Instrument Data Scientists

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Data Management and Scientific Computing Division, ESS

2025-09-03

Science meets DMSC

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Overview

- What is an Instrument Data Scientist?
- Who are the Instrument Data Scientists?
- What do the Instrument Data Scientists know?
- How does one contact an Instrument Data Scientist?

What *is* an Instrument Data Scientist (IDS)?

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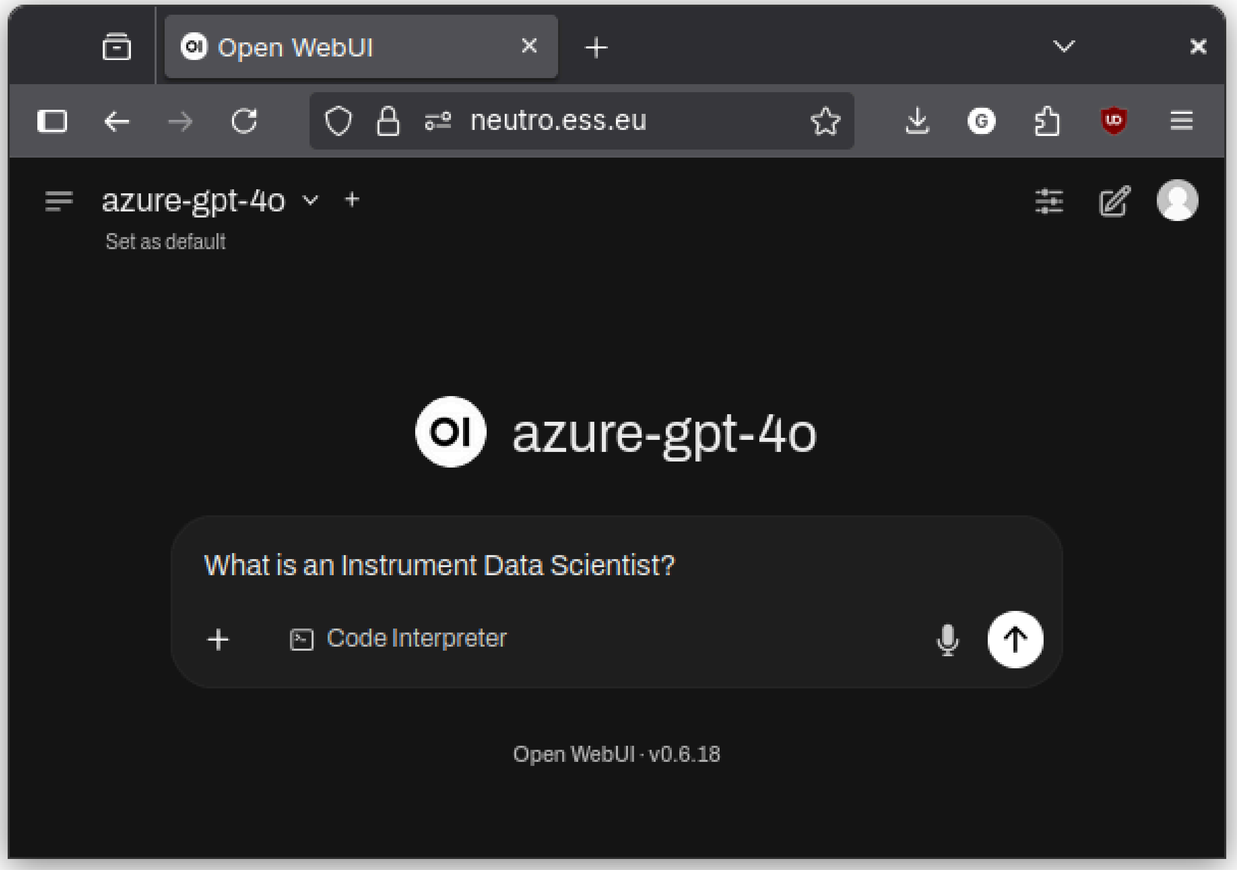


Neutro interpretation of the IDS R2A2

- Bridge instrument teams, users, and the **Data Management and Software Centre** (DMSC)
- Provide expertise in **scientific computing solutions**
    - for neutron scattering experiments
    - and instrument-specific workflows
- Drive efficient and sustainable delivery of data processing pipelines and user-facing tools

Key Responsibilities of an IDS

Interfacing and Collaboration

- **Primary liaison** between instrument teams, technology groups, and the DMSC.
- Actively work with users and teams to address their **scientific computing needs**.

Developing Solutions

- Oversee the **development and maintenance** of data processing pipelines.
- Contribute to **open-source software** projects.
- Provide training on the DMSC software suite to instrument teams and users.

Knowledge Sharing

- Collaborate with other IDSs and DMSC teams to create sustainable solutions.

Expertise and Advocacy

Scientific and Technical Excellence

- Represent DMSC at STAP meetings and **provide expert advice** on data and scientific computing.
- Conduct research, publish results, and present findings at conferences and workshops.
- Maintain accurate and up-to-date instrument models.

User Advocacy

- Assist users in analyzing, processing, and simulating experiment data.
- Actively advocate for the needs of the user community.

Why Instrument Data Scientists matter to ESS

Impact on ESS mission

- IDSs are critical to delivering user-friendly, robust **scientific computing solutions** at ESS.
- Ensure neutron scattering research is equipped with state-of-the-art computing tools for **data modeling, simulation, and processing**.
- Foster a culture of collaboration, sustainability, and **open science**.

Shaping the future of ESS

- IDSs play a pivotal role in transforming data workflows into practical solutions for world-class research.
- By enabling **seamless data pipelines**, IDSs contribute to making ESS the most **advanced neutron source** in the world.

Who are the Instrument Data Scientists?

Céline Durniak
DREAM & BEER

Søren Schmidt
ODIN

Gregory Tucker
BIFROST & CSPEC

Aaron Finke
NMX

Nicolò Paracini
ESTIA

Oliver Hammond
LOKI & SKADI

Iurii Kibalin
MAGIC

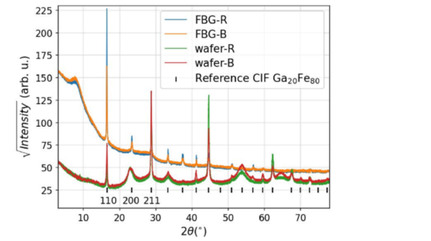
(Oct) Christian Beck
CSPEC & MIRACLES

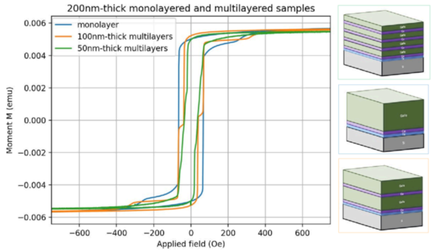
(Nov) Bing Li
TREX

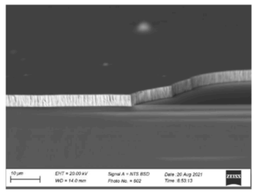
What do the Instrument Data Scientists know?

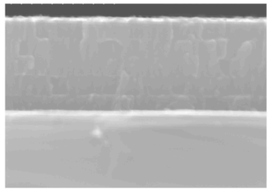
Céline

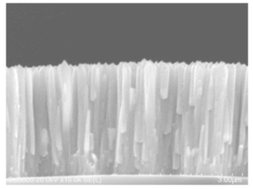
- Magnetostrictive Fe-Ga thin films
- Amorphous materials
- MD simulations







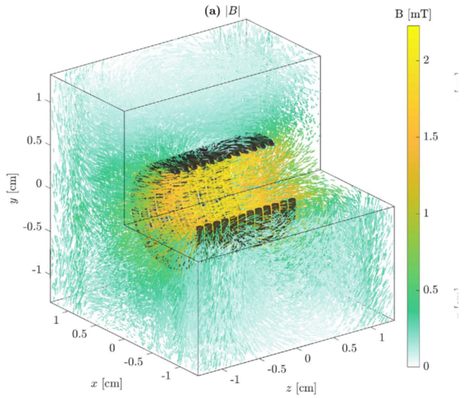




What do the Instrument Data Scientists know?

Søren

- Structural evolution
- Multi-scale/multi modal characterization
- Applied math: pattern recognition, tensor tomography
- ESS SOLID Lighthouse
- Affiliated Professor at DTU Compute



What do the Instrument Data Scientists know?

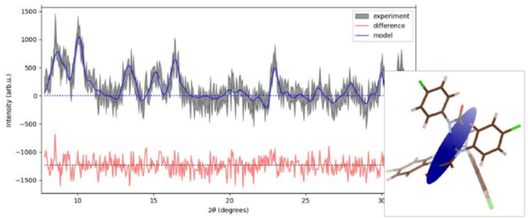
Iurii

Principal Developer of the Crystallographic Library CrysPy

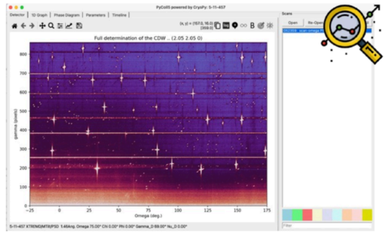
- Data treatment for powders and single crystal samples measured by polarized neutron diffraction.
- Analysis local magnetic anisotropy in molecular magnets, nanoparticles, and related materials.
- I am particularly interested in *advancing this technique for application with pulsed neutron sources*.

Principal Developer of the PyColl5 Software

- Designed for the visualization and analysis of experimental data collected on single-crystal diffractometers at ILL, including D10+, D9, D23, and XTREMED.



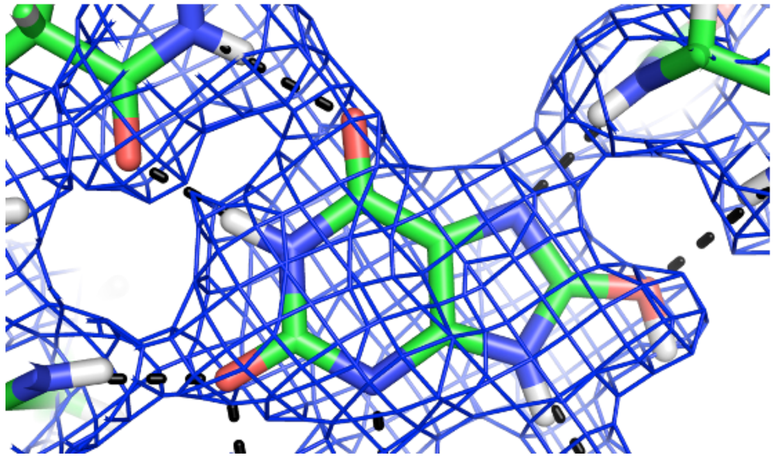
Polarized powder diffraction profile of Co-SMM and magnetization ellipsoid of Co.



PyColl5 interface displaying data collected on XTREMED@ILL.

What do the Instrument Data Scientists know?

Aaron



- Protein and Small Molecule Crystallography
- Physical Organic Chemistry
- Crystallographic Data Collection Strategies
- Algorithms for Processing Reflection Data

What do the Instrument Data Scientists know?

Nico

- bilogical grazing incidence scattering
- model cell membranes
- reflectometry sample environment

What do the Instrument Data Scientists know?

Oliver

- Focused on understanding soft materials with techniques for small angle scattering
- specifically with connections to Ionic Liquids and eutectic solvents
- Adjunct Professor, KTH Royal Institute of Technology

What do the Instrument Data Scientists know?

Interests

- magnetic excitations
- method development for
  - instrument twin simulations
  - data reduction & analysis

Projects

- alternate McStas code generator `mccode-antlr`
- faithful instrument simulations
  - `mcstas-` comps: `readout-master`, `detector-tubes`, `epics-link`, …
  - orchestration: `restage`, `mccode-plumber`, `stacktainer`
  - (BIFROST) calibrated instrument(s): `niess`
- data reduction, reliable $(\boldsymbol{Q},E)$ to (ψ,k_{free}): `undual`
- data analysis, symmetry for cheaper model evaluations: `brille`

What do the Instrument Data Scientists know?

Soft matter inelastic neutron scattering

- the effects of monodispersity vs. polydispersity
- investigation of the kinetically changing samples (e.g. thermal denaturation, crystallization)
- method development for non-standard acquisition modes (FWS on IN16b)

Complimentary scattering techniques user

- SANS
- Xrays
- DLS

What do the Instrument Data Scientists know?

Bing

- Scientific Background:
  - PhD in Condensed Matter Physics (2022). Studied spin dynamics in Magnetic Topological Insulators/Semimetals
  - Computational Instrument Scientist in the Triple-Axis Spectroscopy group in Oak Ridge National Laboratory (2024-2025)
- Expertise:
  - Scientific software development for Inelastic neutron scattering data reduction/analysis
  - Modeling and interpretation of magnetic excitations in quantum magnets
- Research interests:
  - Emergent phenomena in quantum materials arising from the correlation and competition among electronic, lattice, and magnetic degrees of freedom, e.g. chiral magnons, altermagnetism.
  - At ESS, I will focus on integrating instrument development with resolution-aware computational modeling to explore quantum magnets

Contact an Instrument Data Scientist

- (Internal) E-mail alias: ids@ess.eu
- Confluence: confluence.ess.eu/display/IDS
- Slack: #dmsc-ids
- In person

Thanks for listening!
Questions?