DIGITAL TWINS AT MLZ: combining Vitess and McStas with NICOS

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Advanced computer simulations methods for neutron scattering instruments 2025

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MLZ is a cooperation between:

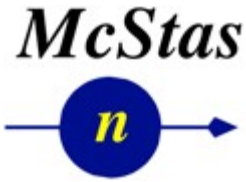
Aim

- Provide a **realistic simulation** of the instrument while using the **real user interface** (ECS of the facility)
- To assess the behavior of the instrument
  - **neutron flux at** sample, e.g. for different settings and different resolution
  - **expected results** with standard samples
  - **time consumption** (not only count, but also move time!)
  - influence of **sample environment** (Al-shields, dark angles etc.)
- For students and new users, **first experience** with performing an experiment at a large scale research facility
- For the facilities, better proposals, better expectations

NICOS
Networked Instrument COntrol System

Monte-Carlo Simulation

with **McStas** and **Vitess**

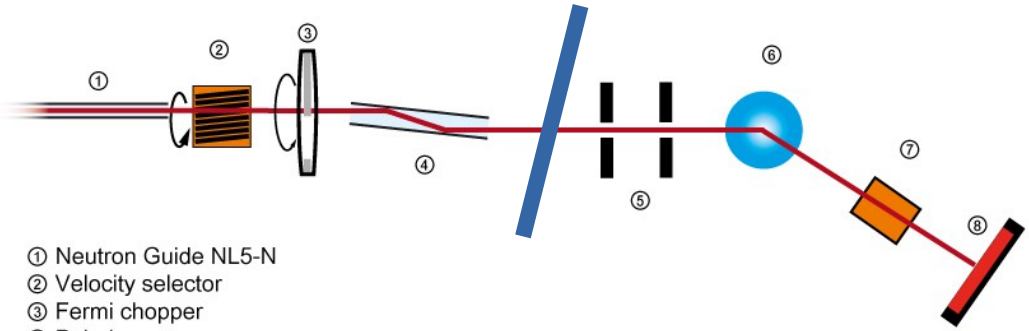


- Common features:
  - instrument as sequence of predefined components
  - simulation run with output to files
- Some differences (instrument definition, GUI, ...)
- Instrument definitions are usually **already available**!
  - but: usually for design/optimization of new instruments/parts
  - need adapt for **new purpose**: more devices
  - commitment of the specialists/scientists required

Implementation in the ECS

- Instrument definition with virtual devices, as far as possible parallel to the real setup
  ⇒ **operation identical** to the real instrument
- Special code, usually connected to detectors, runs a simulation using the position of all virtual devices – results are processed by the ECS as if from real detectors ⇒ **„real“ data files**
- Possibility to **cache** trajectories through seldom-changing instrument parts

  ⇒ Saving time for the detector simulation
- **Validation** required!



① Neutron Guide NL5-N
② Velocity selector
③ Fermi chopper
④ Polariser
⑤ Slit pair
⑥ Hexapod sample table
⑦ Polarisation analyzer (^{3}He)
⑧ Detector

vMARIA

Some implementation details

- **McStas**: Live data extraction uses the **SIGUSR2** „crutch“, which restricts parallelization possibility
  - Also awkward for data expected to be streamed events

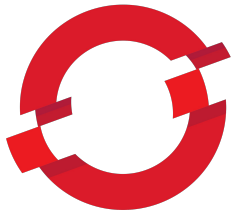
- **Vitess**: Many small changes to Vitess coming together to make digital twins possible/more realistic (talk of K. Lieutenant)
  - saving events to data files in **bunches**
  - defining instruments in **YAML** format, and running using vitess-python, which is easy to interface from NICOS (poster of F. Beule)
  - **live change** of simulation parameters and reset of detectors by propagating events through the pipeline between neutrons

Providing the system to users

- Main target audience are (new) users

  ⇒ system must be **externally available and scalable**

- Potentially large number of parallel instances required per instrument
  - with the possibility to keep private sessions?
- Provide to the outside using Apache **Guacamole** (web browser based interface to VNC)

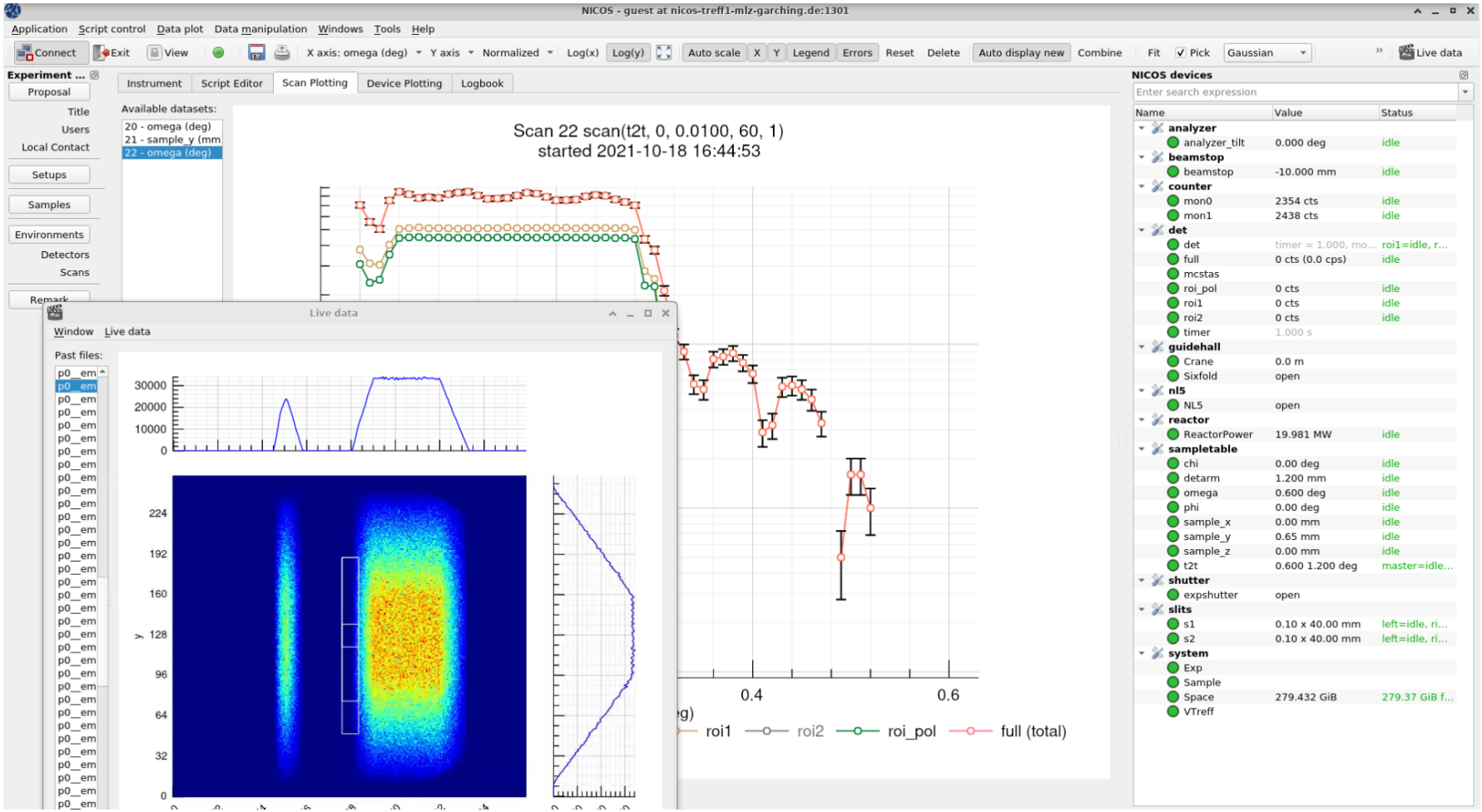


OPENSHIFT

- MLZ: around 10 instruments available, used in **lab courses** since 2021, training for **new scientists**
- Towards bigger scale, cloud based infrastructure

podman

DEMO


NICOS - guest at nicos-treff1-mlz-garching.de:1301
Application Script control Data plot Data manipulation Windows Tools Help
Connect Exit View X axis: omega (deg) Y axis Normalized Log(x) Log(y) Auto scale X Y Legend Errors Reset Delete Auto display new Combine Fit Pick Gaussian Live data
Experiment ...
Proposal
Title
Users
Local Contact
Setups
Samples
Environments
Detectors
Scans
Remark
Instrument Script Editor Scan Plotting Device Plotting Logbook
Available datasets:
20 - omega (deg)
21 - sample_y (mm
22 - omega (deg)
Scan 22 scan(t2t, 0, 0.0100, 60, 1)
started 2021-10-18 16:44:53
0.4
0.6
roi1 roi2 roi_pol full (total)
Live data
Window Live data
Past files:
30000
20000
10000
0
224
192
160
128
96
64
32
0
y
NICOS devices
Enter search expression
Name Value Status
analyzer
analyzer_tilt 0.000 deg idle
beamstop
beamstop -10.000 mm idle
counter
mon0 2354 cts idle
mon1 2438 cts idle
det
det timer = 1.000, mo... roi1=idle, r...
full 0 cts (0.0 cps) idle
mcstas
roi_pol 0 cts idle
roi1 0 cts idle
roi2 0 cts idle
timer 1.000 s
guidehall
Crane 0.0 m
Sixfold open
nl5
NL5 open
reactor
ReactorPower 19.981 MW idle
sampletable
chi 0.00 deg idle
detarm 1.200 mm idle
omega 0.600 deg idle
phi 0.00 deg idle
sample_x 0.00 mm idle
sample_y 0.65 mm idle
sample_z 0.00 mm idle
t2t 0.600 1.200 deg master=idle...
shutter
expshutter open
slits
s1 0.10 x 40.00 mm left=idle, ri...
s2 0.10 x 40.00 mm left=idle, ri...
system
Exp
Sample
Space 279.432 GiB 279.37 GiB f...
VTreff

Further outlook

- Many efforts toward more realistic simulation of **sample**, but also sample environment/shielding

  → Requires work mostly from instrument scientists and domain experts

- Handle **event mode** better; existing plans?
- In general find/define a better and **shared interface** for passing data from simulation to ECS

  → Interest among other groups?

  → What can be reused, what needs to be specific?

Summary

- McStas/Vitess simulations can be combined with the ECS to a „Digital Twin“, to **make advanced simulations accessible** to outsiders
- With realistic sample simulation and validation, enables integration into **scientific workflow**, part of user experience
- Container based solutions allow leveraging **a lot of** industry standard software
- Many improvements possible, collaboration opportunities for the interfaces simulation ↔ ECS

- Don't forget the real experiments ☺

THANK YOU!

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