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Scientific Computing



**CCP-WSI**  
a Collaborative Computational Project  
in Wave Structure Interaction

# OpenFOAM® Parallel Performance Engineering Workshop

Dr Stephen Longshaw

OpenFOAM Parallel Performance Engineering Workshop

Register

Agenda

5 - 6 June 2023

Time TBC

Daresbury Laboratory, Keckwick Lane, WA4 4AD



OpenFOAM

# Introduction to STFC



HM Government



Department for  
Science, Innovation  
& Technology



UK Research  
and Innovation



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# Welcome to Daresbury Laboratory

- One of STFC's 6 UK locations
- One of 2 of the UK's national laboratories
- Home to some of STFC's large facilities and associated activities:
  - Computational Science
  - Supercomputing
  - Particle accelerators
  - Engineering for Science
  - Business Incubation

UK Astronomy Technology Centre  
Edinburgh, Scotland



Polaris House  
Swindon, Wiltshire



Chilbolton Observatory  
Stockbridge, Hampshire



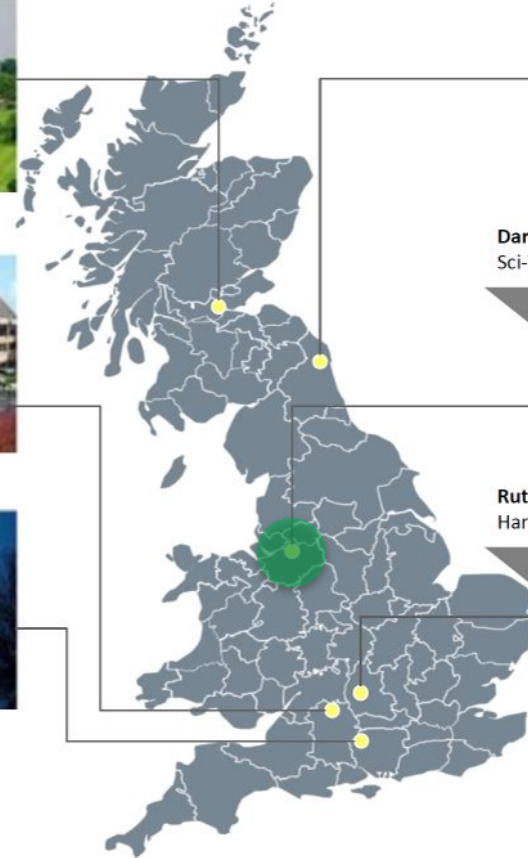
Boulby Underground  
Laboratory  
North Yorkshire



Daresbury Laboratory  
Sci-Tech Daresbury Warrington, Cheshire



Rutherford Appleton Laboratory  
Harwell Didcot, Oxfordshire



# Logistics

- This course will need you to have registered for the virtual teaching environment (referred to as the STFC DAaaS platform):
  - If you have not yet done this, please do it now (if you don't know how please ask)
- There is no fire alarm expected on either day, so if you do hear one then please exit the building immediately
- Course material is self contained within the virtual teaching environment and via GitHub <https://github.com/CCP-WSI/CCP-WSI-OpenFOAM-workshop>
- If you would like to order a taxi then please put your requirements on the provided form as early as possible
- Recommendations of where to get an evening meal will be in the wrap-up

**If you need to leave the room at any point, please make sure you take an access card with you (and then bring it back!)**



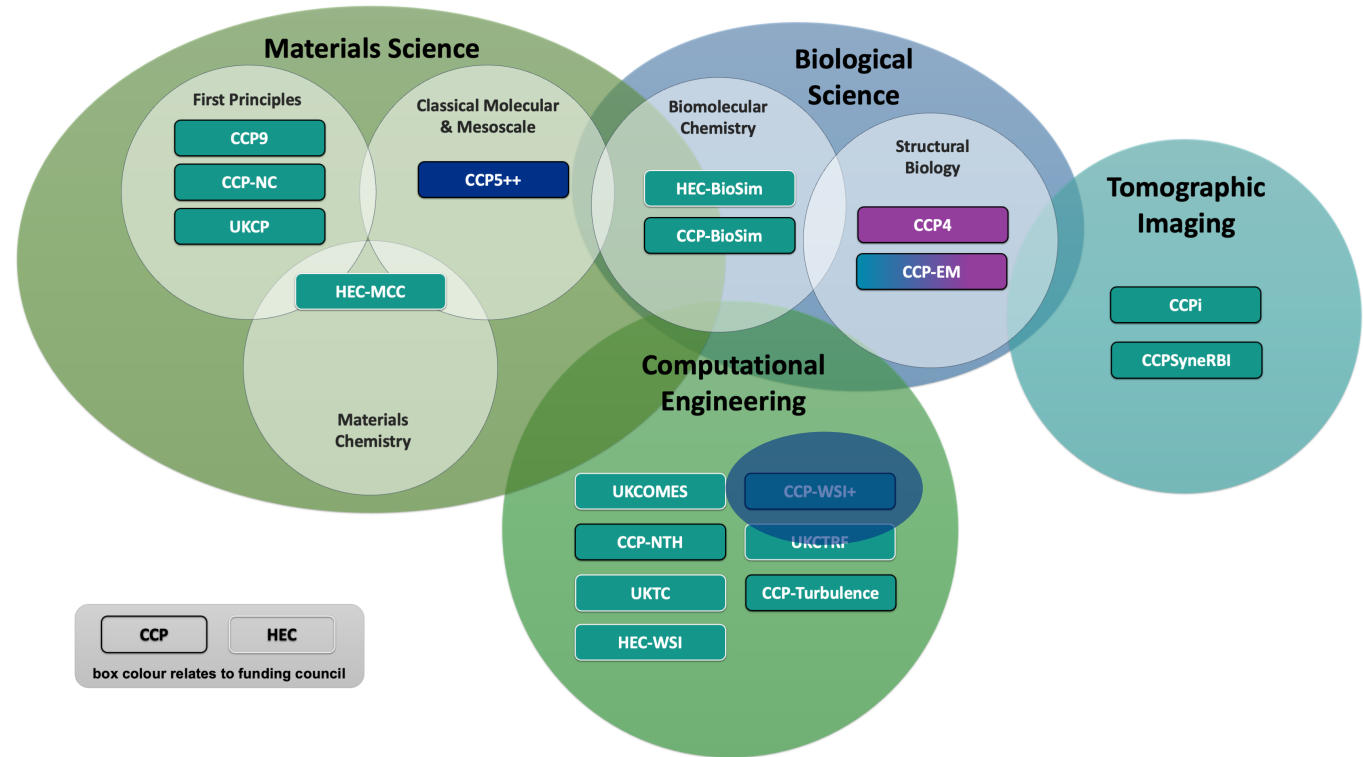
- Collaborative Computational Project on Wave Structure Interaction
- Chaired by Plymouth University
- Founded in 2016 and funded by EPSRC until September 2025
- Community building around computational methods and related software to solve problems related to WSI
- Directly supported by the STFC CoSeC programme to:
  - Deliver training
  - Implement, release and support software
  - Develop new computational modelling and simulation methods

# CoSeC

[www.cosec.stfc.ac.uk](http://www.cosec.stfc.ac.uk)



- The **C**omputational **S**cience **C**entre for Research **C**ommunities
- Around 30 STFC Computational Scientists and support staff
- Provides collaborative and domain-specific computational science support to around 20 CCP and HEC (High-end Consortia) communities across the sciences



- **H**igh **E**nd **C**onsortia on **W**ave **S**tructure **I**nteraction
- New EPSRC funded community running until December 2026
- Chaired by Plymouth University with the same working group as CCP-WSI
- Provides a simple and single point of entry for UK national supercomputing resources for UKRI funded work related to WSI
- Supported by CoSeC around application performance engineering and training
- Visit the HEC website to apply for access to the ARCHER2 service

Call	Closing date	Notes	Application form link
<b>Porting &amp; Benchmarking (PB)</b>	Always open	a short project of 3 months duration with a small number of allocation units for testing scalability	<b><u><a href="#">PB Form</a></u></b>
<b>Code Development (CD)</b>	Always open	a 6-month project with a small allocation for improving software performance	<b><u><a href="#">CD Form</a></u></b>
<b>Project Access (PA)</b> [Summer '23]	21st July 2023	a 12-month project with a large allocation for project runs	<b><u><a href="#">PA Form</a></u></b>
<b>ECR</b>	Always open	Dedicated allocation for early career researchers (ECRs) including training and support	<b><u><a href="#">ECR Form</a></u></b>

# Why Parallel?

- Useful OpenFOAM problems can involve a mesh with 10s of millions of cells
- Calculation of problems with useful mesh sizes can rarely be tackled using a single processor
- Modern workstations typically provide 10-64 cores per CPU, if all are used in parallel then these problems are now tangible
- What about even bigger problems or long time ranges?
- Then we can look to supercomputing resources – the UK national service ARCHER2 has over 750,000 cores available

**OpenFOAM has powerful parallel processing capabilities, but getting good scalability over large core counts is challenging - hopefully this course will help and provide some best practices**



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# OpenFOAM's Parallel Future

- Supercomputing has recently reached an exaflop (equal to over 40 ARCHER2 systems!)
- GPUs form a large part of the available performance
- Attempts to accelerate OpenFOAM using GPUs have happened already with limited success
- General MPI parallel scalability is also often limited compared to other CFD solvers, with solutions reaching 1000s of MPI ranks compared to 10s of thousands
- There are some ongoing large projects such as the EU H2020 exaFOAM project
- General parallel performance is improved incrementally in new releases – keep up to date!

# Agenda

## Day 1

<i>Time (British Summer Time GMT+1)</i>	<i>Title</i>	<i>Format</i>	<i>Person</i>
12:00 – 13:00		Lunch	
13:00 – 13:10	Welcome		Stephen Longshaw
13:10 – 14:00	OpenFOAM Fundamentals	Talk	Omar Mahfoze
14:00 – 14:15		Break	
14:15 – 14:45	Introduction to running OpenFOAM on ARCHER2	Talk	Raynold Tan
14:45 – 15:00	The Virtual Training Environment	Talk & Hands-on	Stephen Longshaw
15:00 – 15:30		Break	
15:30 – 16:45	Moving from Serial to Parallel OpenFOAM cases	Talk & Hands-on	Raynold Tan
16:45 – 17:00	Wrap-up day one	Talk & Feedback	Stephen Longshaw

## Day 2

<i>Time (British Summer Time GMT+1)</i>	<i>Title</i>	<i>Format</i>	<i>Person</i>
09:00 – 09:30	Welcome refreshments		
09:30 – 10:30	Programming Solvers in OpenFOAM	Talk & Hands-on	Wendi Liu
10:30 – 11:00		Break	
11:00 – 12:00	Attendee Support Session	Discussion	All
12:00 – 13:00		Lunch	
13:00 – 14:00	Parallel Programming in OpenFOAM	Talk & Hands-on	Xiaohu Guo
14:00 – 14:30	Dynamic Load Balancing with OpenFOAM	Talk	Xiaohu Guo
14:30 – 14:45		Break	
14:45 – 15:15	OpenFOAM Based Code Coupling	Talk	Stephen Longshaw
15:15 – 15:30	Wrap-up & close	Talk	Stephen Longshaw



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# Questions?