

# A Digital Twin for Neutron Instruments

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



- ▶ 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

The screenshot displays the 'D11 settings' window within the Instrument Control Gui. The interface includes a menu bar (File, View, Hardware, Settings, Command, Editor, Spy, User, Zoom, Help) and a sidebar with tabs for Hardware, Settings, and Execution. The 'Settings' tab is active, showing a tree view of instruments with 'D11 settings' selected. The main panel contains the following settings:

- Collimation:** Wanted position 8.0 m, Actual position 0.0 m
- Measurement type:** Scattering
- Attenuator:** 3 (72.23)
- Diaphragms:** no.1: 3 (15 x 15) 0.5 m, no.2: 7 (28.5 x 31) 1.5 m, no.3: 7 (38 x 55) 5.5 m, no.4: 2 (50 x 55) 10.5 m, no.5: 2 (50 x 55) 20.5 m
- Wavelength:** Wanted 6.00 Å, Actual 0.0 Å
- Detector:** Wanted 2.00 m, Actual 0.00 m
- Beamstop:** Wanted beamstop number Beamstop 1, Current beamstop number 1
- Bx:** 253.00 mm, Actual 0.00 mm
- By:** 0.00 mm, Actual 0.00 mm
- Q Range:** Q min 0.03010 Å<sup>-1</sup>, Q max down 0.46058 Å<sup>-1</sup>, Q max up 0.38717 Å<sup>-1</sup>

An 'Internal use' panel is visible in the bottom right, showing 'Alarms' (fc1), 'End of Launch Pad', and 'LaunchPad' (State: Idle, Remain. Estim. Time: ---:--). The ILL logo is at the bottom right of the 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

The screenshot displays the McStasSimulation software interface. The top menu bar includes File, View, Hardware, Settings, Command, Editor, Spy, User, Zoom, and Help. The 'Settings' tab is active, showing a tree view on the left with 'McStasSimulation' selected. The main panel shows the following settings:

- Active:**
- Sample:**
  - Material: Vanadium
  - Shape: Sphere
  - Thickness(m): 0.0000
  - Radius (m): 0.0200
- Sample files:**
  - Sample support: None
- Simulation:**
  - Quick simulation
  - Clear cache

An 'Internal use' panel is visible in the bottom right, showing 'Alarms' with 'fc1' and 'End of Launch Pad', and 'LaunchPad' with 'State: Idle' and 'Remain. Estim. Time: ---:--'.

## 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

File View Hardware Settings Command Editor Spy User Zoom Help

Hardware Settings Execution

Instruments

- Acquisition
  - Counts
    - CountCam
    - Count**
    - KineticCount
  - SampleSequencer
  - Scans
  - Setting
    - Title
  - Axis
  - Beam parameters
    - Attenuator
    - BeamStop
    - Collimations
    - Diaphragm
    - IN6Wavelength
    - ReactorPower
    - Selector
    - Setting
      - Wavelength
      - D11 settings
      - CheckSPR
  - Sample environment
  - Tools

REC Count

Subtitle test5

1.00 h m s

Repetitions 1

Save data  
 ListMode

More options

Summary

Status: 0 %

Finishing at Still 0 h 0 m 0 s

Loop 0 / 1

RUN 0

MultiDet:	0.000 (	0 c/s)
MultiDetLeft:	0.000 (	0 c/s)
MultiDetRight:	0.000 (	0 c/s)
Monitor 1:	0.000 (	0 c/s)
Monitor 2:	0.000 (	0 c/s)

Internal use

Alarms

- fc1
- End of Launch Pad

LaunchPad

State: Idle

Remain. Estim. Time: ---:--

Internal use

▶

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

# Virtual acquisition

File View Hardware Settings Command Editor Spy User Zoom Help

Hardware Settings Execution

Instruments

- Acquisition
  - Counts
    - CountCam
    - Count**
    - KineticCount
  - SampleSequencer
  - Scans
  - Setting
  - Title
  - Axis
  - Beam parameters
    - Attenuator
    - BeamStop
    - Collimations
    - Diaphragm
    - IN6Wavelength
    - ReactorPower
    - Selector
    - Setting
      - Wavelength
      - D11 settings
      - CheckSPR
  - Sample environment
  - Tools

REC Count

Subtitle test5

1.00 h m s

Repetitions 1

Save data  
 ListMode

More options

**Summary**

Status: Counting 58%

Finishing at  
Still: 0 h 0 m 0 s  
Loop: 1 / 1

RUN 30356

MultiDet:	0.000 (	0 c/s)
MultiDetLeft:	0.000 (	0 c/s)
MultiDetRight:	0.000 (	0 c/s)
Monitor 1:	0.000 (	0 c/s)
Monitor 2:	0.000 (	0 c/s)

Op Link Down

Internal use

Alarms

- fc1
- End of Launch Pad

LaunchPad

State: Idle  
Remain. Estim. Time: --:--:--

Internal use

Play button icon circled in blue

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

# Virtual acquisition

File View Hardware Settings Command Editor Spy User Zoom Help

Hardware Settings Execution

Instruments

- Acquisition
  - Counts
    - CountCam
    - Count**
    - KineticCount
  - SampleSequencer
  - Scans
  - Setting
    - Title
  - Axis
  - Beam parameters
    - Attenuator
    - BeamStop
    - Collimations
    - Diaphragm
    - IN6Wavelength
    - ReactorPower
    - Selector
    - Setting
      - Wavelength
      - D11 settings
      - CheckSPR
  - Sample environment
  - Tools

REC Count

Subtitle test5

1.00 h m s

Repetitions 1

Save data

ListMode

More options

Summary

Status: Idle 100%

Finishing at

Still 0 h 0 m 0 s

Loop 1 / 1

RUN 30356

MultiDet :	5.648E05 (	0 c/s)
MultiDetLeft :	772.000 (	0 c/s)
MultiDetRight :	911.000 (	0 c/s)
Monitor 1 :	0.000 (	0 c/s)
Monitor 2 :	0.000 (	0 c/s)

Op Link Down

Internal use

Alarms

- fc1
- End of Launch Pad

LaunchPad

State: Idle

Remain. Estim. Time: --:--

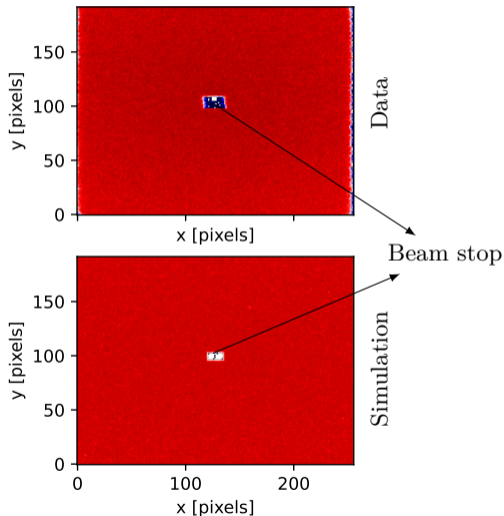
Internal use

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

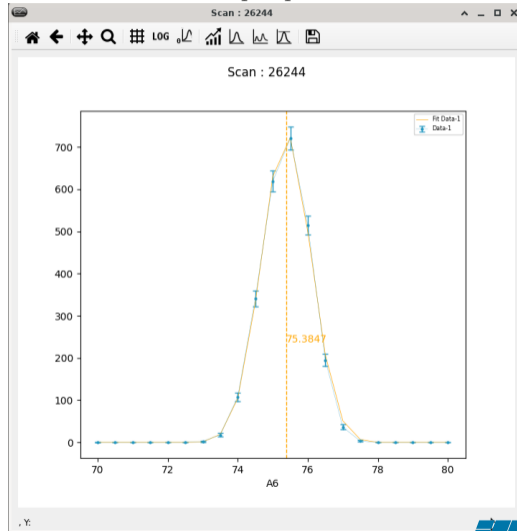


# Simulation result

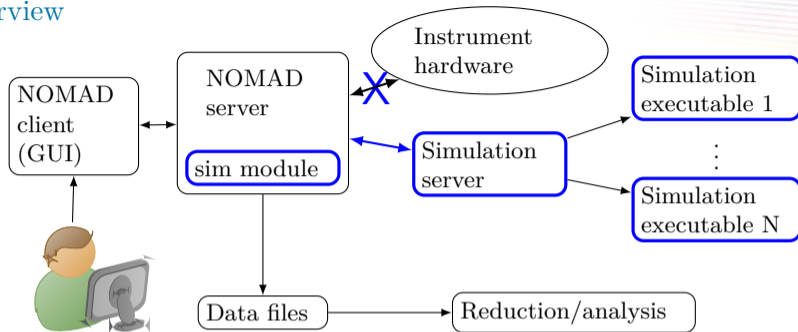
Scattering on empty sample holder



Scan: one simulation per point



# Overview

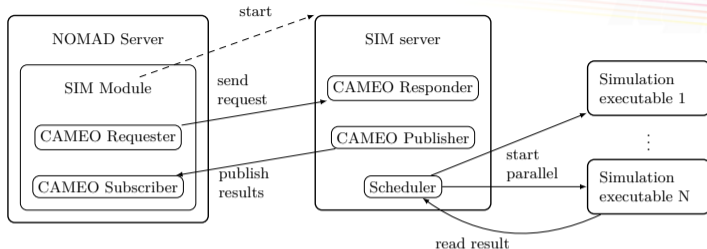


Software divided into:

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



NOMAD's client module:

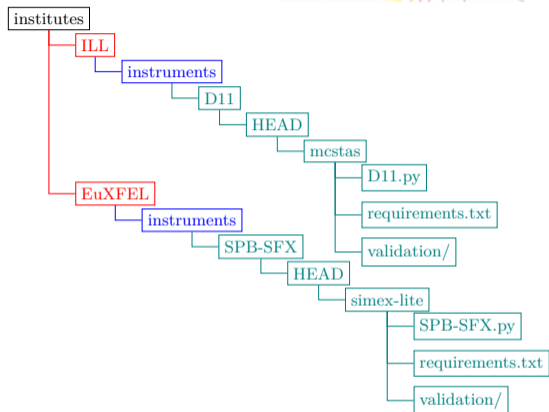
1. Starts the SIM server
2. Collects settings and create a request using the SIM client API
  - ▶ API guarantees format of request message
3. Send the request message (JSON format)
4. Waits for simulation result (or error)
5. Retrieve the simulation status and result

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.

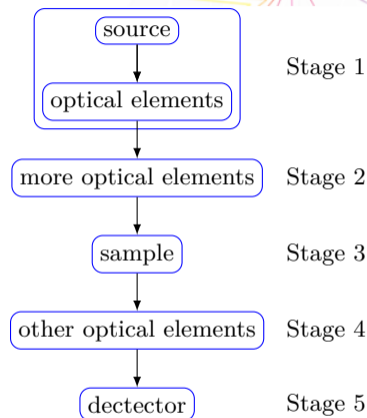


## Simulation staging and smart scheduler

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

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





## 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

