Data Management and Software Centre and the plans for powder diffraction software

Céline Durniak

Data Reduction, Analysis and Modelling group
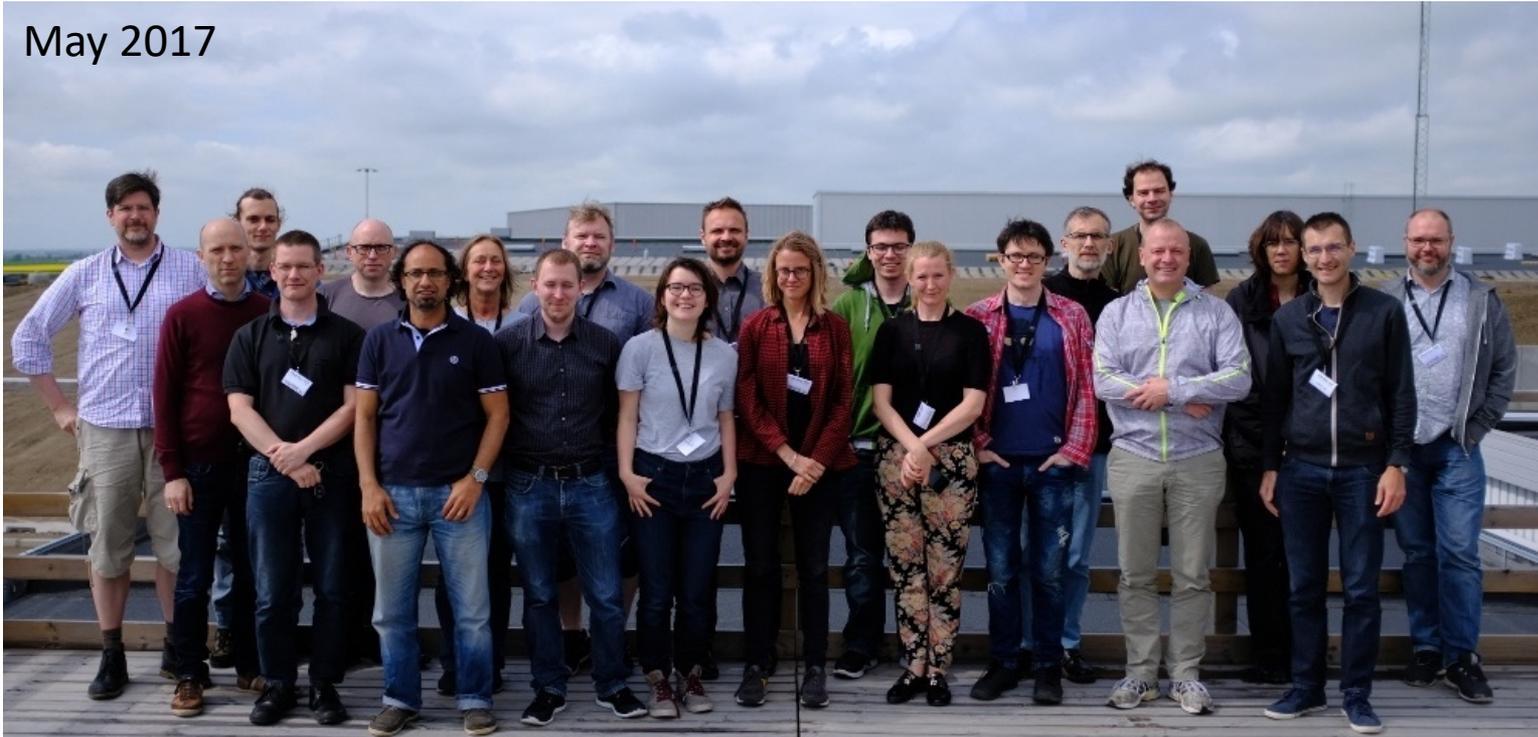
DMSC

Copenhagen Denmark

26 June, 2018
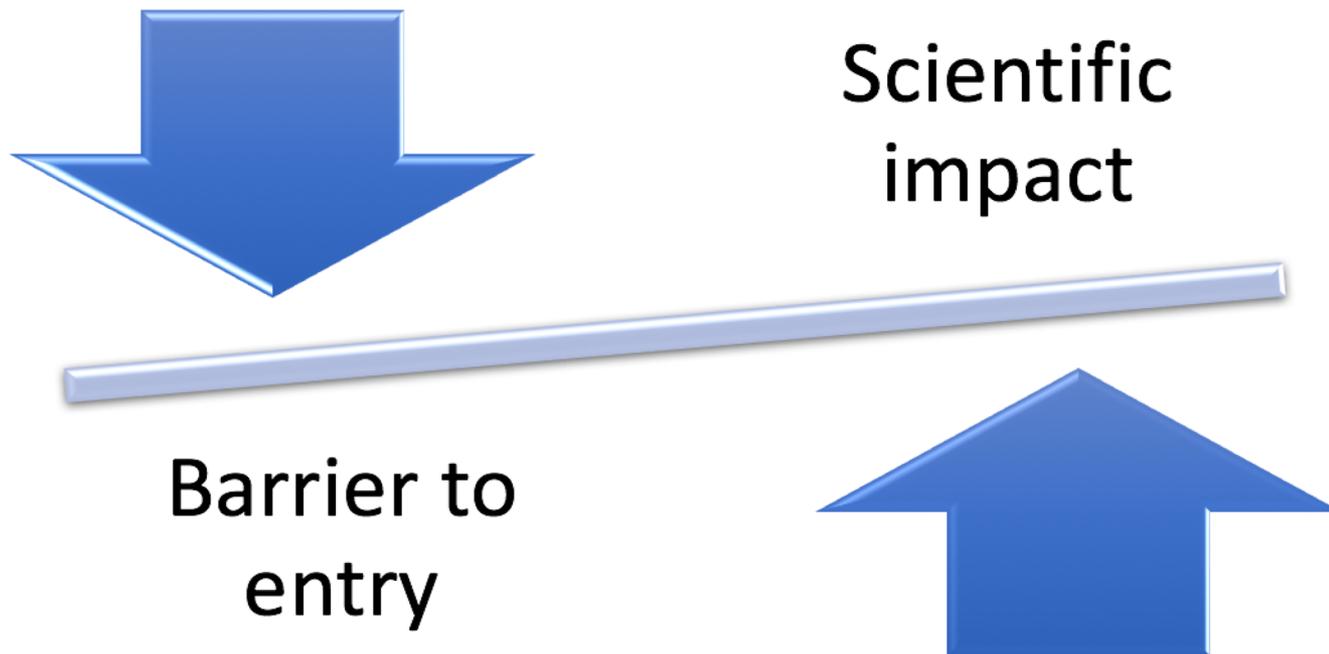
The team

May 2017

June 2018: 24 staff members in Copenhagen, Denmark

Background in physics, chemistry, biophysics, modelling and software development
- Additional staff at ISIS, PSI and MLZ
- Joint post docs with universities and other facilities (externally funded)

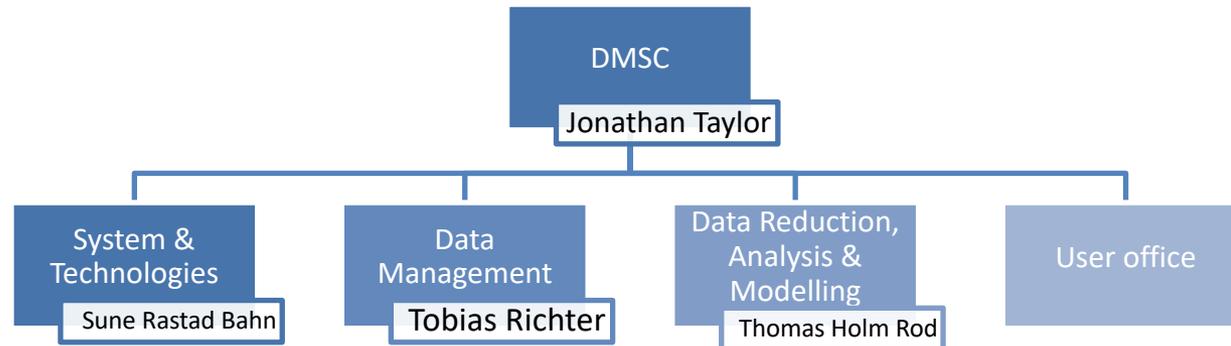- Minimise the time it takes to understand experimental data

Scientific impact

Barrier to entry

- Maximise the scientific impact and scientific success of ESS

DMSC organized according to scope

```
                        DMSC
                   Jonathan Taylor
        ┌─────────────┬─────────────┬─────────────┐
   System &        Data         Data Reduction,    User office
   Technologies    Management    Analysis &
                                 Modelling
   Sune Rastad Bahn  Tobias Richter   Thomas Holm Rod
```

Integrated data processing pipeline – software stack and partners

Software

| Experiment control | Stream events & meta data | Data reduction | Data visualization | Data analysis | Data management |

Partners

technique-dependent
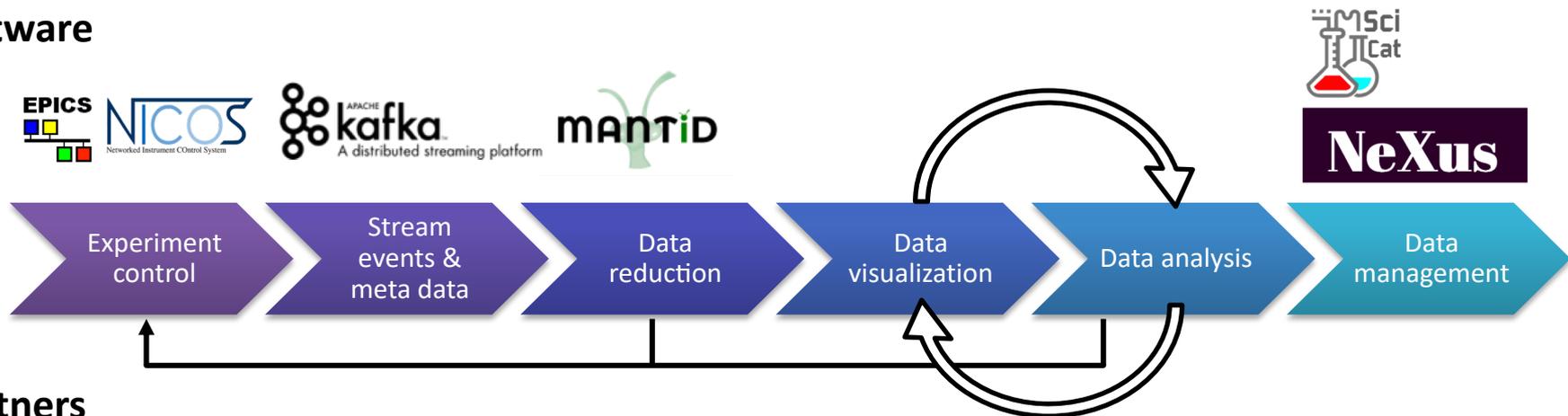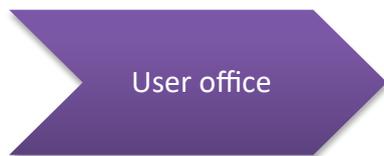
Make *integrated* data processing pipeline work smoothly and seamlessly

For each step: provision *maintainable* software

For data analysis: build on *existing* software / frameworks

User office

User interface before / during / after experiment

Before experiment
- Virtual simulations using *McStas*
- User Office

During experiment
- Real time plots for data collection / reduction / simple analysis

After experiment
- Remote desktops to access / process data
- Jupyter notebooks
- Web interfaces (SciCat)

EUROPEAN
SPALLATION
SOURCE

Need for many **different** and **independently** developed software packages

Methods

- Fitting to models, specific for each technique and science
- Molecular dynamics simulations
- Spin dynamics simulations
- Quantum chemistry methods
- Tomography incl. for ToF
- Monte Carlo simulations
- Machine learning methods…

Challenges

- Technical debt
- Single-point of failure
- Lack of standards
- Not open-source software

Software development

- Poor documentation – if any
- *Not* user-friendly
- Is not inter-operable
- Users are diverse

User experience

ESS will support ~15 programs for analysis

Expert user   User   First time user   Software developer

ESS strategy for maintainable and user-friendly software

ESS should be able to maintain, sustain and (rapidly) extend chosen software.

Focus on *few* existing programs and ensure:

- Modularization / APIs
- CLI (Python) & GUI
- Facilitate 3rd party contributions
- Fully open source and free
- Quality assurance (testing)
- Documented both for users and developers
- No single point of failure
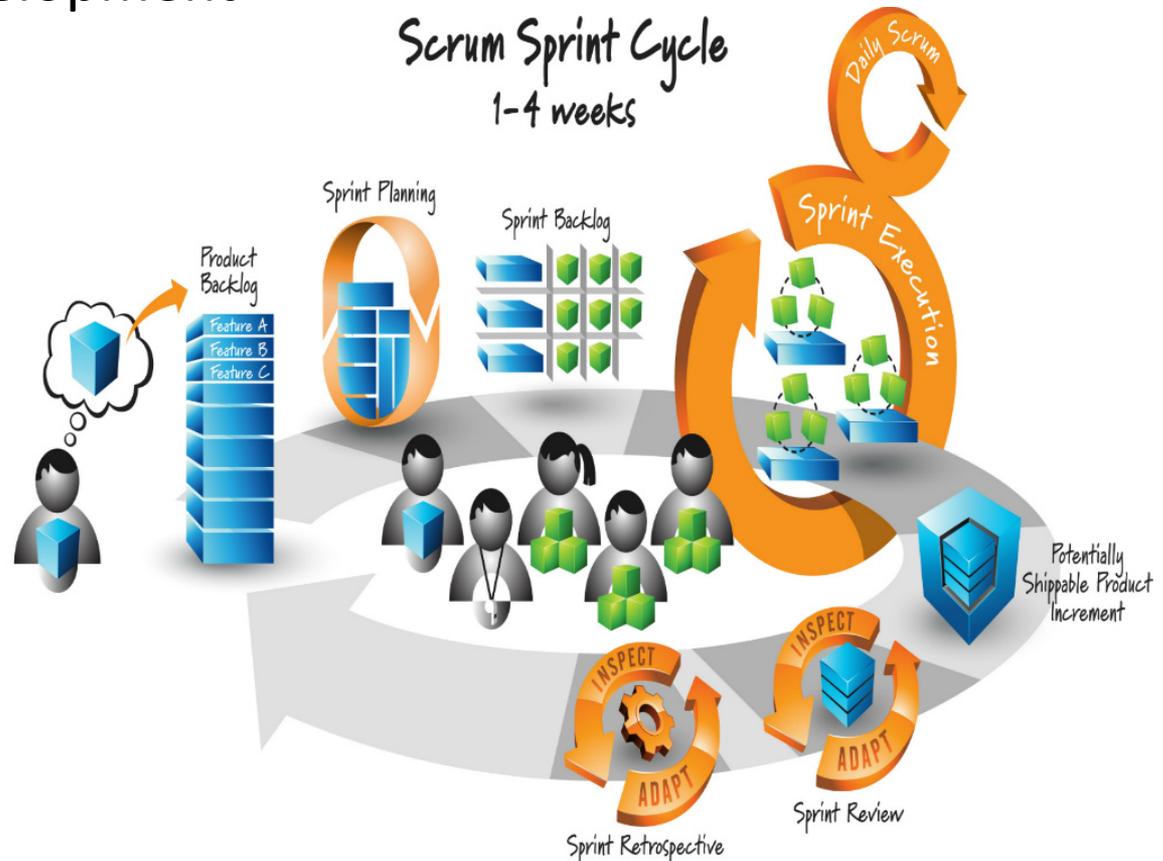- Widely used (preferably the standard)

Standard & Guidelines

Preferred languages

- *ESS may install software not maintained by ESS*
- *Users are free to use their own (analysis) software solutions*

Software development methods & tools

- For example in Data Analysis and Modelling group
  - Agile software development

Scrum Sprint Cycle
1-4 weeks

Daily Scrum

Sprint Planning

Sprint Backlog

Sprint Execution

Product Backlog
Feature A
Feature B
Feature C

Potentially Shippable Product Increment

INSPECT
ADAPT
Sprint Retrospective

INSPECT
ADAPT
Sprint Review

Software development methods & tools

- For example in Data Analysis and Modelling group
  - Agile software development
  - Code under version control

Software development methods & tools

- For example in Data Analysis and Modelling group
  - Agile software development
  - Code under version control
  - Build system **Jenkins**
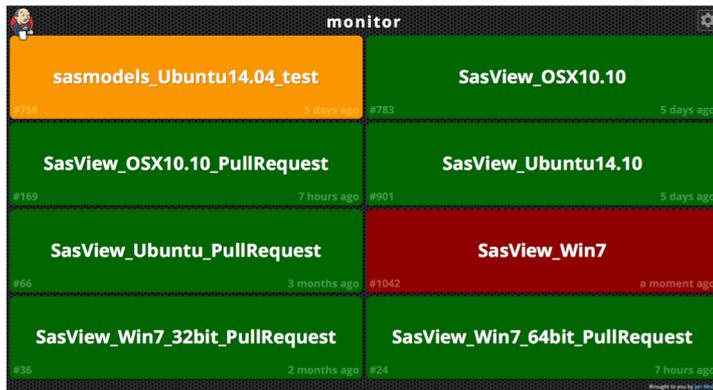
Data Analysis & Modelling collaborations & funding

EUROPEAN SPALLATION SOURCE

Construction project

1 project
(1 post doc
@ Chalmers)

CHALMERS

2 projects
(1 post doc @ LU,
1 post doc @ ISIS)

Vetenskapsrådet

Interreg
Öresund-Kattegat-Skagerrak
European Regional Development Fund

EUROPEAN UNION

ESS & MAX IV:
Cross Border
Science and Society

MAX4ESSFUN: 2
projects (2 x 6 months)

HORIZON 2020

SINE2020

Inter-operability

Technique	Software	Responsible
Standard & Guidelines		ISIS
Data reduction	MANTID	ILL, FZJ, PSI
Imaging	MuhRec / KipTool	PSI (LLB + ESS)
SANS	SasView	ESS
Reflectometry	BornAgain	FZJ
QENS	MANTID	ILL and ISIS

Data Reduction Analysis and Modelling software development

Interfacing

Future developments
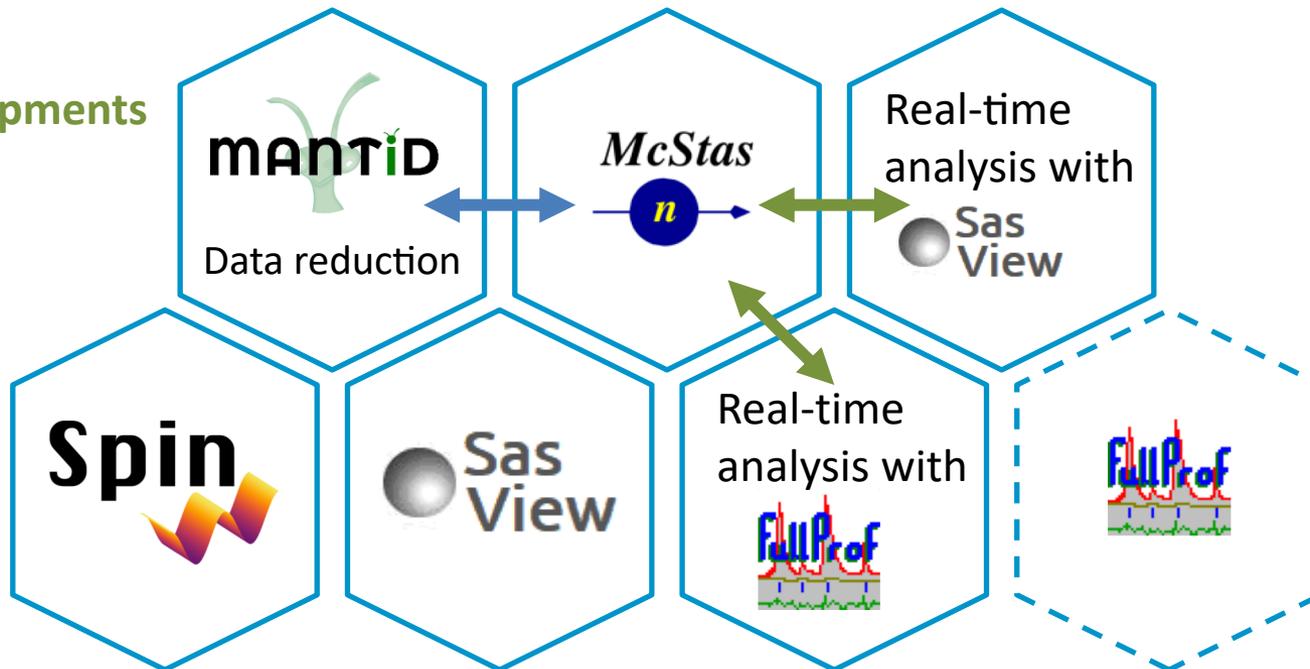
Powder diffraction

Diffractometers at the ESS

engineering

NMX
single crystal

BEER

MAGIC
single crystal

DREAM
powder

HEIMDAL
powder
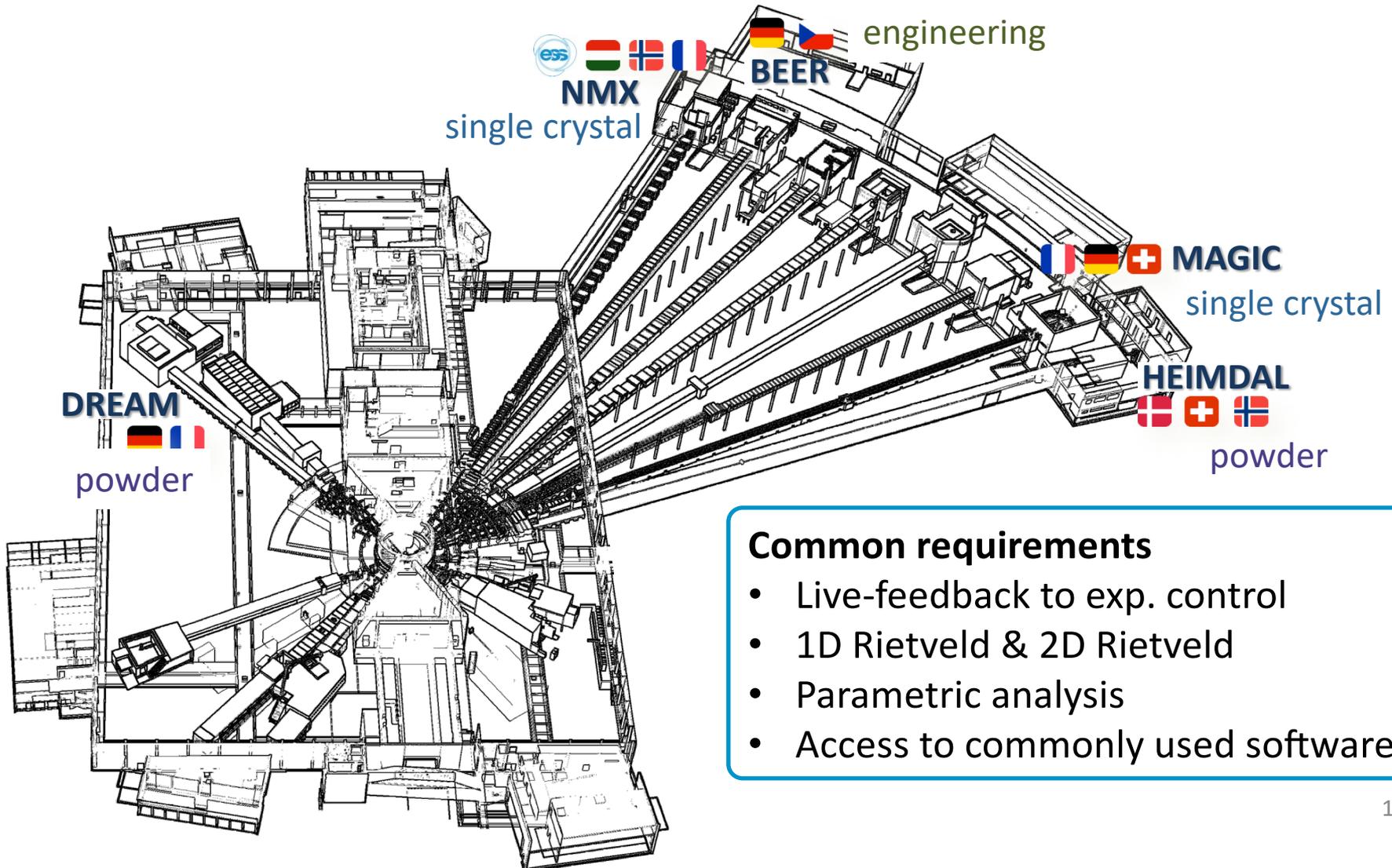
Common requirements
- Live-feedback to exp. control
- 1D Rietveld & 2D Rietveld
- Parametric analysis
- Access to commonly used software

Analysis of powder diffraction data

"Rietveld" programs	Language(s)
FullProf	Fortran
Jana2006	Fortran
GSAS II	python / Fortran
Maud	Java → C++
Topas	

"real space" programs		Language(s)
Small-box	pdfgui	python
	Diffpy-cmi	python
Large-box	RMCProfile	Fortran
	Rmc++	C++

Preferred solution

Work with *ILL* to convert *FullProf* into sustainable software:

- Fully Open Source
- Python scripting interface
- Qt based GUI

- Modularize
- Documentation
- Quality assurance

- 2D Rietveld

and make other major codes available as well

Proof-of-concept
real-time analysis powder diffraction data
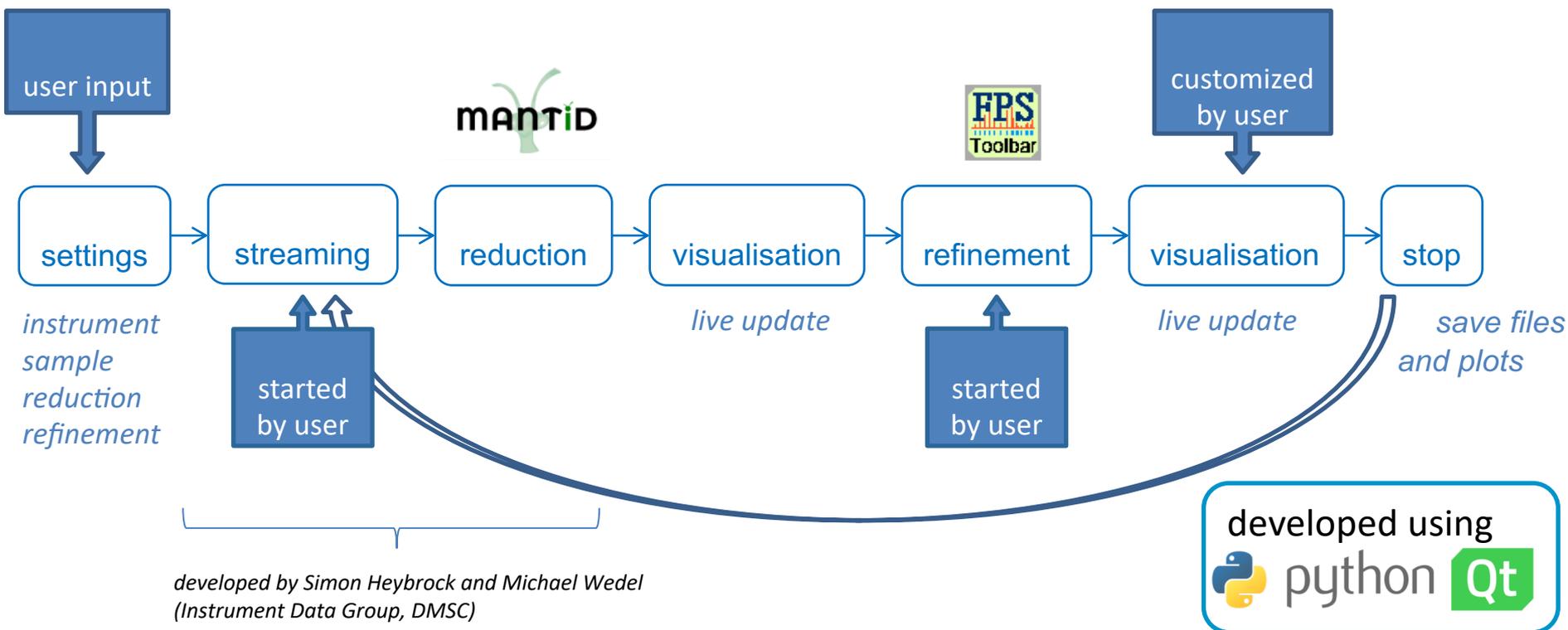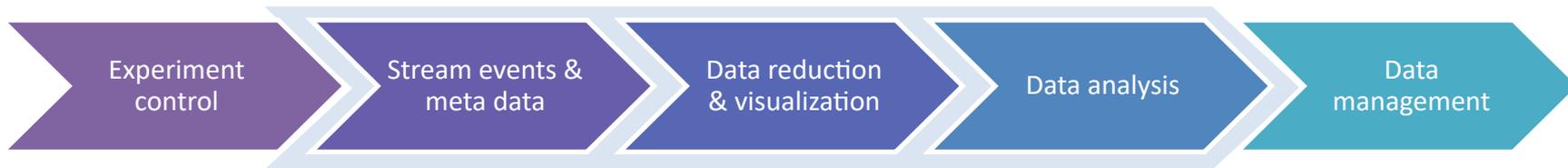
Restrictions: Simple analysis (one dimensional, limited number of refined parameters)

GUI of proof-of-concept

Training for Staff – keep up-to-date with techniques

- Participation to neutron experiments

D4

NOVA

POWGEN

- Programming language courses / conferences

- User experience course

UX course at DMSC Feb 2018

Upcoming events

July
16-19
Visit ILL - collaboration with Juan Rodriguez Carvajal

September
12
Satellite workshop on single crystal diffraction
Lund, Sweden

November
5-8
Neutron experiment on Engineering diffractometer

November
6
Data curation workshop at DMSC