EXCALIBUR PROJECT NEPTUNE – ADMINISTRATION AND SUMMARY

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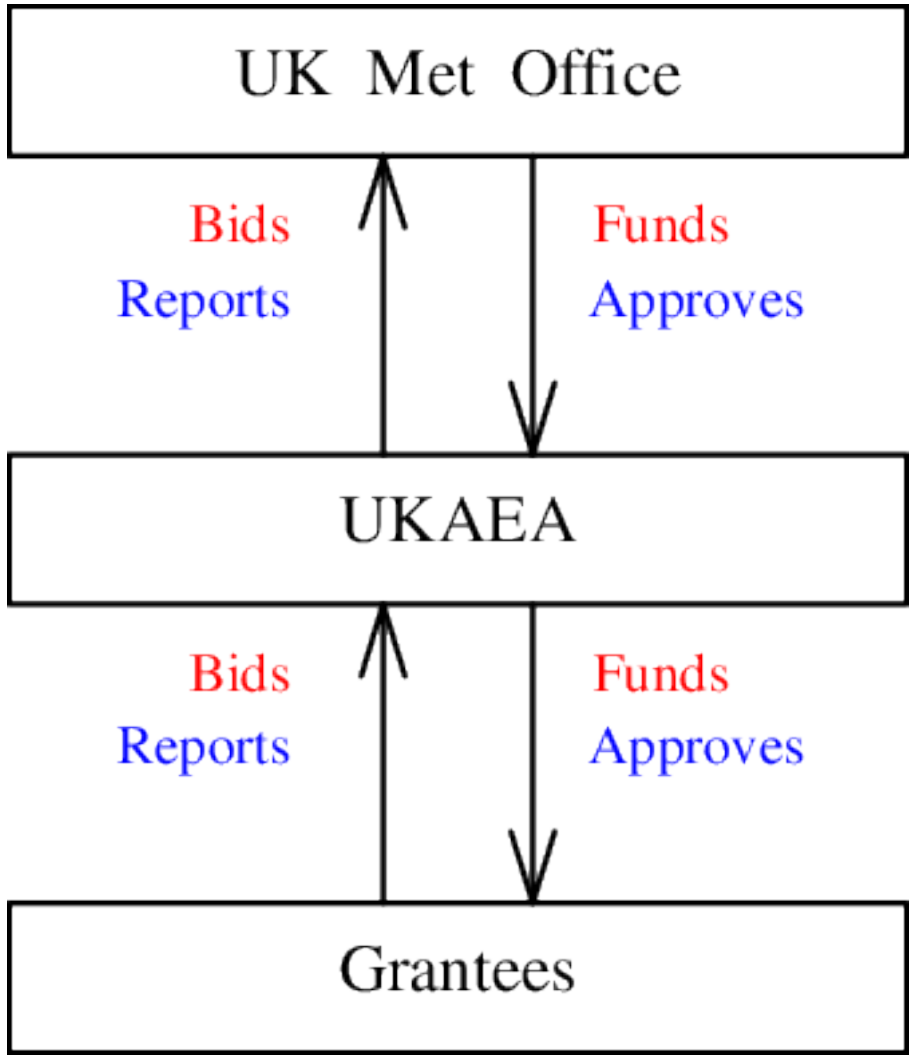
Cosener's House, 5th September 2022

UK Atomic Energy Authority

Contents

1. Relationships
2. Reporting
3. Current grant, proxyapps
4. Website as collaboration tool

1. NEPTUNE relationships



Bids – tenders have to be issued, bids “marked”

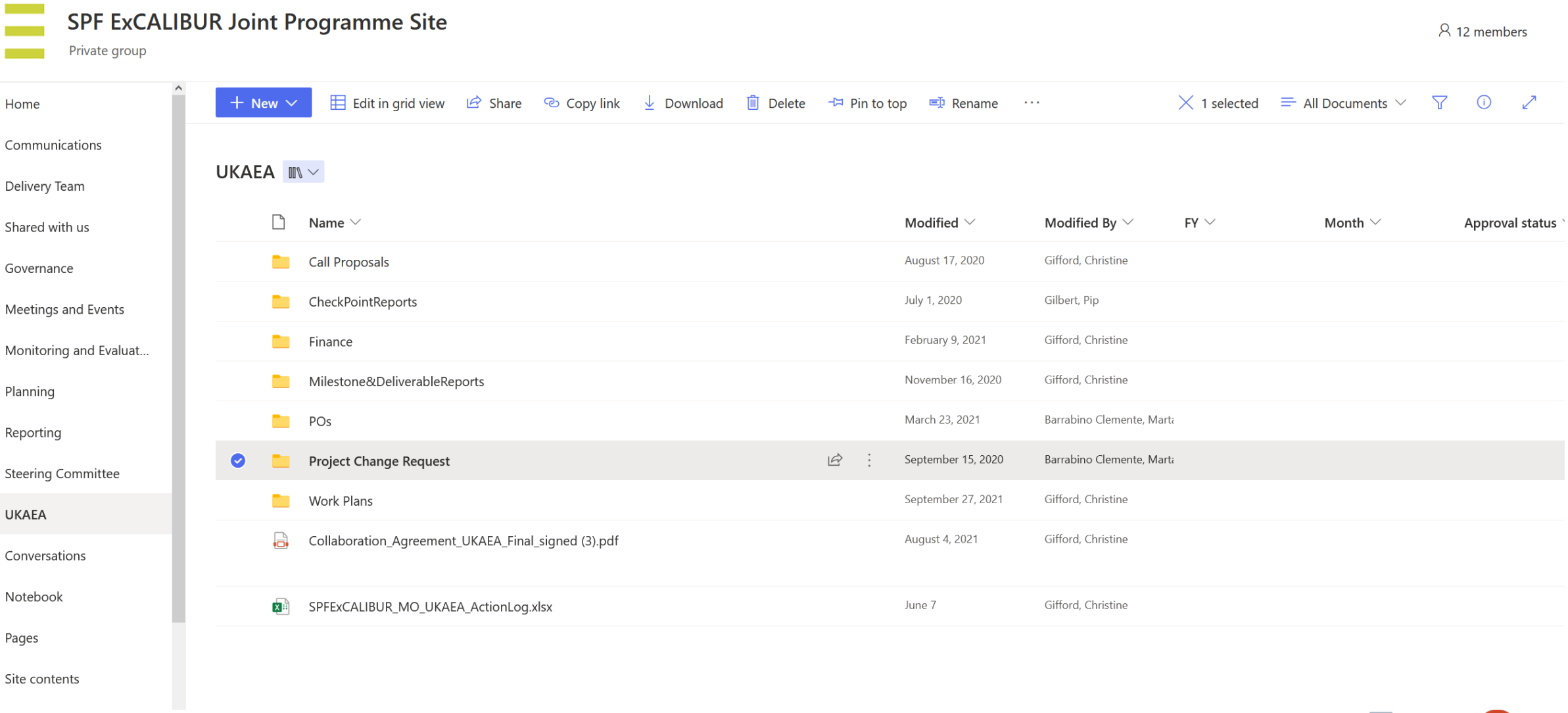
UKAEA Reports

1. Administrative docs - 13
2. Technical reports - 54
3. Periodic (Monthly) Checkpoints
    1. RAG *Red-Amber-Green* One line report /task and traffic light.
    2. “Impact” covers software developed and training

Grantees Reports

1. Administrative docs – Contract change requests only
2. Technical – 31 items at FY end
    1. Reports – c.50
    2. Software as repo/ “merge request”
3. Periodic (Monthly) based on fortnightly meetings
    1. RAG *Red-Amber-Green* One line report /task and traffic light.
    2. “Impact”

2. UKAEA Reporting to Met Office



ExCALIBUR Project Neptune (XPN)

Links

Restricted access:
https://metoffice.sharepoint.com/sites/SPFExCALIBURJointProgrammeExt/UKAEA
Presentations (recent) https://ukaeauk.sharepoint.com/sites/ExCALIBUR-NEPTUNE

Named access only:
LaTeX source, biblio & pictures https://git.ccfe.ac.uk/warter/excalibur-wa access on request to UKAEA
Software and documents https://github.com/ExCALIBUR-NEPTUNE (17 repos, 6 public – send me your github handle to access all.)
https://github.com/ExCALIBUR-NEPTUNE/Documents/
../reports 49 grantees' reports by PO number
../meetings 6 workshop reports
../tex Out-of-date version of excalibur-wa/tex

Public:
Developer web-site https://mbukaea.github.io/main.html (for evaluation, link will change soon, bits only skeletal), public, but link to named access only (Error 404 otherwise)
Nektar++ https://www.nektar.info/getting-started/

ExCALIBUR-NEPTUNE github

https://github.com/orgs/ExCALIBUR-NEPTUNE/repositories?type=all

Search or jump to... / Pull requests Issues Marketplace Explore

ExCALIBUR-NEPTUNE

Overview | Repositories 17 | Projects | Packages | Teams 5 | People 33 | Settings

Find a repository... | Type | Language | Sort | New repository

NESO-Spack Public
Spack repository for installing NESO components and dependencies.
Python 0 1 0 0 Updated 3 days ago

performance-portability-for-fusion Private
0 0 0 0 Updated 3 days ago

NESO Public
C++ MIT 0 1 29 3 Updated 9 days ago

NESO-Particles Public
C++ MIT 1 0 0 0 Updated 12 days ago

MathsSupport Private
TeX 0 0 14 0 Updated 16 days ago

nekmesh-python-demo Private
Demonstration of Python API for NekMesh
Python 0 0 0 0 Updated 19 days ago

nektar-1d-sol Private
Test solver based on 1D SOL equations
C++ 0 0 0 0 Updated on 21 Jul

nektar-driftwave Public
C++ 0 1 2 1 Updated on 26 May

https://github.com/orgs/ExCALIBUR-NEPTUNE/repositories?type=all

Documents Private
Bid documents, calls, reports and supporting documents for ExCALIBUR-NEPTUNE.
TeX BSD-3-Clause 0 3 1 3 Updated on 14 May

nektar-cwipi Private
Repository for Nektar++ CWIPI coupling example proxyapp
C++ 0 0 0 1 Updated on 7 Apr

minepoch Public
Fortran BSD-3-Clause 2 0 5 0 Updated on 3 Mar

Cross-Cutting-Organisation Private
A central repo for organising work that touches multiple codes / repos / workflows
MIT 0 0 0 0 Updated on 14 Feb

private_repo_test Private
0 0 0 0 Updated on 21 Jan

NektarPIC Private
MIT 0 0 0 0 Updated on 26 Nov 2021

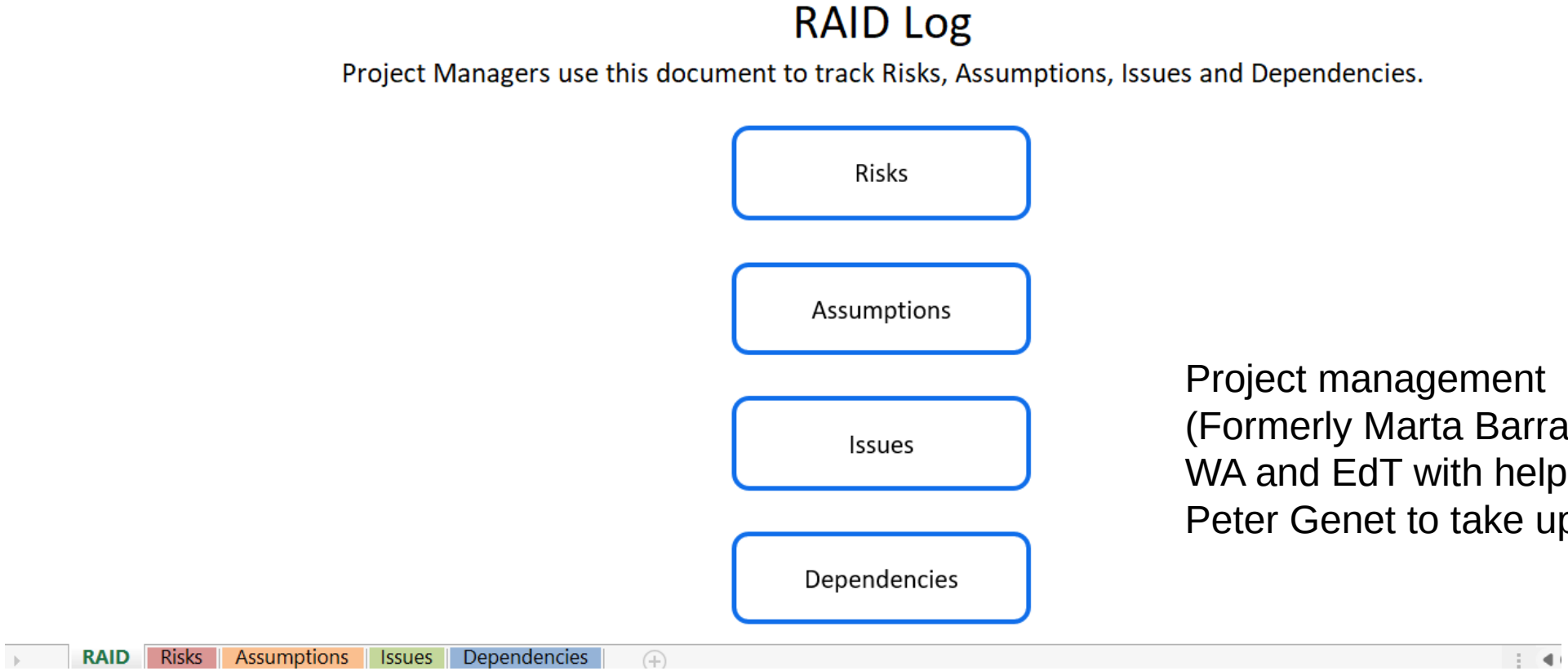
nektar-diffusion Private
Nektar++ diffusion solver
C++ 0 0 0 0 Updated on 25 Nov 2021

roundtable Private
Performance testing tool for the ExCALIBUR NEPTUNE project
Python MIT 0 0 0 0 Updated on 1 Apr 2021

Neptune Public
BSD-3-Clause 0 2 0 0 Updated on 18 Jan 2021

RAID for Project Management

Spreadsheet with 4 pages



Project management
(Formerly Marta Barrabino-Clemente)
WA and EdT with help from Juan Palomo-Frias,
Peter Genet to take up PM role this month

Software development uses repo based system instead

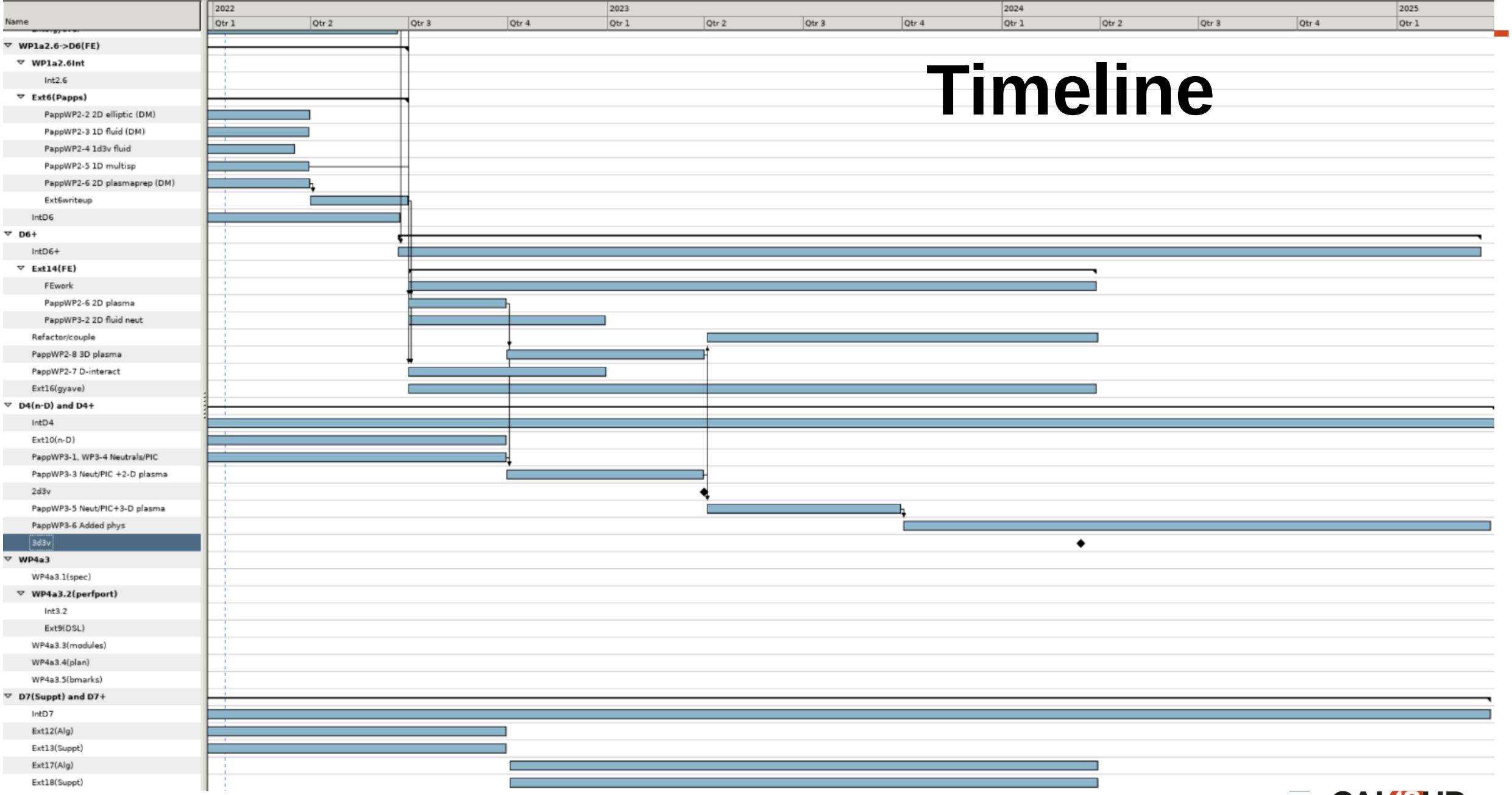
Breakdown by Task

No.	Task Title	Lead
1d	Project and Collaboration Management	– Rob Akers
4c	High-dimensional Models : includes particles	– James Cook
5c	Uncertainty Quantification	– Wayne Arter
6c	Finite element models	– Ed Threlfall (to present)
7c	Support and Coordination	- Vacant

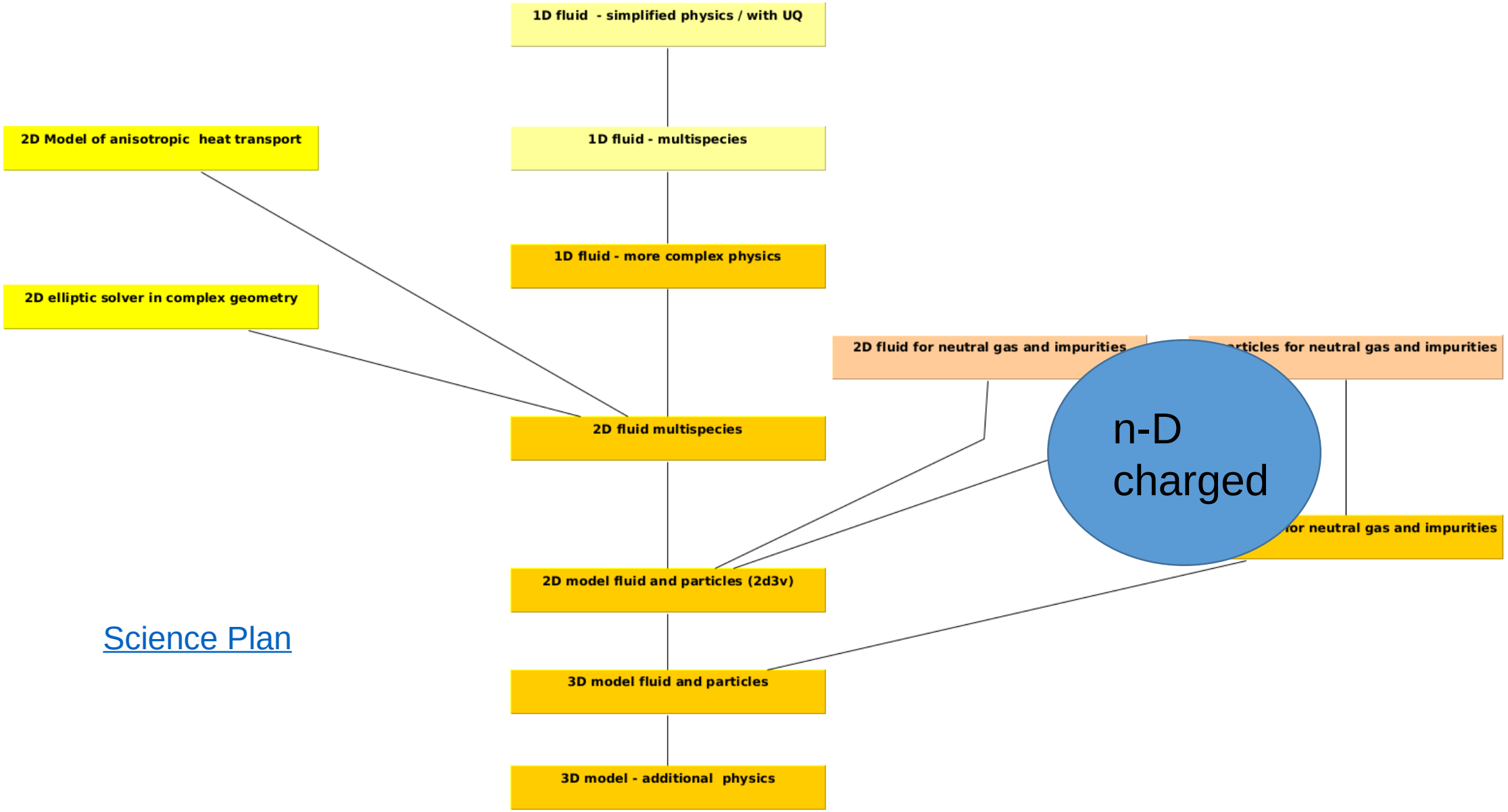
- Task lead may call on other lead and NEPTUNE staff to do the work
- Tasks 5 and 6 are primarily to enable UKAEA to act as intelligent customer,

Task 4 to write software and Task 7 to act as integrator

Timeline



Development as a Sequence of Proxyapps



[Science Plan]

4. Tour of developers' website - management

https://mbukaea.github.io

Executive Summary – website designed following a review of technical literature / websites / book by Eben Hewitt

Business design – so everyone understands the context

Software development - after Ben Dudson, based on his experiences of the BOUT++ development
7.2 Frequency of meetings, version control, repositories, workflow
9 Documentation & testing.

Design Justification File – based on reports produced to-date. Need to download
https://github.com/ExCALIBUR-NEPTUNE/Documents/
and index contents by desktop search engines such as DocFetcher or Recoll

Development Principles

Important principles

General: Communication and good design, and how to achieve (Eben Hewitt)

Use case → requirements, using IETF* conventions

MECE** lists

….

N.B. Developer website has material on “object recognition”

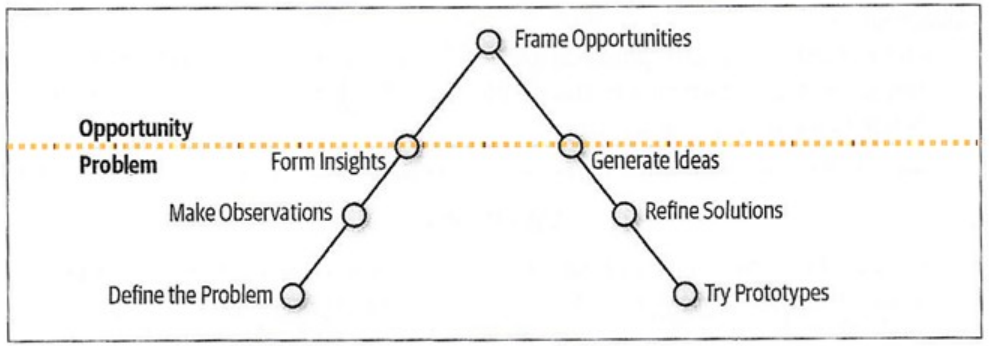
UQ: Write once, use many times

Use of conventions, consistent symbology and enforce, *especially* only ASCII in repos

Good interfaces imply reliability

Exascale: Technology (which includes software) will change

- separation of concerns by careful design of code structure (libraries)
- importance of separate mathematical formulation
- always two options, option to make a case to replace one



*Conventions on use of *must, should* etc.

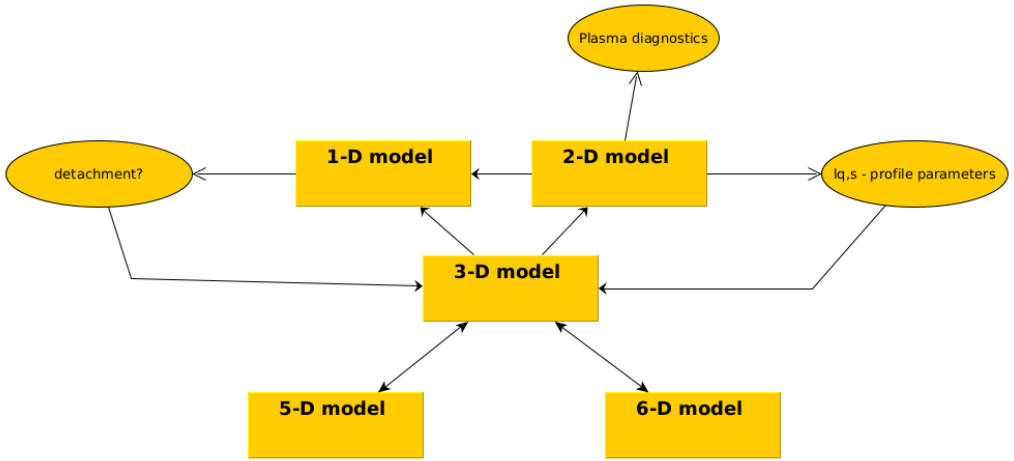
**Mutually Exclusive, Collectively Exhaustive

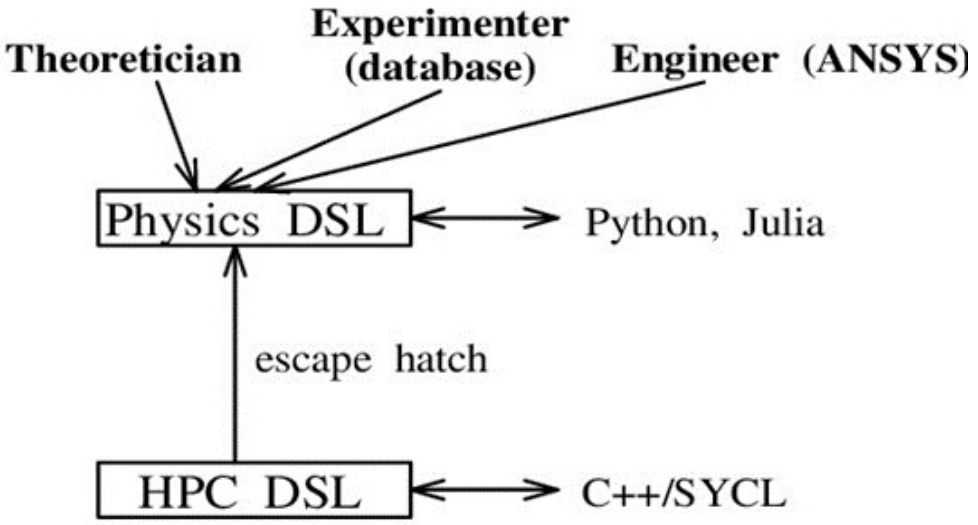
Tour of developers' website - technical

https://mbukaea.github.io

Requirements baseline
- Challenges, what the engineers wanted below (Physicists' wants in TS)
- Use cases, potential users invited to say what they want
- Important note regarding DSLs – two workshops held

Conventions, acronyms and symbols, eg. DSL Domain Specific Language





Summary

Important conclusions

1. Exploited “blank sheet of paper” to produce process for developing opensource software, using opensource tools where possible.
2. Must understand limitations of university contribution to software development.
3. Choice of DSL can be fraught.

Achievements to-date, at approx. 55% spend (80% spend committed)

- UKAEA and Grantees produced 100 tech. reports (c.50 each, say 2-3 books),17 repositories, significant updates to Nektar++ library.
- UKAEA has run NEPTUNE mini-symposium at PP22, and 4 workshops
- Presented at ExCALIBUR workshops