A Digital Twin for Neutron Instruments

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Objectives

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

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)

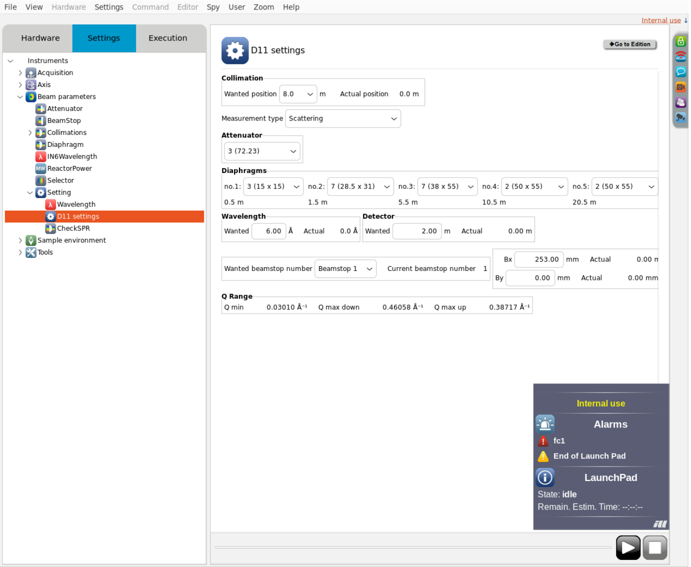
Analysis: improve analysis with better understanding of some background sources and uncertainties (e.g. effect of a possible mis-alignment)

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

Design Requirements

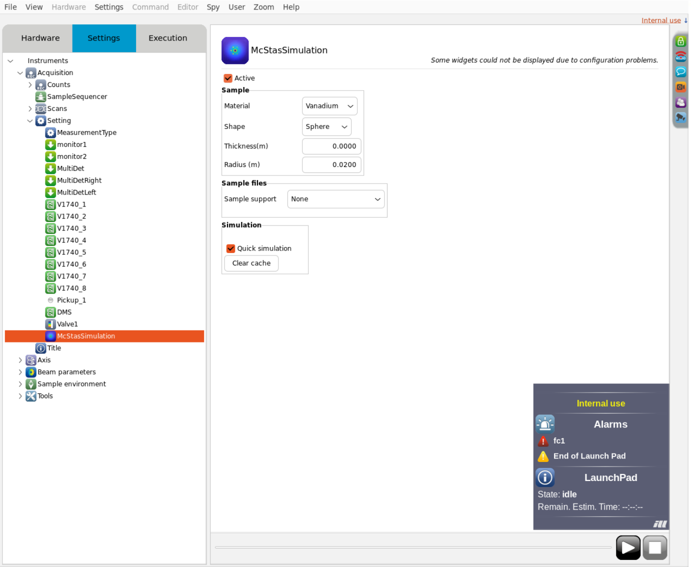
- usable by users with **no knowledge** in neutron physics
- use the **familiar interface** of instrument control to configure and start acquisition
- simulated data must be treated as the real data → written to disk in **same format**
- use **state-of-the-art** simulation software (McStas)
- provide instrument description for public use (McStas experts not using the Digital Twin)
  - possible feedback from power users

Instrument Control Gui



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

Specific module for simulation settings



Sample settings

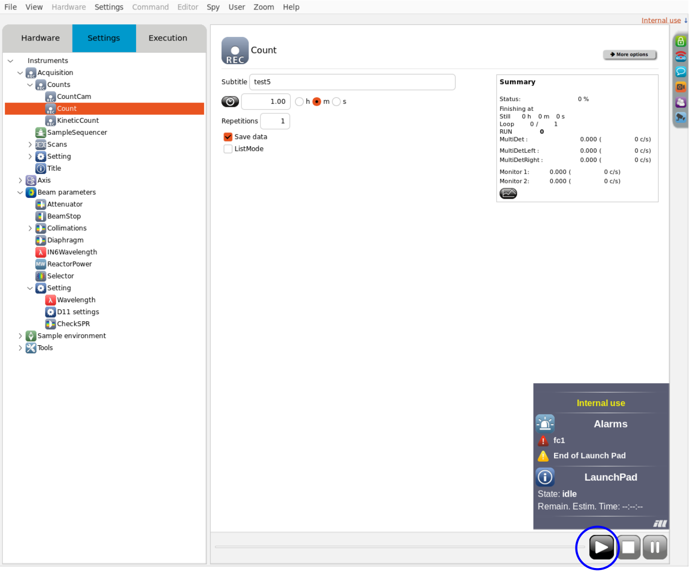
- shape and size
- material or information about scattering probability from theoretical calculations

Sample holder from list of pre-configured or custom

- shape and size
- material

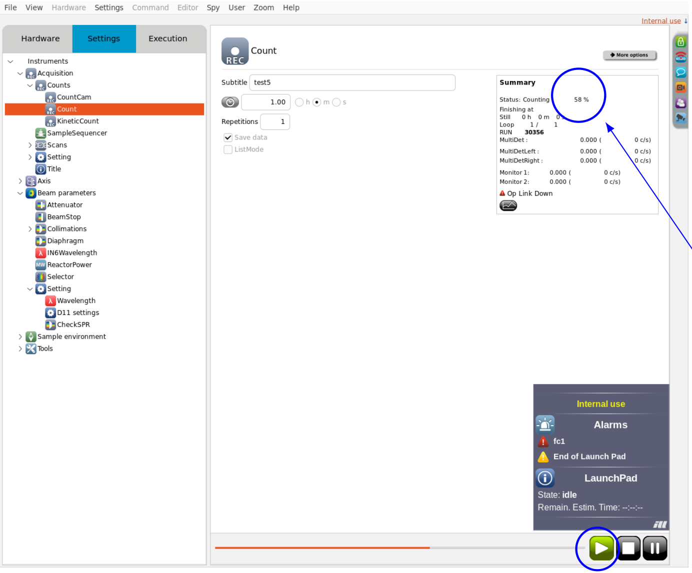
Sample environment from list of those available for the instrument

Virtual acquisition



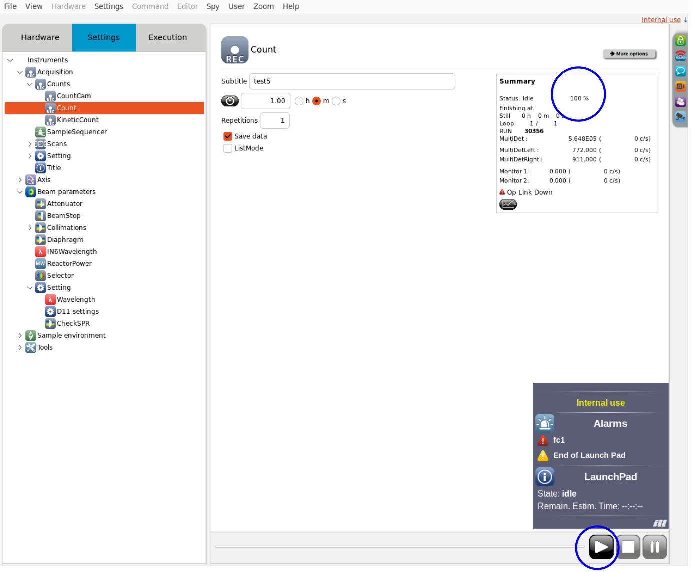
- User can then start a simulation as used to do with the experiment.

Virtual acquisition



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

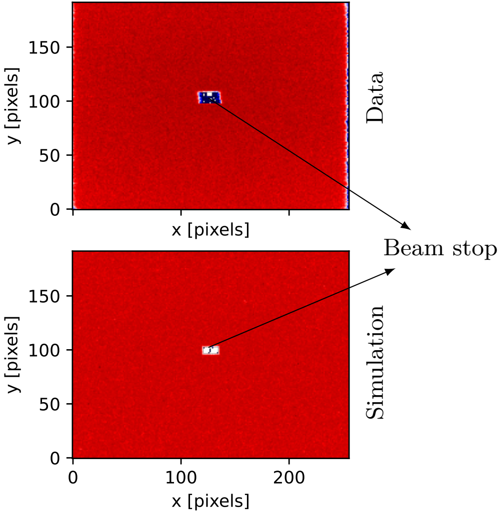
Virtual acquisition



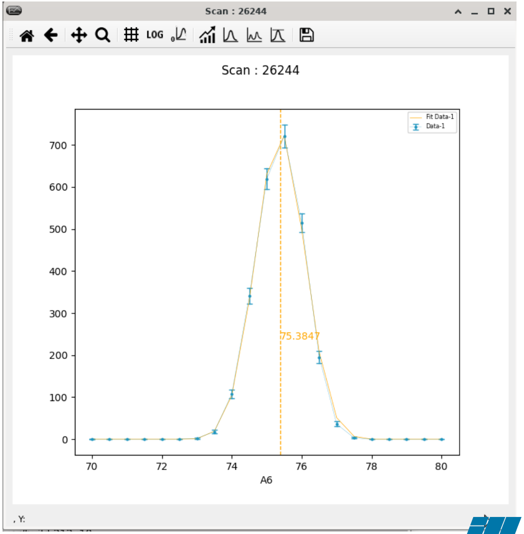
- User can then start a simulation as used to do with the experiment.
- Feedback on progress
- Results available at completion

Simulation result

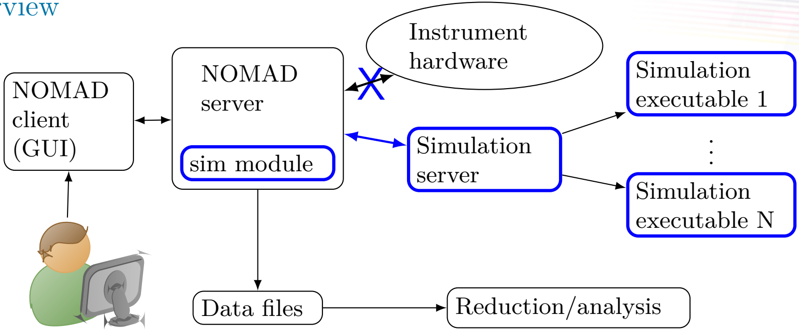
Scattering on empty sample holder



Scan: one simulation per point



Overview



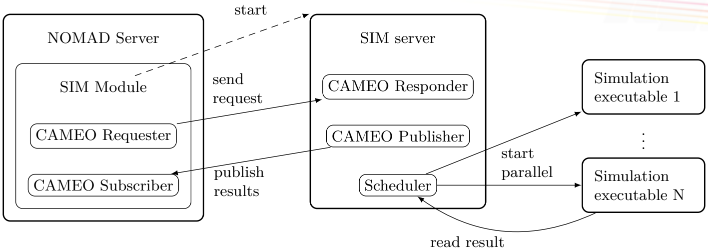
Software divided into:

1. C++ client API
   (used by the NOMAD server's sim module)
2. SIM server
3. instrument simulation executables

CAMEO middleware provides:

- APP management (start/stop) also on remote machines
- Communication between managed APPs with high level Requester-Responder/Publisher-Subscriber patterns implementation using ZMQ

Communications and interactions



NOMAD's client module:

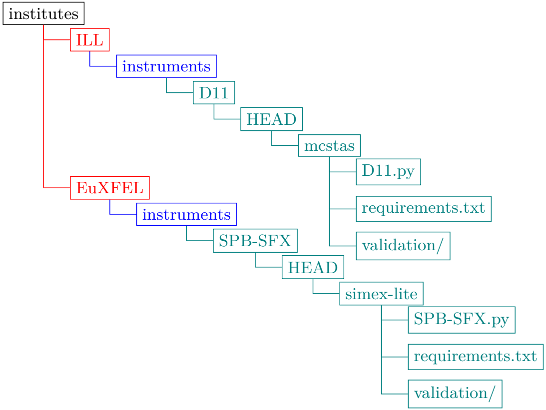
1. Starts the SIM server
2. Collects settings and create a request using the SIM client API
   - API guarantees format of request message
3. Send the request message (JSON format)
4. Waits for simulation result (or error)
5. Retrieve the simulation status and result

SIM Server:

- process incoming simulation requests
- assign UID to the request (messages's hash)
- prepare the scheduler with simulation settings
- the scheduler starts multiple instances of the simulation executables in parallel
- retrieve and merge from disk the results
- publish the simulation results

Simulation executable

- use state-of-the-art neutron ray-tracing software: Mcstas (ANSI C)
- Instrument description
  - in python using McStasScript and libpyvinyl libraries
  - retrieved from “instrument description repository” (github)
- Instrument executables compiled and binary packages created and installed on execution machines.

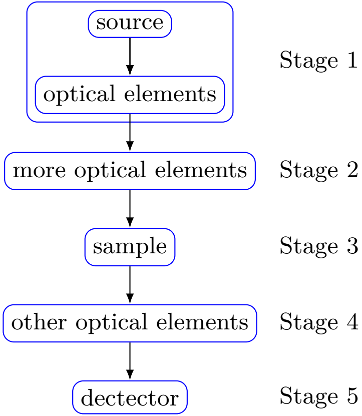


Simulation staging and smart scheduler

Difficult to compete with ILL's high flux:
simulation time much larger than acquiring real neutrons for high scattering scamples.

Mitigations:

- optimize instrument description in simulation
- CPU parallelization vs GPU
- divide the simulation in stages (different executables)
- map instrument settings to different stages
- re-use previously simulated stages, re-running those with changed parameters



Summary

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)

Further steps:

- develop a detector description validation scheme
  → tests comparing real data and simulation for some well understood samples
- reduce simulation time: tune and optimize parallelization

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Additional material

Simulation server diagram