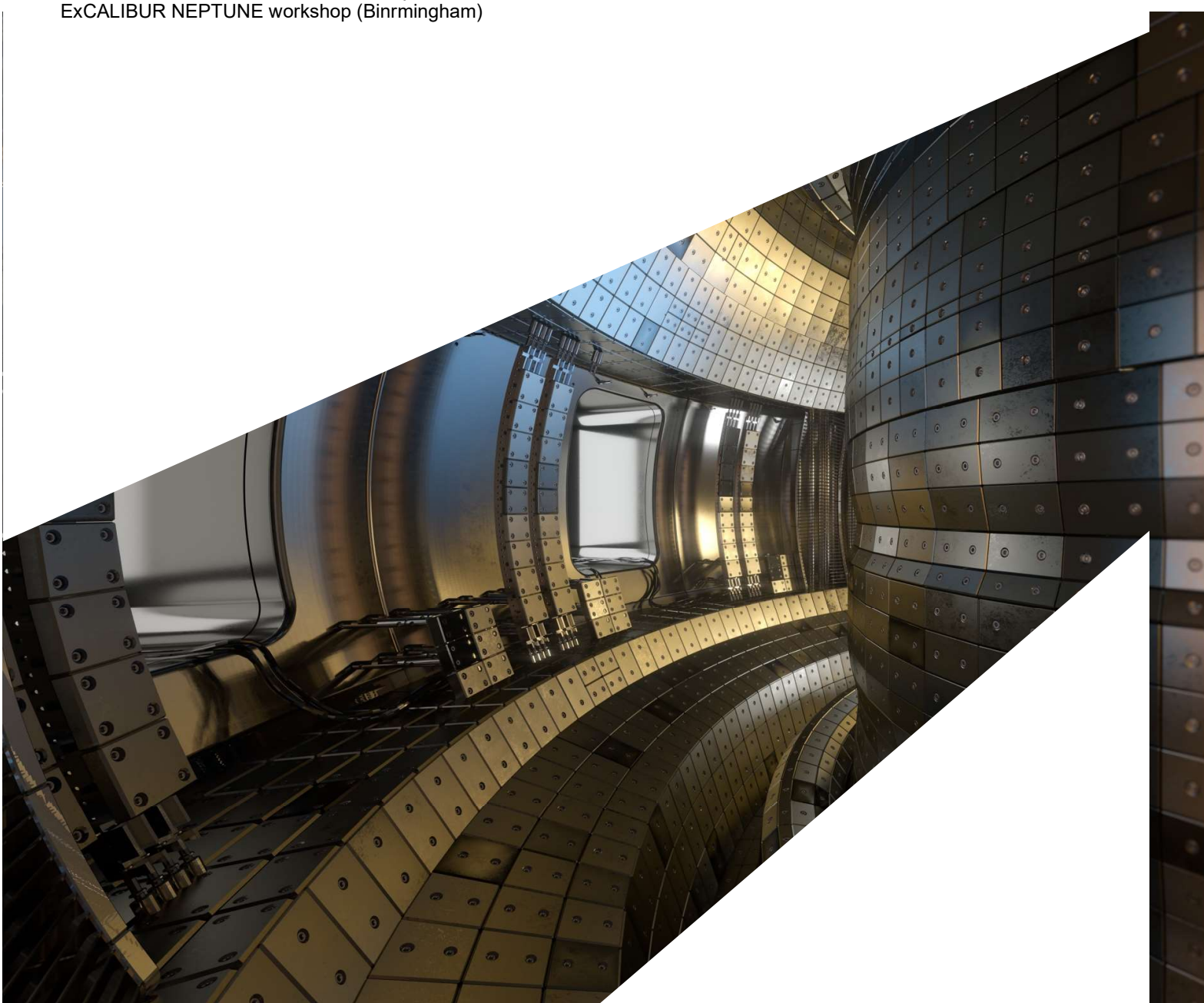
UK Atomic Energy Authority

ExCALIBUR

Summary of Discussion Sessions Workshop, 05-02-2020

Abstract

This document contains a short summary of the discussion sessions of the 05-02-2020 ExCALIBUR NEPTUNE workshop (Binrmingham)



UKAEA REFERENCE AND APPROVAL SHEET

	Client Reference:	
	UKAEA Reference:	CD/EXCALIBUR-FMS/0007
	Issue:	1.00
	Date:	14 February 2020
Project Name: ExCALIBUR Fusion Modelling System. Version 1.10 – modifications in response to reviewer recommendations.		

	Name and Department	Signature	Date
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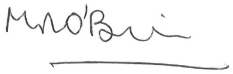
Approved By:	Martin O'Brien* MSSC		14/02/2020

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Summary of discussion sessions

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:

- 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 ETASC aims? (ETASC is related European fusion project that UKAEA participates in)
- identifying suitable intermediate proxy apps
- identify UQ and consider validation process

Gyrokinetics:

The discussion has 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, basic data flow
- open field lines easier as electrostatic potential set by sheath, closed line region need vorticity equation
- the session agreed there was potential to employ Gkeyll for comparison to problems solved using the hp spectral method
- coupling to fluid model longer term aim

Impurities

The discussion pointed to the need to explore suitable numerical methods to handle low plasma density, a large number of species, etc.

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 it create a pedestal as the neutrals in an open field line region, can carry momentum.
- wouldn't be the fastest way to develop a general physics model base, but can provide a basic understanding theory deliverable

Atomic physics/detachment

Both gyrokinetic and fluid theories fail in 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 Eirene.
- accuracy of atomic data

2 Algorithms

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

The following topics were considered to be important:

1. Higher order mesh generation
2. Connected particle and fluid calculation
3. Multi-precision approaches – it was felt that could be left until later if "separation of concerns" adequately implemented
4. Diffusion coefficient with very high (~10^6 ?) 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 1D hyperbolic equation with strong sources and sinks, with spectral accuracy, compare with chebfun solution
7. Elliptic solver issues – compare pre-conditioners? How good is algebraic multigrid?
8. Data compression

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 associate with the module being developed. 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 is using the formal roles such as validation, performance, maintenance tester and manager. The process oversight is done informally by the senior developers. A large scale project (biological tissue simulation) has 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. Exascale computation capability comes in handy for the extra numerical work that is needed. However, the interpretation of the results needs deep domain knowledge. Model errors could be larger than any other error.

Separation of concerns, Domain specific languages, 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 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 on 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.