Mantid Developer Meeting and User Workshop

Report of Contributions

https://indico.stfc.ac.uk/e/mantid_meetings

Contribution ID: **1** Type: **not specified**

Visitor Badging

Monday, 3 November 2025 08:30 (30 minutes)

Receive badges at the Visitor Centre

Please note this is separate from registering for the facility. Please allow enough time for facility registration before Visitor Badging.

Badges will be required for lunch.

Session Classification: Developers Meeting - In Person

Contribution ID: **2** Type: **not specified**

Welcome

Monday, 3 November 2025 09:00 (15 minutes)

TBC

Session Classification: Developers Meeting - In Person

Contribution ID: **3** Type: **not specified**

Overview

Monday, 3 November 2025 09:15 (15 minutes)

An overview of the developer meeting and what to expect

Presenter: FOXLEY, Sarah (STFC)

Session Classification: Developers Meeting - In Person

Contribution ID: **4** Type: **not specified**

Icebreaker

Monday, 3 November 2025 09:30 (30 minutes)

Split into groups for the icebreaker Two Truths, One Lie

Session Classification: Developers Meeting - In Person

Contribution ID: **5** Type: **not specified**

Tours/Facility updates

Monday, 3 November 2025 10:20 (1h 40m)

TBC

Session Classification: Developers Meeting - In Person

Contribution ID: **6** Type: **not specified**

Hackathon of Hackathons - Introduction

Monday, 3 November 2025 13:00 (30 minutes)

Talk from Caila about recent Hackathon at ISIS and set up for the activity

Presenter: FINN, Caila (STFC)

Session Classification: Developers Meeting - In Person

Contribution ID: **7** Type: **not specified**

Hackathon of Hackathons - Part 1

Monday, 3 November 2025 13:30 (1h 15m)

Presenter: FINN, Caila (STFC)

Session Classification: Developers Meeting - In Person

Contribution ID: **8** Type: **not specified**

Hackathon of Hackathons - Part 2

Monday, 3 November 2025 15:15 (1 hour)

Includes feedback and summary

Presenter: FINN, Caila (STFC)

Session Classification: Developers Meeting - In Person

Contribution ID: **9** Type: **not specified**

Prep for Tuesday code camp

Monday, 3 November 2025 16:15 (30 minutes)

Presenters: PETERSON, Peter (Oak Ridge National Laboratory); FOXLEY, Sarah (STFC)

Session Classification: Developers Meeting - In Person

Contribution ID: **10** Type: **not specified**

Recap of previous day

Tuesday, 4 November 2025 09:00 (15 minutes)

Presenter: FOXLEY, Sarah (STFC)

Session Classification: Developers Meeting - In Person

Contribution ID: **11** Type: **not specified**

Code Camp

Tuesday, 4 November 2025 09:15 (2h 45m)

Attendees need to bring a laptop capable of making changes to Mantid or have access to a remote machine that can.

The exact topics for the code camps are dynamic and will be determined by the attendees during the meeting.

Presenters: PETERSON, Peter (Oak Ridge National Laboratory); FOXLEY, Sarah (STFC)

Session Classification: Developers Meeting - In Person

Contribution ID: **12** Type: **not specified**

Autoreduction and Live Reduction using Mantid at ORNL

Tuesday, 4 November 2025 13:30 (15 minutes)

Presenter: BACKMAN, Marie (Oak Ridge National Laboratory)

Session Classification: Developers Meeting - Hybrid

Contribution ID: **13** Type: **not specified**

Texture in Mantid

Tuesday, 4 November 2025 13:45 (30 minutes)

Demonstration and Discussion of the current state of play of texture reduction in mantid

Presenter: BRIDGER, Andy (STFC)

Session Classification: Developers Meeting - Hybrid

Contribution ID: **14** Type: **not specified**

Data Management at CSNS

Tuesday, 4 November 2025 13:00 (30 minutes)

In this presentation, we would share the development of the data management pipeline in CSNS. CSNS provides the users with a one-stop service for data-related tasks from experiments to post-experiment activities. Different online and offline data analysis programs are developed according to the requirements of various neutron spectrometers. A unified data portal was developed to meet the analytical needs of a wide range of scientific users.

Presenter: ZHANG, Junrong (China spallation neutron source)

Session Classification: Developers Meeting - Hybrid

Contribution ID: **15** Type: **not specified**

Release notes in Mantid

Tuesday, 4 November 2025 14:15 (20 minutes)

Presenter: MACIEL PEREIRA, Gui (STFC)

Session Classification: Developers Meeting - Hybrid

Contribution ID: **16** Type: **not specified**

Unwrapping NAPI

Tuesday, 4 November 2025 15:05 (15 minutes)

Most files used for neutron data in Mantid use the NeXus format (.nxs), which specifies a common file structure for neutron, X-ray, and muon scattering data. For many years, Mantid has relied on the NeXus API (NAPI) to handle all elements of reading and writing. However, NAPI development is no longer supported, and the API has not been updated in almost a decade. To move Mantid forward, we need to take ownership of our own file IO. Major work for releases 6.13 and 6.14 completely removed reliance on NAPI, building a new framework in HDF5 directly. This talk will cover the new system, caveats to maintaining it, and also mention the difficult process of phasing out highly prolific legacy code.

Presenter: BOSTON, Scott (Oak Ridge National Laboratory)

Session Classification: Developers Meeting - Hybrid

Contribution ID: **17** Type: **not specified**

Mantid in a Browser: a greener alternative to cloud servers?

Tuesday, 4 November 2025 15:20 (20 minutes)

Most major facilities using Mantid run data analysis servers for their users. In many cases these are cloud-based virtual machines (VMs) which are allocated to a single user. The specifications of these VMs are often defined by the most computationally expensive tasks required so in many simpler cases they are underused. Furthermore they are often idle as users are waiting for data or simply forget to shut down the VMs when they are done. The advantage of these systems is that users don't have to install any software or to download their data. This can also be achieved more efficiently with a file server (for the data) and a WebAssembly/Javascript app where the computations are carried on the user's own computer. In this presentation I show how the Mantid Framework can be compiled to WebAssembly (wasm)[1] and run in-browser using the Pyodide Python distribution. Some Mantid GUI interfaces were ported by using a wrapper layer which replaces qtpy with code which translates the PyQt/PySide calls to Javascript using the OS.js environment. This saves having to compile Qt and PySide to wasm (which is possible). The disadvantage of this approach is that it is limited to 4GB of memory as wasm is a 32-bit platform, but the target here is for less compute-intensive "first look" applications. The prototype implementation also does not support threading although this is possible with wasm. [1] https://github.com/mducle/micromantid

Presenter: LE, Duc (STFC)

Session Classification: Developers Meeting - Hybrid

Contribution ID: **18** Type: **not specified**

Data Handling for Mantid Consuming Workflows

Tuesday, 4 November 2025 15:40 (15 minutes)

A presentation detailing the methodology SNAPRed (https://github.com/neutrons/SNAPRed) used to approach handling of run data, its ancillary data objects, and how this interacts with the Mantid API.

Presenter: WALSH, Michael

Session Classification: Developers Meeting - Hybrid

Contribution ID: **19** Type: **not specified**

Dependency Management and Cybersecurity

Tuesday, 4 November 2025 15:55 (20 minutes)

Presenter: PETERSON, Peter (Oak Ridge National Laboratory)

Session Classification: Developers Meeting - Hybrid

Contribution ID: **20** Type: **not specified**

Recap of previous day

Wednesday, 5 November 2025 09:00 (15 minutes)

Presenter: FOXLEY, Sarah (STFC)

Session Classification: Developers Meeting - In Person

Contribution ID: **21** Type: **not specified**

Code Camp

Wednesday, 5 November 2025 09:15 (2h 45m)

Session Classification: Developers Meeting - In Person

Contribution ID: **22** Type: **not specified**

Lightening Talks

Wednesday, 5 November 2025 13:00 (1h 45m)

TBC

Session Classification: Developers Meeting - Hybrid

Contribution ID: **23** Type: **not specified**

Lightening Talks

Wednesday, 5 November 2025 15:45 (45 minutes)

TBC

Session Classification: Developers Meeting - Hybrid

Contribution ID: **24** Type: **not specified**

Close out

Wednesday, 5 November 2025 16:30 (30 minutes)

Presenters: PETERSON, Peter (Oak Ridge National Laboratory); FOXLEY, Sarah (STFC)

Session Classification: Developers Meeting - Hybrid

Contribution ID: **25** Type: **not specified**

Welcome

Thursday, 6 November 2025 10:00 (5 minutes)

For the User Meeting

Presenter: GRIFFIN, Hannah (STFC)

Session Classification: User Meeting (Hybrid)

Contribution ID: **26** Type: **not specified**

Introduction

Thursday, 6 November 2025 10:05 (10 minutes)

Presenter: COTTRELL, Stephen (STFC)

Session Classification: User Meeting (Hybrid)

Contribution ID: **27** Type: **not specified**

Technical Working Group Report

Thursday, 6 November 2025 10:35 (20 minutes)

Presenter: PETERSON, Peter (Oak Ridge National Laboratory)

Session Classification: User Meeting (Hybrid)

Contribution ID: **28** Type: **not specified**

Discussion

Thursday, 6 November 2025 10:55 (20 minutes)

Presenters: MARKVARDSEN, Anders (STFC); PETERSON, Peter (Oak Ridge National Laboratory); COTTRELL, Stephen (STFC)

Session Classification: User Meeting (Hybrid)

Contribution ID: **30** Type: **not specified**

Future Role of the Science Working Group

Thursday, 6 November 2025 11:15 (10 minutes)

Discussion session

Presenter: MARKVARDSEN, Anders (STFC)

Session Classification: User Meeting (Hybrid)

Contribution ID: **31** Type: **not specified**

Future of the User Meeting

Thursday, 6 November 2025 11:35 (10 minutes)

Part of the SWG discussion session

Presenter: COTTRELL, Stephen (STFC)

Session Classification: User Meeting (Hybrid)

Contribution ID: **32** Type: **not specified**

Discussion (Role of SWG)

Thursday, 6 November 2025 11:45 (15 minutes)

Presenter: MARKVARDSEN, Anders (STFC)

Session Classification: User Meeting (Hybrid)

Contribution ID: **33** Type: **not specified**

Thoughts about the SWG from the chair

Thursday, 6 November 2025 11:25 (10 minutes)

Presenter: SOKOLOVA, Anna (ACNS, ANSTO)

Session Classification: User Meeting (Hybrid)

Contribution ID: **34** Type: **not specified**

Mantid as a Project

Thursday, 6 November 2025 10:15 (20 minutes)

Presenter: MARKVARDSEN, Anders (STFC)

Session Classification: User Meeting (Hybrid)

Contribution ID: **35** Type: **not specified**

Discussion (Mantid Project)

Session Classification: User Meeting (Hybrid)

Contribution ID: **36** Type: **not specified**

Automation and/or Streaming of Mantid Data Treatments

Thursday, 6 November 2025 13:30 (20 minutes)

Session Classification: User Meeting (Hybrid)

Contribution ID: **37** Type: **not specified**

Texture Analysis (ISIS/PSI collaboration)

Thursday, 6 November 2025 14:10 (15 minutes)

Presenter: MALAMUD, Florencia (Paul Scherrer Institut)

Session Classification: User Meeting (Hybrid)

Contribution ID: **38** Type: **not specified**

Development of a Machine Learning Algorithm for WISH (ISIS application)

Thursday, 6 November 2025 14:25 (10 minutes)

Session Classification: User Meeting (Hybrid)

Contribution ID: **39** Type: **not specified**

Mantid Update from the CSNS

Thursday, 6 November 2025 15:40 (20 minutes)

Session Classification: User Meeting (Hybrid)

Contribution ID: **40** Type: **not specified**

Mantid Update from the ILL

Thursday, 6 November 2025 15:20 (20 minutes)

Presenter: ROLS, Stephane (Institut Laue Langevin)

Session Classification: User Meeting (Hybrid)

Contribution ID: **41** Type: **not specified**

Mantid Update from the SNS

Thursday, 6 November 2025 15:00 (20 minutes)

Session Classification: User Meeting (Hybrid)

Contribution ID: **42** Type: **not specified**

Mantid Update from the MLZ

Thursday, 6 November 2025 16:00 (20 minutes)

Presenter: KOSHCHII, Oleksandr (Forschungszentrum Juelich)

Session Classification: User Meeting (Hybrid)

Contribution ID: **43** Type: **not specified**

Mantid Update from ISIS

Thursday, 6 November 2025 13:50 (20 minutes)

Session Classification: User Meeting (Hybrid)

Contribution ID: **44** Type: **not specified**

Closeout

Thursday, 6 November 2025 16:20 (15 minutes)

Presenters: MARKVARDSEN, Anders (STFC); COTTRELL, Stephen (STFC)

Session Classification: User Meeting (Hybrid)

Contribution ID: **45** Type: **not specified**

Modernizing Scientific Software Documentation: From Qt Assistant to QtWebEngine in Mantid

Tuesday, 4 November 2025 16:15 (15 minutes)

Presenter: DINGER, Darsh (Software Engineer at SNS (ORNL))

Session Classification: Developers Meeting - Hybrid

Contribution ID: **46** Type: **not specified**

Beyond Conda: Pixi and the Future of Scientific Python Environment Management

Tuesday, 4 November 2025 16:30 (15 minutes)

Scientific software projects increasingly combine Python with C++, GPU toolkits, and other native dependencies, creating challenges for reproducibility, deployment, and cross-platform support. Traditional tools—Conda, Poetry, uv, Hatch, and PDM—address parts of this problem but leave gaps in speed, determinism, or multi-language integration. Pixi, a new environment manager built on Conda and conda-forge, combines multi-language package support with modern Rust-based performance and reproducibility features. It installs compiled libraries and compilers alongside Python packages, automatically maintains lockfiles, and ensures deterministic environments across Linux, macOS, and Windows. Pixi's high-performance solver accelerates dependency resolution while unifying Conda and PyPI packages. For deployment, Pixi offers portable environment archives, lightweight single-binary installs, and official container support, simplifying CI/CD pipelines and reducing environment drift. Compared to alternatives, Pixi provides speed, reproducibility, and multi-language capabilities that make it especially suited for scientific and HPC workflows.

Presenter: ZHANG, Chen (Oak Ridge National Laboratory)

Session Classification: Developers Meeting - Hybrid

Contribution ID: **47** Type: **not specified**

Close out

Tuesday, 4 November 2025 16:45 (15 minutes)

Presenter: FOXLEY, Sarah (STFC)

Session Classification: Developers Meeting - Hybrid

Contribution ID: **48** Type: **not specified**

Coderabbit: Worth using?

Wednesday, 5 November 2025 15:05 (5 minutes)

A 5 minute lightening talk

Presenter: BORREGUERO CALVO, Jose (ORNL)

Session Classification: Developers Meeting - Hybrid

Contribution ID: **49** Type: **not specified**

Discussion around using AI in Mantid

Wednesday, 5 November 2025 15:10 (35 minutes)

Following on from Jose's Coderrabbitai lightening talk we will open the floor to a general discussion on developers using AI in Mantid.

Session Classification: Developers Meeting - Hybrid

Contribution ID: **50** Type: **not specified**

Correcting spin leakage in ToF full polarisation analysis SANS experiments

Thursday, 6 November 2025 14:35 (10 minutes)

Presenter: ALBA VENERO, Diego (STFC)

Session Classification: User Meeting (Hybrid)