that showed much promise. VA reminded WA that STFC are finalizing an agreement with UKAEA (via Rob Akers) which will allow for wide-ranging future collaboration.

WA explained that a major concern of NEPTUNE is coupling continuum (3-D/5-D) to particle representations: he is interested in any insights for handling these mixed representations (domain decomposition is relevant in this context). ST replied that she has worked on a project involving coupling and that one concern was whether to use an off-the-shelf or an in-house coupler; somebody she knew (Philipa) has worked on coupling fluids / particles. WA replied that UKAEA had examined off-the-shelf options and that nothing had stood out; he also made the point that UKAEA's theorists were very busy. ST opined that our problem probably required a 'niche' coupling solution. WA made the point about there being a lack of coherent theory regarding overlap regions for the different representations (eg. size of overlaps or convergence properties) and again cited domain decomposition as a related area; there is potential for future discussion in this direction.

WA asked whether ST or VA had any questions. The reply was largely in the negative; ST reiterated that she is endeavouring to link to other parts of the NEPTUNE project. There was a brief discussion of STFC and UKAEA plans to return to office working (of some sort) prior to WA closing the meeting.

Acknowledgement

The support of the UK Meteorological Office and Strategic Priorities Fund is acknowledged.

References

[1] S. Thorne. Priority Equations and Test Cases. Technical Report 2047353-TN-01, UKAEA Project Neptune, 2021.

[2] V. Alexandrov, A. Lebedev, E. Sahin, and S. Thorne. Linear systems of equations and preconditioners relating to the NEPTUNE Programme: A brief overview. Technical Report 2047353-TN-02, UKAEA Project Neptune, 2021.