



# Instrument Data Scientists

PRESENTED BY GREG TUCKER

2023-10-05

# Agenda



- 1 Instrument Data Scientists

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- 2 Role of the Instrument Data Scientist

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- 3 Scientific subject matter expertise

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- 4 Potential interactions with DTU & UCPH

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# Instrument Data Scientists



Small Angle  
Scattering



Wojciech Potrzebowski

Diffraction



Celine Durniak

Imaging



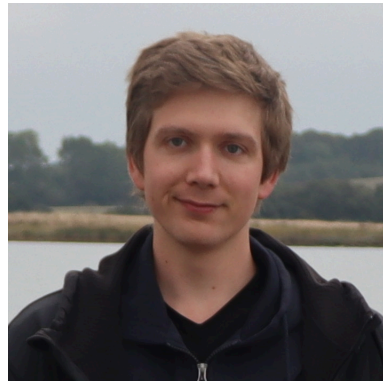
Søren Schmidt

Spectroscopy



Gregory Tucker

Macromolecular  
Crystallography



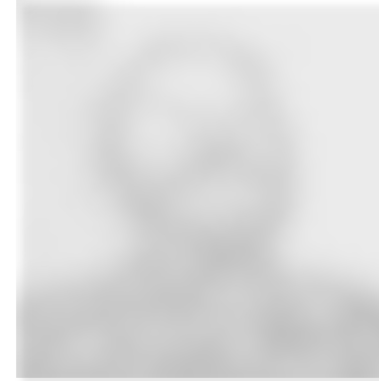
Justin Bergmann

Reflectometry



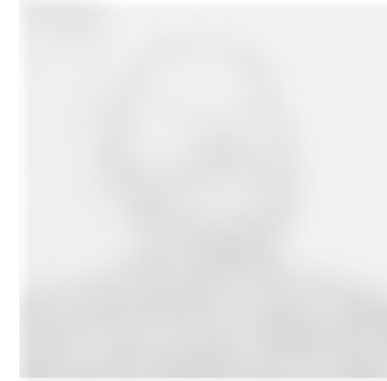
Your Name Here ([Now](#))

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

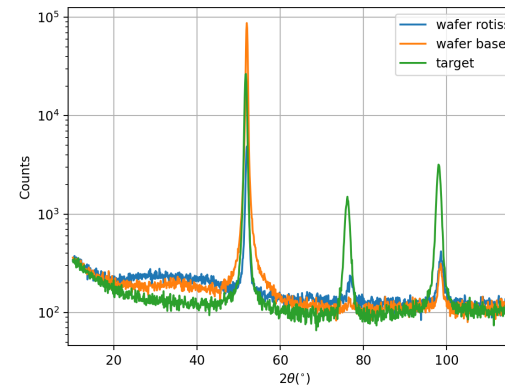
- Provide direct support to the experimental program advancing the cutting-edge of their domain
- Assist facility users with the analysis of collected data
- Create and maintain a world-leading user program as part of their respective instrument teams

# Scientific subject matter expertise



## Celine Durniak - Diffraction

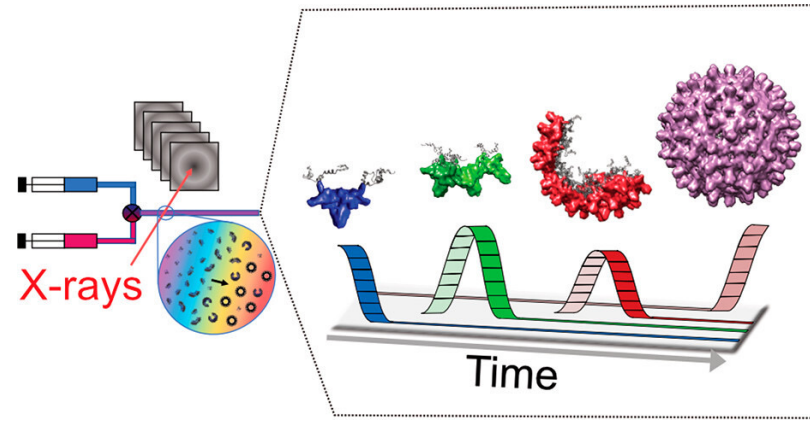
- Magnetostrictive GaFe thin films
- amorphous materials
- MD simulations
- QENS



# Scientific subject matter expertise

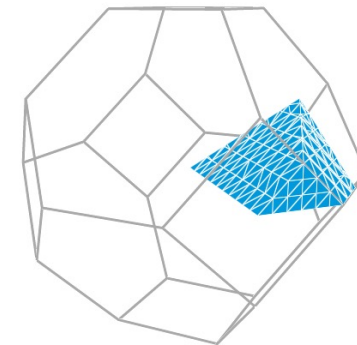
## Wojceich Potrzebowski - SANS

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



## Gregory Tucker – Neutron Spectroscopy

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

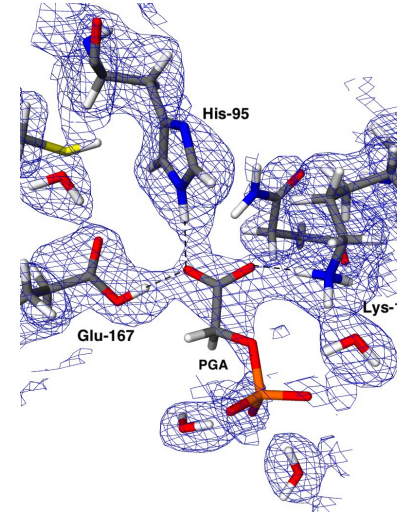


# Scientific subject matter expertise



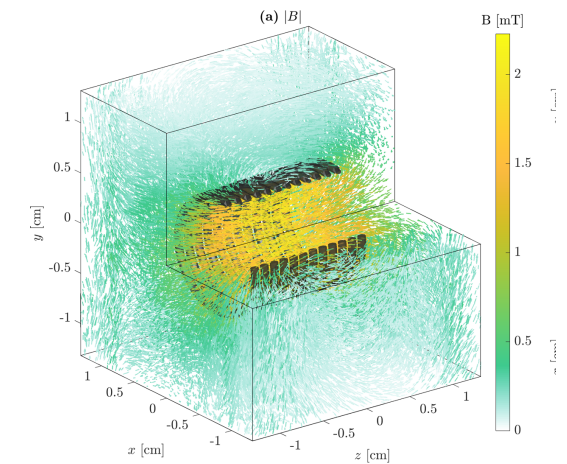
## Justin Bergmann – Single Crystal Diffraction

- 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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