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PaNOSC Closing Event

Paving the way towards the PaN FAIR Data Commons

29-30 November 2022

Grenoble - France

VINYL Simulations – post-project plans

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29/11/2022

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Introduction

Aim of WP5 - ViNYL

- **Vi**rtual **N**eutron and X-ra**y** **L**aboratory
- Harmonize simulation codes for neutron and x-ray experiments
- Agree on dataformats
    - For transfer of signal between codes
    - For detector results

- Led by Carsten Fortmann-Grote

- Chose Python packages with OpenPMD and Nexus data

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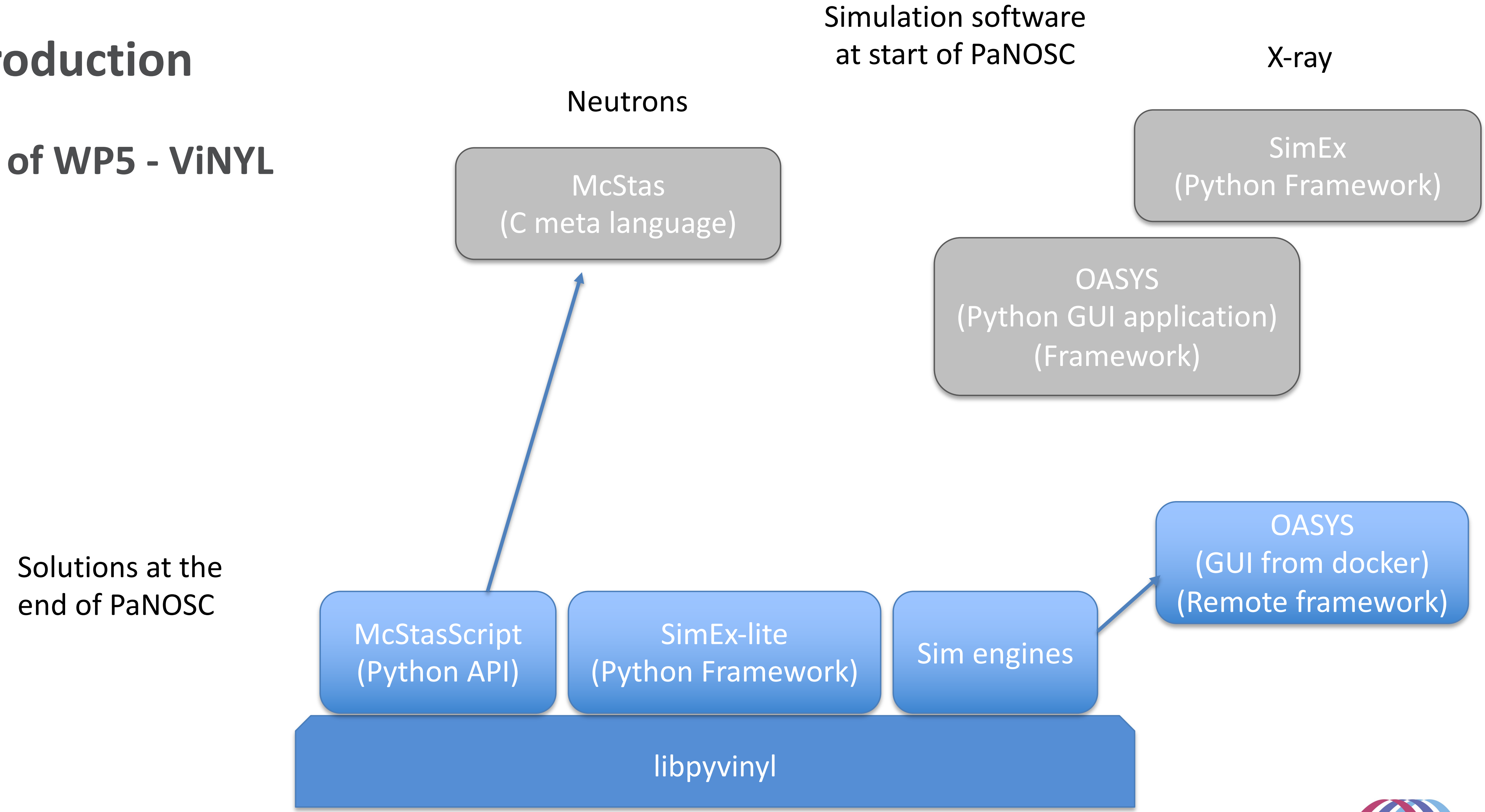
Introduction

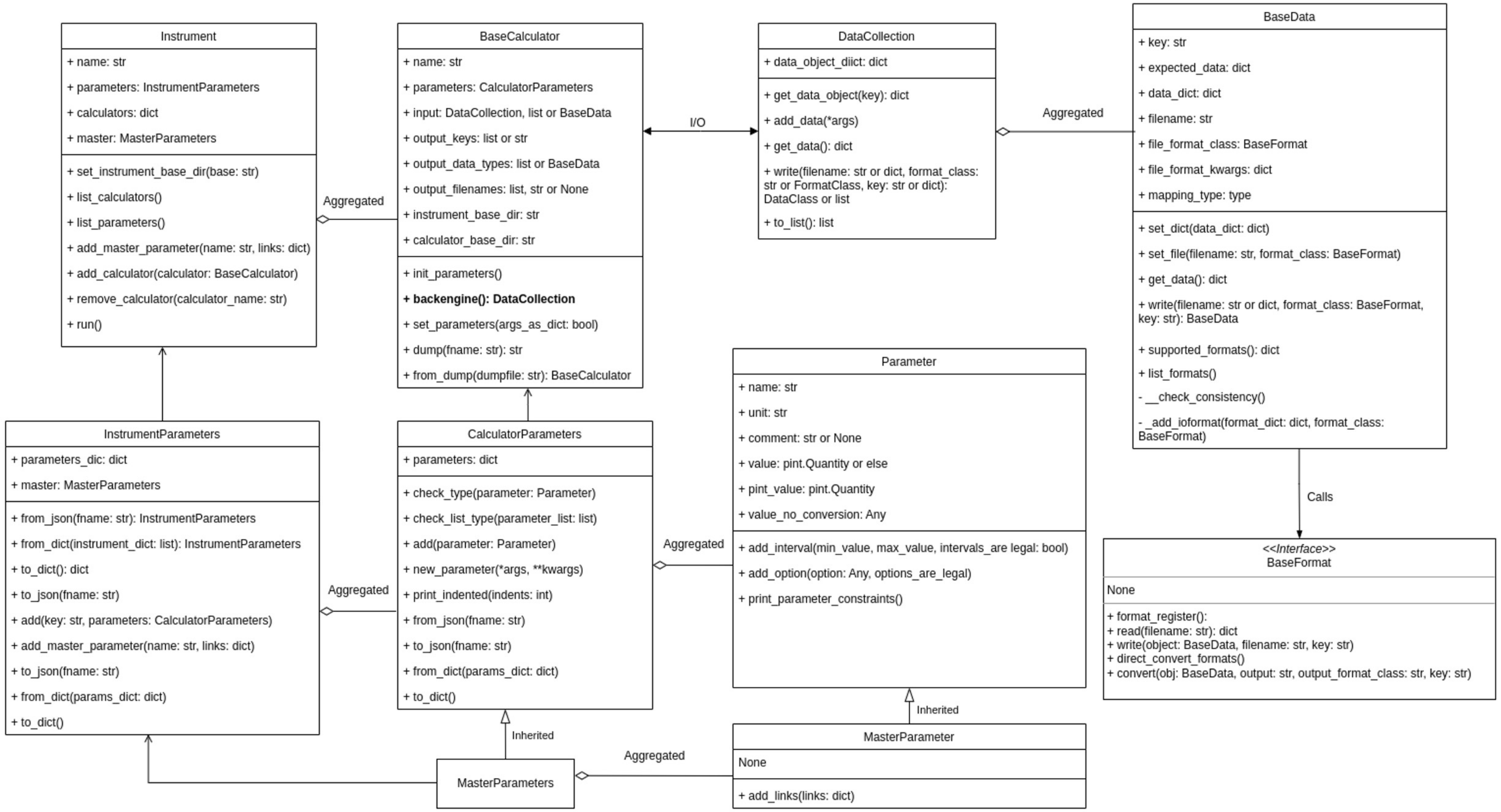
Aim of WP5 - ViNYL



libpyvinyl

Juncheng E, Shervin Nourbakhsh, Mads Bertelsen, Carsten Fortmann-Grote

Libpyvinyl class overview



- Harmonize the user interfaces for **neutron** and **X-ray** simulation
- Base classes:
  - BaseCalculator
  - BaseData
  - BaseFormat
- Auxiliary classes:
  - Parameter
  - CalculatorParameters
  - DataCollection
  - Instrument
- It provides the developers of start-to-end simulation platforms in neutron and X-ray community with a framework to integrate various backengine software.
- It reduces the effort needed to integrate their software to a start-to-end simulation platform for simulation software developers.

https://github.com/PaNOSC-ViNYL/libpyvinyl

A simple usage example:
https://github.com/PaNOSC-ViNYL/libpyvinyl/tree/master/tests/integration/plusminus

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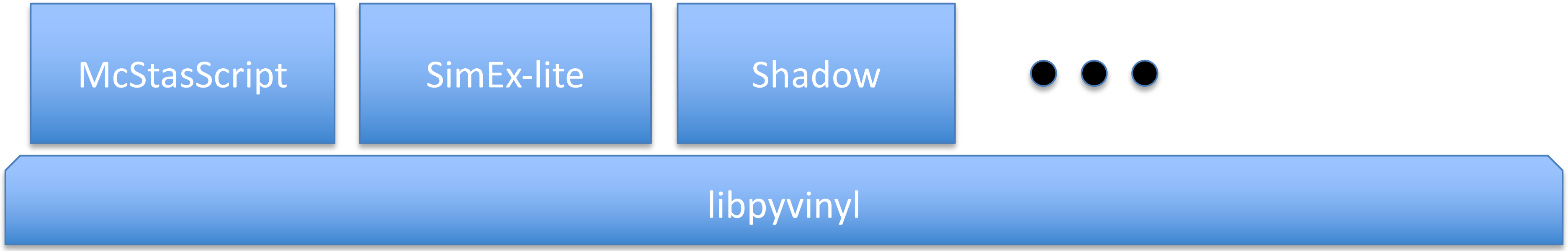
libpyvinyl

Juncheng E, Shervin Nourbakhsh, Mads Bertelsen, Carsten Fortmann-Grote

libpyvinyl is a dependency

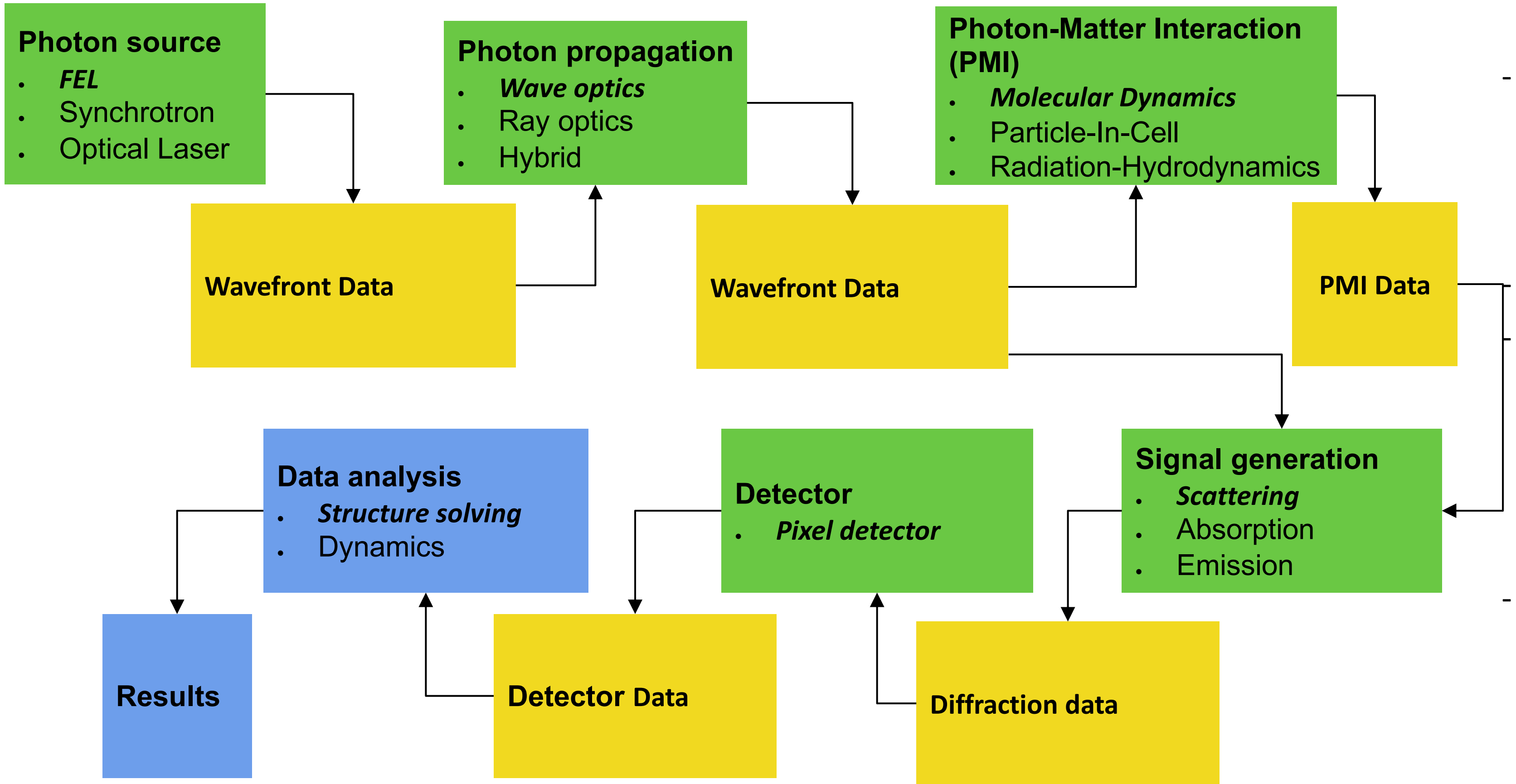
- libpyvinyl is a starting point for packages
- Provides base classes for
  - Parameters
  - Calculator
  - Data



SimEx-lite

Juncheng E, Carsten Fortmann-Grote

Package overview - Workflow



- It is the core package of the SIMEX platform providing the calculator interfaces and data APIs.

- It is built based on **libpyvinyl**
- A **calculator** can be easily constructed within SimEx-Lite with the definition of the corresponding **data class** and the **format class.**

- Users can choose which backengine software to implement to make the installation minimal per needs.

Calculators
Data interfaces

https://github.com/PaNOSC-ViNYL/SimEx-Lite

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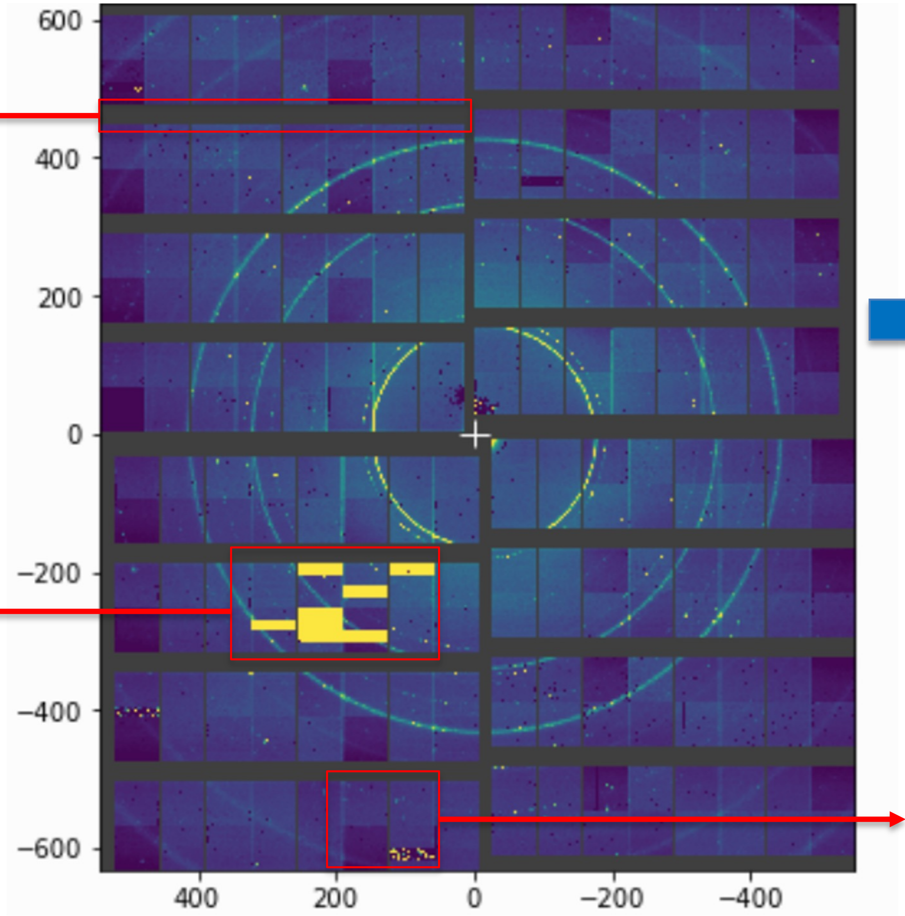
SimEx-lite

Serial Crystallography Simulation and Analysis

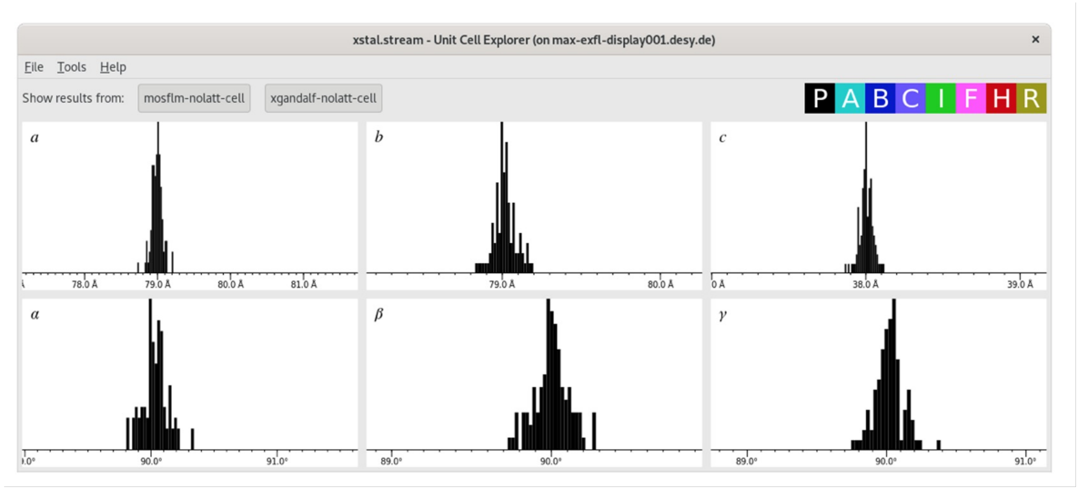
Panel gaps

Masks



Noise

Demonstrate the effects of noise, panel gaps and masks on the results of crystallography analysis with SimEx simulation diffraction pattern results



Scenarios:

- New researchers want to get hands-on experience of data processing for serial crystallography.
- Starting from a working example of a simulation coupled to an analysis pipeline.
- Explore how different experimental conditions and different analysis options affect the results.

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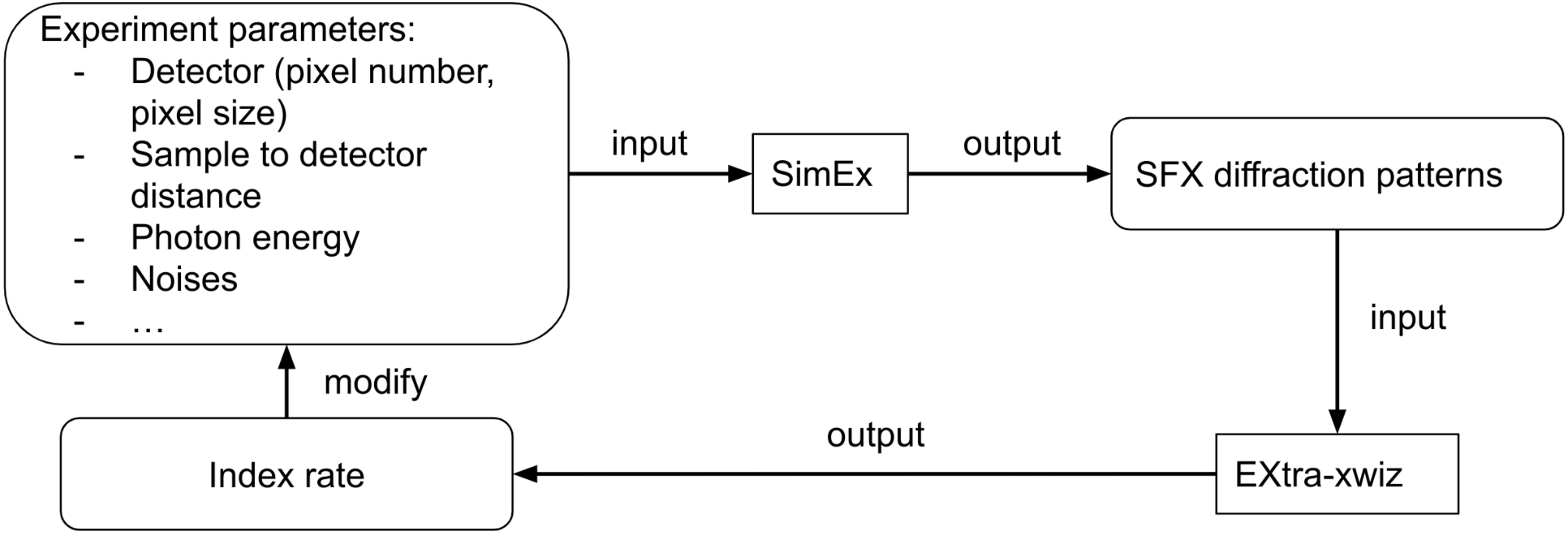
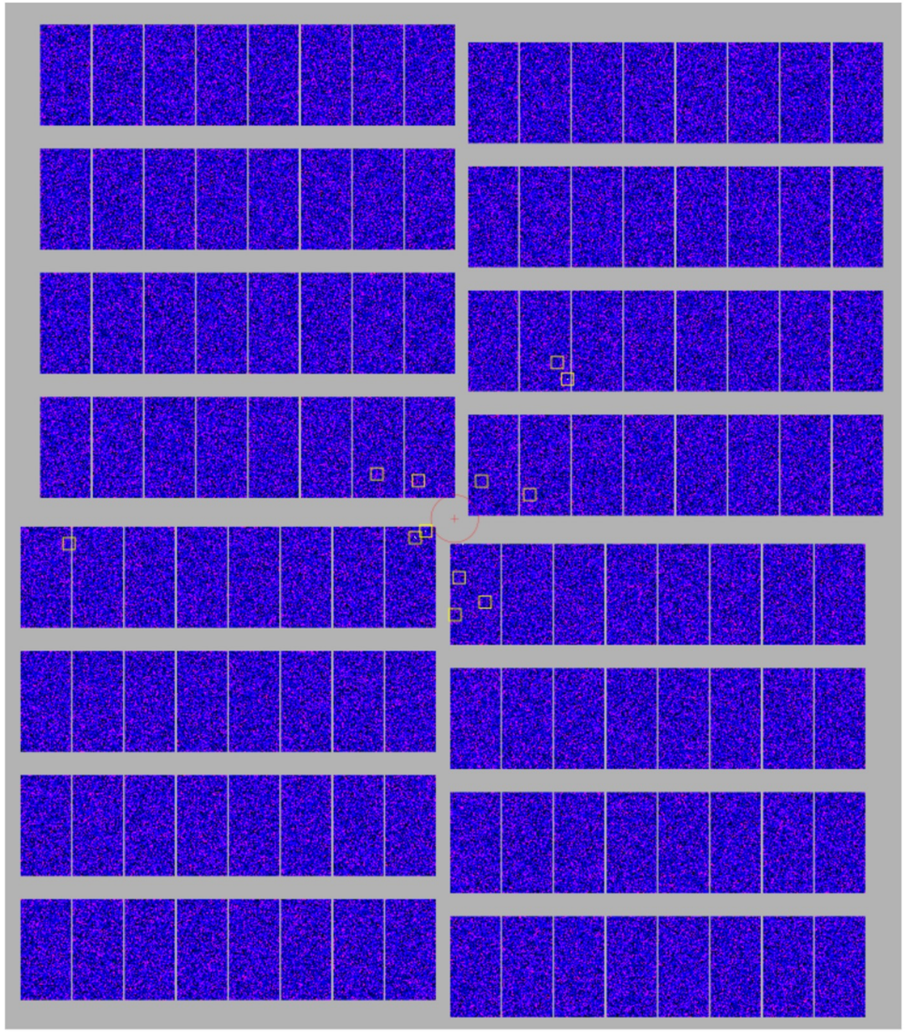
SimEx-lite

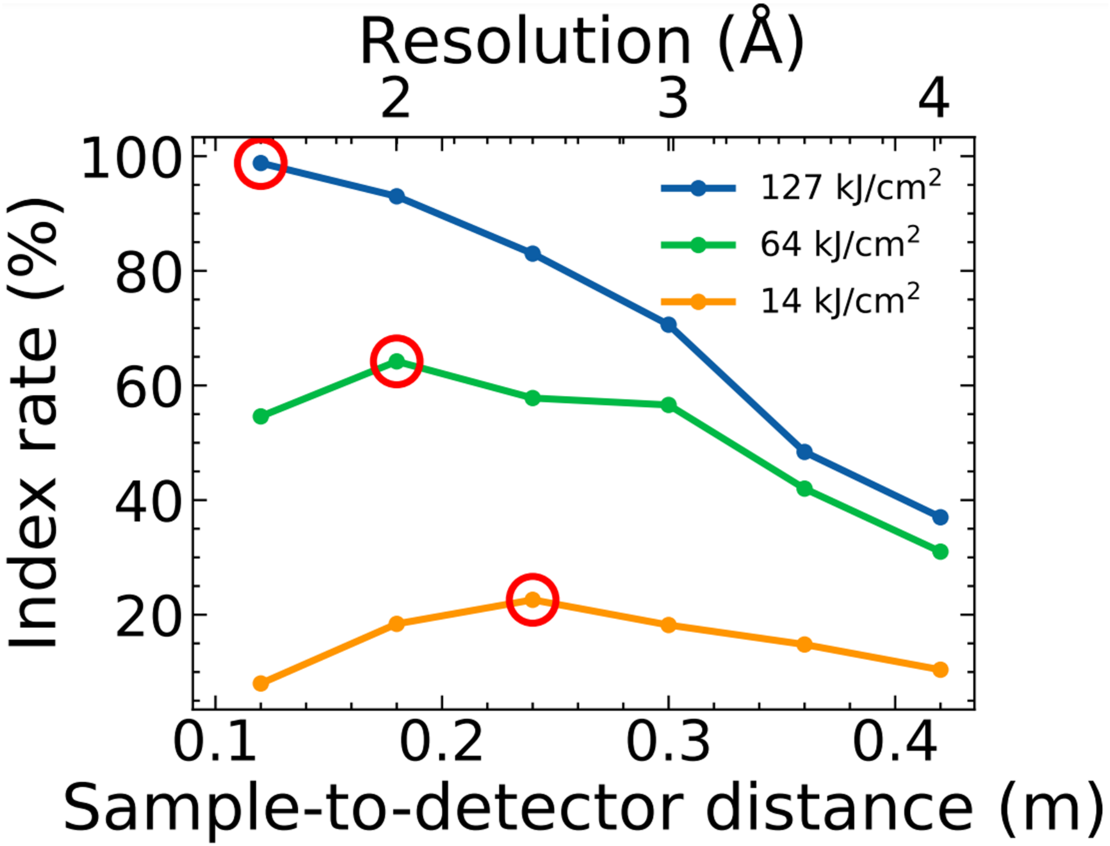
Optimize sample to detector distance in different energy densities



SimEx-lite

Optimize sample to detector distance in different energy densities





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SimEx-lite

Scientific publications

Structural Dynamics ARTICLE scitation.org/journal/sdy

Expected resolution limits of x-ray free-electron laser single-particle imaging for realistic source and detector properties EP ← **Editor's pick**

Cite as: Struct. Dyn. **9**, 064101 (2022); doi: 10.1063/4.0000169
Submitted: 7 September 2022 · Accepted: 31 October 2022 ·
Published Online: 16 November 2022

View Online Export Citation CrossMark

Juncheng E,[1] Y. Kim,[1] J. Bielecki,[1] M. Sikorski,[1] R. de Wijn,[1] C. Fortmann-Grote,[1,2] J. Sztuk-Dambietz,[1] J. C. P. Koliyadu,[1] R. Letrun,[1] H. J. Kirkwood,[1] T. Sato,[1] R. Bean,[1] A. P. Mancuso,[1,3,a)] and C. Kim[1,b)]

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scientific reports

Check for updates

OPEN

Effects of radiation damage and inelastic scattering on single-particle imaging of hydrated proteins with an X-ray Free-Electron Laser

Juncheng E[1], Michal Stransky[1,2], Zoltan Jurek[3,4], Carsten Fortmann-Grote[1,5], Libor Juha[6,7], Robin Santra[3,4,8], Beata Ziaja[2,3] & Adrian P. Mancuso[1,9]

The papers are based on the simulation of photon-matter interaction, scattering process and detector response within the framework of SIMEX.

E, J. et al. Sci Rep 11, 17976 (2021) doi:10.1038/s41598-021-97142-5
E, J. et al. Structural Dynamics 9, 064101 (2022) doi:10.1063/4.0000169

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OASYS

Manuel Sanchez del Rio, Aljosa Hafner

Project overview

- ✓ OASYS = OrAnge SYnchrotron Suite
- ✓ A common platform to build synchrotron-oriented User Interfaces ***that communicate***
- ✓ The upper layer of the application presented to the user
- ✓ Open Source & Python technology

Luca Rebuffi, Manuel Sanchez del Rio (2017)
OASYS (OrAnge SYnchrotron Suite) : an open-source graphical environment for x-ray virtual experiments
Proc.SPIE 10388: 10388-10388. http://dx.doi.org/10.1117/12.2274263

https://oasys-kit.github.io/

U.S. DEPARTMENT OF ENERGY
Argonne NATIONAL LABORATORY
Elettra Sincrotrone Trieste
BERKELEY LAB Bringing Science Solutions to the World
ESRF The European Synchrotron
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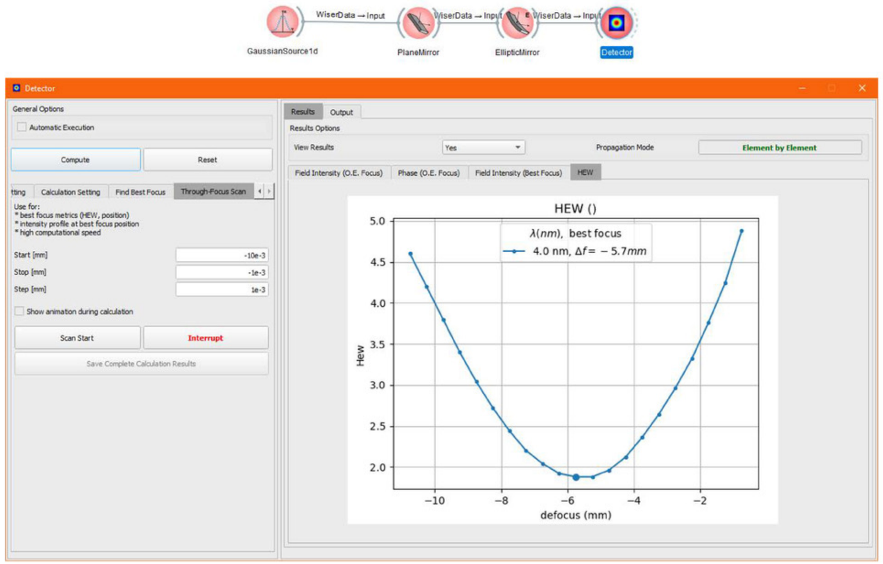
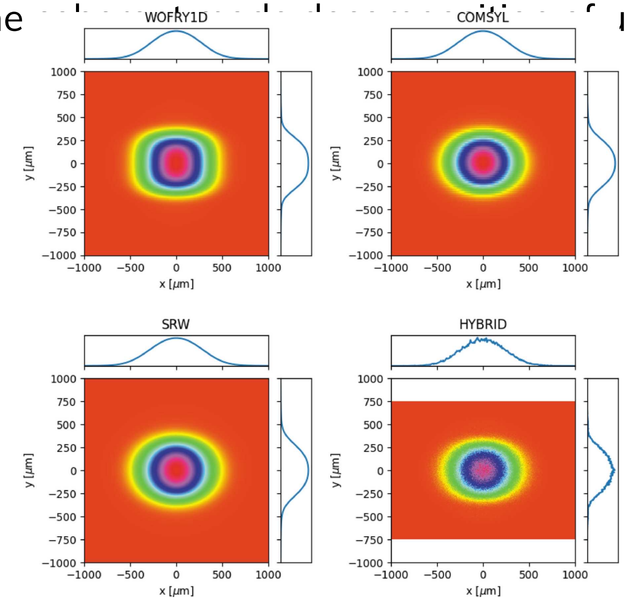
OASYS

Wiser and COMSYL

Main code developments - Require **high-performance computing** resources and benefit from **remote deployments**:

- **Wiser** code for numerical integration of wave propagation:
  Allows for precise metrology simulations, correctly taking into account shape and roughness contributions at various length scales.
- **COMSYL** (COherent Modes for SYnchrotron Light):
  … the … undulator radiation in a storage ring.





- M. Manfredda et al. *Advances in Computational Methods for X-Ray Optics V*. Vol. 11493. International Society for Optics and Photonics. SPIE, 2020, 114930B. DOI: 10.1117/12.2568574
- M. Glass et al. *EPL (Europhysics Letters)* 119.3 (Aug. 2017), p. 34004. DOI: 10.1209/0295-5075/119/34004
- M. Sanchez del Rio et al. *Journal of Synchrotron Radiation* 29.6 (Nov. 2022), pp. 1354–1367. DOI: 10.1107/S1600577522008736.

OASYS

Remote usage

Main challenge: OASYS is a GUI program built in PyQT. How to run it in the browser? As a **Jupyter hub plug-in**!

- **Deployed** easily as a **Docker container** and can be used within an existing Jupyter hub instance
- **Remote repository workspace downloader** has been **developed as a widget**
- Used together with WP8 for th … ssfull … ol

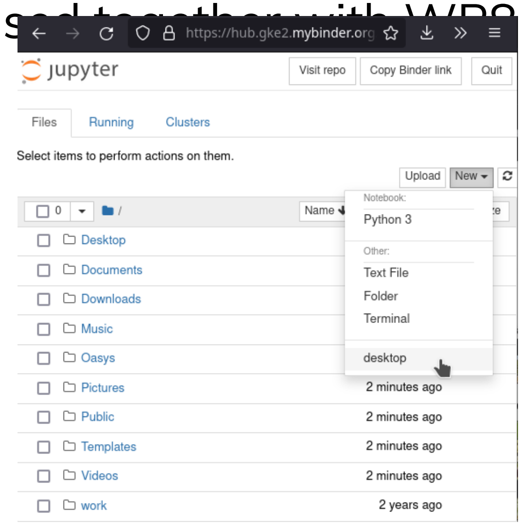


Figure: Select and run a desktop environment from within Jupyter hub.

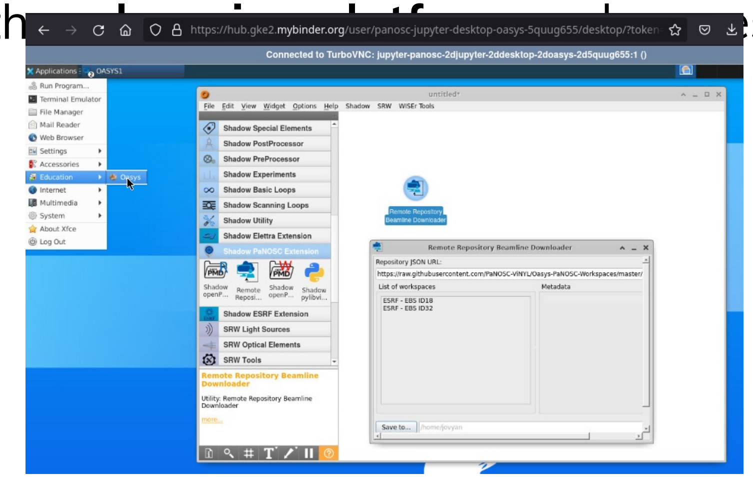


Figure: OASYS GUI envrionment inside a web browser.

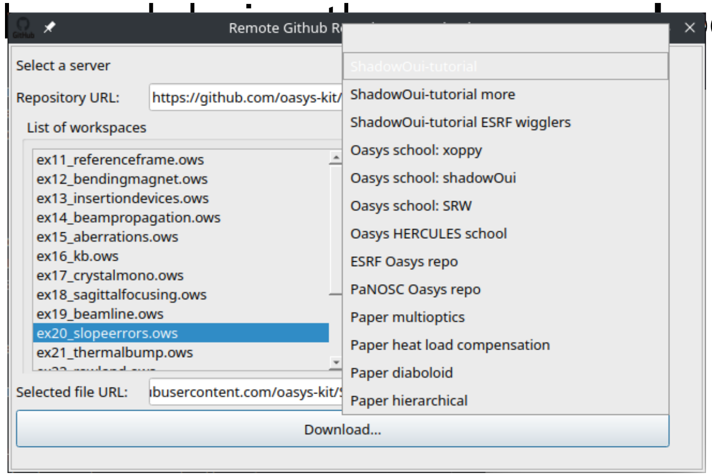


Figure: Remote repository downloader widget showing a selection of curated workspaces available.

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OASYS

Other developments – openPMD and link to SimEx

- **Deliverable D5.1**: contributions to openPMD standard for ray-tracing
- **Synergy of WP5 simulation codes**: link between diffraction simulations and beamline optics
  - OASYS-SimEx Widget **developed and available**
  - **OASYS PaNOSC toolbox** contains all the tools developed in the project and is available for installation through the built-in add-on manager as OASYS1-PaNOSC package

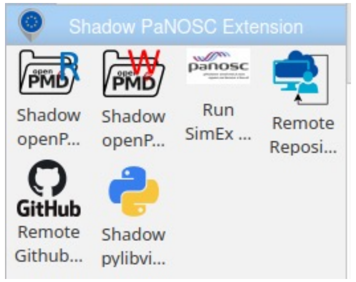


Figure: OASYS PaNOSC toolbox.

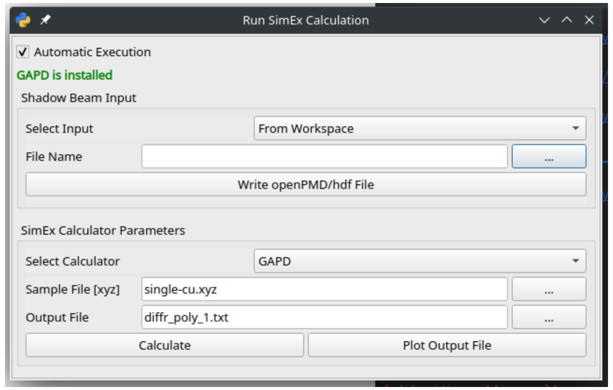


Figure: SimEx interaction widget showing the GAPD calculator.

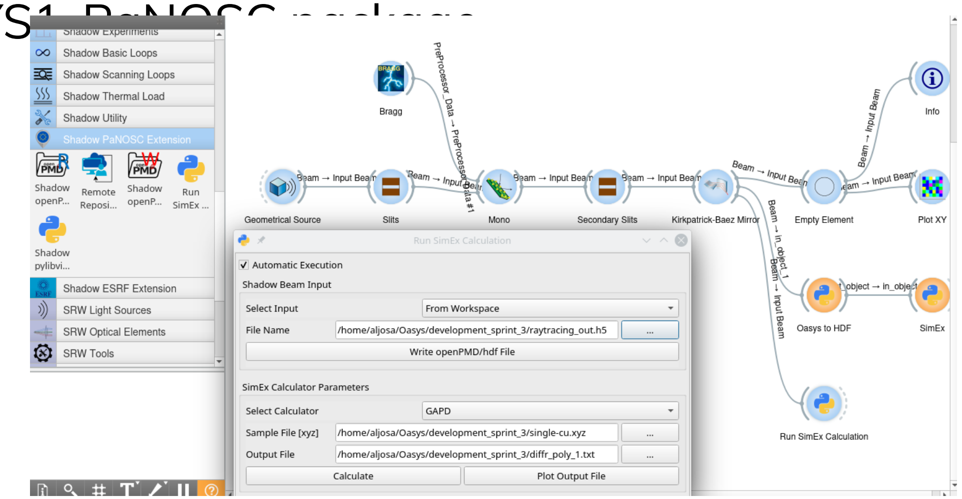
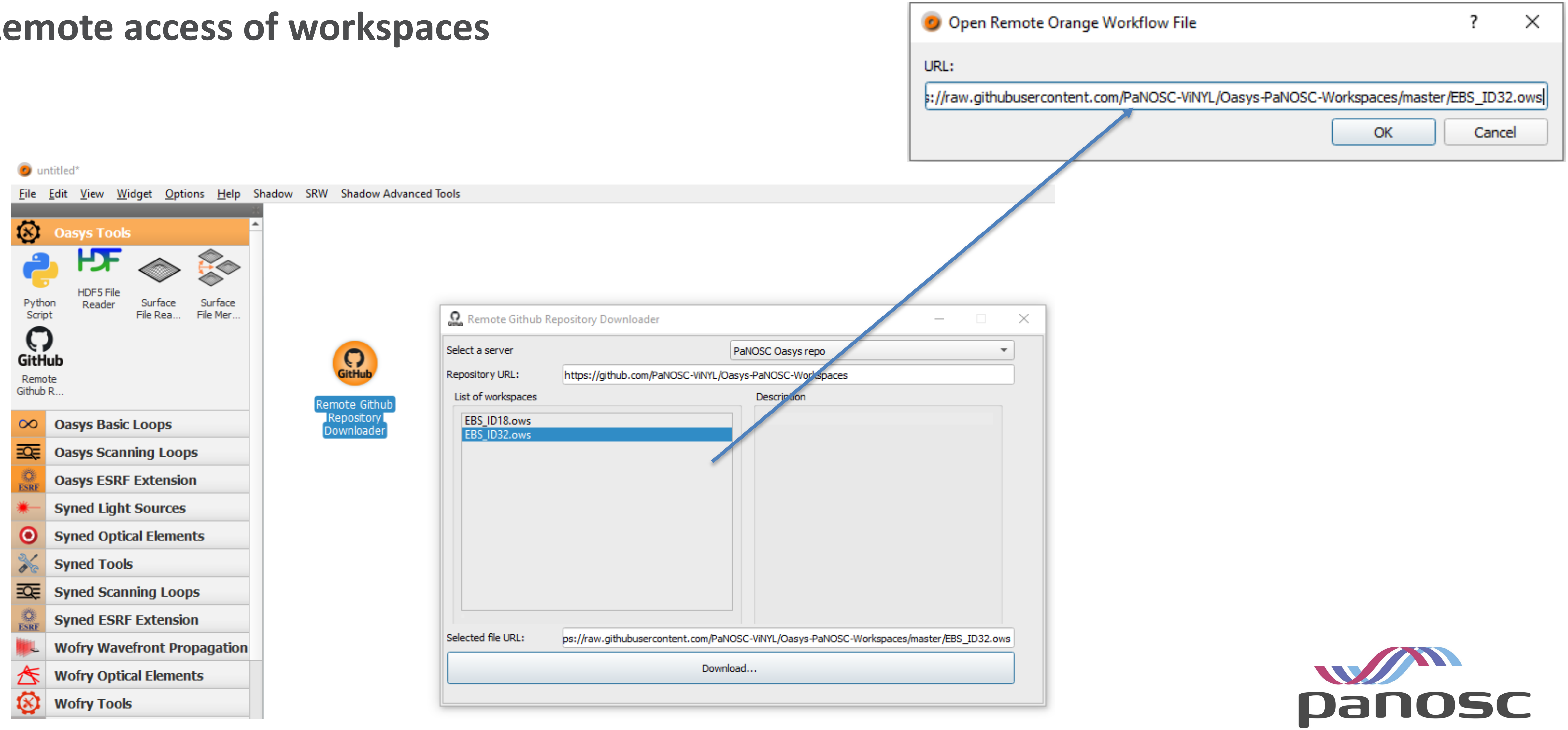


Figure: Seamless workflow from beamline optics to diffraction simulations within the OASYS GUI.

OASYS

Remote access of workspaces



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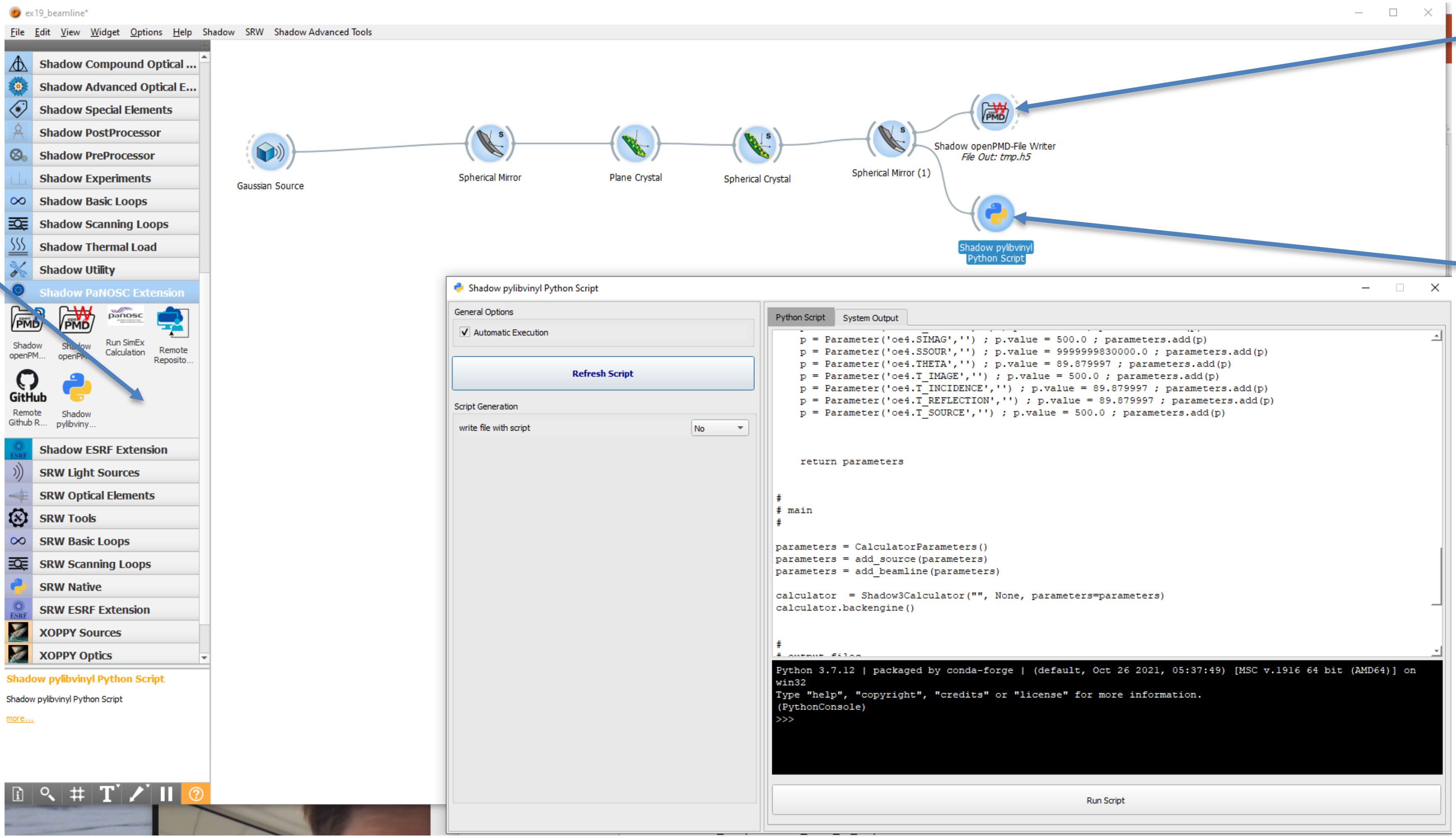
OASYS

PaNOSC tools for SHADOW simulations

PaNOSC add-on



OpenPMD writer

Script using libpyvinyl

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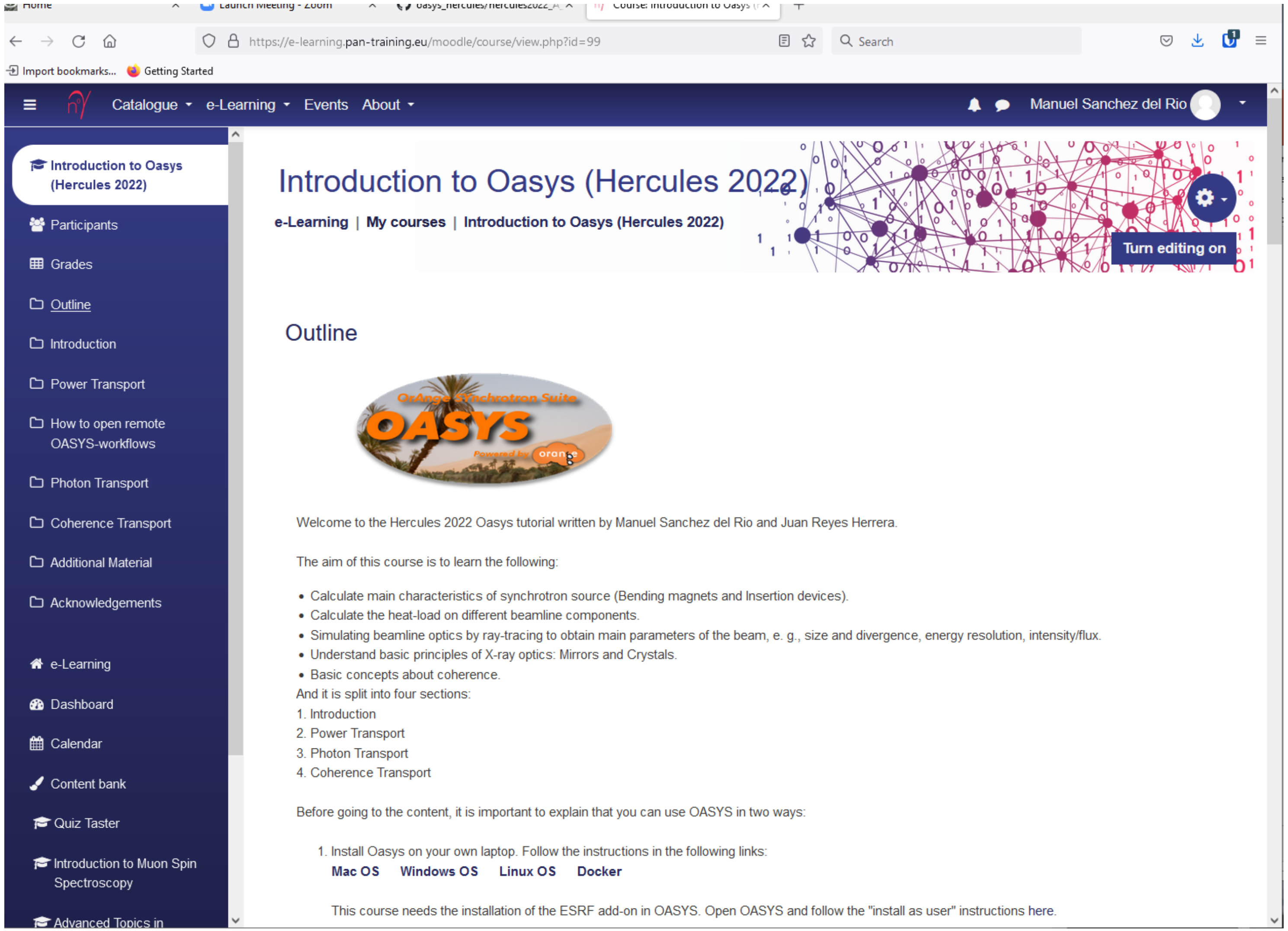
OASYS

E-learning course on pan-training.eu



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McStasScript

Mads Bertelsen

Overview

- API for popular instrument simulation tool McStas
  - Describe instrument to be simulated
  - Get help and overviews
  - Run simulations
  - View data
  - Get data as numpy arrays
  - Use widgets

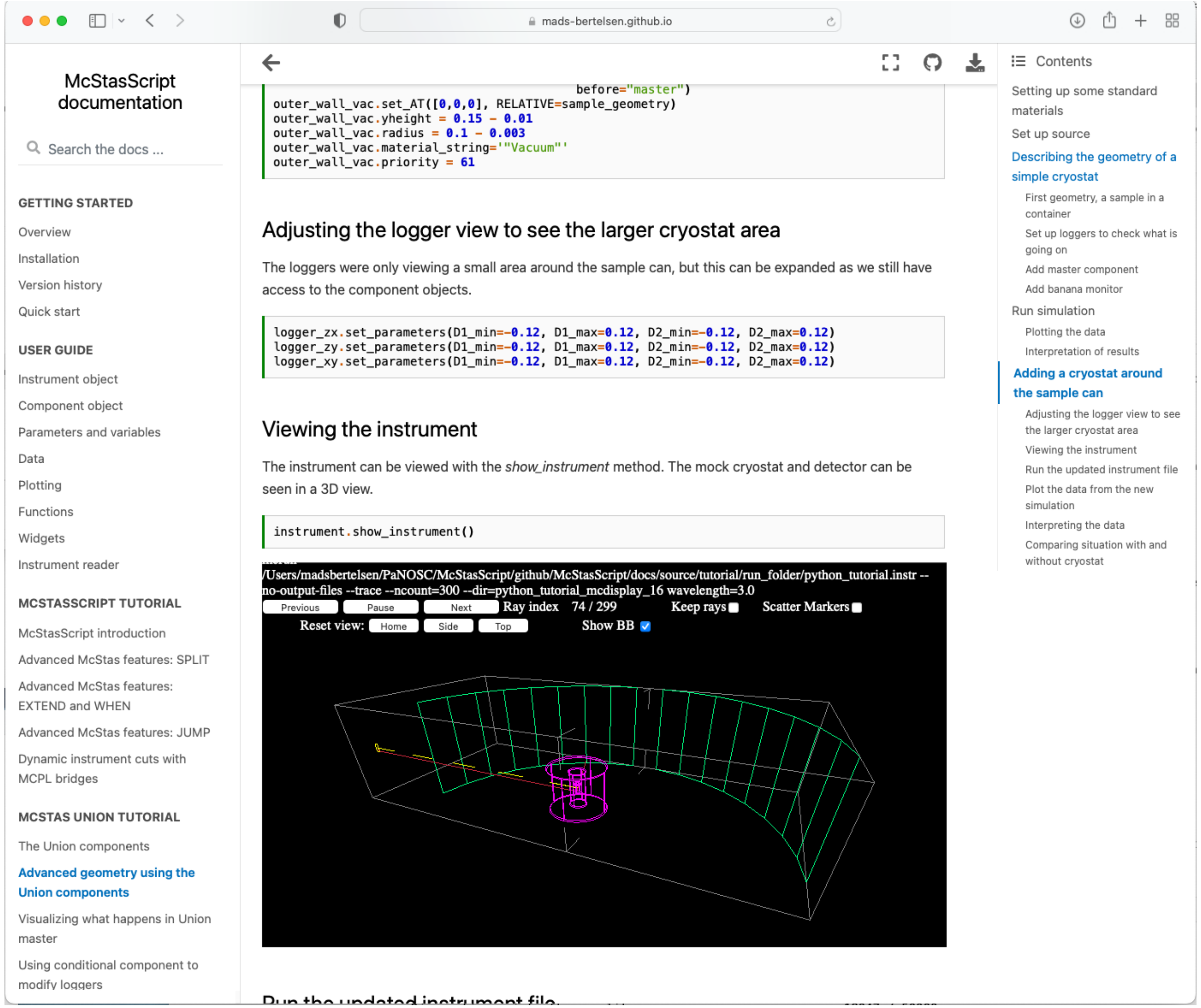
```
guide = instr.add_component("guide", "Guide_gravity")
guide.set_parameters(w1=0.05, h1=0.05, m=2, G=-9.82, l=10)
guide.set_AT(2.0, RELATIVE=src)

slit = instr.add_component("slit", "Slit")
slit.radius = 0.03
slit.set_AT(guide.l + 0.2, RELATIVE=guide)

sample = instr.add_component("sample", "PowderN")
sample.set_AT(0.1, RELATIVE=slit)
sample.set_parameters(radius=0.015, yheight=0.05,
                      reflections='"Na2Ca3Al2F14.laz"')

data = instr.backengine()
```

McStasScript

Documentation

- Documentation
  - Install guide - pip
  - Configuration – set a few paths
  - Quick guide
  - Tutorials
  - Reference

- All as jupyter notebooks



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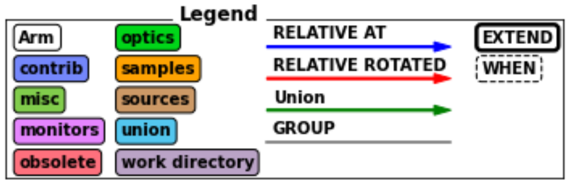
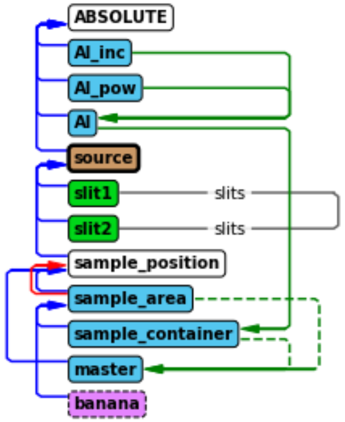
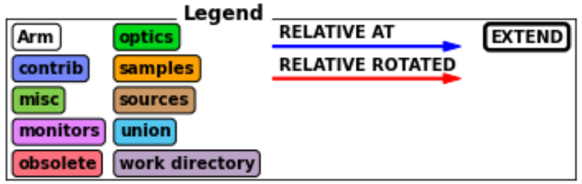
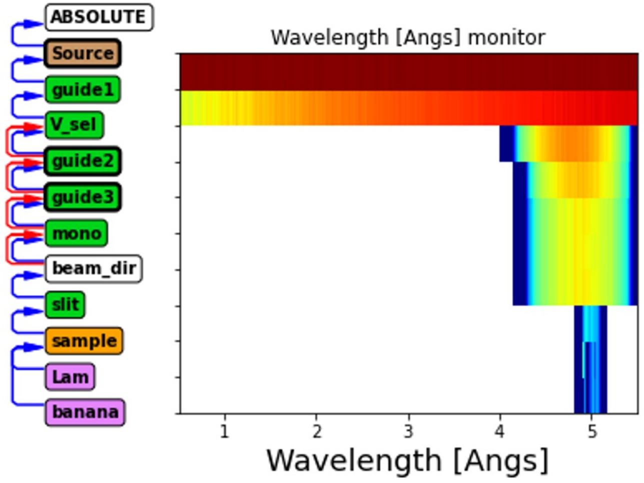
McStasScript

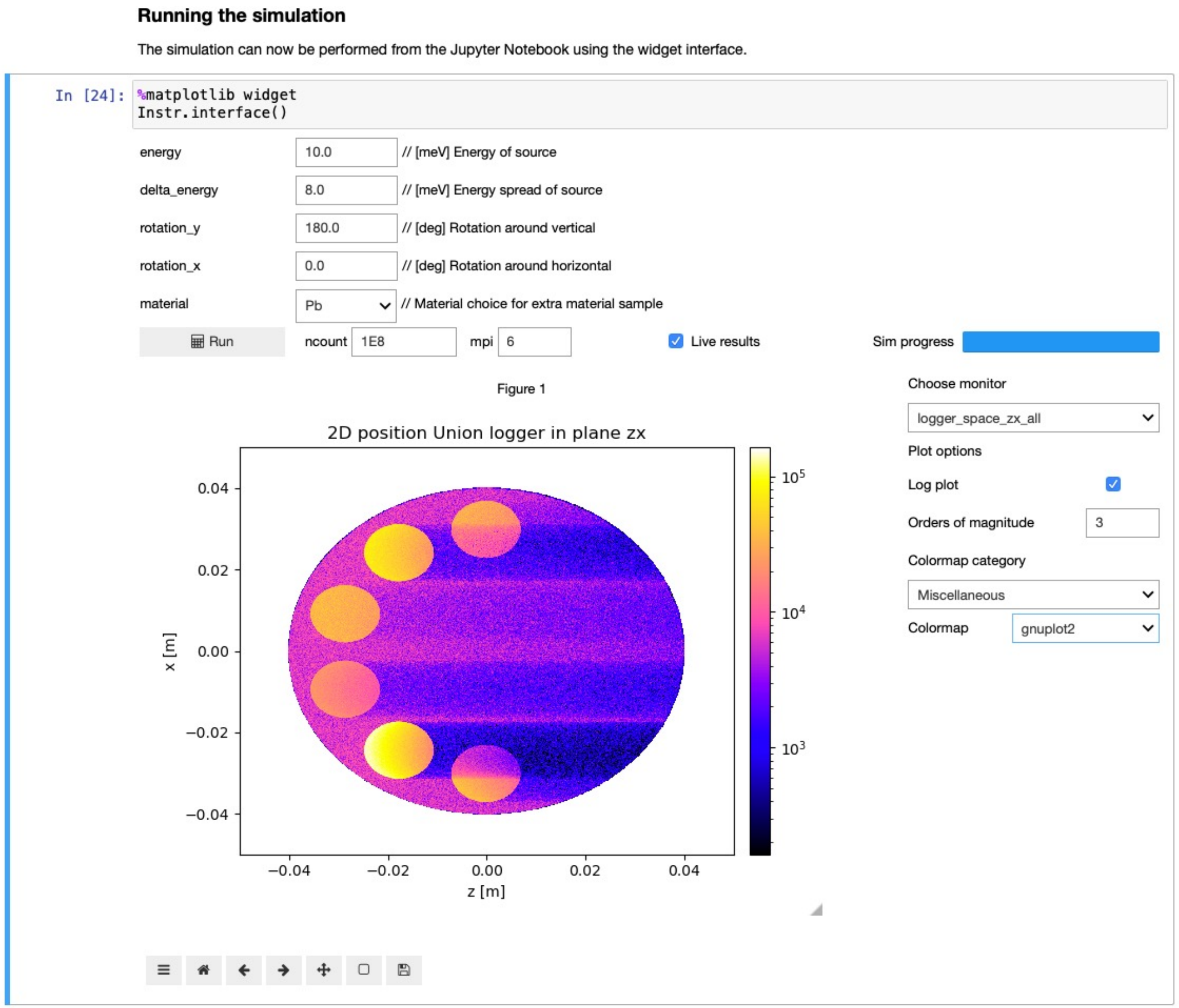
Diagrams and widgets











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Instrument repository

Shervin Nourbakhsh

Overview

GIT stores instrument descriptions in the form a Python scripts following the libpyvinyl API.
Advantages of GIT:

- History of changes
- Integrated issue tracking system
- Automatic workflows for validation
- Openly accessible
- Free hosting
- Easy to clone, fork for special needs of the RIs

Sustainability

- Instrument description maintained by instrument experts at Ris
- Users contributing with validations and debugging

A dedicated python API is developed to allow end users (especially those not knowing git) to access the instrument description.

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Instrument repository

Instrument repository API

- Setup the API

```
from instrumentdatabaseapi import instrumentdatabaseapi as API
repo = API.Repository()
repo.init()
```

- Load the instrument and units
  - Institute name
  - Instrument name
  - Version: HEAD for the current or date of last day of validity YYYY-MM-DD
  - Flavour: if different alternative descriptions are possible (e.g. detailed vs simplified)

```
myinstrument = repo.load("ILL","ThALES" , "HEAD", "mcstas", "full", dep=
                                    False)
import pint
ureg = pint.get_application_registry()
```

- Set simulation settings

```
myinstrument.set_instrument_base_dir("/tmp/ThALES_scan/")
myinstrument.sim_neutrons(500000)
myinstrument.set_seed(654321)
```

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Instrument repository

Instrument repository API

- Set instrument parameters:

```
myinstrument.master["a2"] = myinstrument.energy_to_angle(4.98 * ureg.meV)
myinstrument.master["a4"] = 60 * ureg.degree
```

- Set sample parameters:

```
myinstrument.set_sample_by_name("vanadium")
myinstrument.sample_cylinder_shape(0.005, 0.01)
```

- Run simulations

```
np = (21 - 1) / 2
dEI = 0.05
import numpy
myinstrument.force_compile(false)
outputs = []
for energy in numpy.arange(4.98 - np * dEI, 4.98 + np * dEI, dEI):
  myinstrument.master["a6"] = myinstrument.energy_to_angle(energy * ureg.
                                  meV)
  myinstrument.run()
  outputs.append(myinstrument.output)
```

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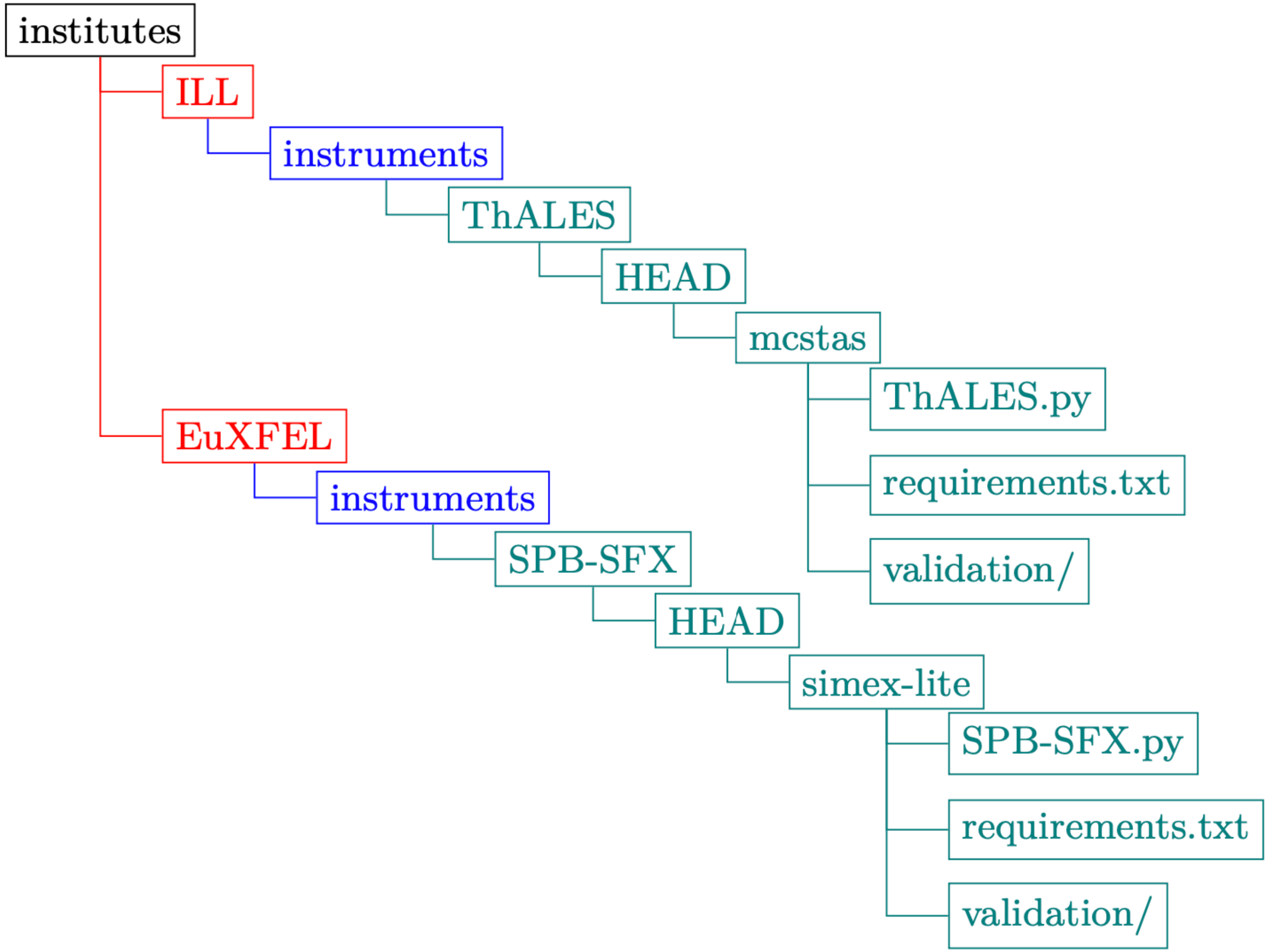
Instrument repository

Instrument repository structure



Digital Twin

Shervin Nourbakhsh

Overview

General idea of a Digital Twin

It is a digital replica of the physical elements of an instrument that can be controlled and provide feedback as the real instrument.

It can be implemented at different levels of fidelity to replicate the features that one is interested in.

Ingredients of Digital Twin at ILL

- An instrument fully described in the *instrument database*
- The physics of the sample provided by the user via Sqw files or other formats
- A set of sample environments fully described
- The data acquisition system (Nomad) used for both real and simulated data
- An application manager (Cameo) providing also basic communication patterns

A simulation server:

- processing simulation requests
- scheduling and parallelizing the simulation
- reading and sending the results to Nomad

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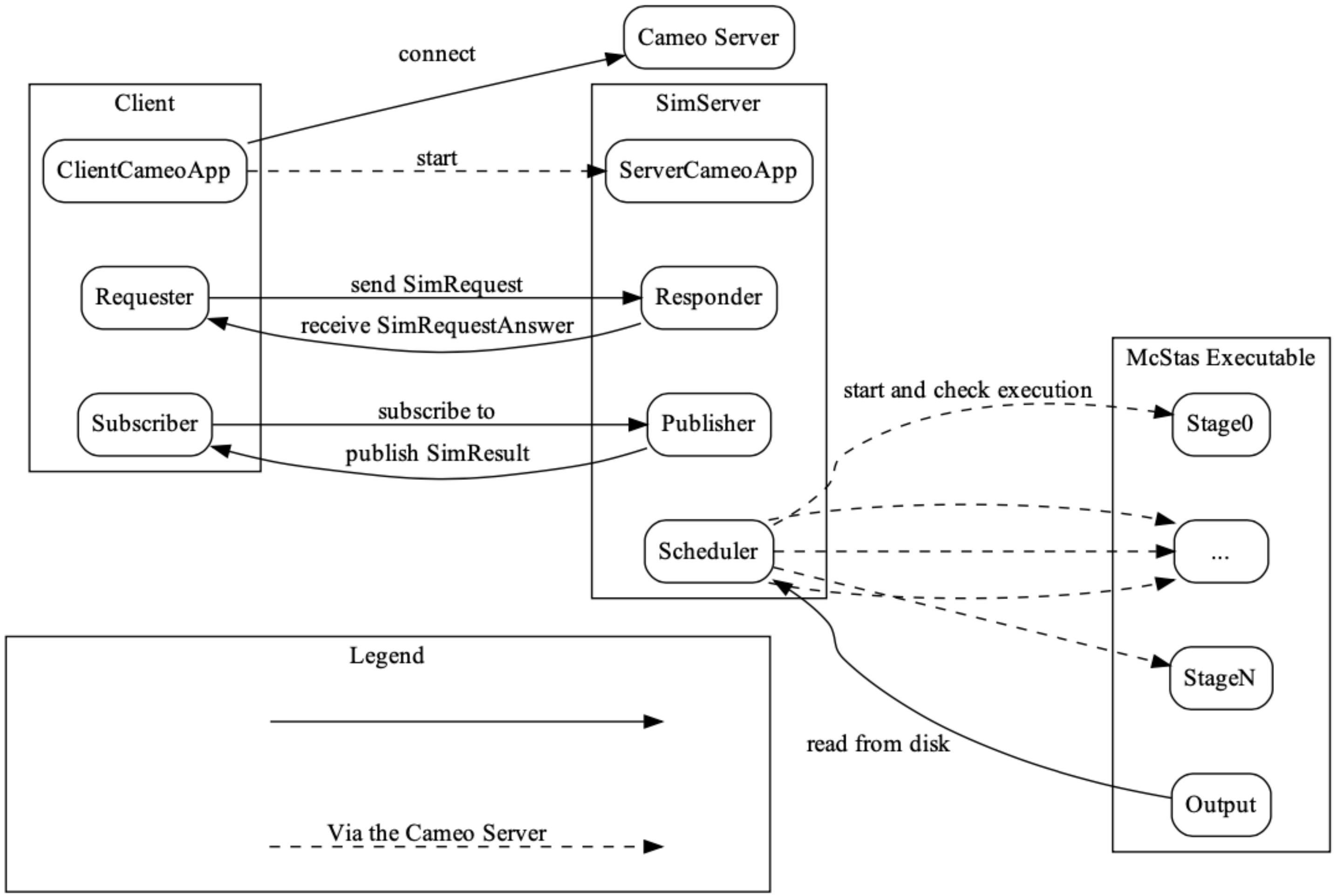
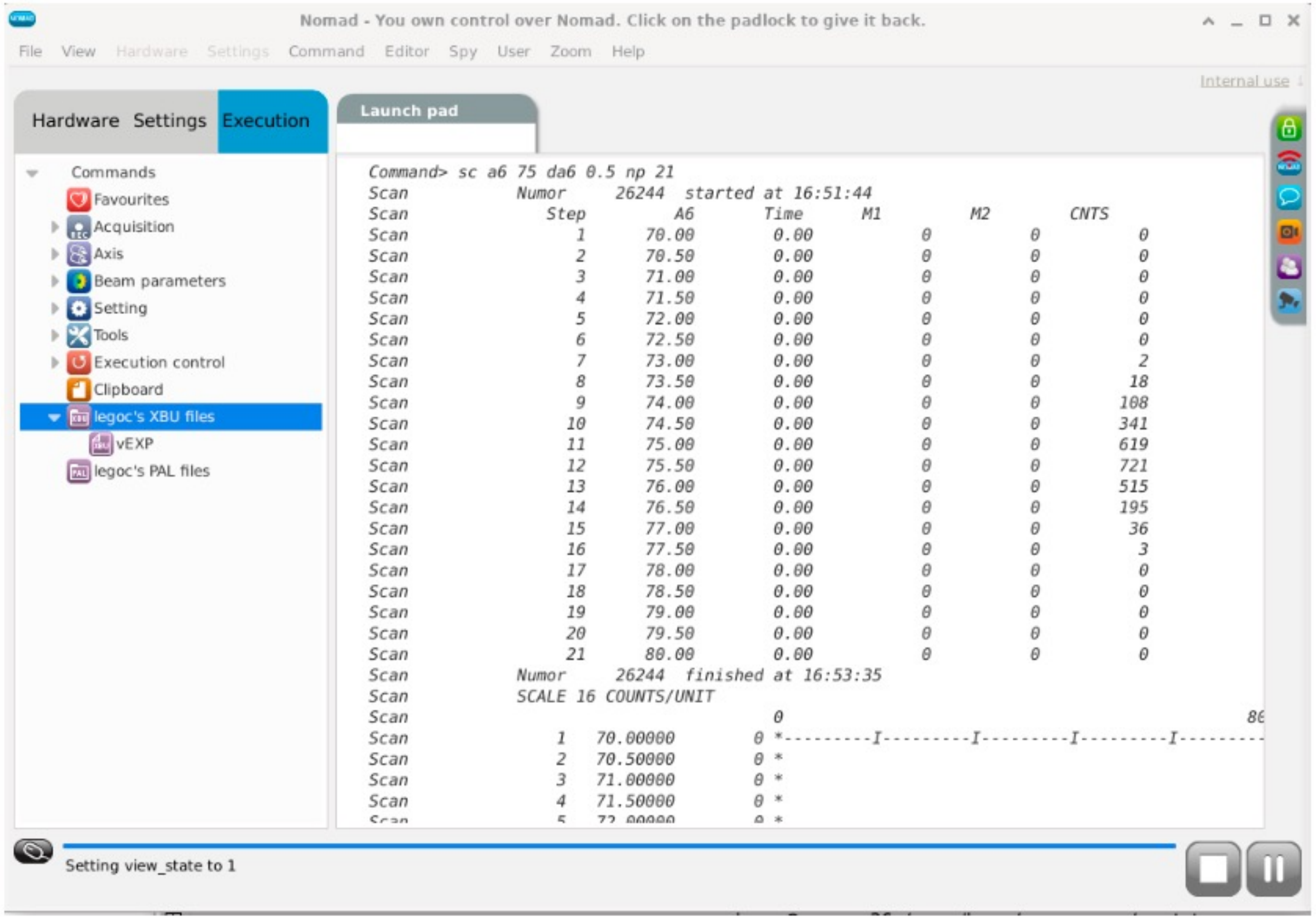
Digital Twin

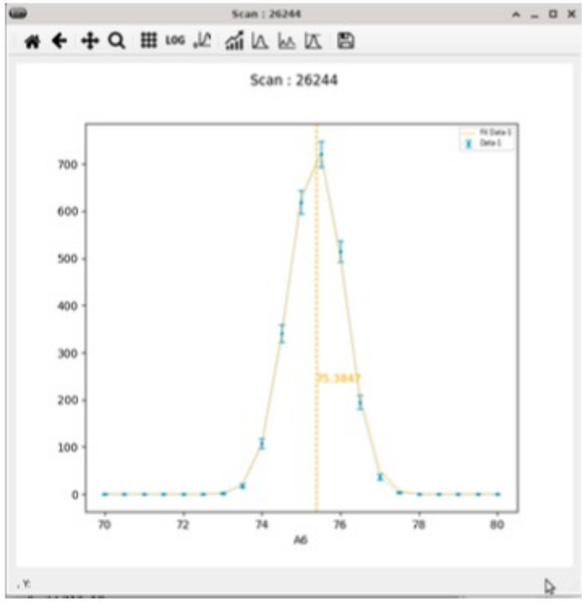
ILL system overview



Digital Twin

Results in Nomad

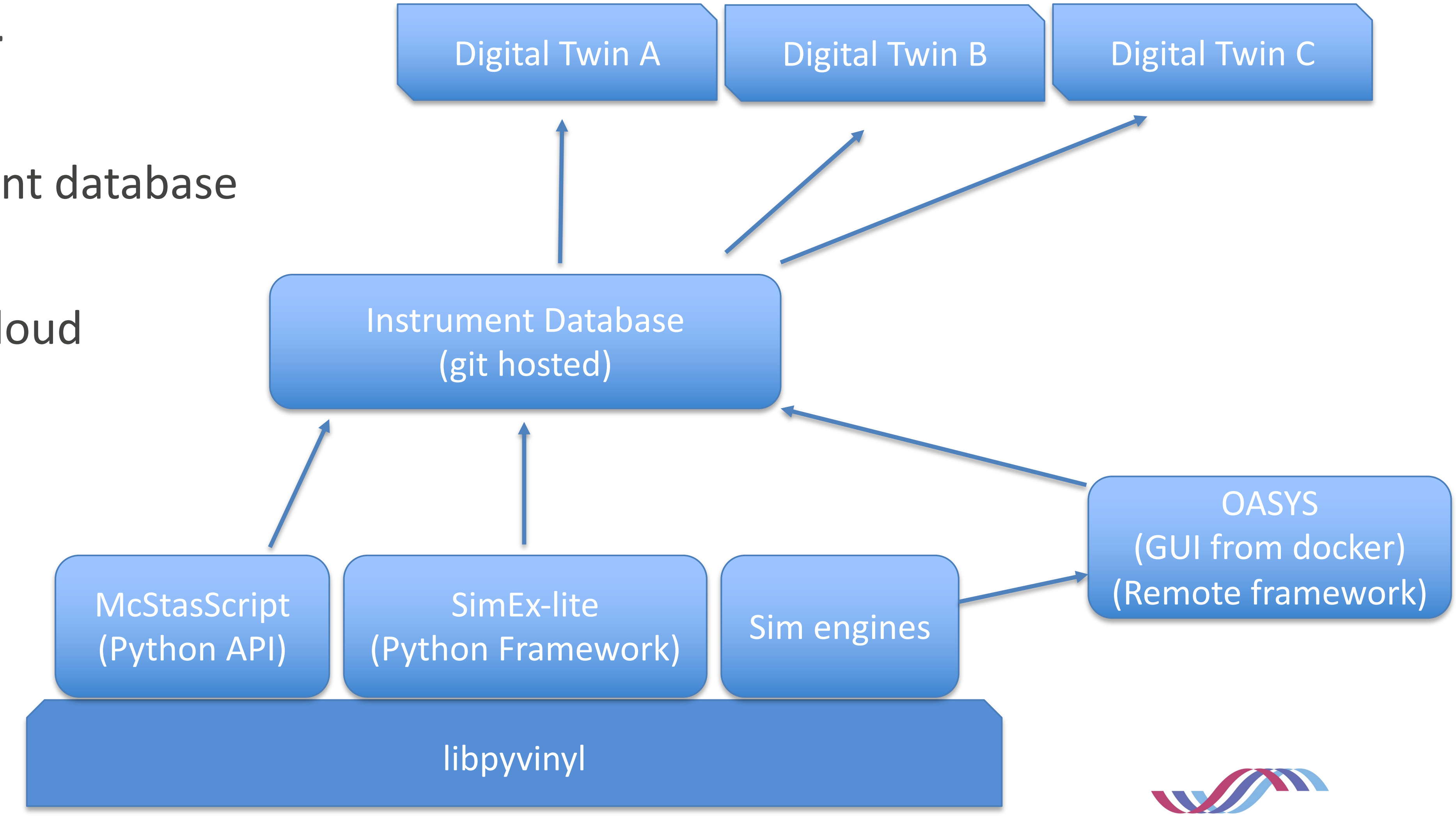




Summary

Result of WP5 - ViNYL

- Common instrument database
- Interoperability
- Can be hosted in cloud



Sustainability

Future for the developed software

- All packages have developers interested in continuing support
- Reduced level compared to PaNOSC

Package	Current	After PaNOSC
libpyvinyl	Juncheng, Shervin, Mads, Carsten	Juncheng, Mads, Carsten
Instrument DB	Shervin	Mads
McStasScript	Mads	Mads
SimEx	Juncheng, Carsten	Juncheng, Carsten
Oasys	Aljosa, Manuel	Manuel

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Paving the way towards the PaN FAIR Data Commons
29-30 November 2022
Grenoble - France

Thank you

Mads Bertelsen
Mads.Bertelsen@ess.eu

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