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**ExCALIBUR   
  
NEPTUNE: Report on Y1 2020 External Workshop  
  
Towards Milestone M1.1.1b (REPORT1)**

**Abstract**

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

**UKAEA REFERENCE AND APPROVAL SHEET**

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# Introduction

This report summaries the outcomes of the first “open” workshop of the ExCALIBUR NEPTUNE project (see Science Plan CD/ExCALIBUR-FMS/0001), which was held in Birmingham on 5th Feb 2020. This workshop was an important part of the Y1 Requirements Capture exercise included in Activity 1.

The workshop objective was to engage the UK academic community in order to improve NEPTUNE user and system requirements, and to present our vision for collaboration and the procedures set in place by ExCALIBUR for collaborative work. A significant effort was expended in building a straw person plan that was mature enough to engage the community, and ensure that all potential partners are fully aligned in their thinking and ambition.

The workshop lasted 1 day and was organised in two main parts. In the first part the UKAEA NEPTUNE project team gave four presentations. The first described the aims and organisation of NETPUNE and the overarching ExCALIBUR programme. It was followed by 3 short technical presentations on the three main activitiess that NEPTUNE plans to covers in Y1 and 2. More details on the presentations are in the next section of this document.

The second part of the workshop consisted of three parallel discussion sessions that were each associated with one of the three technical presentations. Specific discussion subjects for these sessions were set in the technical presentations. Attendees were also provided with a detailed pre-reading list and information, together with a redacted Y1-2 Activity Draft Plan (document CD/ExCALIBUR-FMS/0006). In each discussion session careful notes were collected by assigned colleagues from UKAEA.

The attendees included delegates from both from the academic and UKRI community (notably STFC). The full list of participants, with affiliations, is in the Annex.

# Presentations session

This section presents short summaries of the NEPTUNE team presentations. The full presentations can be made available to the ExCALIBUR board upon request.

### **P1. ExCALIBUR: NEPTUNE**

Presenter: Rob Akers

This presentation described briefly the objectives of the ExCALIBUR project, its top level organisation and the place of NEPTUNE within this structure. An outline of the physics case, as per the Science Plan CD/ExCALIBUR-FMS/0001 was also presented. The funding available for external calls, together with the Activities Draft Plan were also briefly described.

**P2. Edge Plasma Physics – some outstanding challenges**

Presenter: Debasmita Samaddar

This presentation described the challenges of tokamak boundary simulations - what has been done so far internationally and what NEPTUNE aims to achieve in order to build an actionable framework targeting Exascale class supercomputing. The tokamak plasma edge is a particularly difficult part of the fusion plasma to simulate, given the many different and competing physics processes, many plasma, impurity and neutral particle species, and widely varying length and timescales – a classic highly coupled, multi-scale, multi-physics challenge.

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

Presenter: Wayne Arter

This presentation underlined some of the numerical modelling challenges raised by the tokamak first wall geometry and edge physics. The properties required by candidate numerical schemes were discussed. The NEPTUNE team recognises the need to draw upon the experience of other computer modelling communities (many of whom were represented at the meeting), in particular to provide options for algorithms suitable for the several difficult simulation challenges in this project.

**P4. Requirements engineering and elements of design for NEPTUNE**

Presenter: Lucian Anton

This presentation went into some detail around the Software Engineering challenges for Computational Science and Engineering (CSE) codes. As the complexity of the CSE codes increases, modern software engineering methods are needed to provide CSE software with performance, portability, maintainability, capability, extensibility, reliability in a sustainable way. The current literature (which has been extensively reviewed as part of the Y1 requirements gathering exercise) emphasizes the need for a detailed system requirements and their in depth analysis for a successful project. A rational design approach based upon a standardized software requirements specification was proposed for NEPTUNE.

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 ensure effective co-design and to find the best available solutions for performance portability, scalable implementation of models, data management and user programing frameworks.

1. **Discussions session**

This section summarises the conclusion of the three parallel discussion sessions. The sessions had two parts, before and after coffee. In the first part, attendees were assigned to one of the three sessions, based upon their research profiles; in the second part, attendees were free to go to whichever session they preferred (most decided to stay with their assigned session).

The summaries that follow are based on notes taken by different UKAEA staff and therefore vary somewhat in style and detail. They inevitably include several instances of specialist fusion and computational science jargon including the names of existing codes; if explanation is required, the authors of this report can of course be approached.

## **Session 1: Physics models**

In this session the discussion was focused on the selection of the referent model for numerical implementation. At the beginning XGC (a well-known gyrokinetic code simulating the plasma edge) was analysed, the session agreed that is not an actionable code. The magnetic fusion community uses a number of gyrokinetic (GK) codes – but except for a very few such as XGC and Gkeyll, most of their simulations are restricted to the core plasma, rather than the edge plasma that is the focus of NEPTUNE.

**Fluid models:**

The discussion produced the following recommendations or points worthy of further investigation around a fluid solver referent model:

* potential for fluid/GK region matching procedure
  + identify a fluid approach with good performance for the suitable regions, which includes turbulence “consistently”
* can this fluid model also support E-TASC aims? (E-TASC is related European fusion project that UKAEA participates in – to develop the European Boundary Code)
* the project must identify suitable “intermediate” proxy apps
* and similarly identify the scope of UQ and consider at length the validation process

**Gyrokinetics:**

The discussion produced the following observations and suggestion for a GK proxyapp:

* could start with full-f, simple geometry, simple mesh, open field line region, 2D GK proxyapp to demonstrate modelling of edge region where the open magnetic field lines touch the metal surface – the divertor: establish the basic data flow
* open field lines are easier as electrostatic potential is set by sheath, closed field line region needs vorticity equation
* the session agreed there is potential to employ Gkeyll (PPPL code, RO Greg Hammett) for comparing against the hp-spectral method
* coupling to fluid models should be considered a longer term aim (certainly not in Y1 and Y2 of the project).

**Impurities:**

The discussion pointed to the need to explore suitable numerical methods to handle low plasma density, a large number of species, etc. Rob Akers (ExCALIBUR NEPTUNE PI) is scheduled to give a talk to the Atomic Physics Community at CCPQ (Atomic and Molecular Data Needs for Plasma Applications - workshop funded jointly by Collaborative Computational Projects CCPQ and CCP-Plasma 1-3 April 2020 at the Culham Centre for Fusion Energy, United Kindom). This will act as an opportunity to engage this community and prepare them for future calls around the NEPTUNE Impurity Solver.

**Neutrals:**

Typically neutral particles are not included in gyrokinetics, whereas fluid approaches treat them differently from ions. An initial exploration could be done along the following lines:

* include basic charge exchange operator in a simple GK code with simple geometry
* to consider how this affects the core, can such a code form an edge “pedestal” due to the neutrals in the open field line region carrying momentum in and out of the plasma?
* such an approach wouldn’t be the fastest way to develop a general physics model basis, but could provide a basic understanding of the theory as a deliverable.

**Atomic physics/detachment:**

Both gyrokinetic and fluid theories fail in so-called “detachment studies” due to insufficient handling of atomic/molecular reactions. The discussion concluded that further exploration is needed for the following:

* suitable numerical methods and study of what reactions are handled in current codes – mainly the EIRENE code.
* accuracy of atomic data – uncertainty in this data is guaranteed to play a key role in how actionable a future exascale edge plasma code/platform will be, so a detailed understanding of the uncertainties and how to include them through rigorous Uncertainty Quantification techniques and tools will be essential.

## **Session 2: Algorithms**

The main outcome of this session was that proxy-apps or other input could be requested via contracts from universities. However, it was recognised that not all possible topics could be covered, and that some topics were not specific to fusion/NEPTUNE and might well be provided from the UKRI call if not on the critical path for NEPTUNE. Conversations revealed that some universities have consultancy companies that could interface to academics to provide quickly a small amount of consultancy (weeks, even months depending on staff/teaching ratio).

The following topics were considered to be important:

1. Higher order mesh generation (both due to the critical 2 degree angle problem at plasma-material interface, but also because higher order methods are deemed to scale well (as identified by the US ECP CEED Programme)
2. Connected particle and fluid calculations
3. Multi-precision approaches – it was felt that these could be left until later if a "separation of concerns" methodology is adequately implemented
4. Diffusion coefficients with a very high ratio (e.g. a million) of parallel to perpendicular asymmetry
5. Time integration in problems with a wide range of timescales, implicit PIC as a challenge with/without enslavement
6. Solution of the 1D hyperbolic equation with strong sources and sinks, with spectral accuracy, perhaps comparing with chebfun solution
7. Elliptic solver issues – pre-conditioners and algebraic multigrid
8. Data compression (ubiquitous)

After identifying the most important issues, there followed a wide ranging discussion which included:

1. A long dialogue/argument around spectral element versus AMR, their pros and cons.
2. Agreement that we need to establish a “hierarchy of complexity” and start with simple mini-apps or similar (technology demonstrators? literature review?) to address individual aspects and only later (a) go up in dimensions and (b) see if different elements can be integrated together.
3. Start from Rayleigh-Benard problem and gradually add in the required complexities (WA) based upon Wilczynski et. al. reference (student supervised jointly by Fulvio Militello and Wayne Arter).
4. It is essential to have iterations with the other two groupings (plasma in particular, the equations aren’t clear!) – there would need to be compromises!
5. Origin/reduction of noise in particle treatments (a ubiquitous, well known challenge)
6. Met Office has been good at specifying problems. GungHo is good…
7. We should look at iterative approaches – including mixed/multi precision
8. Design in adjoint from the start. Basically, for solving the adjoint problem once, you can compute certain outputs for a range of parameters. Using surrogates could would make this less of an issue.
9. UQ is very important and where possible needs to be embedded from the start.
10. I/O compression will be essential for big simulations – in some cases only limited physics and engineering output will be of interest from the simulations. Can surrogate models do data compression adequately?
11. What do people know of developments in the commercial as opposed to academic sphere?
12. Can UKAEA second staff to work in/with universities? – We would certainly like to as this would certainly aid co-design; we are currently focusing upon building an internal core team however.
13. Can we draw upon other funding (e.g. for PhD students – but they’re only useful for long-term parts of NEPTUNE).
14. Another workshop near the end of 2020 should be scheduled to compare notes on progress with the various elements across the entire NEPTUNE project together with other projects within the overarching ExCALIBUR programme. It will be interesting to see if there are common challenges that we should explore across NEPTUNE with Met Office as well as the EPSRC part of the programme.

## **Session 3: Software Engineering**

Topics discussed in this session:

**Short term contracts:**

The general opinion was that short-term contracts are not ideal because of the large overheads and the constraints of hiring practices of academia e.g. agree that some percentage of FTE will be funded rather than assert that the contract finishes inside a specified number of months.

**Requirements gathering / documentation:**

The attendees who are involved in developing and maintaining public CSE applications are following an informal process, with the accent on modularisation and API specification. No Software Requirements Specification document is used. It was suggested to check publicly available requirements documents for CSE software projects.

**Automated testing procedure:**

Attendees involved in large scale software developments acknowledged that the unit testing procedure is embedded in their development team culture, in order to ensure software sustainability and the efficiency of the development process. The developer has to produce the test associated with the module being developed – this will influence our design of the 3rd party defrayed contracts. The testing needs to be done across platforms, compiler versions and vendors and sometimes operating systems. Automation tools are used to support these processes. None of the attendees were using formal roles such as validation, performance, maintenance tester or manager. Process oversight is typically done informally by senior developers. Large scale projects (e.g. biological tissue simulation) have certain tasks, such as verification, assigned to distinct groups.

**Uncertainty Quantification:**

The attendees pointed to several UQ techniques that can be used, intrusive should be designed into the project from the start (e.g semi-intrusive or Multi-Level Monte Carlo). Exascale computation capability will come in handy for the extra numerical work that will be needed. However, the interpretation of the results will need deep domain knowledge. Model errors could be larger than any other error within the proposed simulations.

**Separation of concerns, Domain Specific Languages (DSL), programming models:**

DSL were commended as a good solution for separation of concerns and complexity management, however they come with their own cost. One has to support the associated code generators. One has to mitigate the risk of DSL project termination, if this is done by a third party. Met Office is collaborating with STFC on code generator systems and they are also developing internal expertise for GungHo. It was mentioned that Kokkos is transferring some of its idioms in the C++ standard. No code generator for nodes with different architectures is universal. There is the risk of vendor lock in.

**Fault tolerance:**

Large scale applications might need to consider recovering from single node failure and continue the computation. The implementation used by Nektar++ based upon MPI functionality was presented in detail.

**Hardware availability:**

The HPC systems currently available to the UK academic community and their near-term upgrades were reviewed together with their access policies. ExCALIBUR has a small fund for hardware – UKAEA is engaging with those leading this part of the project to ensure hardware-software co-design is in place.

# Concluding remarks

The attendees were from those institutions and departments which we believe are the most relevant for the success of NEPTUNE.

After the workshop we received a number of expressions of interest from attendees (these also said they welcomed and enjoyed the event). UKAEA is not engaging in a dialogue with these individuals so as not to compromise the tender process.

All presentations were followed by questions and discussions which pointed to the fact that we covered the most relevant topics. The discussion sessions have shown that the problems we have put forward in physics, algorithms and software engineering are interesting for the community and that there is a fertile ground for cooperation. Useful information was gathered for the requirements capture process. It was noted that a number of decisions “in-session” would have to be subject to further consideration by UKAEA regarding their practicality and timing.

The main points that emerged from the workshop will now be considered by UKAEA and incorporated (as is deemed appropriate) in the calls for tender for contracts to be placed to support the NEPTUNE project early in Y2. A Prior Information Notice (PIN) is in preparation to warm up the market.

The travel arrangements and venue logistics all went very smoothly – we can consider the venue again for further community workshops.

# Annexe

## **Attendees list**

Individuals were allocated to one of the 3 discussion sessions described above. In the table our first and second choices for their allocation are given – in most cases they went to the first choice, but not always so as to ensure that the sessions were of roughly equal size. The session codes are D: Plasma Physics (led by Debasmita Samaddar), W: Algorithms (Wayne Arter) and L: Software Engineering (Lucian Anton).

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| 1st |  | 2nd | 1st |  | 2nd |
| D | Felix Parra Diaz  University of Oxford | W | W | Stefan Guettal  University of Manchester | L |
| W | Patrick Farrell  University of Oxford | D | L | David Silvester  University of Manchester | W |
| D | Steve Tobias  University of Leeds | W | W | Spencer Sherwin  Imperial College London | L |
| L | Paul Milewski  University of Bath | W | L | Chris Cantwell  Imperial College London | W |
| W | Eike Mueller  University of Bath | L | W | Nikos Nikiforakis  University of Cambridge | D |
| L | Peter Coveney  University College London | W | D | Steve Millmore  University of Cambridge | W |
| L | Ben Dudson  University of York | D | Float | Nigel Wood  Met Office | Float |
| L | Peter Hill  University of York | D | L | Paul Selwood  Met Office |  |
| L | Simon McIntosh-Smith  University of Bristol | W | Float | Rob Akers  UKAEA | Float |
| W | Tom Deakin  University of Bristol | L | L | Lucian Anton  UKAEA | L |
| W | David Moxey  University of Exeter | D | D | Debbie Samaddar  UKAEA | D |
| W | Xiaohu Guo  STFC | L | W | Wayne Arter  UKAEA | W |
| D | Wei Wang  STFC | W | W | Martin O'Brien  UKAEA | W |
| D | Joseph Parker  STFC | L | L | James Cooke  UKAEA | L |
| D | Ben Mcmillan  University of Warwick | W |  | Emma Palmer  UKAEA |  |
|  |  |  | D | Sarah Newton  UKAEA | D |

## **Workshop agenda**

Below is the agenda for the meeting.

**Fusion Modelling System ExCALIBUR Workshop**

Wednesday 5th February 2020

Hyatt Regency, 2 Bridge Street, Birmingham, B1 2JZ, UK

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| --- | --- |
| AGENDA | |
| 09:30 – 10:00 | Coffee |
| 10:00 – 10:30 | Welcome and Introduction by Rob Akers, UKAEA |
| 10:30 – 11:00 | Physics talk by Debasmita Samaddar, UKAEA |
| 11:00 – 11:30 | Numerics talk by Wayne Arter, UKAEA |
| 11:30 – 12:00 | Software Engineering Talk by Lucian Anton, UKAEA |
| 12:00 – 13:15 | Lunch |
| 13:15 – 14:15 | Group Discussion |
| 14:15 – 14:45 | Coffee Break |
| 14:45 – 15:30 | Group Discussion |
| 15:30 – 16:00 | Summary of Group Discussions and Closing Remarks |