Into the future: ILL Endurance program

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Table of contents

Introduction

- Since 1972, Institut Laue-Langevin (ILL) operates a high flux reactor as the centre for leading edge neutron science and technology
- 40 instruments, 500 employees, 1200 experiments / year

- Two decade campaign of improvements to continue providing world-class facility for neutron research
- Endurance phase 2 ensures continued output of quality science on 16 updated instruments
- Better Analysis Software Tools for ILL Experiments (BASTILLE) project part of this effort, aiming to bring full Mantid support for 19 instruments at the ILL

Outline

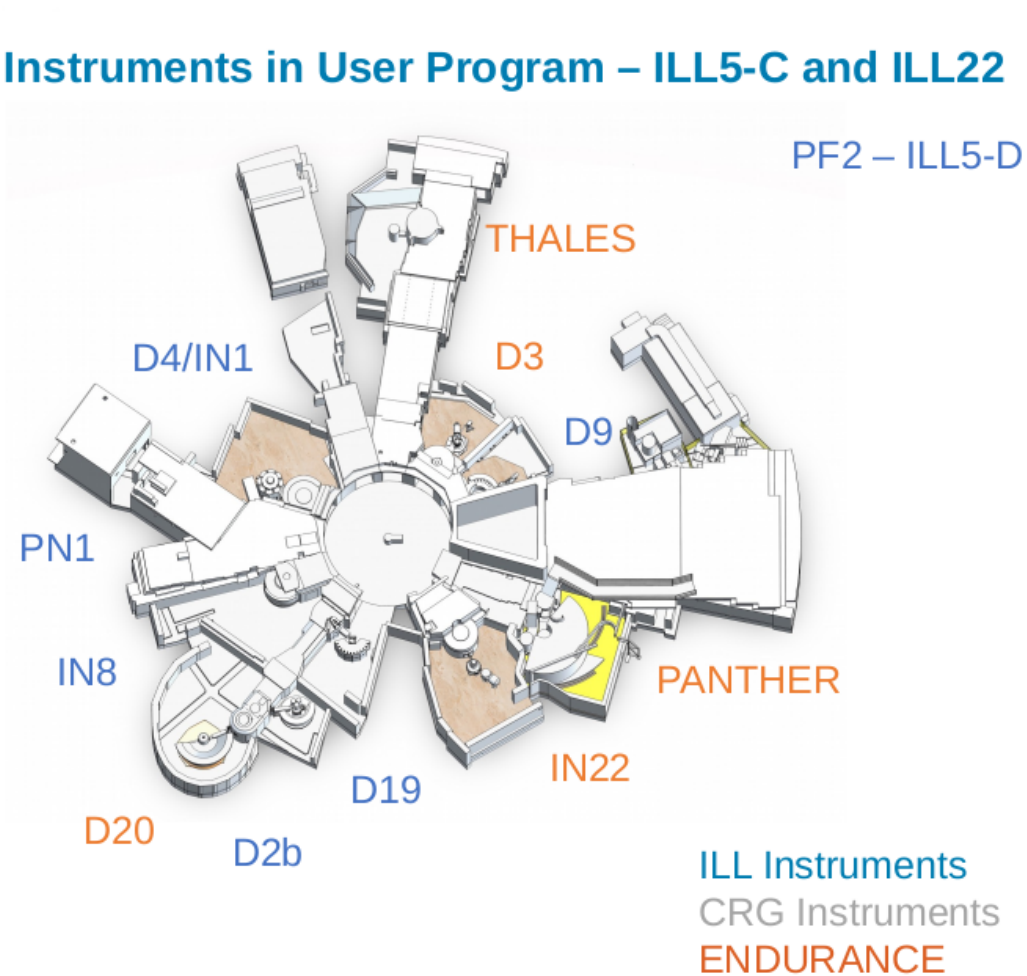
Millenium program

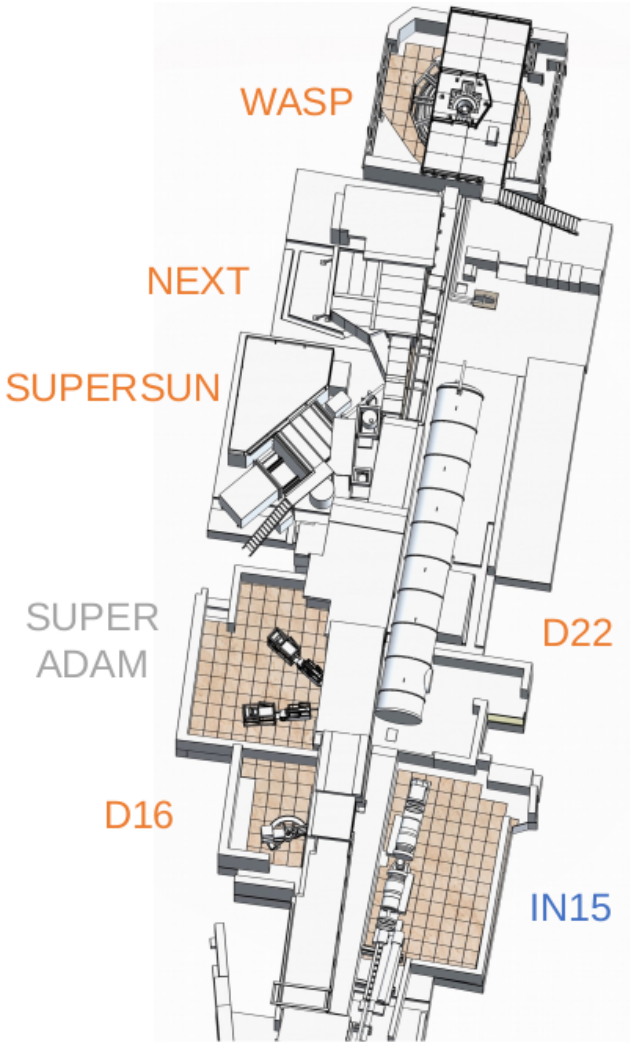
- Two stages: 2001-2008, and 2009-2018
- Strategy for the continual improvement of the infrastructure
- Significant upgrades to neutron guides and instruments, profited from technological advancements in detectors and monochromators
- 25 instruments built or upgraded
- Average detection rate was improved by a factor 25, overall efficiency by a factor of 19

Endurance overview

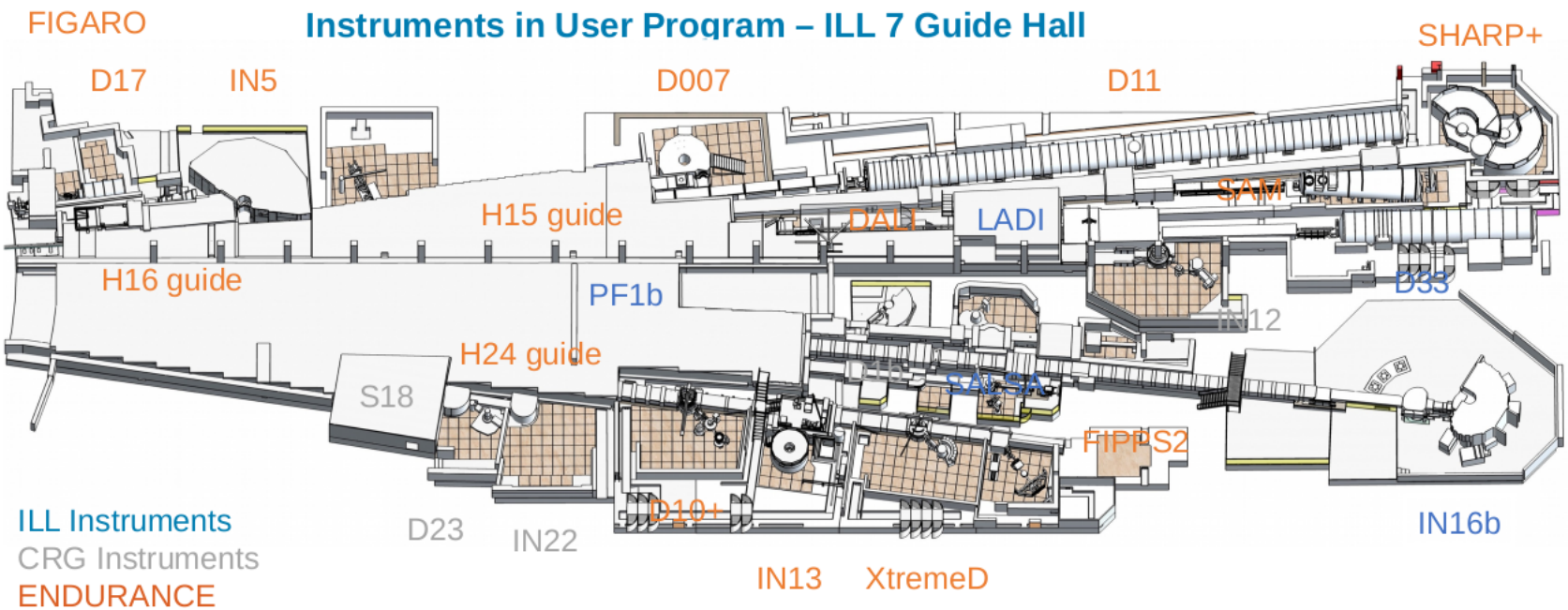
- Builds on Millenium investment
- Ensure ILL instruments and supporting infrastructure satisfy user community expectations well up to 2030
- Extending and opening opportunities in fields of magnetism, material science, soft matter, biology, and particle physics
- Timeline from 2016 to 2023, most projects complete or nearing
- Special attention to maintain constant operational budget

Endurance overview





Endurance overview



Outline

Endurance: phase 1

- Spanned 2016-2019, partially overlapping with Millenium
- Improvements to instruments: D10+ (diffraction), FIPPS (spectrometer), IN13+ (indirect), PANTHER (TOF), RAINBOWS (spectrometer), SuperSUN (ultracold neutron source)
- Updated beamlines: H23/H24, H1/H2, H16
- Nesse: sample environment equipement development
- Bastille: Inititated software improvements; introduction of Mantid
- Biggest gain: PANTHER (factor 60 in efficiency)

Outline

Endurance: phase 2

- Timeline 2019-2023, most projects completed or nearing
- Updates in D11, D22, SAM (SANS), IN20 (triple-axis), LADI-B (Quasi-Laue spectrometer), IM2020-NeXT (reflectometer), RAMSES (TOF)
- Later phase 2: FIPPS (spectrometer), D19 (diffraction), RAINBOWS (spectrometer), WASP (spin-echo), D007 (polarised diffraction/spectroscopy), Laasi311 (high-Q analysers), Marmot (analyser)
- Corner stone of Endurance phase 2: upgrade to cold neutrons beamline H15, serving 6 instruments, expected gain 2-4 times
- Nesse2: continuation of new standards for sample environment
- Bastille2: Further software improvements and consolidation

Bastille

- Provide modern data analysis framework
- Harmonize user experience across instruments and facilities
- Replace the common legacy solution, Lamp, with Mantid
- Mantid: internationally developed framework (jointly by ISIS Neutron and Muon Facility and the Oak Ridge National Laboratory), for data manipulation, visualisation, and analysis
- Maintainable solution, written in C++ and Python, with robust testing and developed according to industry standards
- Bring Mantid support to 21 instruments across various techniques: SANS, direct and indirect geometry inelastic spectrometers, TOF reflectometers, polarised and unpolarised diffractometers

Outline

Bastille phase 1

- One Tessella consultant (2 yr) + 3 time-limited contracts (3 yr)
- From initial feasibility investigation, through requirement capture to development of production-quality data reduction workflows, all in Mantid framework
- Data reduction workflows implemented in Mantid for: TOF spectrometers (IN4, IN5, IN6, Panther), backscattering spectrometer (IN16B), scanning powder diffractometers (D20, D2B), TOF reflectometers (D17, Figaro), and SANS (D11, D22, D33)
- Contributions to general Mantid development

Outline

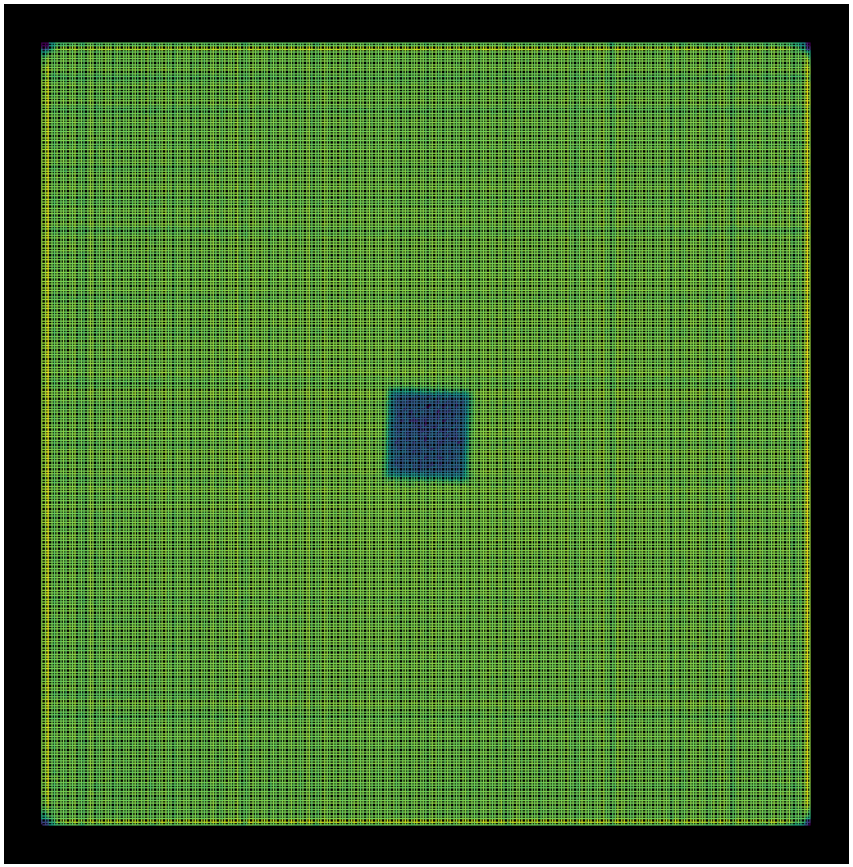
Bastille phase 2

- Currently ongoing, nearing completion by year-end
- One senior developer + three time-limited contracts
- Consolidate and improve the work done during phase 1, promote further adoption
- Continue implementation for remaining 9 instruments: D1B, D3, D4, D16, SALSA, IN13, Lagrange, XtremeD
- Development of common GUI for data reduction (DrILL), and specialised solutions if necessary (ScanExp for D16)
- Extend tools for raw data visualisation (RdExp), and plotting (Superplot)
- Support event mode data and kinetic measurements
- Participation in global improvement of framework (instrument view)

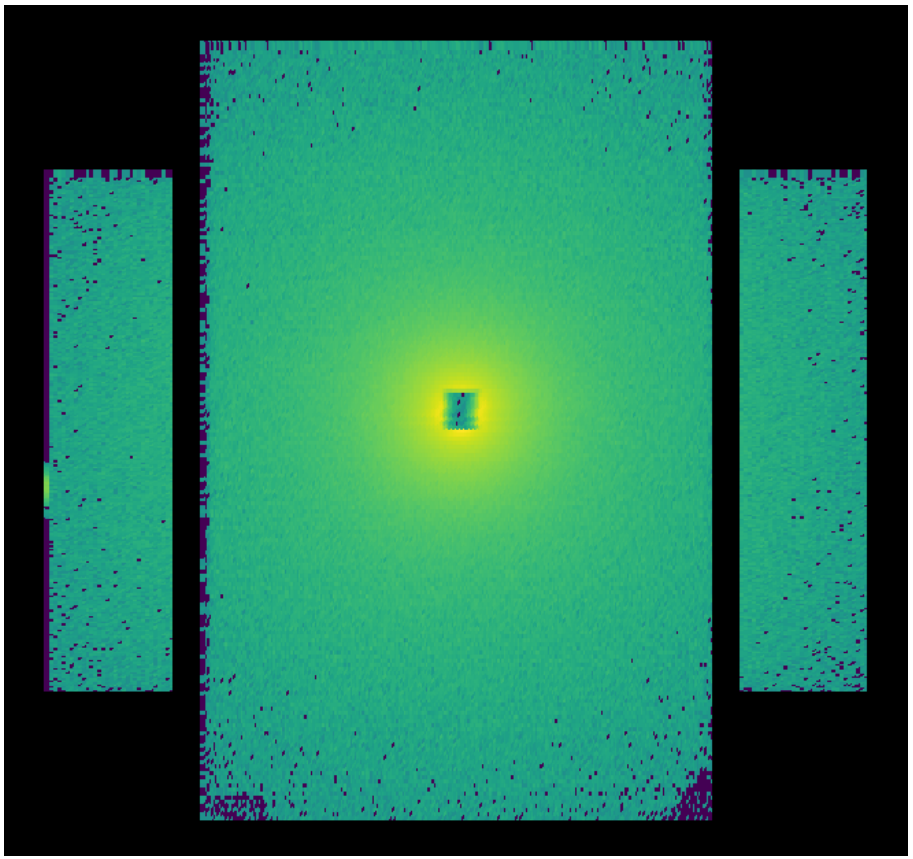
New and updated algorithms

- ILL-focused:
  - Several new AutoProcess algorithms: *DirectILLAutoProcess*, *SANSILLMultiProcess* streamlining data reductions
  - Dedicated NeXus loaders for polarised neutrons (D7), strain (SALSA), diffractometer (XTremeD), scan measurements for direct geometry (PANTHER, SHARP)
  - Component separation (nuclear coherent, spin-incoherent and magnetic) of polarised neutron cross-sections via *D7AbsoluteCrossSections*
- General purpose:
  - *Stitch* replacing *Stitch1DMany* and *Stitch1D* (v3) for reactor-source needs
  - *GenerateLogbook* for automated electronic logbook generation from metadata

Evolving instruments: D11 & D11B



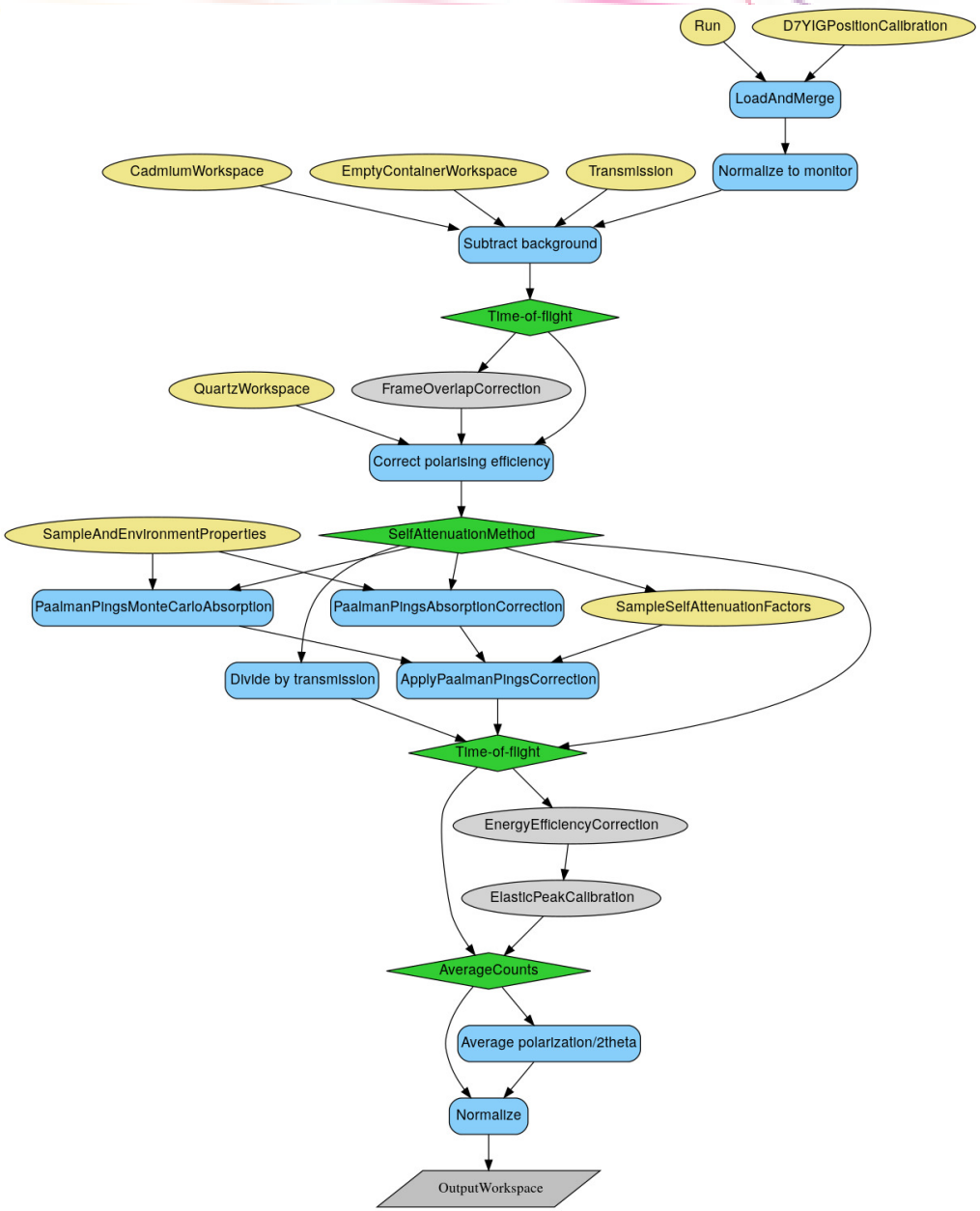
D11 instrument measurement; 256 x 256 pixels



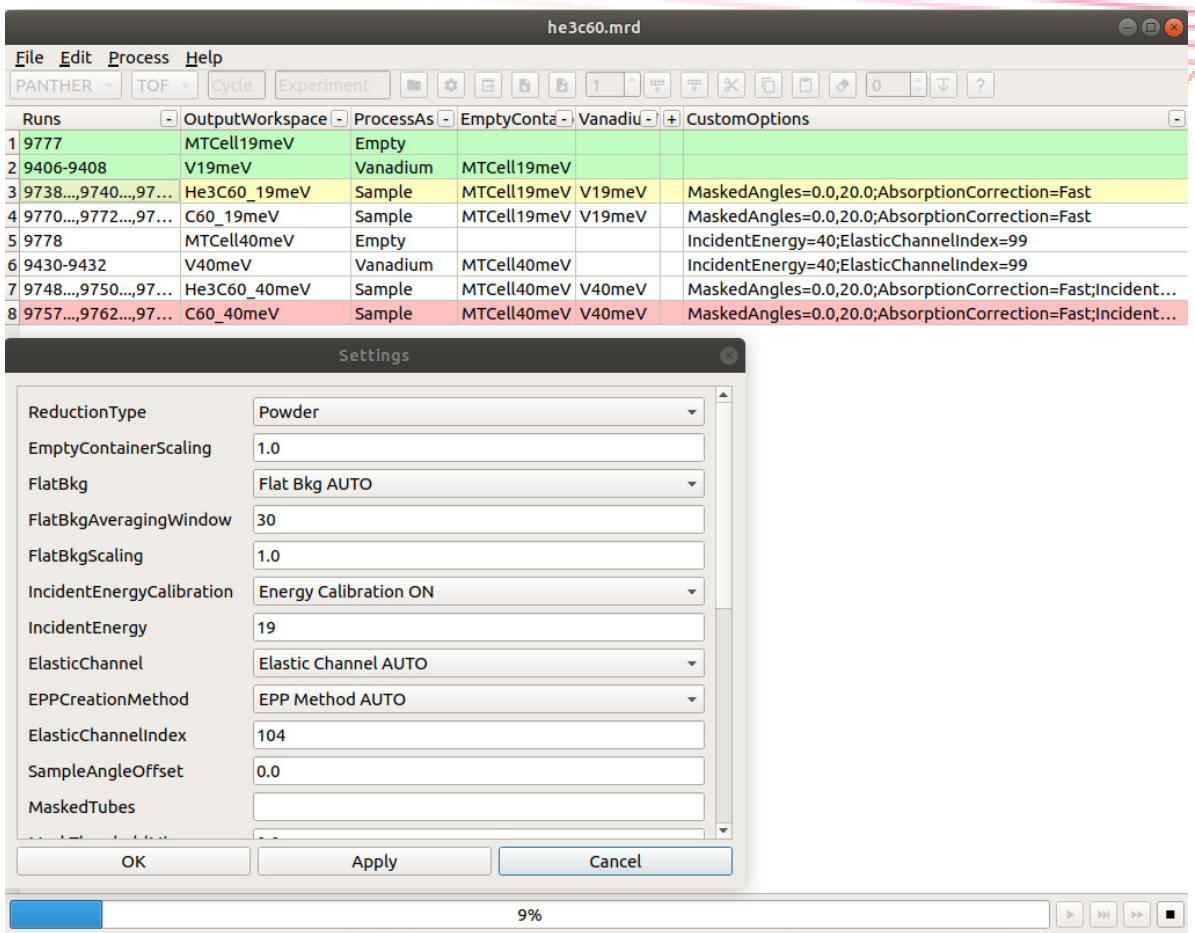
D11B: two new panels, higher granularity

New workflows

- Polarised neutron data reduction (D7, *D3L*, *D007*)
- Kinetic SANS (D11, D22)
- Strain measurement (SALSA)
- Continuous integration and deployment of local branch: GitLab CI + Docker → Singularity @ VISA

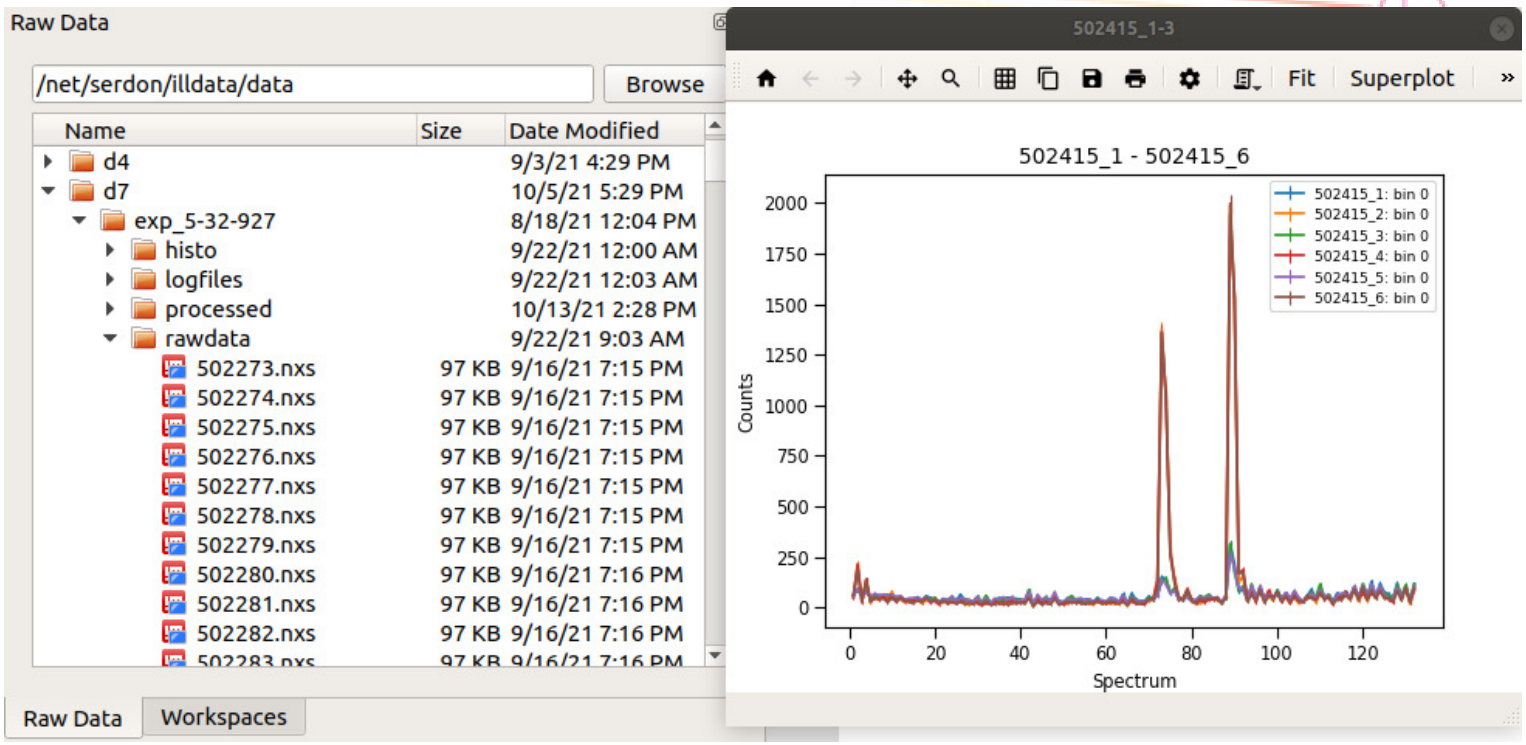


New GUIs: DrILL



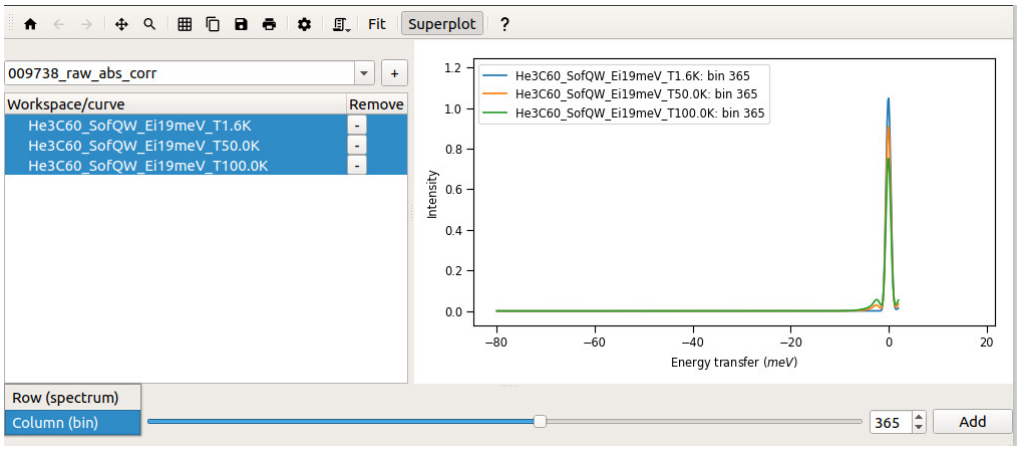
- Spreadsheet GUI to reduce large number of samples
- Interfaces to autoprocess algorithms
- Supports SANS, direct-geometry TOF, and reflectrometry
- Implemented in PyQt and Python

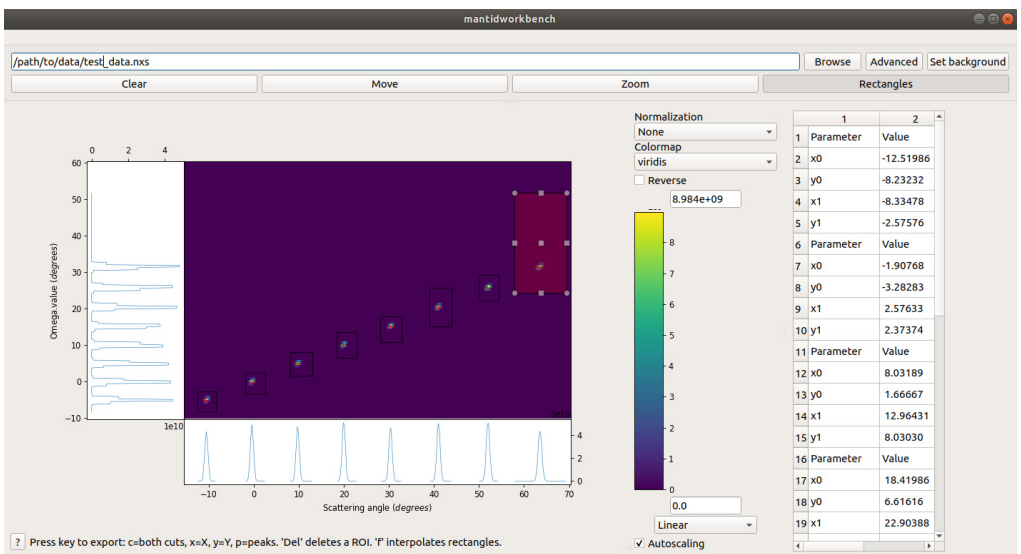
New GUIs: RdExp



- Allows browsing directory tree and visualise raw data with one click
- Most adapted visualisation selected per technique out of 1D spectrum/bin plots, 2D colorfill maps, instrument view, slice view
- Default to instrument view

New GUIs: Splot, ScanExp, WorkspaceCalculator





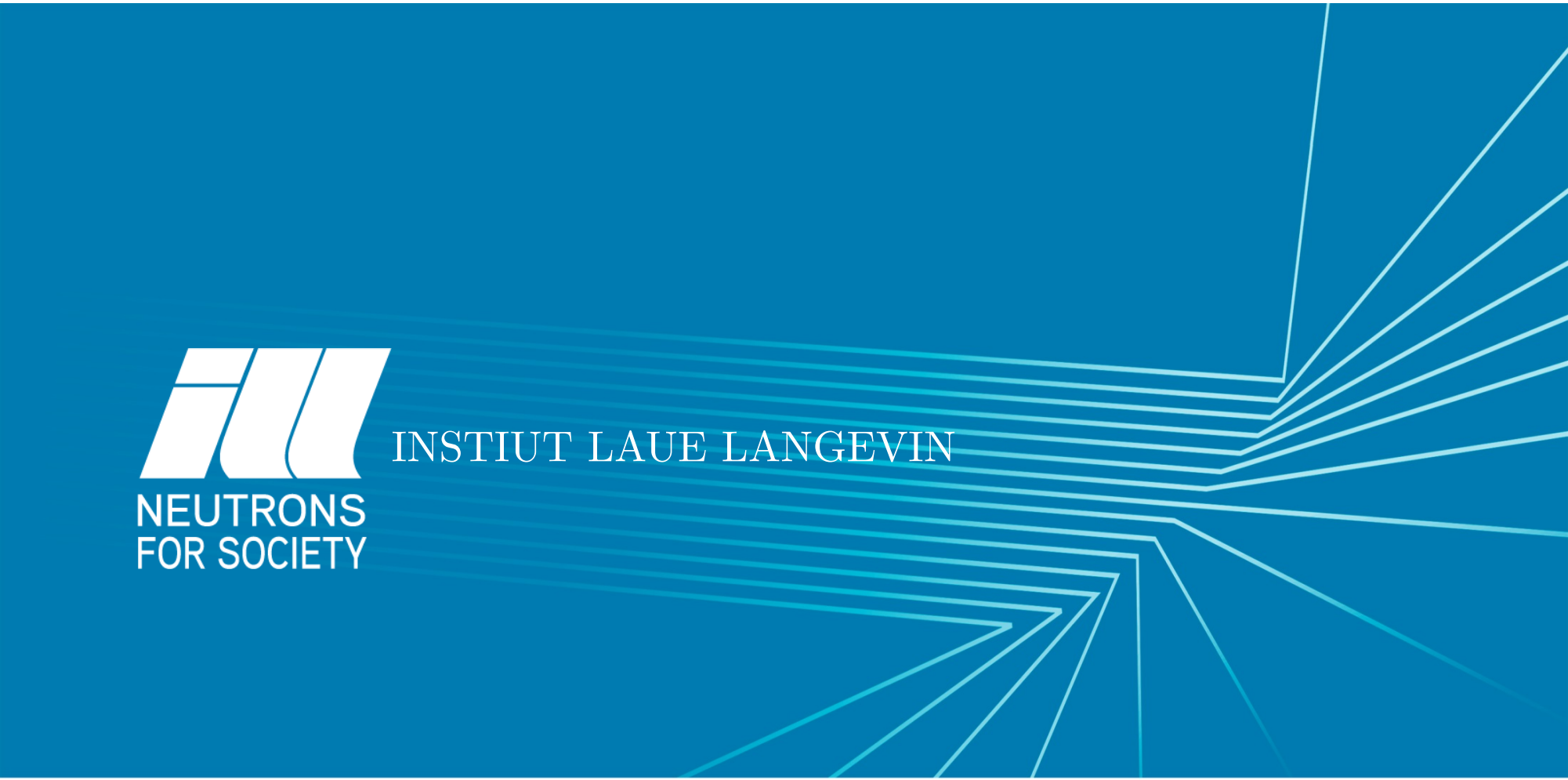
- Superplot: quick overplotting of multiple distributions
- Scanexplorer: aid for data reduction and analysis of multilayer scans at D16
- WorkspaceCalculator: minor widget to ease binary calculations on workspaces

Future plans

- Consolidation and maintenance of ILL algorithms developed during Bastille phase 1 and 2
- Continuous implementation of new features and quality of life improvements for ILL users
- Automatic filling of DrILL table for entire experiment
- Automatic data reduction in near real time
- Contributions to Mantid project within the resources available (2 permanent developers)
- Intergovernmental convention extended to 2033
- FILL2030 - The Future of the ILL beyond 2030

Conclusions

- ILL positioned to support superb neutron research for users into 2030s
- 16 instruments already upgraded, constructed, or scheduled to be ready in the nearest future
- Average gain in efficiency of factor 10
- Program on schedule despite pandemic and human resources disruptions
- Mantid already supported on 19 instruments across main ILL techniques out of 21 foreseen for this stage
- Future works focused on maintenance and expansion of existing features, notably the automatic reduction


NEUTRONS
FOR SOCIETY
INSTIUT LAUE LANGEVIN

Backup slides

Endurance project table phase 1

PROJET	DESCRIPTION	DELIVERY
FIPPS	New fission product γ-ray spectrometer	2016
FIPPS	Anti-Compton detectors	2018
RAINBOWS	White-beam reflectometer option	2017 (Proof of principle)
D17	Guide & chopper upgrade	2018
PANTHER	Thermal neutron chopper spectrometer	2019
H16/IN5	Guide and beam focusing optics	2019
SUPERSUN	Next-generation ultra-cold neutron source	2019
D3 liquids	Wide angle detector & polarization analysis	2019
H24	Thermal neutron guide renewal	2020
D10+	Single cristal diffractometer	2020
IN13+	Backscattering spectrometer (CRG)	2020
XtremeD	New extreme condition powder & single crystal diffractometer	2020
H1-H2	Beam tube renewal	2020
IN20	Velocity selector	2020
NESSE	Sample environment equipment	2016 - 2019
BASTILLE	Data treatment software	2016 - 2019

Endurance project table phase 2

PROJET	DESCRIPTION	DELIVERY
D11	Large area detector	2021
D22++	Wide angle detector	2021
D16	Wide angle detector	2021
D20c	Replacement detector	2021
IN20	Monochromator and multianalyser/detector	2021
LADI-B	Second protein crystallography station	2019
IM2020 -NeXT	Public imaging beam line	2020
H15	Guide design	2019
NESSE2	Sample environment equipment	2019 - 2023
BASTILLE2	Data treatment software	2019 - 2023

Endurance project table phase 2 H15

PROJET	DESCRIPTION
H15	Guide renewal
D7+	Primary spectrometer
D11	Beam collimation
RAMSES	Primary spectrometer of SHARP (ex. IN6)
SAM	SANS instrument (CRG)
GAPS	TAS instrument (CRG)

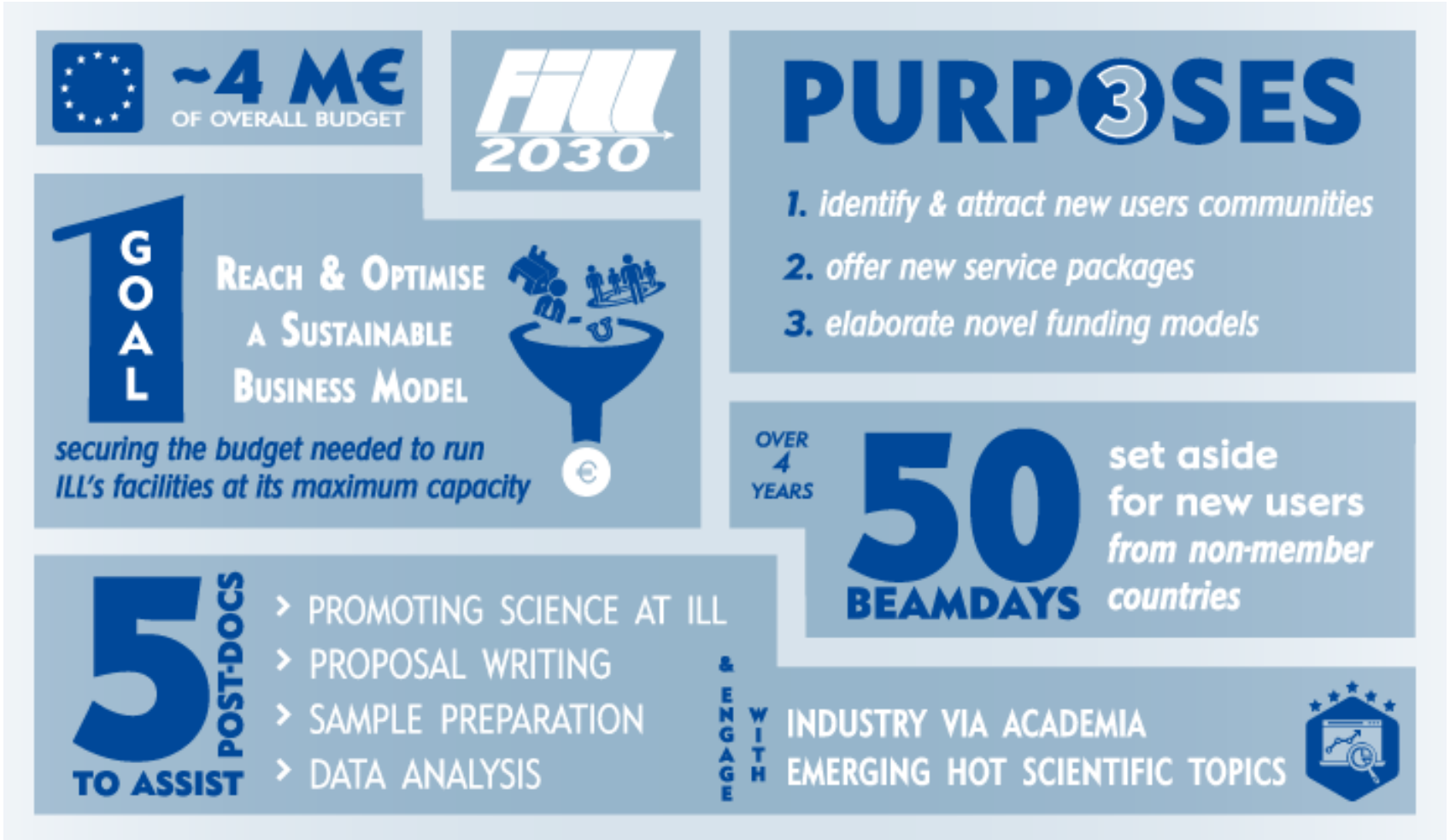
Endurance project table phase 2 2020-2023

PROJET	DESCRIPTION
FIPPS	Gas filled magnet: mass spectrometer
D19	High count rate detector
RAINBOWS	Implementation on D17/FIGARO
WASP	Extra detectors & time-of-flight option
LAASI311	High-Q, Si311 analysers for IN16
MARMOT	Multiplexing analyser and detector for ThALES

NESSE

- Provide and maintain best experimental capabilities at ILL
- Sample levitation techniques of melted samples
- High pressure: Paris-Edinburgh presses (20 GPa) and cryostat
- Soft-matter research: humidity chambers, stopped-flow systems, rheometers
- High magnetic fields: 15 T

Fill30


~4 M€
OF OVERALL BUDGET
FILL 2030
PURPOSES
1. identify & attract new users communities
2. offer new service packages
3. elaborate novel funding models
1 GOAL
REACH & OPTIMISE A SUSTAINABLE BUSINESS MODEL
securing the budget needed to run ILL's facilities at its maximum capacity
OVER 4 YEARS
50 BEAMDAYS
set aside for new users from non-member countries
5 POST-DOCS TO ASSIST
› PROMOTING SCIENCE AT ILL
› PROPOSAL WRITING
› SAMPLE PREPARATION
› DATA ANALYSIS
& ENGAGE WITH INDUSTRY VIA ACADEMIA EMERGING HOT SCIENTIFIC TOPICS