

**ExCALIBUR   
  
NEPTUNE: Report on Y1 2019 Internal Workshop  
  
Towards Milestone M1.1.1a**

**Abstract**

This report summaries the Y1 2019 UKAEA internal workshop, as part of the ExCALIBUR NEPTUNE Y1 Requirements Capture activity.

**UKAEA REFERENCE AND APPROVAL SHEET**

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# Introduction

As part of the ExCALIBUR NEPTUNE Y1 Requirements Capture (under Activity 1), an internal workshop was organized within the UKAEA. The aim of this workshop was to kickstart the Requirements Capture exercise of the Fusion Modelling System Use Case as outlined in Science Plan CD/EXCALIBUR-FMS/0001. This internal workshop was designed to be followed by an external workshop in February 2020 that would include participants from across the UKAEA, including those outside of the magnetic fusion community but who possess valuable skills and knowledge relevant to the project. This internal workshop only included UKAEA staff, covering a wide range of specialities such as physics, engineering and software development. Attendees were selected to ensure that a broad range of potential users are part of the co-design of the system.

The full day workshop had a twofold goal of requirements capture from real users/developers of magnetic fusion codes as well as to inform this user community around the planned outcomes of the NEPTUNE project. The workshop was held at Culham Science Centre and comprised eight presentations, each being followed by extensive discussions. There were also intermittent breaks to encourage dialogue.

# Presentations session

This section presents short summaries of the workshop presentations, the full presentations can be made available to the ExCALIBUR board / Met Office upon request. A brief summary of each is given below.

### **P1. ExCALIBUR: Exascale Computing Algorithms & Infrastructures Benefitting UK Research – Overview**

Presenter: R. Akers

This presentation described briefly the objectives of the ExCALIBUR project, its overarching goals, high level organisation and governance and outlined the place of NEPTUNE within this structure. The presentation outlineed the physics case from the draft Science Plan that is the focus of project NEPTUNE. The funding available was discussed, together with an activities straw person plan (which would later become the Activity Plan for Y1-2).

**P2. Strategy and development of the European Edge Code**

Presenter: Fulvio Millitello

This presentation described the European Boundary Code (EBC) – a project running in parallel with NEPTUNE but funded by EUROFusion as part of European Theory and Advanced Simulations Coordination TSVV E-TASC programme. The EBC project (in which UKAEA is heavily involved) aims to create a code on a short timescale that will simulate the edge of the plasma, in line with the long term goal of the NEPTUNE project. The main problems in plasma physics being investigated in E-TASC and the methods pursued were specified along with possible synergies with other projects.

**P3. Computational physics and engineering for fusion at Exascale**

Presenter: W. Arter

This presentation underlined some of the numerical modelling challenges raised by the tokamak first wall geometry and edge physics. Candidate numerical schemes were discussed.

**P4. Productive HPC software**

Presenter: J. Cook

This presentation listed some of the work done by the Research Software Engineers at Culham. Some of the challenges faced by them were described which would most likely have to be addressed as part of NEPTUNE. Neptune may also benefit from UKAEA RSE resources where a lot of issues in simulating edge plasma physics are already being investigated.

**P5. Common Obstructions to Effective Simulation**

Presenter: C. Jones

This presentation, based upon an “engineer’s” view (as a primary user of the infrastructure) listed the challenges faced in simulations involved in fusion engineering. Issues such as discontinuities, transients as well as time dependence were described. The fact that magnetic fusion is a multi-physics problem was highlighted. This talk gave a great insight into long term software requirements for the platform.

**P6. Excalibur – the Physics challenges**

Presenter: D. Samaddar

This presentation described the challenges of tokamak boundary simulations along with a brief review of an existing literature review to date.  This information at a later date, combined with information from the Feb 5th open workshop in Birmingham would feed in to the overall NEPTUNE system requirements. The plasma edge is a particularly difficult part of the tokamak to simulate, given the many different and competing physics processes combined with many plasma, impurity and neutral particle species, and widely varying length and timescales.

**P7. Requirements engineering and elements of design for NEPTUNE**

Presenter: L. Anton

This presentation went into some detail around the Software Engineering challenges for Computational Science and Engineering (CSE) codes in the NEPTUNE class. As the complexity of CSE codes increases, modern software engineering methods are needed to provide CSE software with adequate performance, portability, maintainability, capability, extensibility and reliability in sustainable way. The current literature emphasizes a need for a detailed requirements capture process and subsequent in depth analysis for a successful project. A rational design approach based upon standardized software requirements specification was proposed for NEPTUNE and discussed at length.

Elements of software design at three abstraction levels: front end, middle layer and back end were presented. For each of them we need to collaborate with the community to find the best available solutions for performance portability, scalable implementation of models, data management and user programming frameworks.

**P8. An Exascale optimised storage system**

Presenter: S. de Witt

This presentation primarily described big data management and object storage by optimizing novel hardware which were parts of two H2020 projects called SAGE and SAGE2 (led by Seagate). Although the SAGE projects at face value seem unrelated to the proposed Y1 and Y2 activities of NEPTUNE, the outcome of both projects can be synergized in the long term to maximize use of exascale computing. Caution was urged around the potential I/O bottlenecks that will likely be encountered at the Exascale (we know for example that codes based upon the Nektar++ library are typically I/O limited).

1. **Summary and Concluding remarks**

The attendees at the internal workshop were all from UKAEA. There were representations from various departments including physics, engineering and software development. Although four presentations were directly related to NEPTUNE (it’s project plan, physics, algorithms and software), the presentations covered a wide range of topics. Some of the talks reported issues and findings in other parallel projects – which might contribute to steer the direction of NEPTUNE. Moreover, the meeting with the wide range of experts with some of them being potential users of codes generated by NEPTUNE and others offering resources that may contribute to the success of NEPTUNE was very motivating and formed a string basis for the design of the Activity Y1-2 straw person plan and the subsequent Feb 5th Open Workshop. This internal workshop also helped achieve the aim of informing the fusion community within UKAEA around the scope and ambition of the ExCALIBUR project.

1. **Annexe**

**Excalibur UKAEA Internal Workshop**

* Location: Phoenix Room
* Date: 10:00 to 16:00 - 16 December 2019

**Agenda:**

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| --- | --- |
| 10:00 – 10:30 | R. Akers - *ExCALIBUR: Exascale Computing Algorithms & Infrastructures Benefitting UK Research – Overview* |
| 10:30 – 11:00 | F. Militello - *Strategy and development of the European Edge Code* |
| 11:00 – 11:30 | Coffee / tea |
| 11:30 – 12:00 | W. Arter - *Computational physics and engineering for fusion at Exascale* |
| 12:00 – 12:15 | J. Cook - *Productive HPC software* |
| 12:15 – 13:00 | Lunch (on your own) |
| 13:00 – 13:15 | Coffee/tea |
| 13:15 – 13:45 | C. Jones - *Common Obstructions to Effective Simulation* |
| 13:45 – 14:15 | D. Samaddar – *Excalibur – the Physics challenges* |
| 14:15 – 14:45 | L. Anton - *Requirements engineering and elements of design for NEPTUNE* |
| 14:45 – 15:15 | S. de Witt: *SAGE – An Exascale optimised storage system* |