



Instrument Data Scientists

PRESENTED BY GREG TUCKER

2023-10-05

Agenda



- 1 Instrument Data Scientists
- 2 Role of the Instrument Data Scientist
- 3 Scientific subject matter expertise
- 4 Potential interactions with DTU & UCPH

Instrument Data Scientists



Small Angle
Scattering



Wojceich Potrzebowski

Diffraction



Celine Durniak

Imaging



Søren Schmidt

Spectroscopy



Gregory Tucker

Macromolecular
Crystallography



Justin Bergmann

Reflectometry



Your Name Here ([Now](#))

Spectroscopy Too



Your Name Here (Later)

...



Your Name Here (Later)

Role of the Instrument Data Scientist (IDS)



Science

- developing data science and data analysis methods
 - advancing the cutting-edge of their domain
- establishing a scientific research programme

Project management

- DMSC deliverables to their respective instrument teams
- Participate in the construction projects of their respective instruments

User support

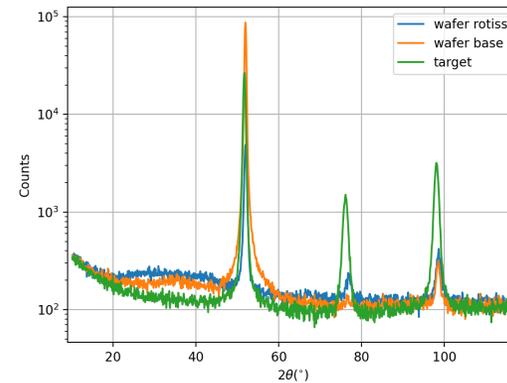
- Provide direct support to the experimental program advancing the cutting-edge of their domain
- Assist facility users with the analysis of collected data
- Create and maintain a world-leading user program as part of their respective instrument teams

Scientific subject matter expertise



Celine Durniak - Diffraction

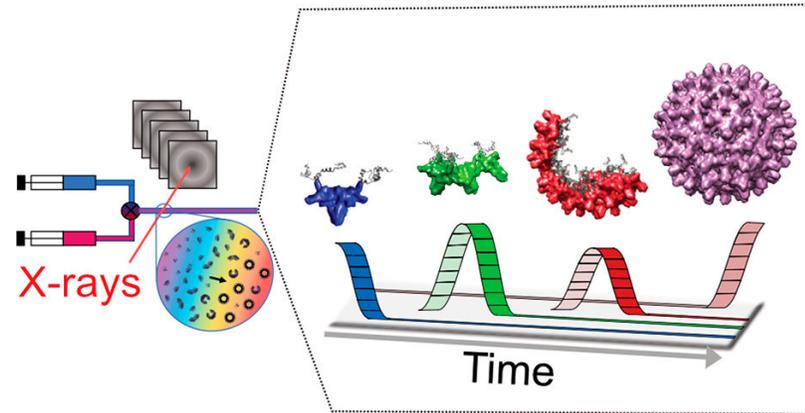
- Magnetostrictive GaFe thin films
- amorphous materials
- MD simulations
- QENS



Scientific subject matter expertise

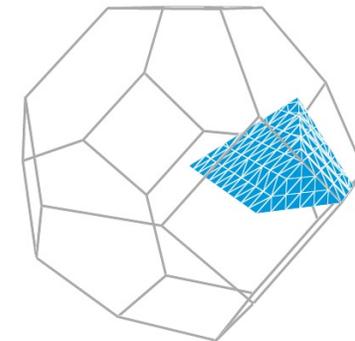
Wojceich Potrzebowski - SANS

- Self-assembly
- Viruses
- Bayesian statistics
- Atomistic simulations
- Multimodal analysis
- SasView



Gregory Tucker – Neutron Spectroscopy

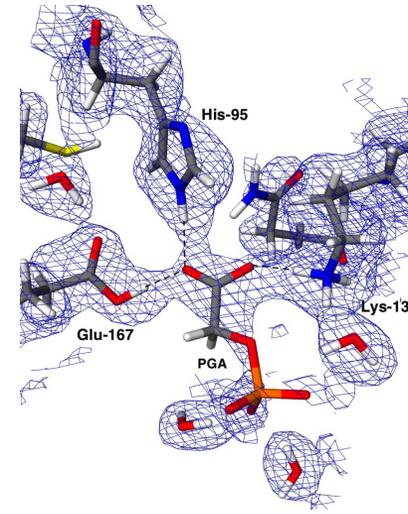
- inelastic neutron scattering & instrumentation
- Magnetic excitations
- Symmetry for modelling codes



Scientific subject matter expertise

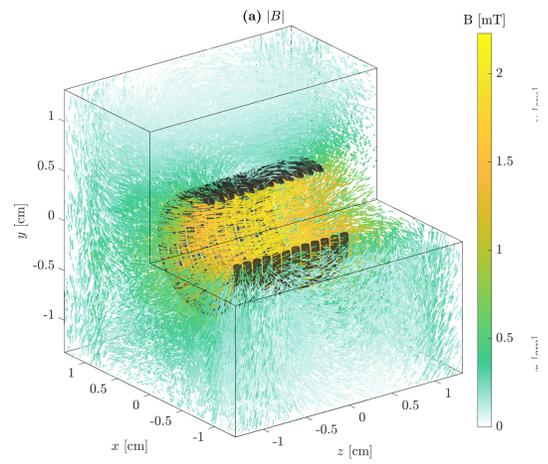
Justin Bergmann – Single Crystal Diffraction

- Protein crystallography
- Accurate hydrogen location
- Element identification



Søren Schmidt – Imaging & Eng. Diffraction

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





Potential interactions with DTU&UCPH (next couple of years)

- Design of experiments
- Method development
- Simulations
- Data analysis
- Already collaborating with Kim Lefmann, E-learning platform (McStas online)
- Future: E-learning courses (e.g. Sasview)
- Open source collaborations – network to other neutron facilities
- Consultants on data science applications
- Co-supervision of Bachelors, Masters, and Ph.D. students



Possibility to involve neutron scattering

Large-Scale Structures	ODIN Imaging Instrument					
	SKADI General Purpose SANS					
	LOKI Broadband SANS					
	Surface Scattering					
	FREIA Horizontal Reflectometer					
	Estia Vertical Reflectometer					
Diffraction	HEIMDAL Powder Diffractometer					
	DREAM Powder Diffractometer					
	Monochromatic Powder Diffractometer					
	BEER Engineering Diffractometer					
	Extreme Conditions Diffractometer					
	MAGiC Magnetism Diffractometer					
NMX Macromolecular Diffractometer						

Spectroscopy	CSPEC Cold Chopper Spectrometer				
	Broadband Spectrometer				
	T-REX Thermal Chopper Spectrometer				
	BIFROST Crystal Analyser Spectrometer				
	VESPA Vibrational Spectroscopy				
	MIRACLES Backscattering Spectrometer				
	High-Resolution Spin-Echo				
	Wide-Angle Spin-Echo				
	Particle Physics Beamline				

	life sciences		magnetism & superconductivity
	soft condensed matter		engineering & geo-sciences
	chemistry of materials		archeology & heritage conservation
	energy research		particle physics



Finish presentation

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