EXCALIBUR PROJECT NEPTUNE – TECHNICAL FRAMEWORK

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Cosener's House, 6th September 2022

UK Atomic Energy Authority

Contents

News

Workshop instead of fortnightly progress meeting

1. Next Progress Meeting 11am, 22nd September. Invitations should have already been received.
2. Purchase Orders for three 2022 tenders should now have been issued.

Summary (from Day 1)

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

ExCALIBUR Project Neptune (XPN)

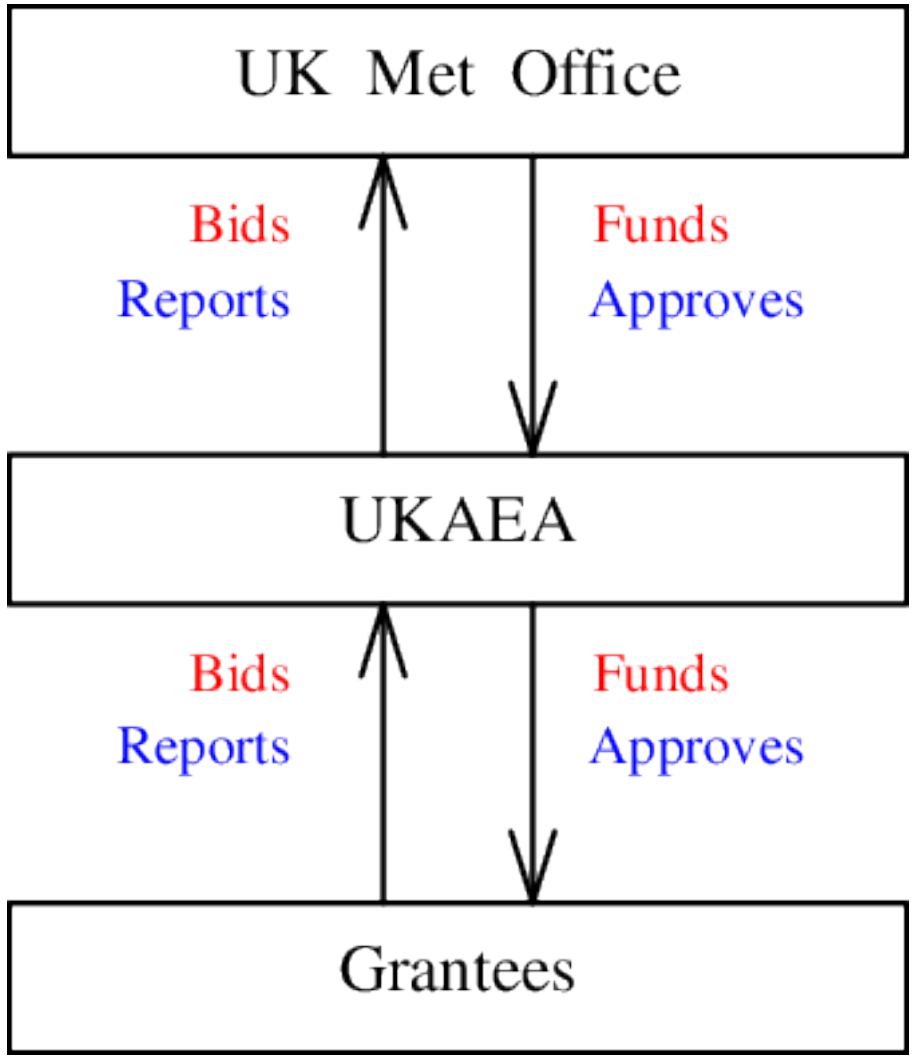
Links

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 for UKAEA only
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 (4 to process)
../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../tex Out-of-date version of excalibur-wa/tex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/

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”

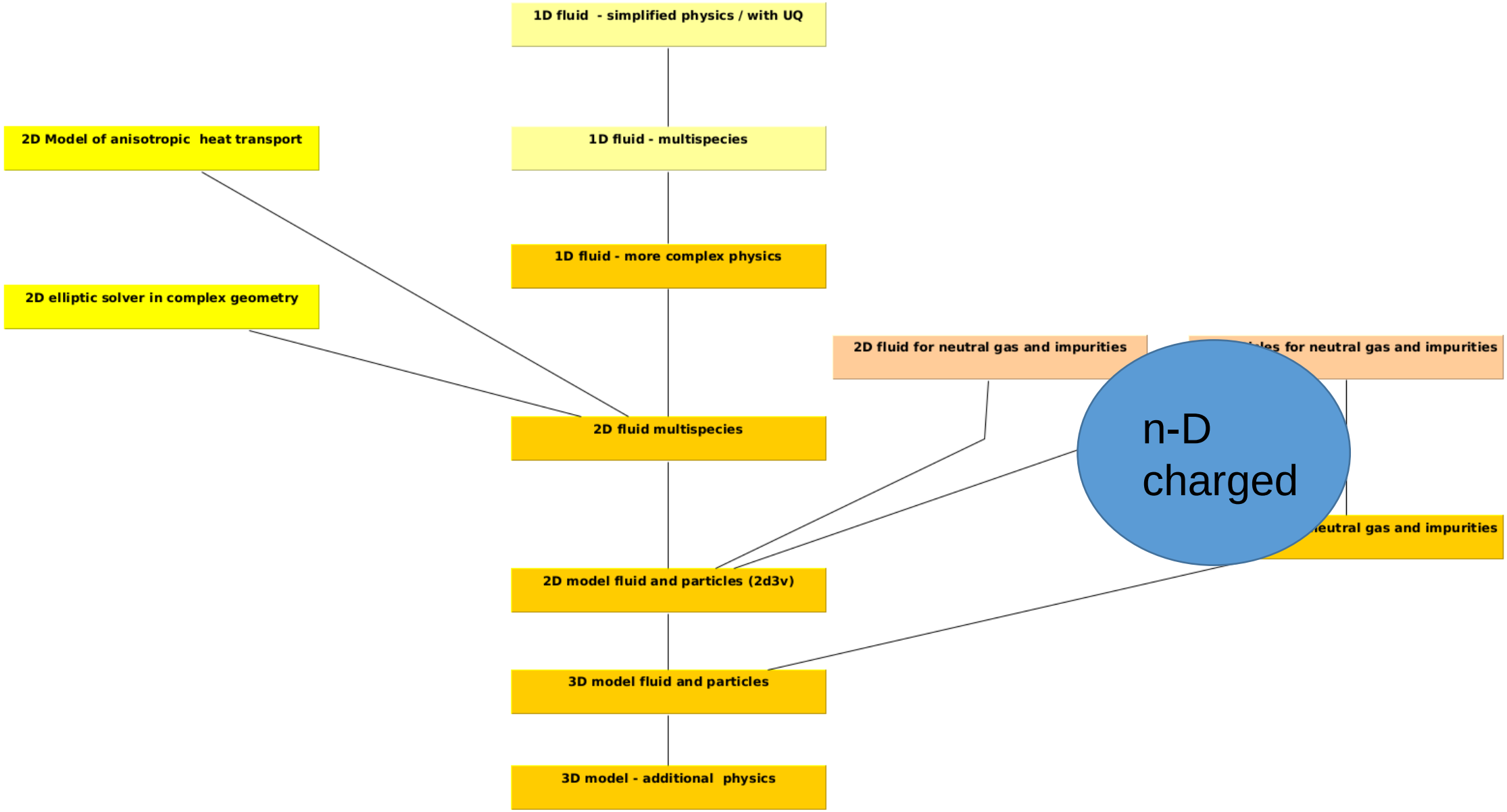
Breakdown by Task

No.	Task Title	Lead	Key staff
1d	Project and Collaboration Management	– Rob Akers	- Wayne Arter
4c	High-dimensional Models : includes particles	– James Cook	- Will Saunders
5c	Uncertainty Quantification	– Wayne Arter	- (Joseph Parker), Ed Threlfall
6c	Finite element models	– Ed Threlfall	- Owen Parry
7c	Support and Coordination	- Vacant	- Matthew Barton

- 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

Development as a Sequence of Proxyapps



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 indexing of contents by desktop search engines such as DocFetcher or Recoll

Development Principles

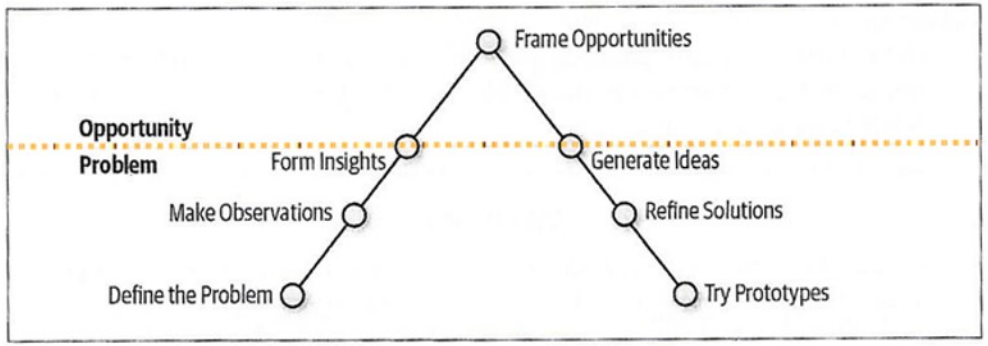
Important principles

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

*Mutually Exclusive, Collectively Exhaustive



Tour of developers' website - technical

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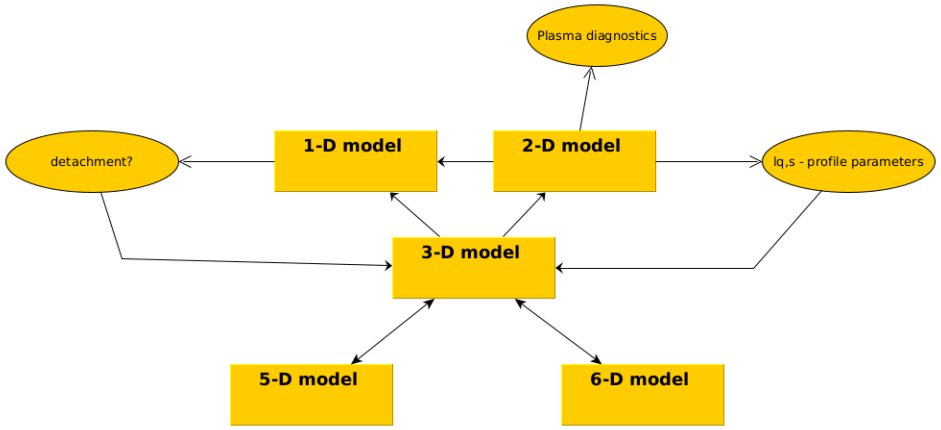
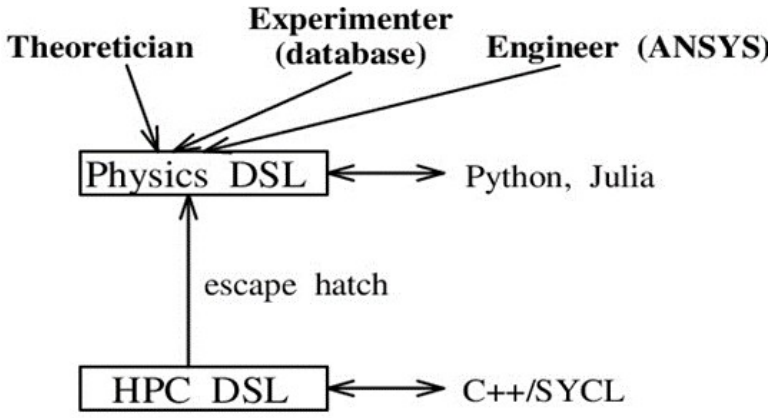
Requirements baseline
- Challenges, what the engineers wanted below (Physicists' wants in TS)
- Use cases, real users invited to say who they are and what they want
- Important note on DSLs – two workshops held

Conventions, acronyms and symbols

To be added
- Importance of spack





Summary

Sessions

UKAEA Technical Presentations	Start time		Time allocated
Presenter - topic			
Wayne Arter - Framework	09:30	Garden Room	20
Ed Threlfall - UQ	09:50		15
Owen Parry – Finite elements at UKAEA	10:05		15
Will Saunders - Particles	10:20		20
James Cook - Particles and Finite Elements	10:40		20
Mid-Morning Tea, Coffee & Biscuits with additional croissants and preserves, plus mixed muffins	11:00	Garden Room	30