

Digital Twin Design and Implementation at the Institut Laue-Langevin

Shervin Nourbakhsh (Institut Laue-Langevin)

NOBUGS 2024

Enrich the offer of user tools with the possibility to run a virtual experiment.

Training:

- ▶ newcomers to the instrument control system
- ▶ users new to a particular instrument, its configuration and capabilities

Settings optimization: study and optimize instrument settings for a specific configuration to maximize some figure of merit (e.g. intensity vs resolution)

Analysis: improve analysis with better understanding of some background sources and uncertainties (e.g. effect of a possible mis-alignment)

Support material: enrich proposals for demanding beam time with results from simulated data with the specific instrument taking into account its capabilities



- ▶ usable by users with **basic knowledge** in neutron ray-tracing and interaction simulation
- ▶ use the **familiar interface** of instrument control to configure and start acquisition
- ▶ simulated data must be treated as the real data → written to disk in **same format**
- ▶ use **state-of-the-art** simulation software (e.g. McStas for neutron ray-tracing)

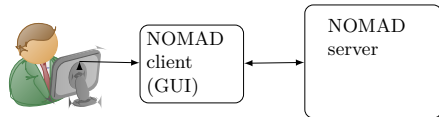
File View Hardware Settings Command Editor Spy User Zoom Help

Hardware Settings Execution

Launch pad

Commands

- Favourites
- Acquisition
 - Counts
 - CountCam
 - Count
 - KineticCount
 - SampleSequencer
 - Scan
 - Setting
 - MeasurementType
 - MultiDet
 - MultiDetRight
 - MultiDetLeft
 - Valve1
 - McStasSimulation
 - Title
 - Axis
 - Beam parameters
 - Attenuator
 - BeamStop
 - Collimations
 - Diaphragm
 - Selector
 - Setting
 - Wavelength
 - D11 settings
 - Sample environment
 - Tools
 - Execution control
 - Clipboard
 - Users' scripts
 - Internal use
 - launch_pad-005708
 - launch_pad-005711
 - launch_pad-005721
 - Shared



- ▶ NOMAD is ILL's Instrument Control System
- ▶ The GUI is a java client connecting to the server
- ▶ NOMAD core is a c++ server
- ▶ from the GUI users can:
 - ▶ control the instrument settings
 - ▶ program the acquisition workflow

Specific module for simulation settings

Sample settings

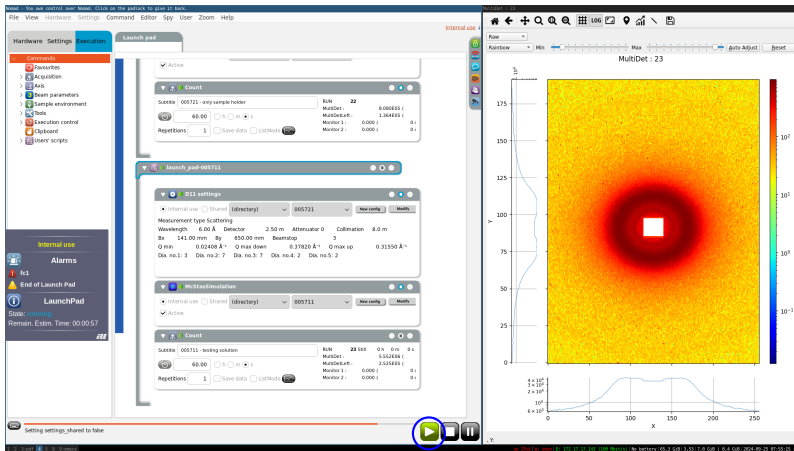
- ▶ shape and size
- ▶ material or information about scattering probability from theoretical calculations

Sample holder

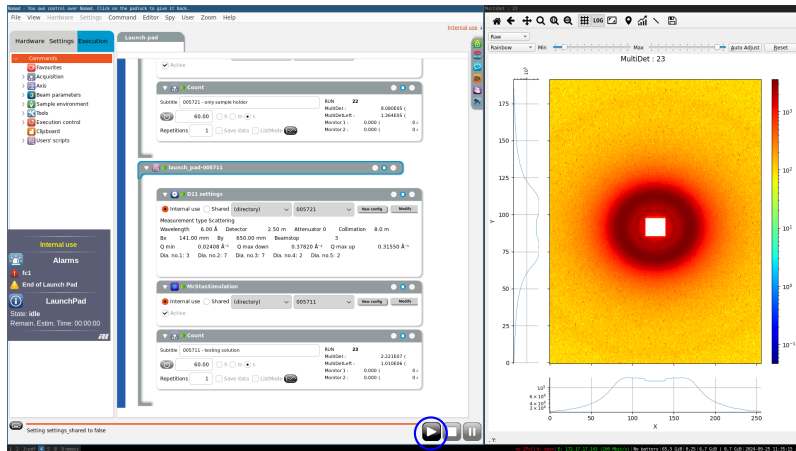
- ▶ shape and size
- ▶ material

The screenshot displays a software interface for virtual acquisition. On the left, a sidebar contains a tree view with categories like 'Commands', 'Acquisition', 'Axis', 'Beam parameters', 'Sample environment', 'Tools', 'Execution control', 'Clipboard', 'Users' scripts', and 'Internal use'. Under 'Internal use', three launch pads are listed: 'launch_pad-005708', 'launch_pad-005710', and 'launch_pad-005711'. The 'launch_pad-005711' is selected. Below the sidebar, an 'Internal use' panel shows 'Alarms' (fc1, End of Launch Pad) and 'LaunchPad' (State: idle, Remain. Estm. Time: 00:03:00). The main window shows a 'Launch pad' list with three entries. The 'launch_pad-005711' entry is expanded, revealing several configuration windows: 'D13 settings' (Internal use, Shared, directory: 005721, New config, Search; Measurement type: Scattering; Wavelength: 6.00 Å, Detector: 2.50 m, Attenuator: 0, Collimation: 8.0 m; D1: 141.00 mm, D2: 650.00 mm, Beamstop: 3; Q min: 0.02408 Å⁻¹, Q max down: 0.37820 Å⁻¹, Q max up: 0.31350 Å⁻¹; D1a no.1: 3, D1a no.2: 7, D1a no.3: 7, D1a no.4: 2, D1a no.5: 2), 'McStasSimulation' (Internal use, Shared, directory: 005711, New config, Search; Active), and 'Count' (Success: 005711 - testing solution; 60.00; Repeats: 1; Save data; List blocks). The interface includes a menu bar (File, View, Hardware, Settings, Command, Editor, Spy, User, Zoom, Help), a toolbar with navigation and search icons, and a status bar at the bottom.

- ▶ User can start a simulation as used to do with the experiment.



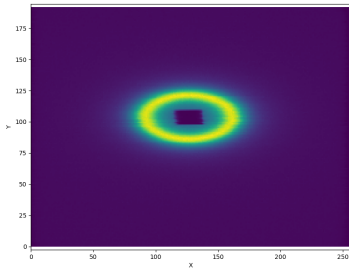
- ▶ User can start a simulation as used to do with the experiment.
- ▶ Feedback on progress



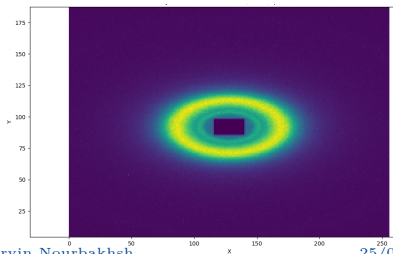
- ▶ User can start a simulation as used to do with the experiment.
- ▶ Feedback on progress
- ▶ Results updated at time intervals

Simulation result

Scattering on calibration sample with sample holder (D11)

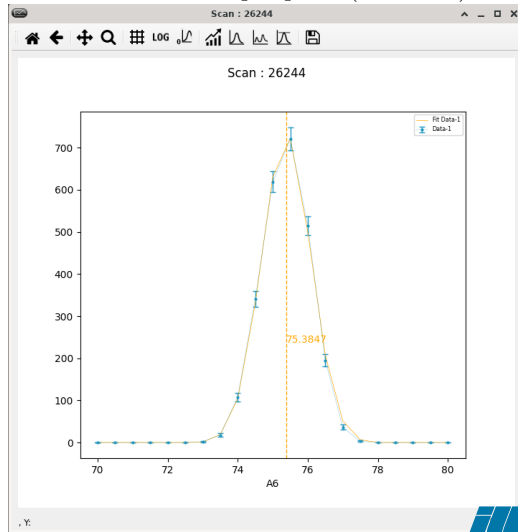


Data
(NeXus)



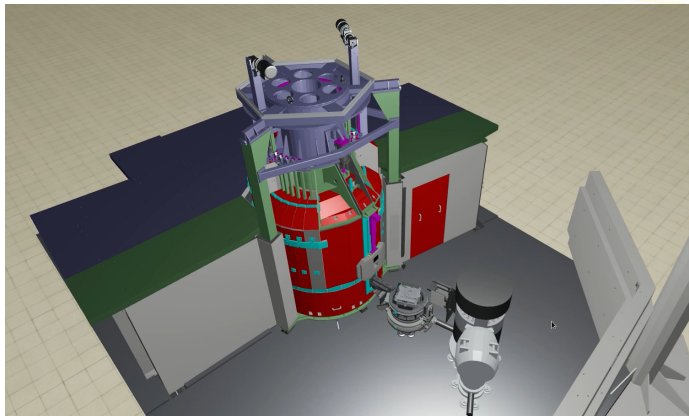
Simulation
(NeXus)

Scan: one simulation per point (THALES)



3D view

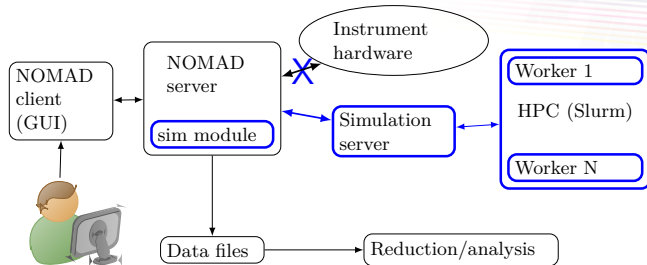
Y. Le Goc et al.



Better understanding of the instrument, its current configuration and possible movements.

- ▶ Live 3D view of current configuration.
- ▶ Animated showing moving parts at change of configuration.

Overview



C++ client API: sends simulation requests with instrument and sample parameters and receives results

SIM server: receives requests, dispatches workers, packs and returns results

Workers on **HPC (Slurm)** running the instrument simulation executables (e.g. McStas)

3D server: receives instrument parameters, generates 3D view in HTML5 page

CAMEO middleware (see Le Goc's poster) provides:

- ▶ APP management (start/stop) also on remote machines
- ▶ Communication between managed APPs

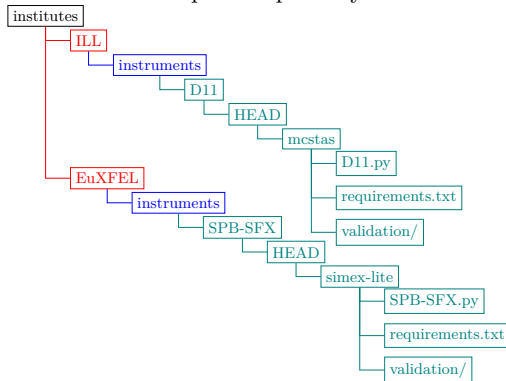
Simulation Executable

- ▶ Workers can run any program to perform the simulation
- ▶ McStas used as state-of-the-art neutron ray-tracing software
- ▶ Instrument description
 - ▶ in Python using **McStasScript**^a and **libpyvinyl** library^b
 - ▶ retrieved from **PANOSC Vinyl** public “instrument description repository” (Github)
 - ▶ usable also in Jupyter notebook
- ▶ Instrument executables compiled for **CPU and GPU** and binary packages created and installed on HPC nodes.

^aMads Bartelsen

^bCarsten Fortmann-Grote, Mads Bertelsen, Juncheng E, Shervin Nourbakhsh

Instrument description repository structure:



Objectives achieved:

- ▶ A prototype setup for a digital twin (DT) at ILL has been developed
- ▶ The DT can be used by users with no knowledge about simulation
- ▶ Data are available in the usual format, ready for reduction and analysis via the normal workflow.
- ▶ The client-server model allows further development of different interfaces to the simulation server (e.g. Jupyter notebooks via python API, or other client program)
- ▶ The parallelization on HCP (Slurm) has been implemented.
- ▶ Workers are flexible to allow different simulation softwares.
- ▶ McStas simulation binaries running on both CPUs and GPUs.
- ▶ 3D live view of the instrument in current configuration and showing movements at configuration change available as a web application.

Further steps:

- ▶ Add non-simulated background from real data.
- ▶ Develop surrogate models (ML) for faster simulations.