ESS Data Management & Software Center

- en dansk del af ESS

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DTU Fysik
Institut for Fysik

The Data Management and Software Centre

- Data Management
- Instrument Control
- Data Reduction & Analysis
- Instrument simulations
- (Theory and simulations)

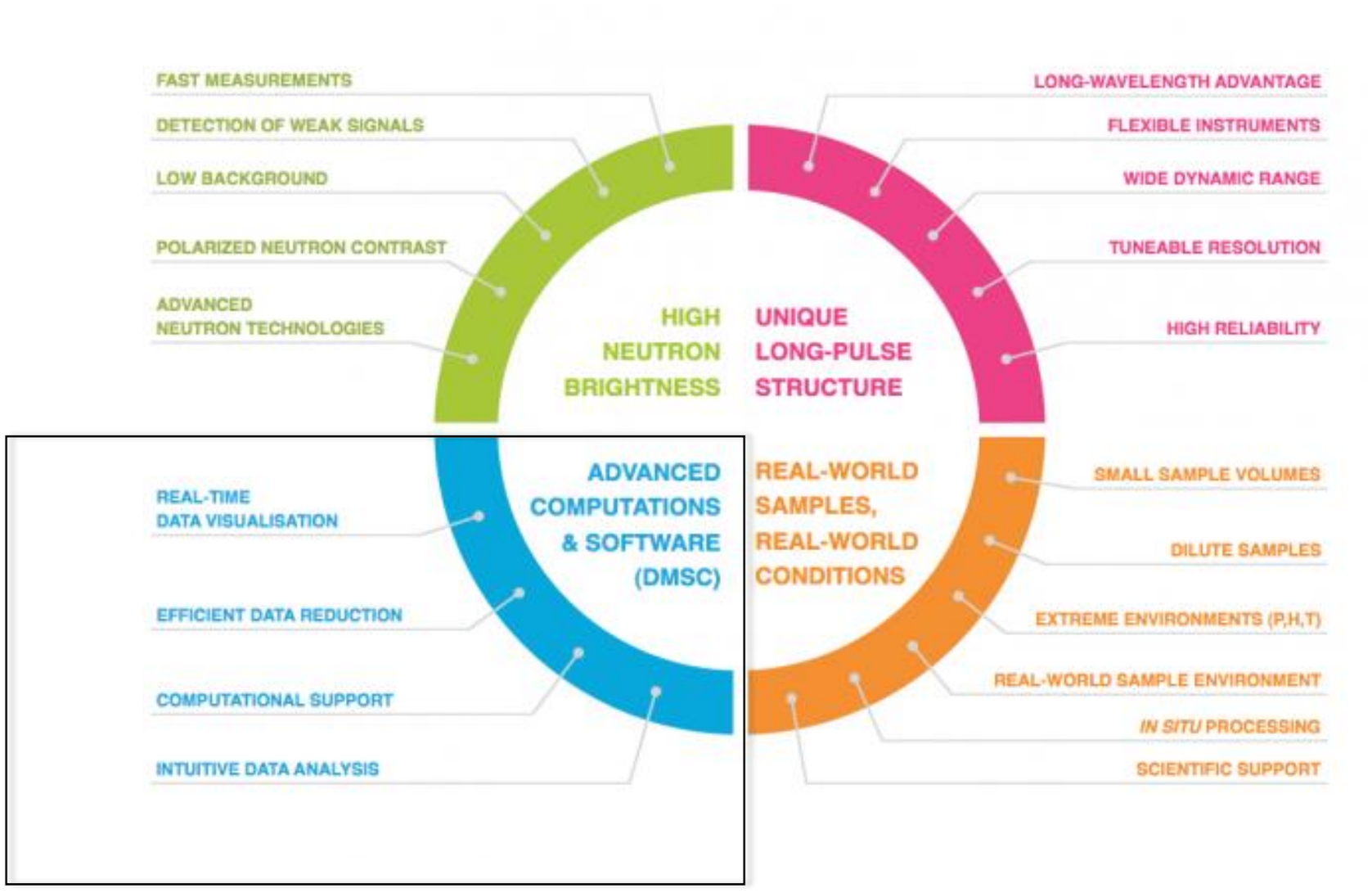
Built on DK competences!

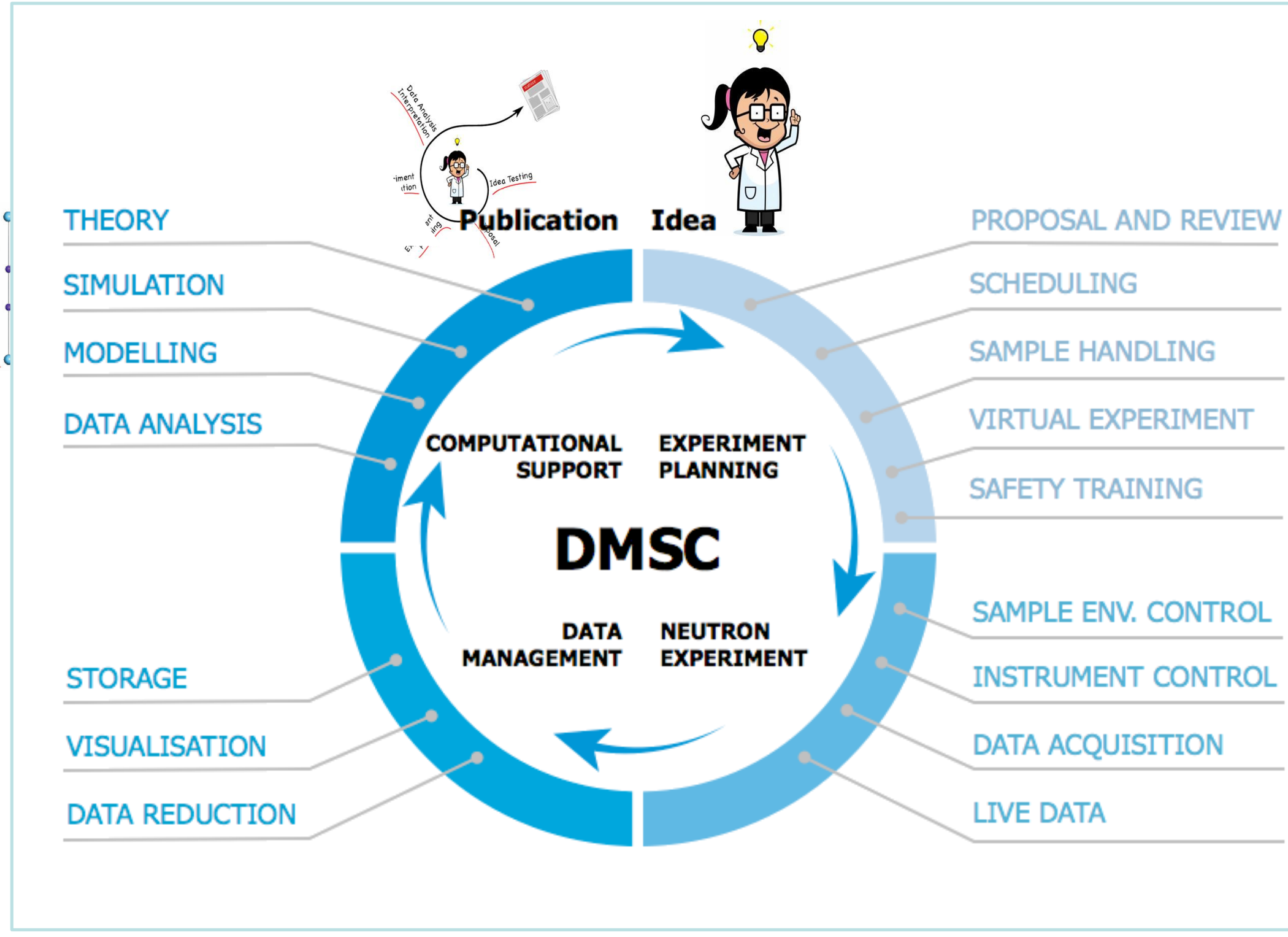
EUROPEAN SPALLATION SOURCE

DTU

Technical Design Report (2013)

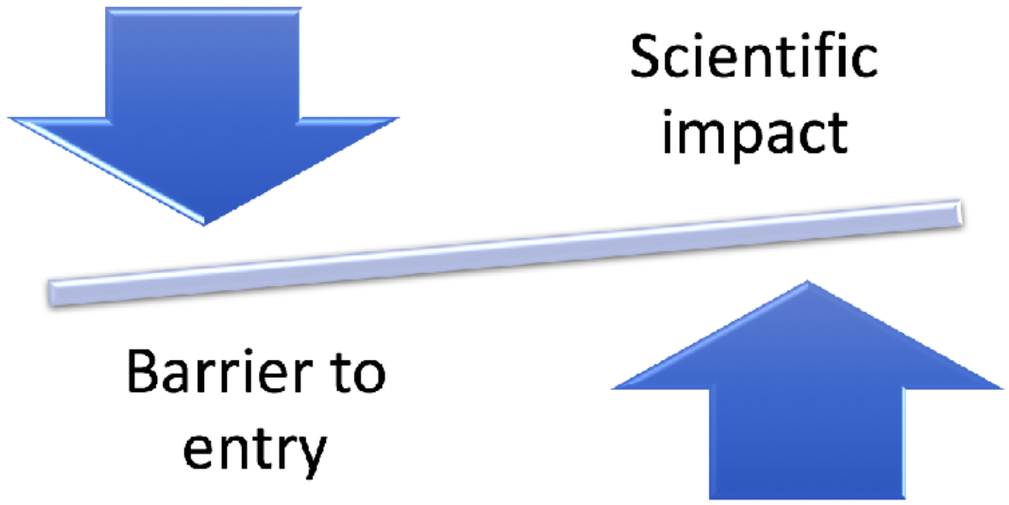
Importance of computing was emphasized already in design phase




Publication
Idea
Data Analysis Interpretation
Idea Testing
THEORY
SIMULATION
MODELLING
DATA ANALYSIS
PROPOSAL AND REVIEW
SCHEDULING
SAMPLE HANDLING
VIRTUAL EXPERIMENT
SAFETY TRAINING
COMPUTATIONAL SUPPORT
EXPERIMENT PLANNING
DMSC
DATA MANAGEMENT
NEUTRON EXPERIMENT
STORAGE
VISUALISATION
DATA REDUCTION
SAMPLE ENV. CONTROL
INSTRUMENT CONTROL
DATA ACQUISITION
LIVE DATA

DMSC objective

Minimize the time it takes to analyze and interpret experimental data



This is particular important for neutron sources due to the cost of producing neutrons

Maximise the scientific impact and success of ESS by serving the needs of both non-expert and advanced users

The user community is diverse – even for each instrument

Non-expert and occasional user (few days/year)

Graphical User Interface

Experienced (daily) or geeky user

python™

MATLAB

Command Line Interface

DMSC

Facility datarates:
~ TB / instrument / day
~ PB / instrument/ year

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TO DO:
Scientific computing and software for ALL of this

NM

HIRACLES

MAGIC

T-REX

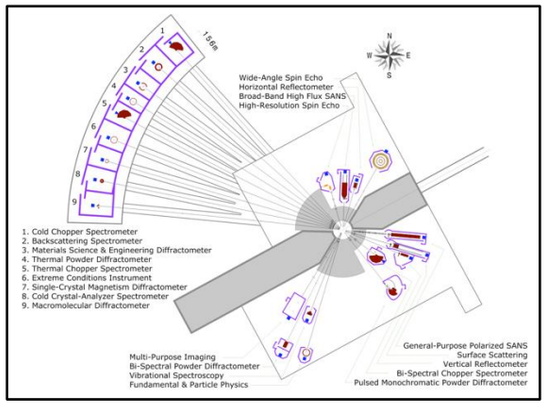
HEIMDAL

ODIN

Data Management

Data Analysis

DMSC's Domain and Interfaces

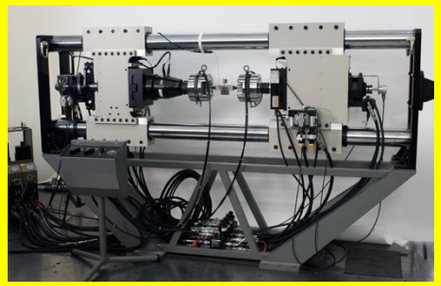


INSTRUMENT TECHNOLOGIES

Choppers

Motion Control

Sample Environment



Fast Sample Environment

Detectors & Monitors

Fast Data Readout

INTEGRATED CONTROL SYSTEMS

Timing

EPICS

Control Box

DATA MANAGEMENT & SOFTWARE CENTRE

Data Aggregator & Streamer

Instrument Control Room

User Control Interface

Mantid
Live, Local & Remote Data Reduction

Data Analysis Interfaces

ESS Server Room

Automated Post Processing

Mantid

DMSC Server Room

We must cater for many different scientific domains

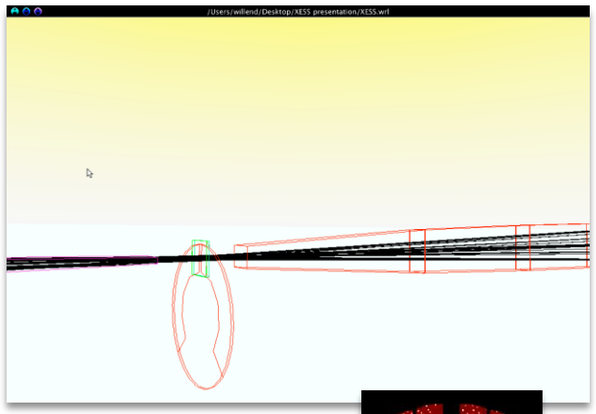
Instr.		Tasks	Programs
ODIN	Im	Computed Tomaggrapy, ToF, diffraction imaging, polarization	➢ MuhRec
BEER, DREAM, HEIMDAL, MAGIC, NMX	Diffraction	➢ 2D Rietveld ➢ Resolution func. ➢ Time-of-flight	➢ FullProf ➢ Esmeralda ➢ Phenix
LoKI, SKADI, ESTIA, FREIA	Large-scale	➢ 2D Fitting ➢ Polarization ➢ Ab initio model	➢ SASView ➢ CCP-SAS ➢ ?
C-SPEC, VOR, T-REX, BIFROST, MIRACL, VESPA	Spectroscopy	➢ Resolution func. ➢ Spin dynamics ➢ Molecular dyn. ➢ DFT	➢ MANTID ➢ VATES/HORACE ➢ SpinW ➢ LAMMPS ➢ VASP

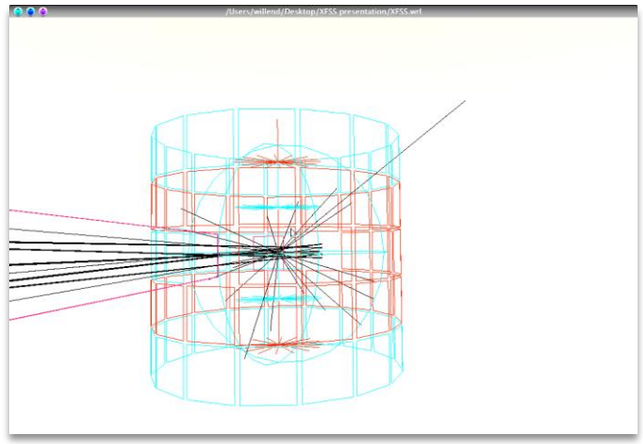
(Incomplete list)

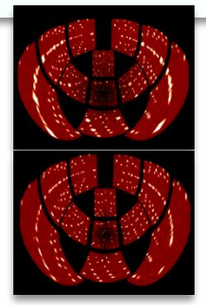
What is McStas used for?

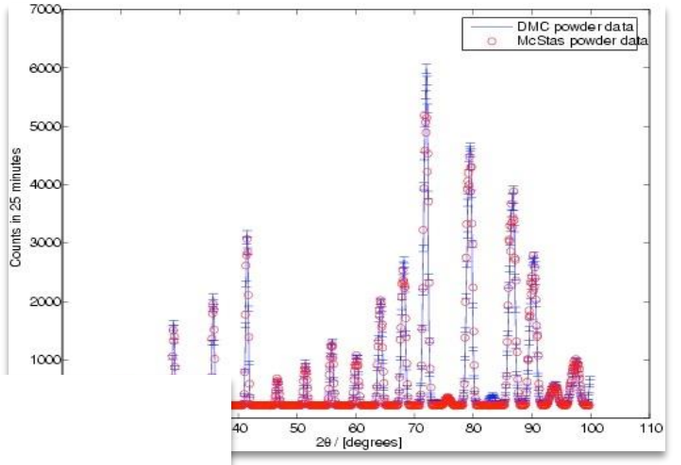
- Instrumentation
- Virtual experiments
- Data analysis
- Teaching

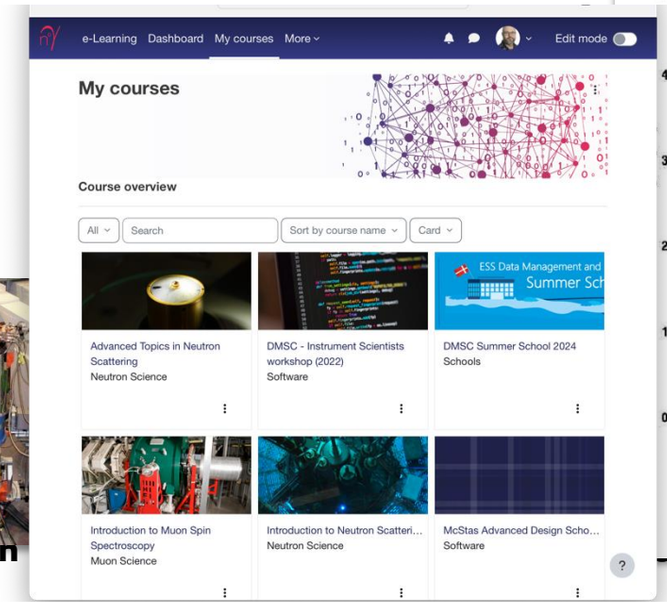
(KU, DTU)

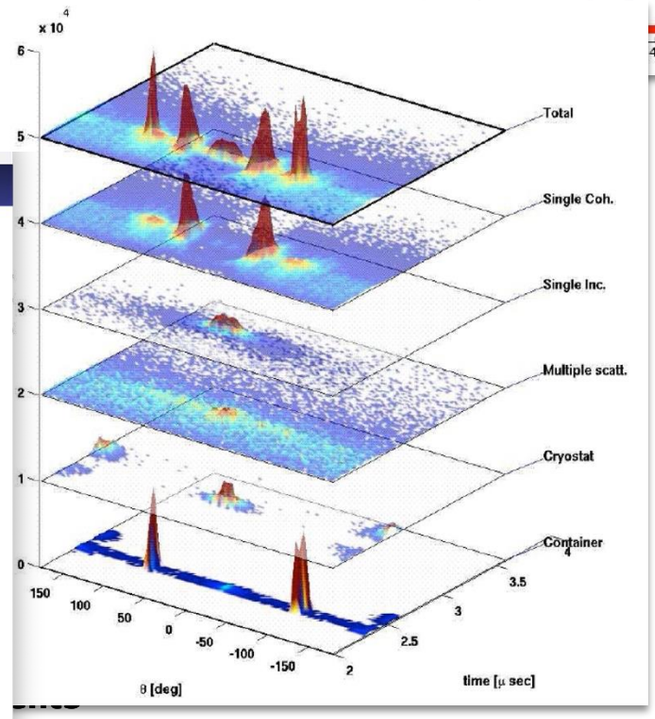


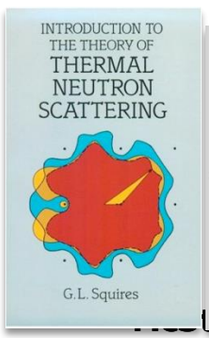


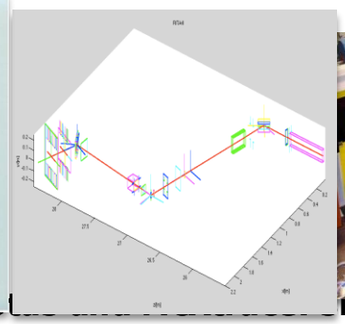












Scientific computing gives understanding

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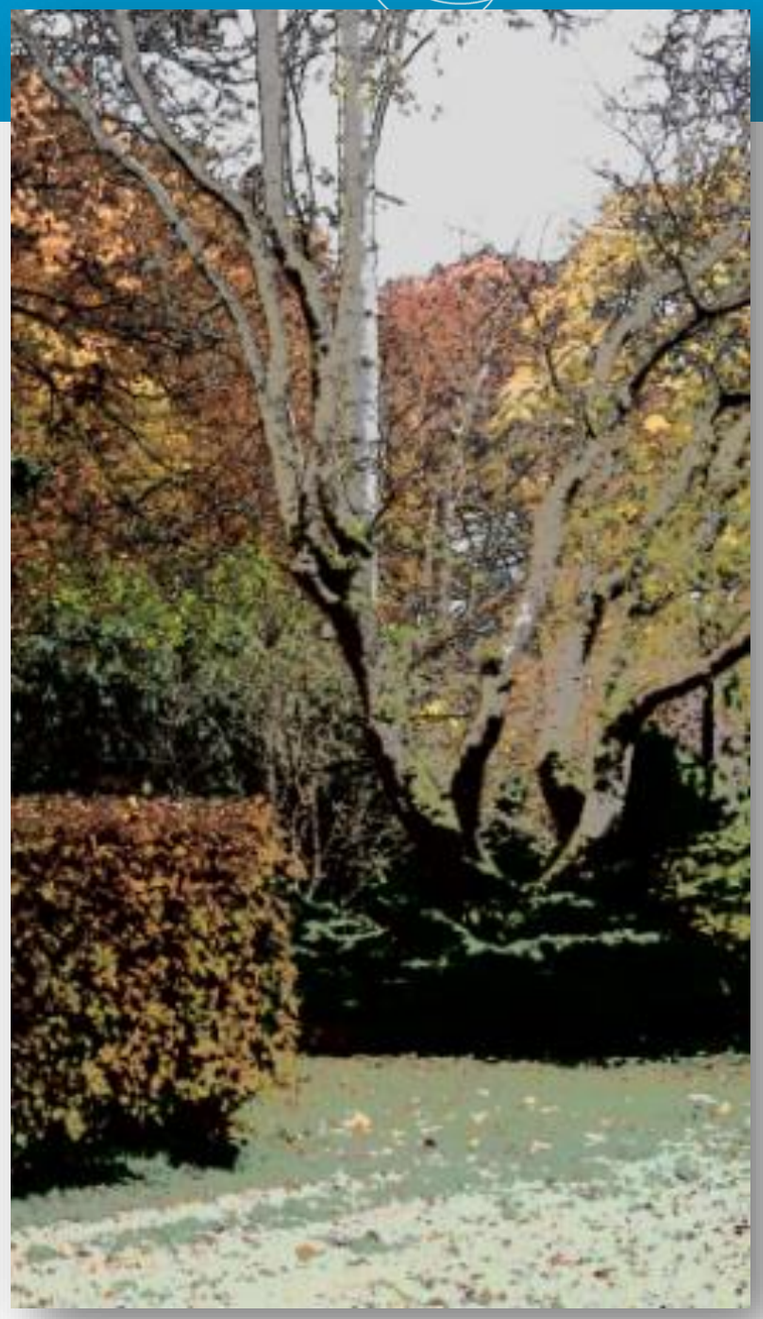
Experiment

An approximate representation of reality

Reality



Modelling

A cartoon representation of reality

Questions