



EXCALIBUR PROJECT NEPTUNE WORKSHOP – INTRO

Rob Akers
Head of Advanced Computing, UKAEA

Cosener's House, Abingdon, 5-6 Sep 2022



**UK Research
and Innovation**



**UK Atomic
Energy
Authority**

MONDAY	Start time	Venue	Time allocated
Badge pickup	09:00	Entrance	60
Welcome Tea & Coffee	09:00	Garden Room	60
Grantees Work-to-date, Chair Wayne Arter			
Introduction, fire precautions (Rob Akers)	10:00	Garden Room	20
Exeter/KCL (Dave Moxey)	10:20		15
Imperial (Chris Cantwell)	10:35		10
York (Steven Wright)	10:45		20
Warwick (Will Saunders as Rapporteur)	11:05		5
UCL (Serge Guillas / Peter Coveney)	11:10		15
STFC (Sue Thorne)	11:25		15
Oxford (Michael Barnes)	11:40		15
Lunch	12:00	Dining Room	60
Grantees depart for Culham Site	13:15 SHARP		
UKAEA Only Session, Chair James Harrison			
Wayne Arter - UKAEA admin and summary	13:30	Garden Room	30
Tea and coffee	14:00	Garden Room	
Ed Threlfall - NEPTUNE Spectral Element Grants	14:30	Garden Room	30
Robert Kingham - Exhaust Code Project, and discussion	15:00		30
Other presentations and discussion	15:30		30
Soft drinks	16:00	Garden Room	
Grantees return from Culham site	16:15		
Grantees Proposed Work, Chair Ed Threlfall			
Exeter/KCL (Dave Moxey)	16:30	Garden Room	30
York Csci+Plasma (Steven Wright)	17:00		20
UCL (Serge Guillas/Peter Coveney)	17:20		20
STFC (Sue Thorne)	17:40		20
Oxford (John Omotani as Rapporteur)	18:00		20
Poster Session	18:30	Thames Room	30
Dinner	19:00	Dining Room	180

Grantees return from Culham site

Exeter/KCL (Dave Moxey)

York Csci+Plasma (Steven Wright)

UCL (Serge Guillas/Peter Coveney)

STFC (Tyrone Rees)

Oxford (John Omotani as Rapporteur)

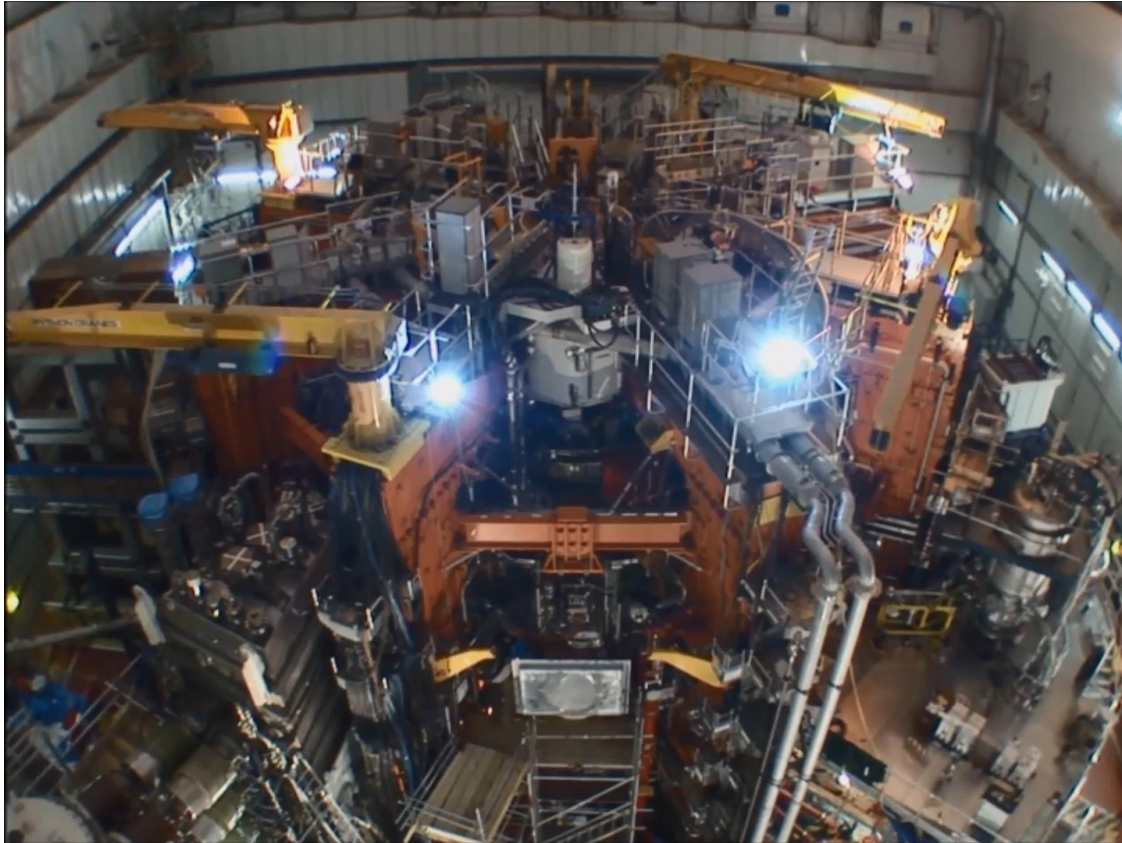
Poster Session

Dinner

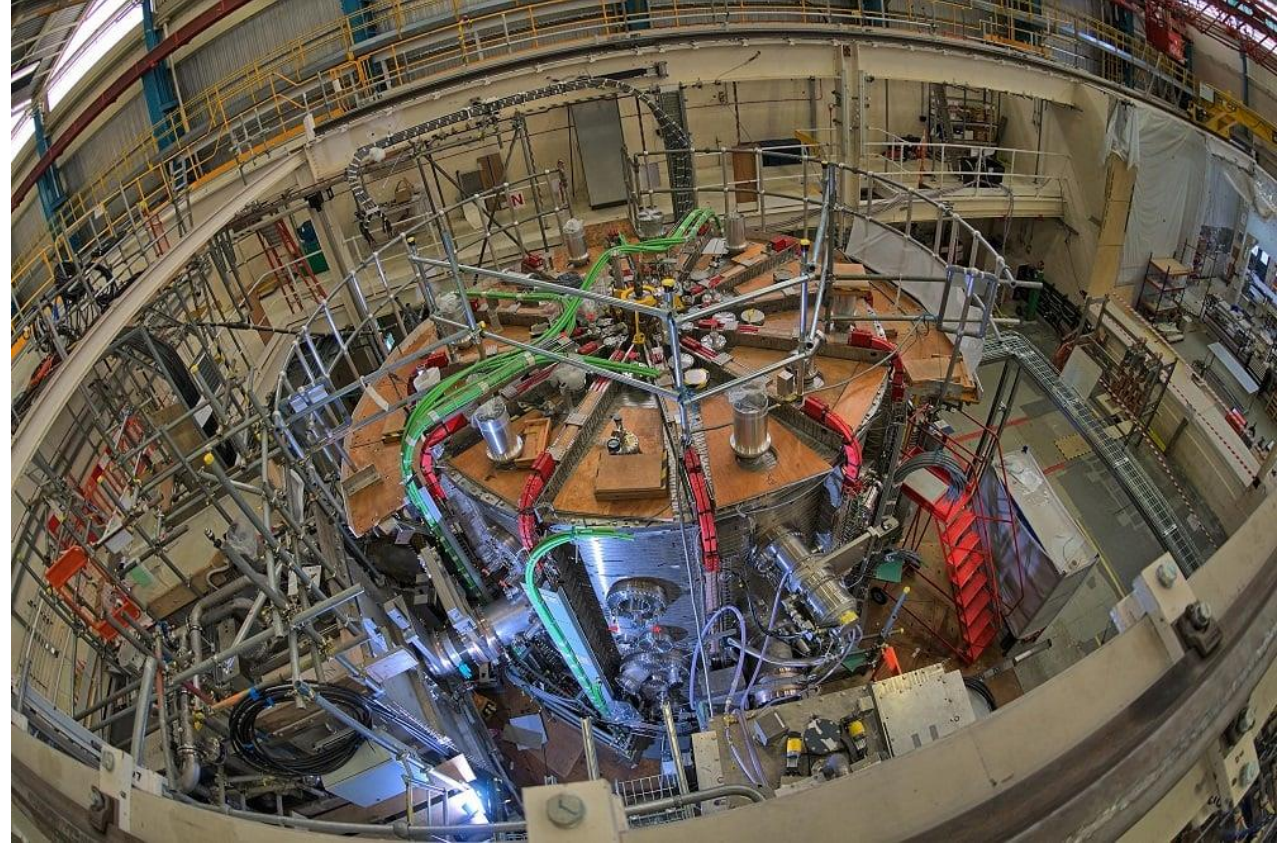


CCFE Tour of the Tokamaks

Departing promptly at **13:15 Today**



JET: Joint European Torus



MAST-U: MAST Upgrade

Details about where to board will be provided later (please see Owen Taylor for more details)

CCFE Tour of the Tokamaks – no inappropriate footwear

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CCFE Tour of the Tokamaks



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General visit information for UKAEA organised tours

- Facemasks are optional during the visit (unless indicated otherwise)
- All visitors will need to bring photo ID to show on arrival to be issued with their site pass to come onto the Culham Site. This needs to be current passport or driving licence.
- We would like to make you aware that there will be a significant amount of walking during the tour, so it is advisable to wear comfortable shoes.
- Please also note that open-toe shoes are strictly forbidden in one of the experimental areas, so please ensure ALL visitors wear covered footwear (no sandals / flip-flops etc).
- Please let us know in advance if you have any special mobility needs so that we can make arrangements for you to visit the facilities.
- Please could you let us know if any of the group have a pacemaker, or an automatic drug dispenser fitted as a medical implant, as this may affect access to some parts of the Culham tour.
- Please let all visitors know they are welcome to take photos at designated areas of the tour – please ask your guide for further information.
- If you or your group would like to share any photos or comments with us on social media, you can find us at @UKAEAofficial on: Instagram, Twitter, Facebook, LinkedIn & YouTube.

13:30 Arrive at reception – Contact Pauline Lawrence (x4846)

13:45 – 14:45 Tour of JET (from K1 foyer)

Group A – Jon Witty (x8071)	Group B – David Middleton-Gear (x6891)
Models Control Room Gallery Remote Handling Assembly Hall	Assembly Hall Remote Handling Control Room Gallery Models

14:45 – 15:00 Walk to MAST

15:00 – 15:40 Tour of MAST

Group A – Sam Gibson	Group B – Scott Allan
Models Control Room Fusion Technology	Fusion Technology Models Control Room

15:40 – 15:50 Walk to K1 Foyer

16:00 Depart as appropriate

CCFE Tour of the Tokamaks



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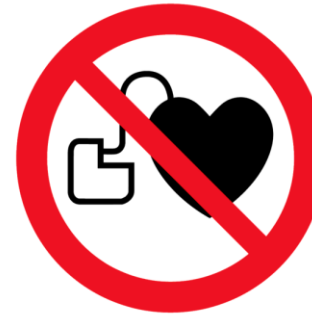


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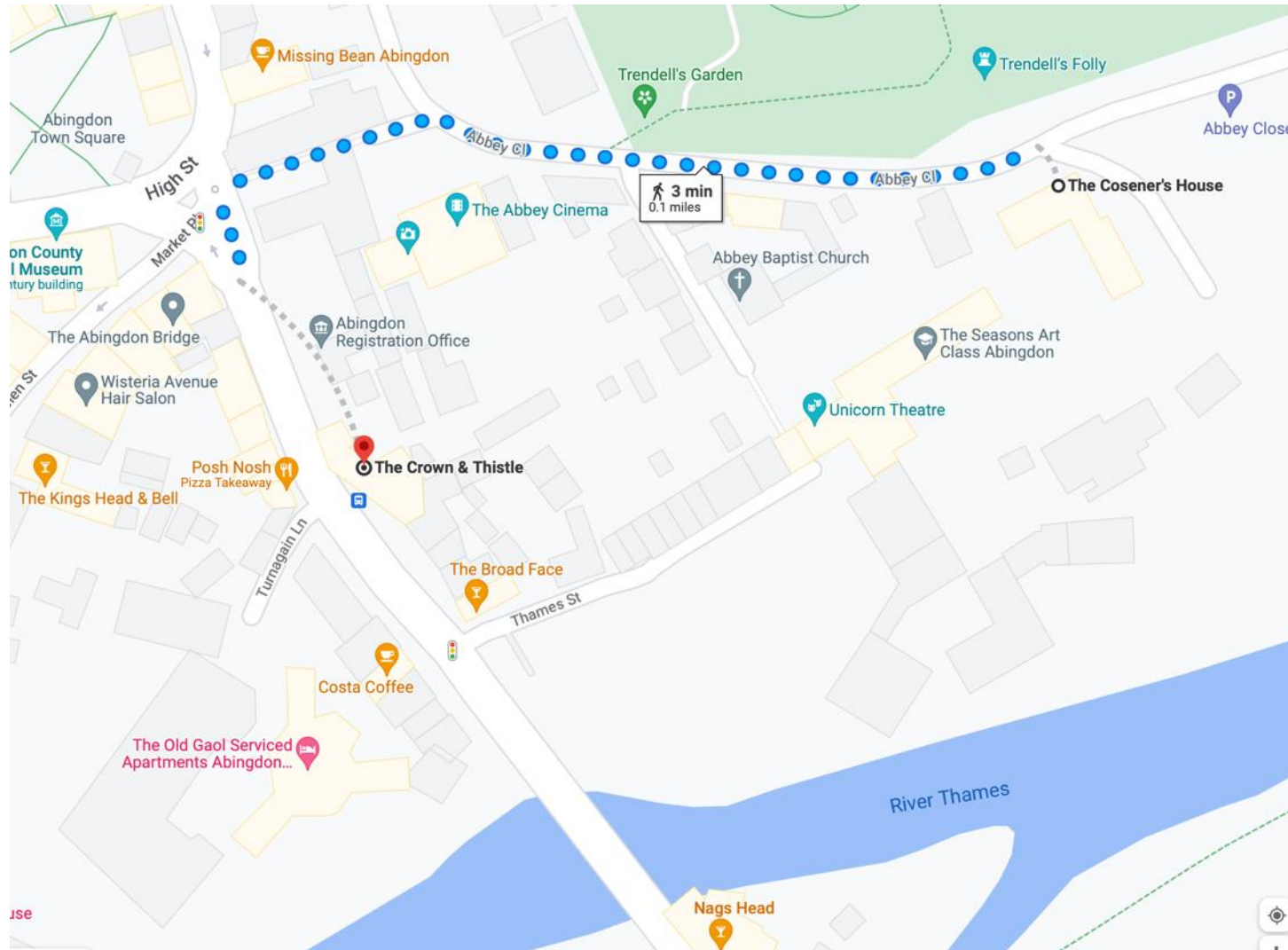


or



**No pacemakers
Strong magnetic
field**

Pick up at the Crown & Thistle Bus Stop, 13:00



Pick up at the Crown & Thistle Bus Stop, 13:00



TUESDAY	Start time	Venue	Time allocated
UKAEA Technical Presentations, Chair Rob Akers			
Framework (Wayne Arter)	09:30	Garden Room	20
VVUQ activities (Ed Threlfall)	09:50		15
Nektar++ working (Owen Parry)	10:05		15
Particles (Will Saunders)	10:20		20
Particles and Finite Elements (James Cook)	10:40		20
Mid-Morning Tea, Coffee & Biscuits	11:00	Garden Room	30
BREAKOUTS across 3 rooms			
Nektar++ (Ed Threlfall - moderator, Owen Parry – assistant)	11:30	Garden Room	90
Particles (James Cook - moderator, Will Saunders – assistant)	11:30	Royse, Guildhall	90
Physics equations – (Sarah Newton moderator, Wayne Arter – assistant)	11:30	Abbey Rm, Guildhall	90
Lunch	13:00		60
UQ – (Ed Threlfall – moderator, Owen Parry – assistant)	14:00	Garden Room	90
Nektar++ - (Will Saunders - moderator, James Cook – assistant)	14:00	Royse, Guildhall	90
Physical data – (Wayne Arter moderator, Matthew Barton – assistant)	14:00	Abbey Rm, Guildhall	90
Tea and coffee	15:00	Garden Room	
Plenary	15:30		30
End	16:00		

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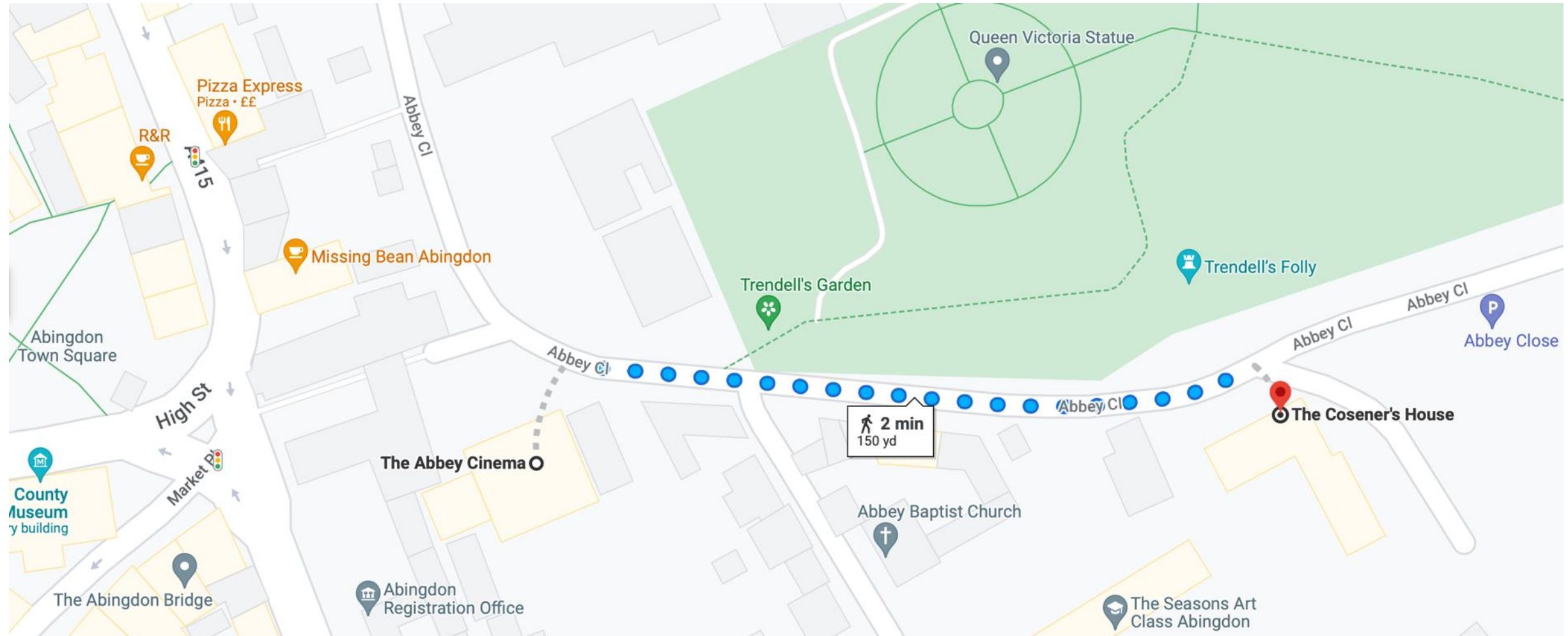


Please sign up to an 11:30 pre-lunch session and a 14:00 post lunch session

UKAEA staff: Amanda Quadling and Fulvio Millitello have asked that you don't all coalesce in one session so please spread out

Tuesday Breakout Sessions – The Guildhall

Entrance through the Abbey Cinema



Tuesday Breakout Sessions – The Guildhall

Entrance through the Abbey Cinema



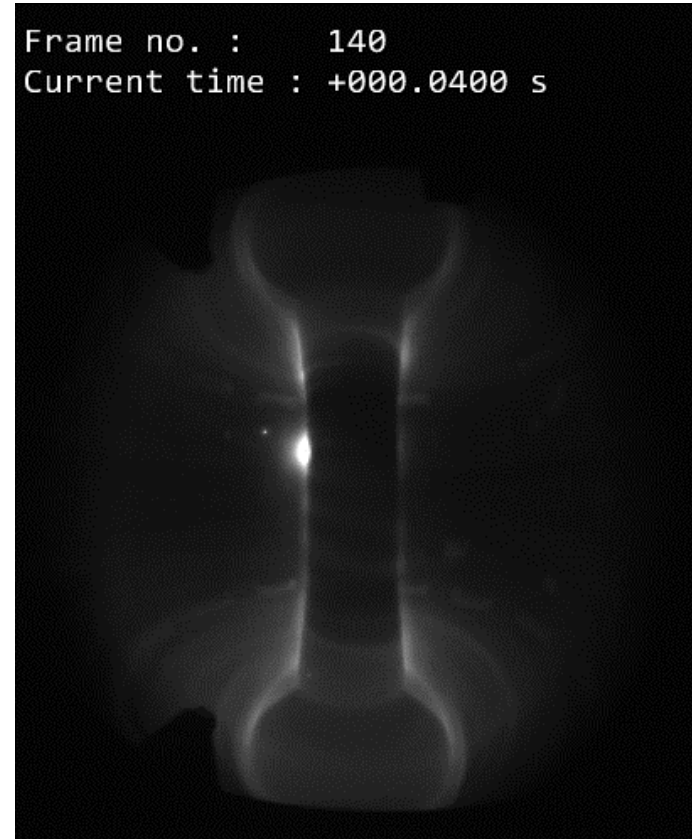
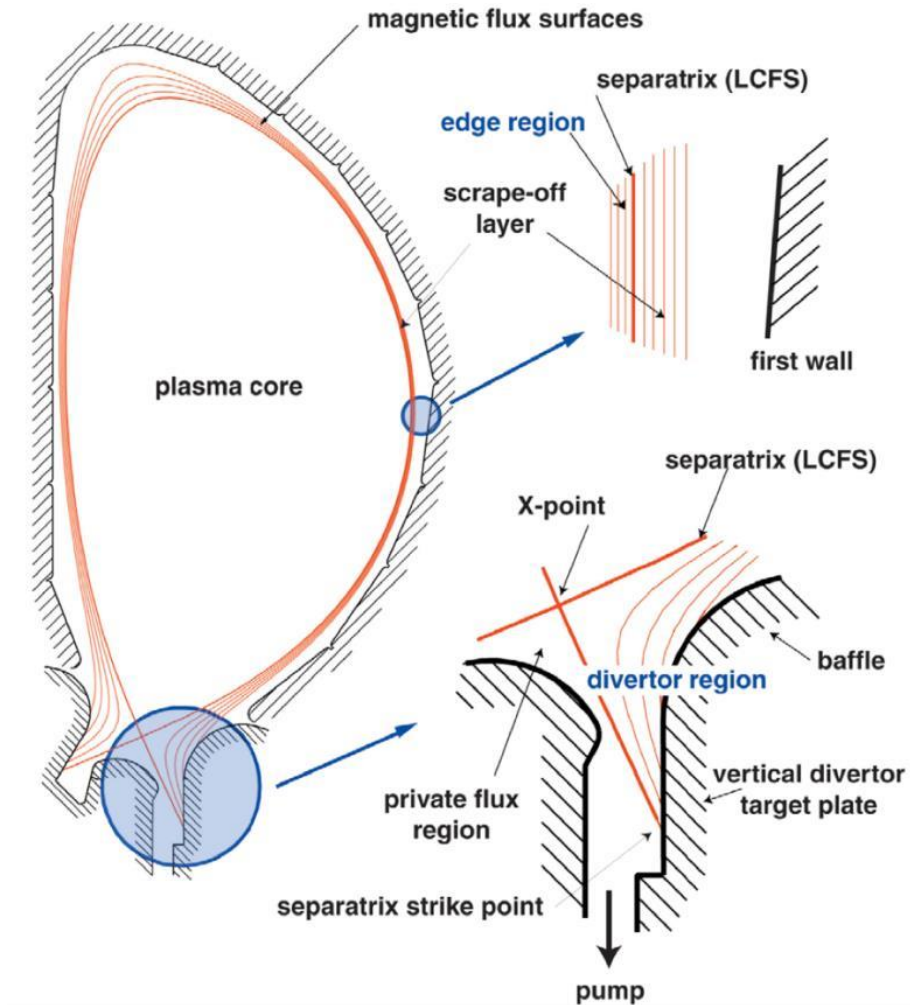


Aims of workshop:

- **Inevitably, we will be looking back at what we have done so far – this is in sharp focus**
- **However, the aim of the workshop is to bring into focus the road ahead, based upon what we have learnt – so we can move forward at speed**
- **Please focus upon coordination, alignment, objectives setting etc.**

NEPTUNE High Priority Use Case

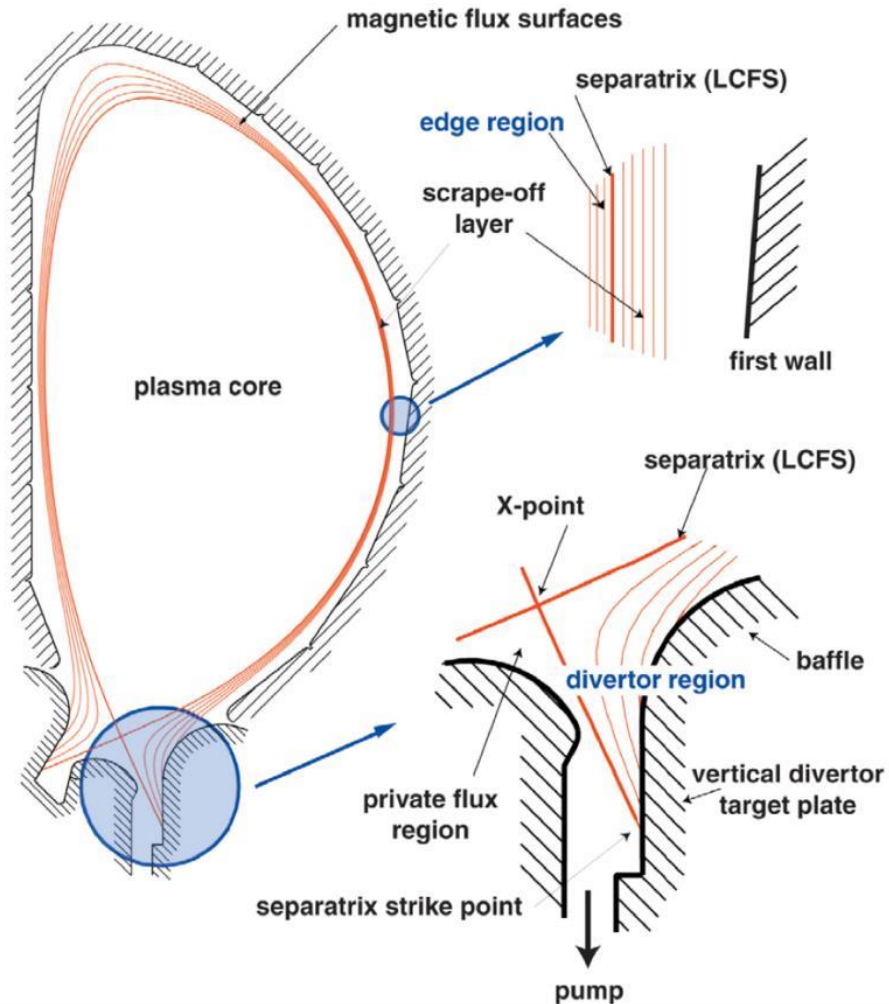
Neutrals and Plasma Turbulence Numerics for the Exascale



~1s long H-mode MAST-U pulse

NEPTUNE High Priority Use Case

Neutrals and Plasma Turbulence Numerics for the Exascale



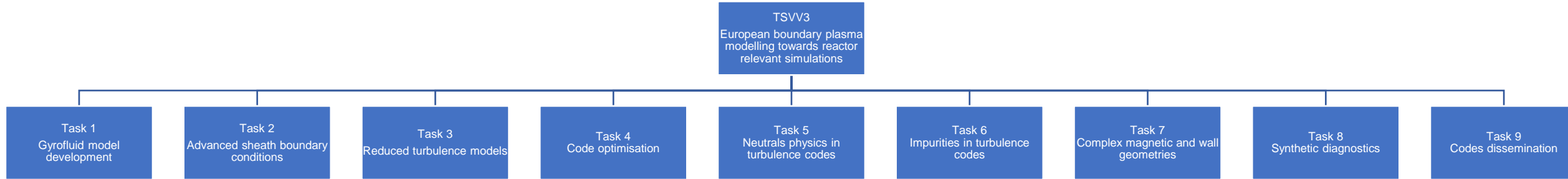
Modelling the plasma edge or ‘exhaust’

- A long established exascale **grand-challenge, Multi-physics, Multi-scale** problem
- Complexity – **turbulence, atomic physics** etc.
- Incomplete mathematics (\$1M Millennium Prize)
- For plasma, kinetic effects can’t be ignored – requires **coupled fluid + particles**

Requires an interdisciplinary rainbow team...

EUROfusion Exhaust Code development

Synergy with NEPTUNE Programme



Task 1: Deriving gyro-fluid models towards reactor relevant applications, including collisional closures, neutrals and impurities

Task 2: Developing sheath boundary conditions for fluid codes and extending their validity to reactor relevant regimes

Task 3: Deriving reduced turbulent transport models (e.g., Reynolds-Averaged Navier-Stokes) of cross-field transport and implementation in existing codes

Task 4: Optimising edge fluid turbulence codes towards future fusion power stations

Task 5: Studying different methods to implement neutrals physics in edge turbulence codes and their coupling

Task 6: Investigating methods to implement impurities in edge turbulence codes (e.g., with Zhdanov closure)

Task 7: Investigating numerical methods to enable modelling of complex magnetic and wall geometries

Task 8: Developing synthetic diagnostics to compare code predictions and experiment, IMAS-ification of code I/O

Task 9: Promoting collaborative development methods to share progress amongst the EUROfusion community as early as possible

NEPTUNE High Priority Use Case – see www.excalibur.ac.uk

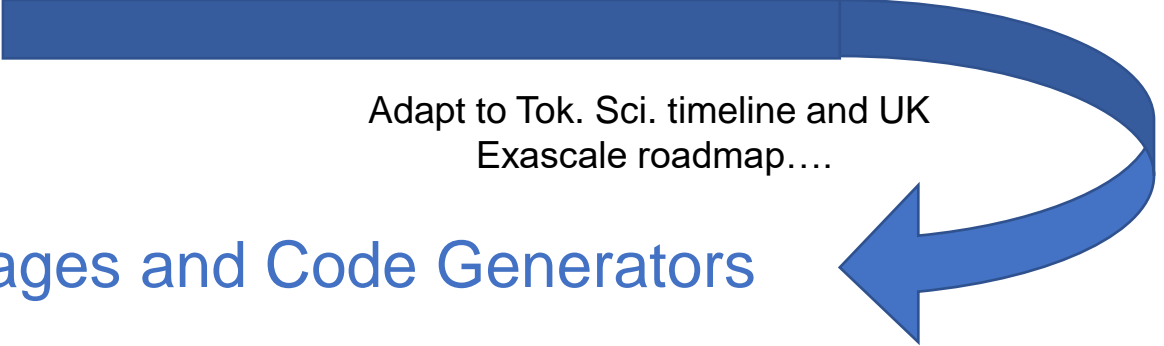
A different approach – research the right way forward from blank sheet of paper

- Performance of Spectral Elements
- Optimal use of Particles
- Study of Uncertainty Quantification Techniques
- Study of Model Order Reduction techniques
- Development of Fluid Referent Model
- Development of gyro-averaged model
- Investigation of Domain Specific Languages and Code Generators
- High Dimensional Models for Neutral Gas and Impurities
- Numerical Representation

NEPTUNE High Priority Use Case – see www.excalibur.ac.uk

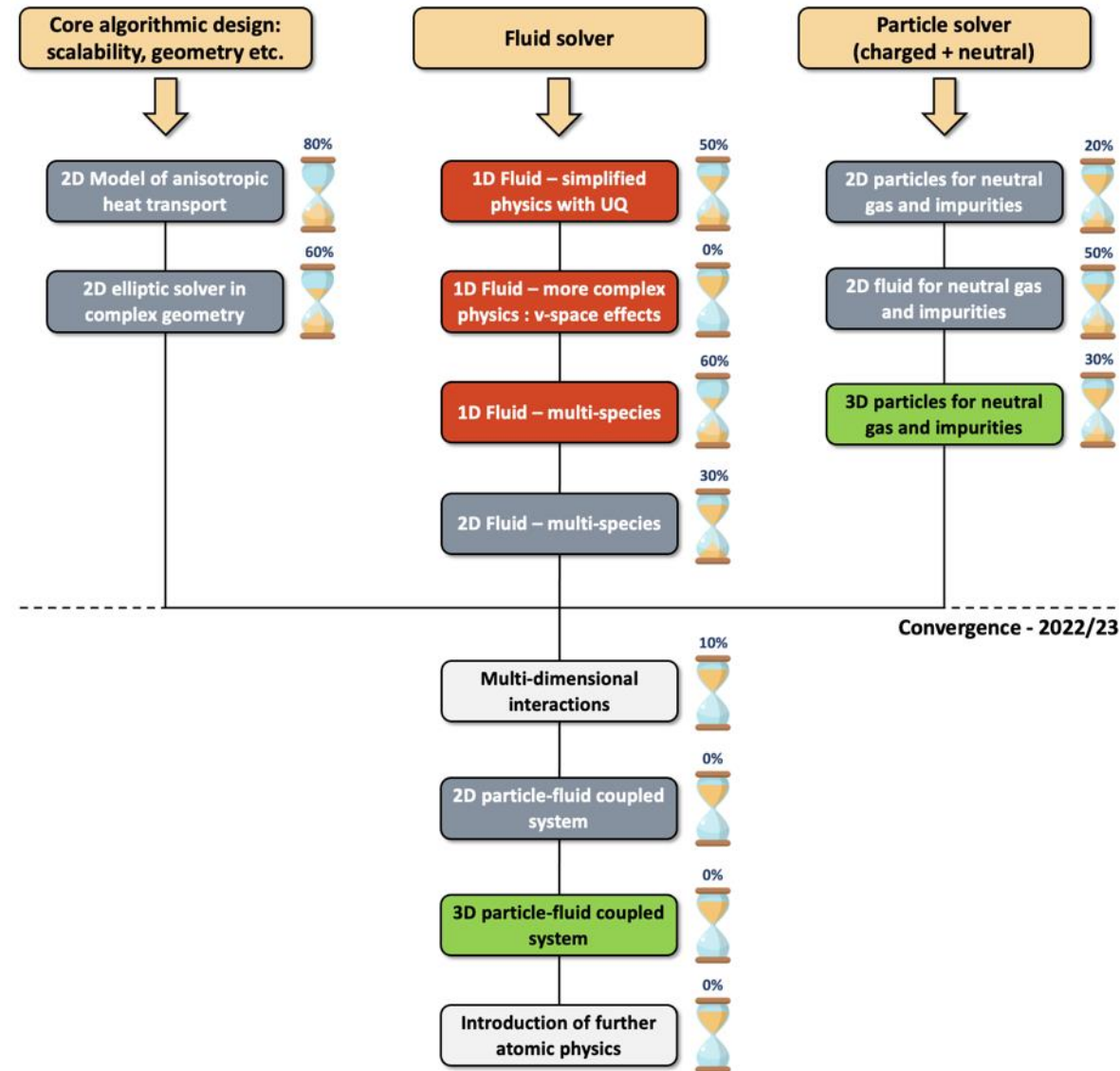
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Adapt to Tok. Sci. timeline and UK
Exascale roadmap....

Development by Proxyapps



Public Relations + Photography



- We need to work harder at our PR – the ExCALIBUR website needs more content...news articles, simulation imagery and also “events” **photographs**
- I have my camera – if anyone does not want their photo taken, please let me know and I will keep you out of the frame
- UKAEA will not use any images from this event without first seeking your consent (we have a special form which we will send out to those appearing in any images that are suitable)

www.excalibur.ac.uk

ExCALIBUR 10

About ExCALIBUR Themes Projects Resources News & Events Contact

Exascale Computing Algorithms & Infrastructures Benefiting UK Research (ExCALIBUR)

ExCALIBUR is a UK research programme that aims to deliver the next generation of high-performance simulation software for the highest-priority fields in UK research. It started in October 2019 and will run through until March 2025, redesigning high priority computer codes and algorithms to meet the demands of both advancing technology and UK research.

ExCALIBUR will achieve this by building on the four pillars:

Separation of Concerns	Co-design	Data Science	Investment in People
The algorithms that encapsulate the mathematics and physics of the problem are separated from the computational science of their implementation.	Holistic design of the software of the entire simulation system involving innovative collaborations between mathematicians, domain scientists and computational scientists.	Research to design new workflows adapted to managing & analysing vast volumes of data ingested and produced by simulations.	Improved RSE career development driven by professional forward-looking approach to scientific software design of simulation codes.

About ExCALIBUR

The programme is led by the Met Office and the Engineering and Physical Sciences Research Council (EPSRC) along with the Public Sector Research Establishment, the UK Atomic Energy Authority (UKAEA) and UK Research and Innovation (UKRI) research councils, including the Natural Environment Research Council (NERC), the Medical Research Council (MRC) and the Science and Technologies Facilities Council (STFC).

[More about ExCALIBUR →](#) [View ExCALIBUR funding →](#) [View ExCALIBUR governance →](#)

Sunak hails supercomputers as key to making UK leader of next generation technology



Suban Abdulla

13 June 2022 · 3-min read



In this article:



Rishi Sunak
British politician (born 1980)



Chancellor Rishi Sunak set out his vision on the first day of the annual London Tech Week conference celebrating the UK's tech sector. Photo: Daniel Leal/WPA Pool/Getty

UK gov taps Google's Ghahramani to head 'Future of Compute' review



Professor Zoubin Ghahramani

The UK government's "Future of Compute" review will be headed up by Zoubin Ghahramani, director of Google Brain and professor at Cambridge University.



Please see Owen Taylor, Wayne Arter, Ed Threlfall or myself if you have any problems...