Work package 5
“Virtual Neutron and X-Ray Laboratory”
–
Workpackage review report to the Project Management Council

Sept. 1st 2021

Carsten Fortmann-Grote, Andy Götz

This project has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement No. 823852

Outline

- Status
- WP5 partners
- Open Issues
- Highlights from the partner RIs
- Conclusions

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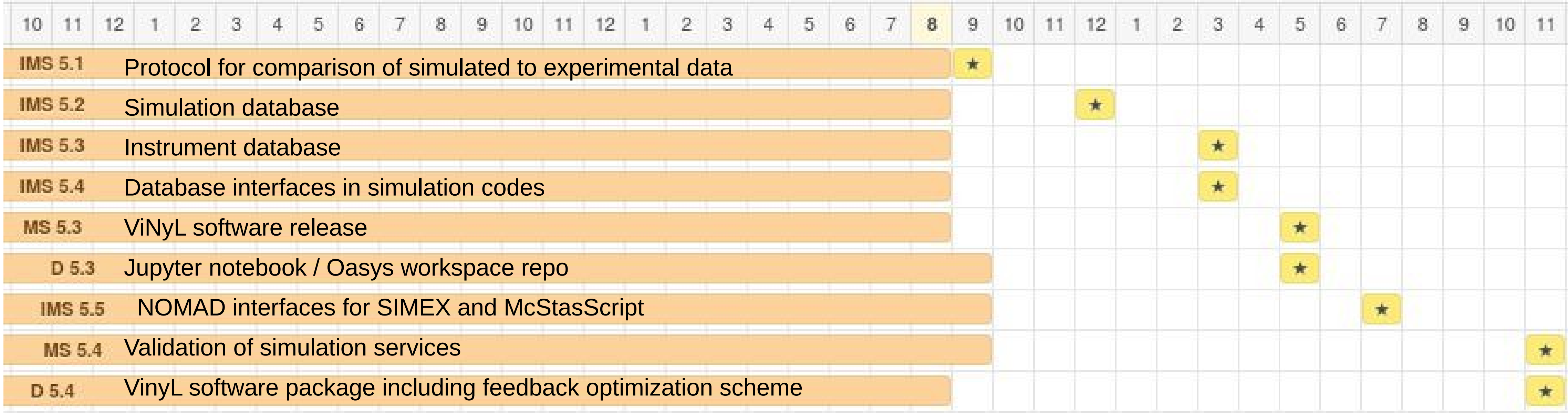
WP5 schedule

Completed items

- MS5.1: Simulation codes in PaNData Software Catalog (5/2019)
- D5.1: OpenPMD domain specific extensions (11/2019)
- MS5.2: Demonstration of simulation services (11/2020)
- D5.2: Release of documented simulation APIs (11/2020)



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WP5 dashboard

Partner	Correspondent	Adopt OpenPMD	Adopt NeXus	integration in PaN Portal /VISA	OASYS is a remote service	COMSYL is a remote service	Collection of simulation Jupyter Notebooks / Oasys Workspacess
ESRF	M. Sanchez-Rio	✓					✓
ILL	Shervin Nourbakhsh	✓	WIP		NA	NA	WIP
ESS	Mads Bertelsen	✓	WIP		NA	NA	WIP
XFEL	C. Fortmann-Grote, Juncheng E	✓	WIP		NA	NA	WIP
CERIC	Aljosa Haffner	✓			✓		✓
ELI	Mousumi Upadhyay Kahaly	✓	NA		NA	NA	WIP
EGI	NA	NA	NA	NA	NA	NA	NA

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WP5 KPIs

Number	KPI description	Value
5.1.1	Number of contributors to ViNYL	9
5.2.1	number of users of ViNYL services at ESRF	0
5.2.2	number of users of ViNYL services at ILL	0
5.2.3	number of users of ViNYL services at XFEL	3
5.2.4	number of users of ViNYL services at ESS	2
5.2.5	number of users of ViNYL services at ELI	0
5.2.6	number of users of ViNYL services at CERIC	2
5.3.1	Number of modules included in ViNYL service	3
5.4.1	Number of partner infrastructures that have used ViNYL service	3
5.5.1	Number of DOIs for simulated data (by counting datasets with "ViNYL" labels on open-access repositories like Zenodo).	5
5.6.1	Number of openPMD standard domain extensions merged into mainline openPMD repository	1

last update: 09/20201

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WP5 partners and responsibilities

- **EuXFEL** (Juncheng E, Carsten Fortmann-Grote)
  - WP lead
  - SIMEX start-to-end photon experiment simulations
  - Simulation API “libpyvinyl”
- **ESS** (Mads Bertelsen, Stella d
  - McStas Neutron Raytraci
  - McStasscript (python wra McStas)
  - Simulation services in par
- **CERIC-ERIC** (Aljosa Haffner)
  - Oasys x-ray optics simulation GUI
  - WISER wavefront propagation code

- Bi-weekly VTC
  - Fridays 1pm
  - Meeting notes on github
- 1-2 code development sprints per year

- **ILL** (Shervin Nourbakhsh)
  - Neutron simulations
  - McStas openPMD IO
  - Integration of simulation services in CAMEO and NOMAD
  - for raytracing data
  - abase
  - dhyay-Kahaly, Gergely
  - (TD)DFT simulations of sample/target properties
  - Testing of simulation services
  - NOMAD deposition

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WP5 open issues

- **Service deployment**
  - Docker containers with simulation API, backengine executables, jupyter notebooks
  - Container building (implement a reliable workflow that we can use)
  - Integration in PaNOSC portal
  - Last year, had support from David Webster (WP6?) who left PaNOSC.
- **Integration with WP4**
  - One of our objectives is to support data analysis through forward simulations and feedback from comparison experiment to simulation.
  - Unclear at the moment how to connect DA and SIM services
  - Should define and then execute a use case
- **Databases:** Currently our “databases” are repositories, plain files, notebooks
  - could benefit from a database expert to put simulation data and instrument parameters into an actual DB

    potentially including a web based frontend and REST/JSON API.
  - Other option: Integration into workflow system that supports dumping and loading of intermediate states
- **Comsyl:** Manuel implemented a 1 D solution to the original 2D problem which greatly reduces computational resource needs → Comsyl 1D can be run on a laptop, no HPC service needed.

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Contributions from ESS

McStasScript

Python API for creating and running McStas simulations, suitable for jupyter notebooks.

- Included McXtrace support

  Now both neutron and x-ray

- Full internal review of code

  Internal review led to many improvements, especially in plotting

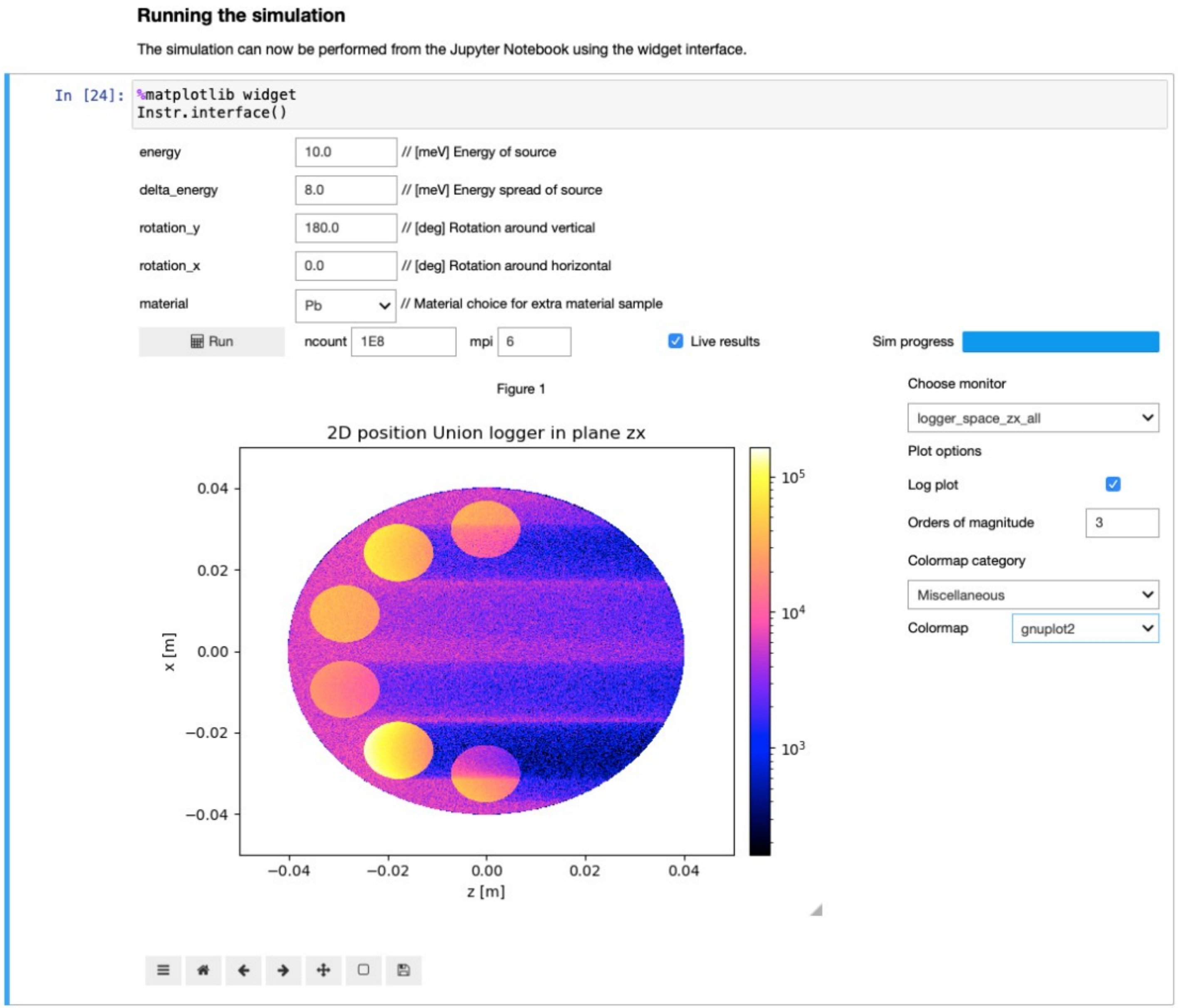
- Widget GUI for jupyter notebooks

  Running simulations and viewing data

  Example shown on the right

- Dissemination:

  Talks at MLZ, PNPI, ESS SWIM meeting, HighNESS school, ISIS school



Contributions from ESS

Instrument database/repository

Deliverable 5.3 requires repository of documented jupyter notebooks.
Group decided to have a git repository with instrument descriptions.

- Parameter system
  - Collected control of all parts of instrument
  - Separate user and expert parameters
  - Allowed ranges for each parameter
  - Implemented in *libpyvinyl*

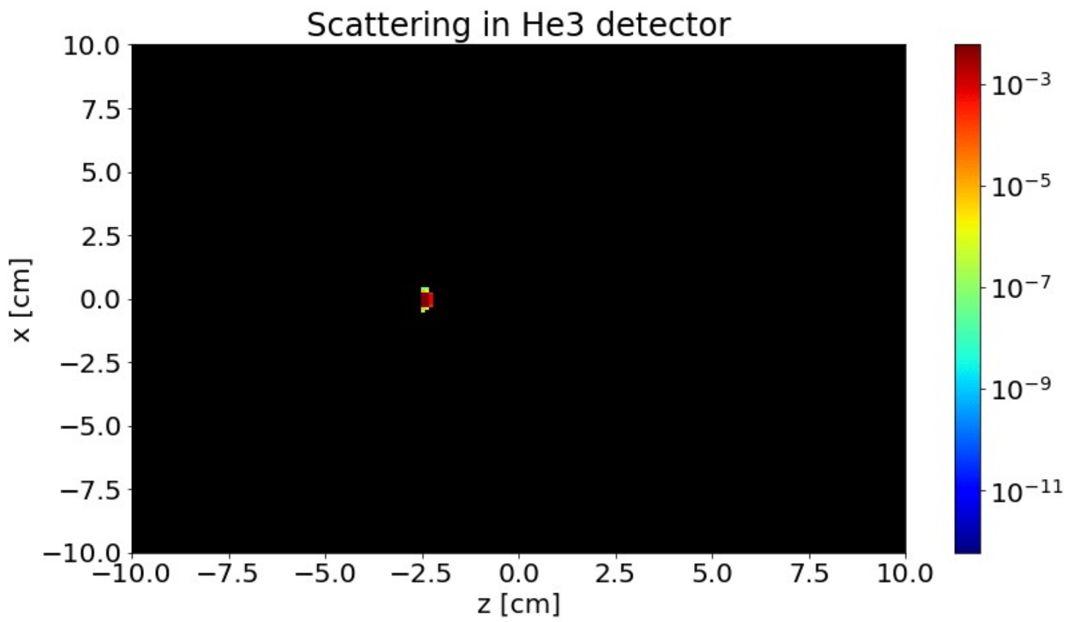
- Instrument repository
  - python modules describing instruments, sample environments and samples
  - Standardized sample position
  - Quality assurance using CI on git upload
  - python module to retrieve desired instrument

Contributions from ESS

Absorption logging in McStas Union

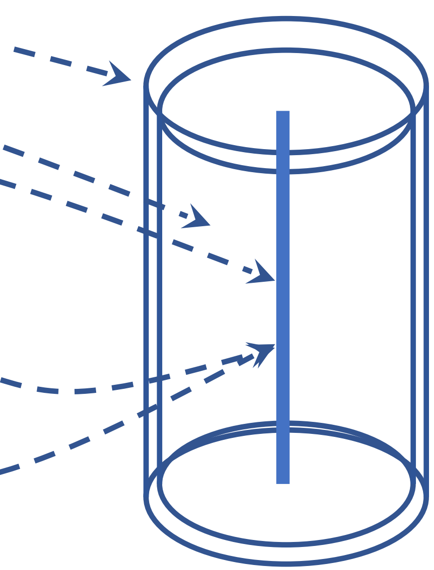
Allow detection of absorption in McStas Union framework,
Which enables simulation of complex detector systems.

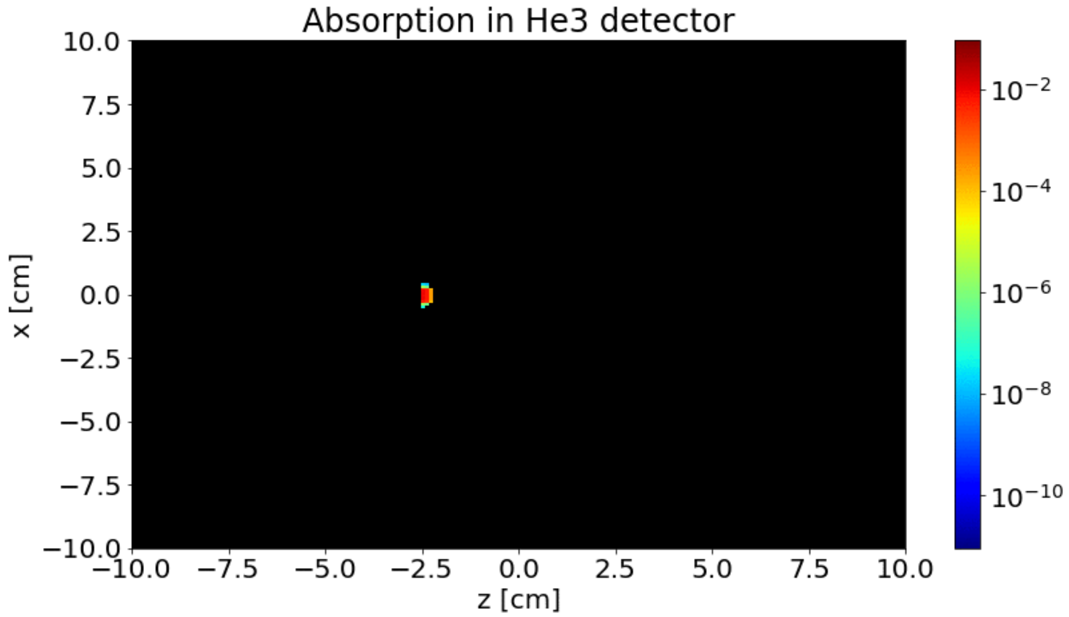
- Record absorbed neutrons in detector materials
- Many types available, event / histogram
- Simulate systematic detector errors and inaccuracies



- Aluminium
- He3
- Detector wire

- Abs_logger_1D_space_tof
- Abs_logger_event





Contributions from ESS

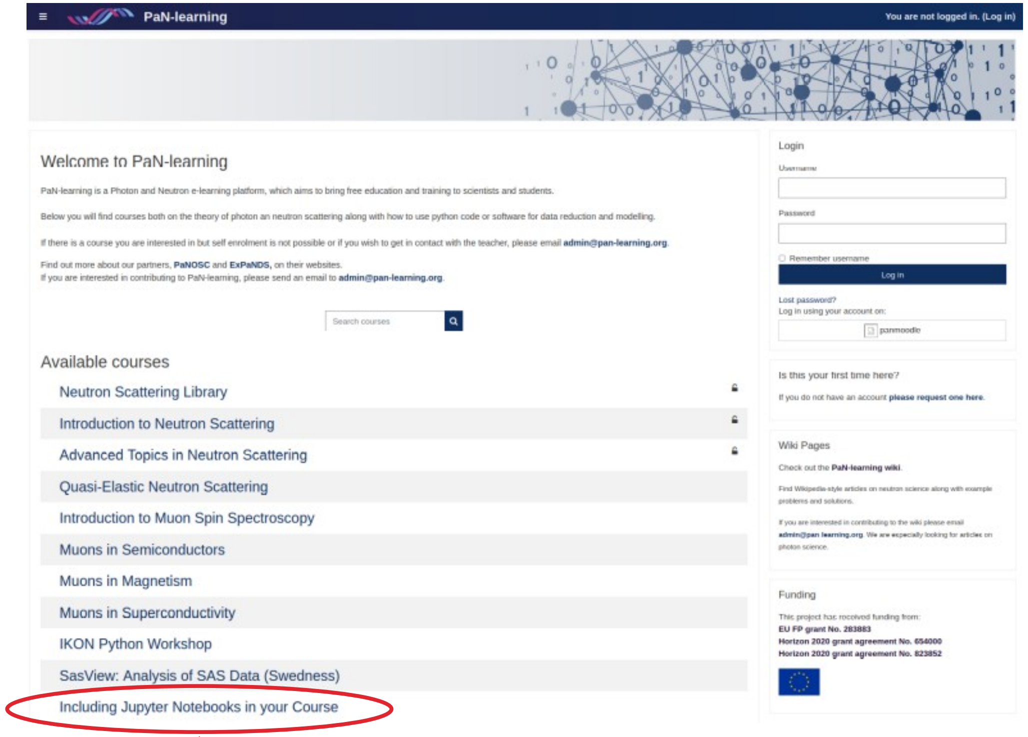
Showcasing simulation software on JupyterHub

- PaN-learning platform is being developed for online learning by WP8.
- Courses can now have a tailored JupyterHub container attached which pulls notebooks directly from github.
- JupyterHub containers are being built with WP5 software pre-installed.
- WP5 are creating notebooks which both provide training for its software and use it to demonstrate scientific principles and experiments.

Task 5.3: Expose photon and neutron beamline optics simulation services for photon and neutron facilities.

Deliverable 5.3: Repository of documented jupyter notebooks and Oasys canvases showcasing simulation tasks executable via JupyterHub or remote desktop

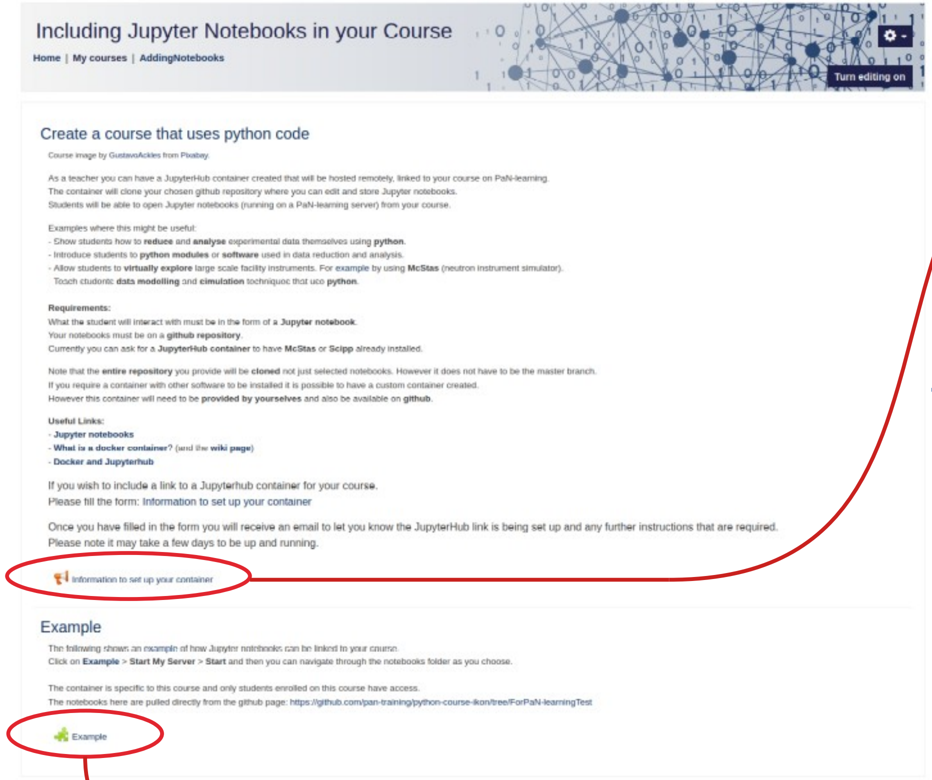
PaN-learning.org: How any teacher could make use of this.



Course for teachers to understand how the process works.

Contributions from ESS

Showcasing simulation software on JupyterHub



Including Jupyter Notebooks in your Course

Home | My courses | AddingNotebooks

Turn editing on

Create a course that uses python code

Course image by GustavoAckles from Pixabay.

As a teacher you can have a JupyterHub container created that will be hosted remotely, linked to your course on PaN-learning.
The container will clone your chosen github repository where you can edit and store Jupyter notebooks.
Students will be able to open Jupyter notebooks (running on a PaN-learning server) from your course.

Examples where this might be useful:
- Show students how to **reduce** and **analyse** experimental data themselves using **python**.
- Introduce students to **python modules** or **software** used in data reduction and analysis.
- Allow students to **virtually explore** large scale facility instruments. For example by using **McStas** (neutron instrument simulator).
  Teach students **data modelling** and **simulation** techniques that use **python**.

Requirements:
What the student will interact with must be in the form of a **Jupyter notebook**.
Your notebooks must be on a **github repository**.
Currently you can ask for a **JupyterHub container** to have **McStas** or **Scipp** already installed.

Note that the **entire repository** you provide will be **cloned** not just selected notebooks. However it does not have to be the master branch.
If you require a container with other software to be installed it is possible to have a custom container created.
However this container will need to be **provided by yourselves** and also be available on **github**.

Useful Links:
- **Jupyter notebooks**
- **What is a docker container?** (and the **wiki page**)
- **Docker and Jupyterhub**

If you wish to include a link to a Jupyterhub container for your course.
Please fill the form: Information to set up your container

Once you have filled in the form you will receive an email to let you know the JupyterHub link is being set up and any further instructions that are required.
Please note it may take a few days to be up and running.

Information to set up your container

Example

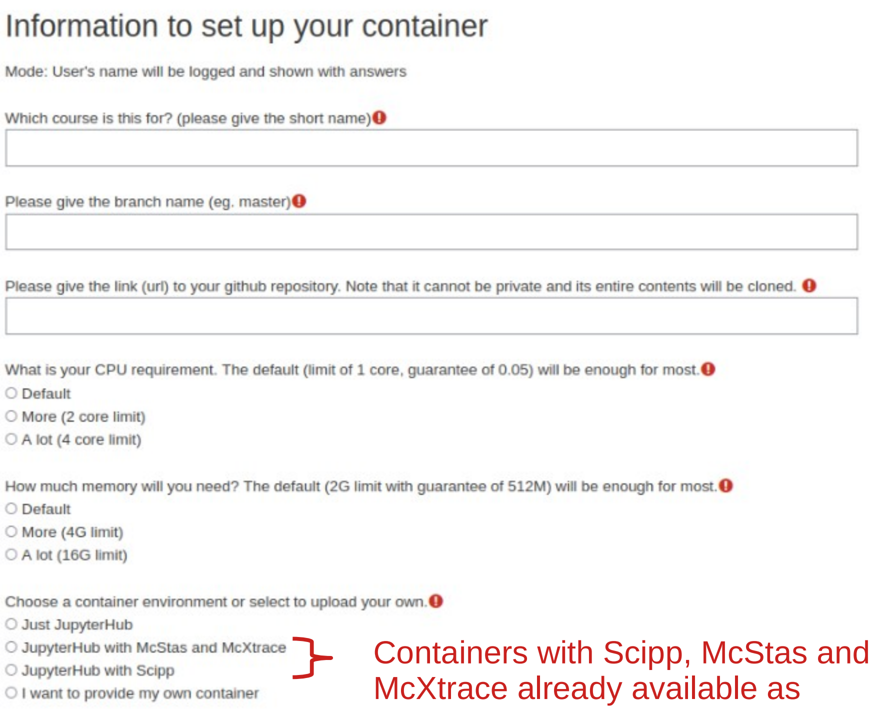
The following shows an example of how Jupyter notebooks can be linked to your course.
Click on **Example** > **Start My Server** > **Start** and then you can navigate through the notebooks folder as you choose.

The container is specific to this course and only students enrolled on this course have access.
The notebooks here are pulled directly from the github page: https://github.com/pan-training/python-course-ikon/tree/ForPaN-learningTest

Example

Teachers only need to fill in a short questionnaire for a JupyterHub link to be set up for them in their chosen course.

Example:
Next slide



Information to set up your container

Mode: User's name will be logged and shown with answers

Which course is this for? (please give the short name)

Please give the branch name (eg. master)

Please give the link (url) to your github repository. Note that it cannot be private and its entire contents will be cloned.

What is your CPU requirement. The default (limit of 1 core, guarantee of 0.05) will be enough for most.
- Default
- More (2 core limit)
- A lot (4 core limit)

How much memory will you need? The default (2G limit with guarantee of 512M) will be enough for most.
- Default
- More (4G limit)
- A lot (16G limit)

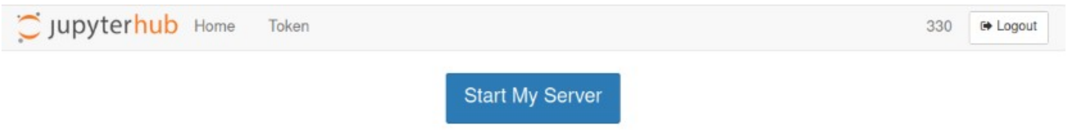
Choose a container environment or select to upload your own.
- Just JupyterHub
- JupyterHub with McStas and McXtrace
- JupyterHub with Scipp
- I want to provide my own container

Containers with Scipp, McStas and McXtrace already available as standard. SimEx soon to be added.

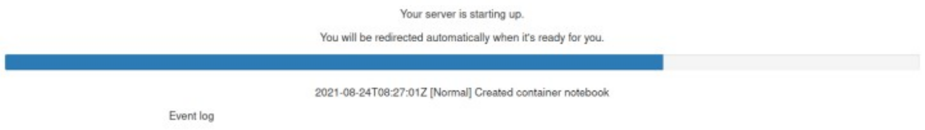
Contributions from ESS

Showcasing simulation software on JupyterHub

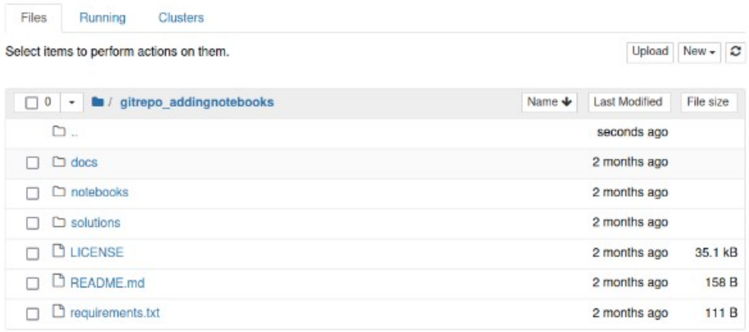
How it works: New tab is opened asking student to start their server.

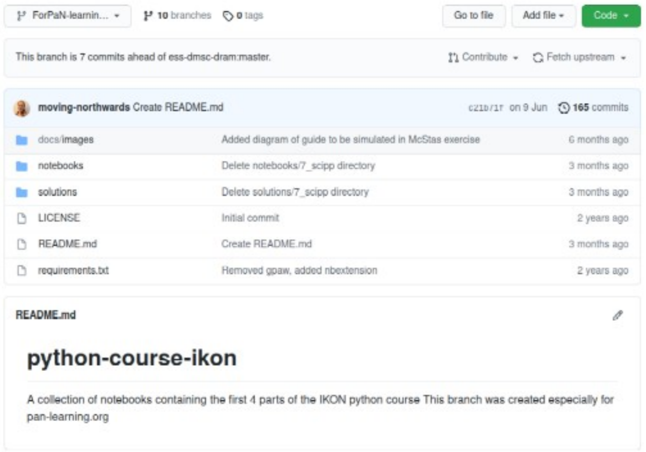


Required container is pulled from DockerHub started for student.



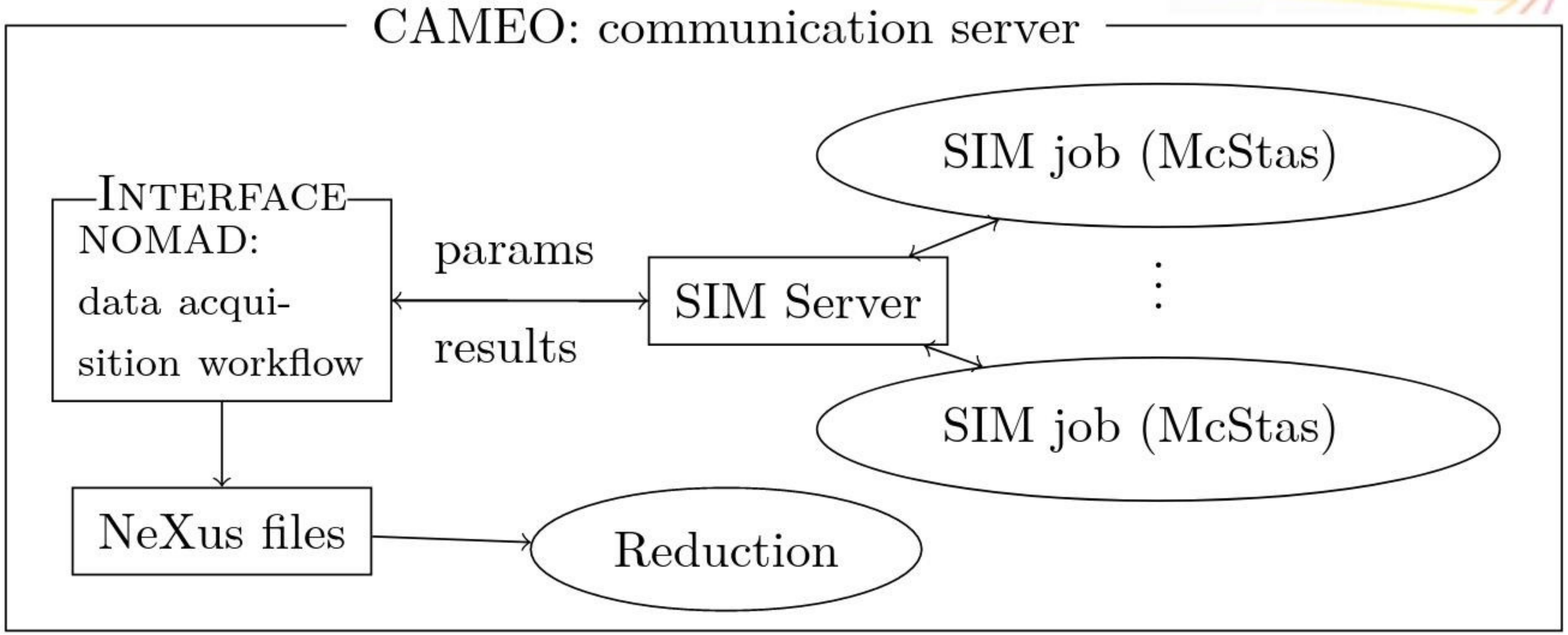
From this example you can see entire github repo (a specific branch can be specified) is cloned into JupyterHub.





Implementation scheme @ ILL (5)

Communication between applications



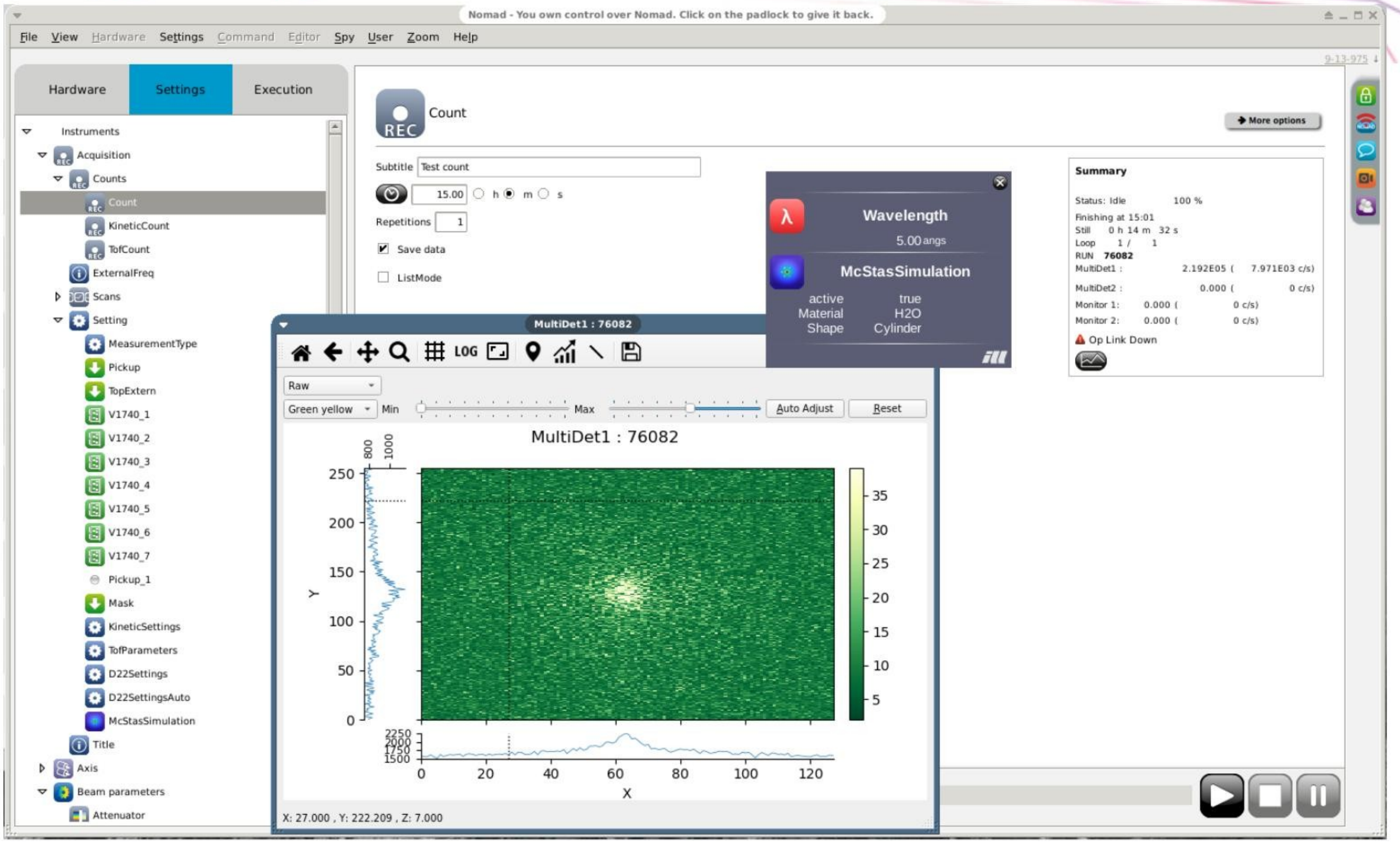
NeXus files:

- NOMAD is in charge of creating NeXus files for both real and simulated data
- Detector image provided by SIM server as a fake data acquisition card

Reduction and analysis:

- Same path as the real data

Working prototype

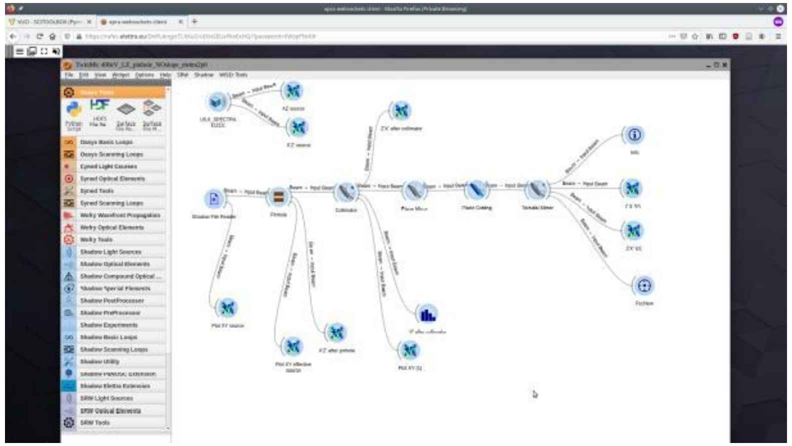


NEUTRONS FOR SOCIETY

CERIC

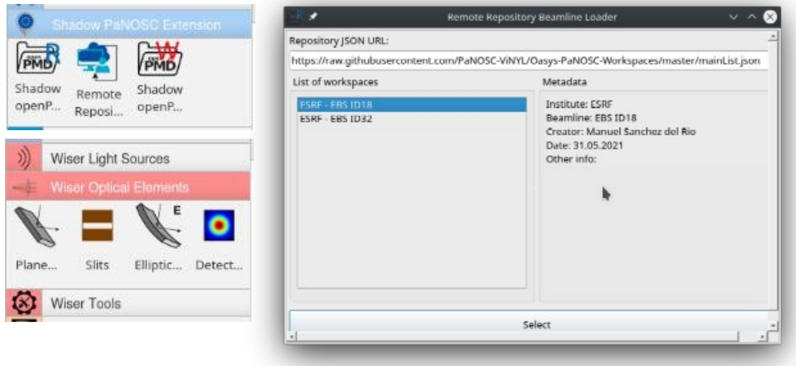
CERIC-ERIC WP5 Deliverables and Milestones

- Ray-tracing openPMD extension, together with example datasets, has been designed and released (D 5.1). Panosc toolbox for Oasys has been created.
- Oasys Wiser wavefront propagation simulation code has been released (D 5.2)
  - Deployment of Oasys as a remote application within CERIC's proposal management system VUO, with the help of RAFEC, developed in WP6. The service is freely accessible to CERIC users on-demand (MS 5.2)
- Reading and loading from a remote repository of documented Oasys beamlines has been developed (IMS 5.4)



Left: Oasys running in the browser.

Right: Remote repository loader from Panosc toolbox.



PaNOSC and ExPaNDS projects have received funding from the European Union's Horizon 2020 research and innovation programme under grant agreements 823852 and 857641, respectively.

panosc
photon and neutron open science cloud

ExPaNDS
European Open Science Cloud Photon and Neutron Data Services

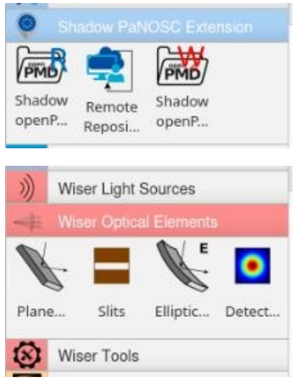
CERIC-ERIC WP5 Other Activities

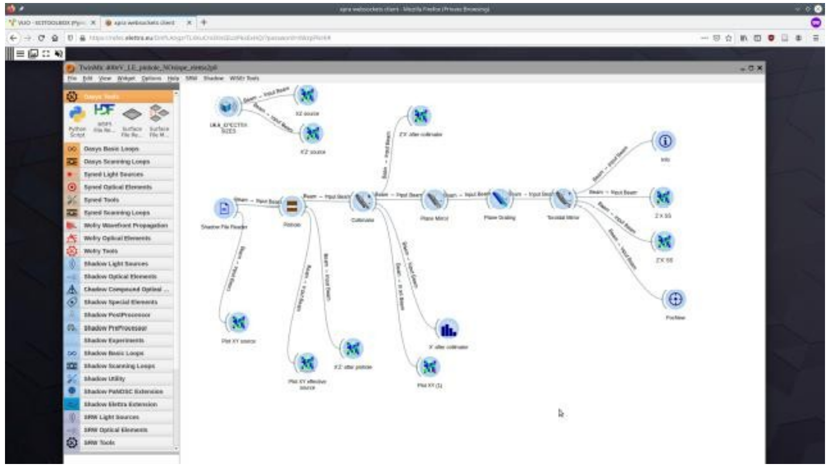
- Use cases:
  - Remote, collaborative access to beamline optics simulations: *https://www.panosc.eu/use-cases/use-case-8-remote-collaborative-access-to-beamline-optics-simulations/*
  - K-B System performance analysis: *https://www.panosc.eu/use-cases/panosc-use-case-12-k-b-system-performance-analysis/*
  - Effects on the spot quality of the mirror error profile and source pointing instability: *https://www.panosc.eu/use-cases/panosc-use-case-13-effects-on-the-spot-quality-of-mirror-error-profile-and-source-pointing-instability/*
- Conference presentations:
  - M. Manfredda, A. Hafner, S. Gerusina, N. Mahne, A. Simoncig, M. Zangrando, L. Raimondi, "WISER wavefront propagation simulation code: advances and applications," Proc. SPIE 11493, Advances in Computational Methods for X-Ray Optics V, 114930B (16 September 2020); https://doi.org/10.1117/12.2568574
  - J. C. E, A. Hafner, T. Kluyver, M. Bertelsen, M. Upadhyay Kahaly, Z. Lecz, S. Nourbakhsh, A. P. Mancuso, C. Fortmann-Grote, "VINYL: The VIrtual Neutron and x-raY Laboratory and its applications," Proc. SPIE 11493, Advances in Computational Methods for X-Ray Optics V, 114930Z (21 August 2020); https://doi.org/10.1117/12.2570378
- Oasys Wiser and Panosc toolbox official releases on PyPI
  - *https://pypi.org/project/OASYS1-oasyswiser/*
  - *https://pypi.org/project/OASYS1-PaNOSC/*

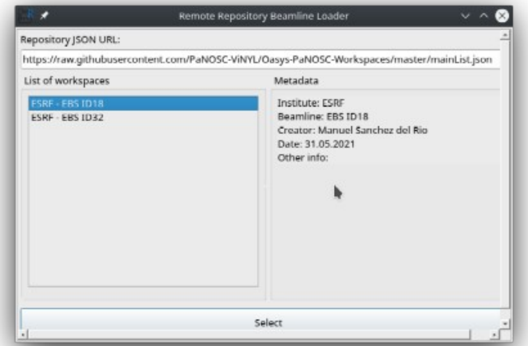
PaNOSC and ExPaNDS projects have received funding from the European Union's Horizon 2020 research and innovation programme under grant agreements 823852 and 857641, respectively.

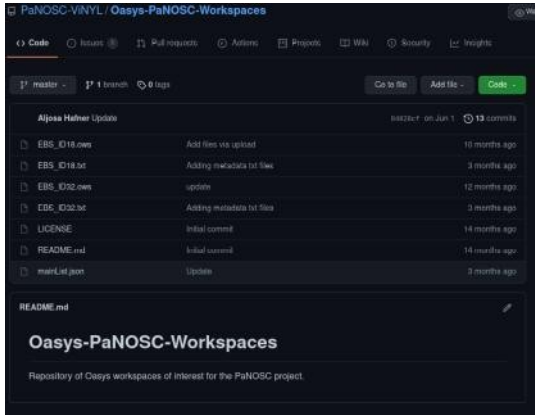
CERIC-ERIC WP5 Summary

- 3 use cases provided by scientific users
- 2 publications in conference proceedings
- Demonstration of Oasys as a remote service
- Remote repository of documented Oasys beamlines (OWS workspaces) with a corresponding interaction widget









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Contributions from European XFEL

- Parameters and instrument (parameters collection) classes were developed for libpyvinyl
  → T5.3, IMS5.3
- Protocol for comparison of raw simulated to raw experimental data → IMS 5.1, T5.4
- A research paper using SimEx for Single-particle imaging experiment simulation, relevant codes can be found on Zenodo (https://doi.org/10.5281/zenodo.5243148) → T5.4

panosc photon and neutron open science cloud

This project has received funding from the EU FP 7 grant number 283883, Horizon 2020 grant agreement No 654000 and Horizon 2020 grant agreement No. 823852.

Protocol for comparison of raw simulated to raw experimental data

Shervin Nourbakhsh, Stella d'Ambrumenil, Juncheng E, Carsten Fortmann-Grote

May 2021

Contents

scientific reports

Accepted

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,*], and Adrian P. Mancuso[1,*]

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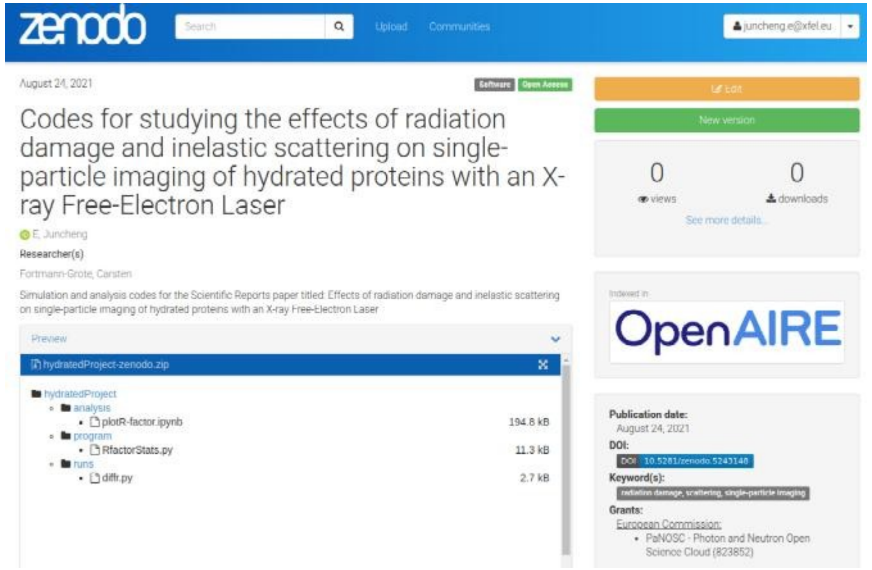
ABSTRACT

We present a computational case study of X-ray single-particle imaging of hydrated proteins on an example of 2–Nitrogenase–Iron protein covered with water layers of various thickness, using a start-to-end simulation platform and experimental parameters of the SPB/SFX instrument at the European X-ray Free-Electron Laser facility. The simulations identify an optimal thickness of the water layer at which the effective resolution for imaging the hydrated sample becomes significantly higher than for the non-hydrated sample. This effect is lost when the water layer becomes too thick. Even though the detailed results presented pertain to the specific sample studied, the trends which we identify should also hold in a general case. We expect these findings will guide future single-particle imaging experiments using hydrated proteins.



zenodo Search Upload Communities juncheng.e@xfel.eu

August 24, 2021 Software Open Access

Codes for studying the effects of radiation damage and inelastic scattering on single-particle imaging of hydrated proteins with an X-ray Free-Electron Laser

E. Juncheng

Researcher(s)

Fortmann-Grote, Carsten

Simulation and analysis codes for the Scientific Reports paper titled: Effects of radiation damage and inelastic scattering on single-particle imaging of hydrated proteins with an X-ray Free-Electron Laser

Preview

hydratedProject-zenodo.zip

- hydratedProject
  - analysis
    - plotR-factor.ipynb 194.8 kB
  - program
    - RfactorStats.py 11.3 kB
  - runs
    - diffr.py 2.7 kB

Edit

New version

0 views 0 downloads

See more details...

Indexed in

OpenAIRE

Publication date: August 24, 2021

DOI: 10.5281/zenodo.5243148

Keyword(s): radiation damage, scattering, single-particle imaging

Grants: European Commission:

- PaNOSC - Photon and Neutron Open Science Cloud (823852)

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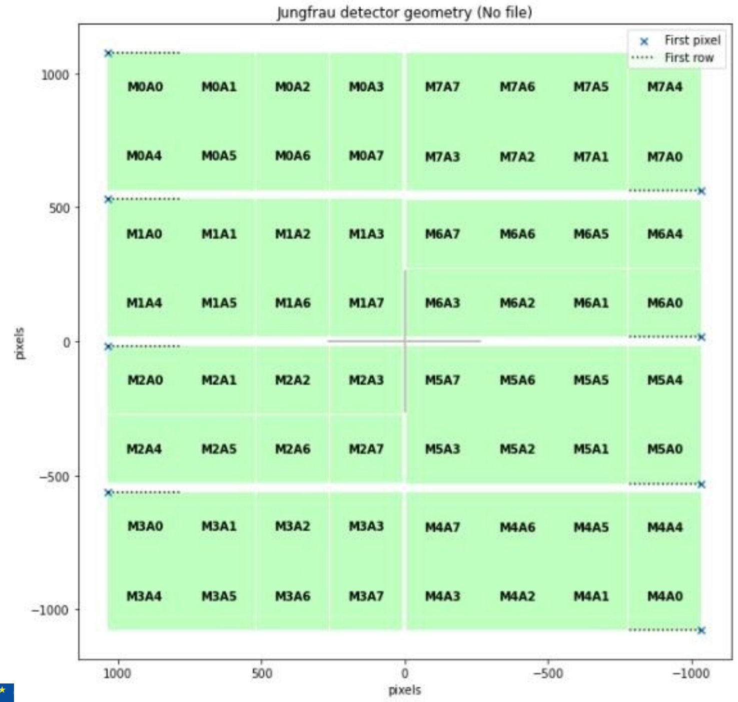
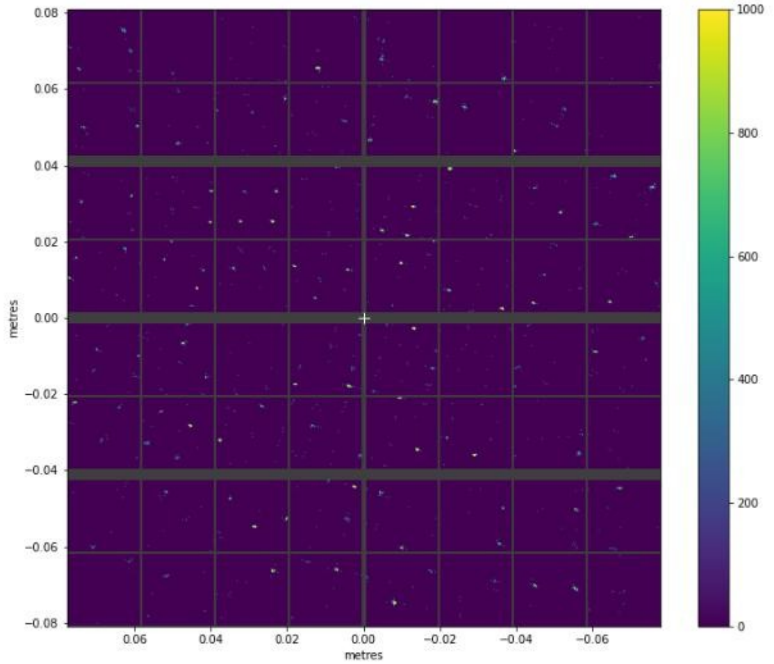
panosc

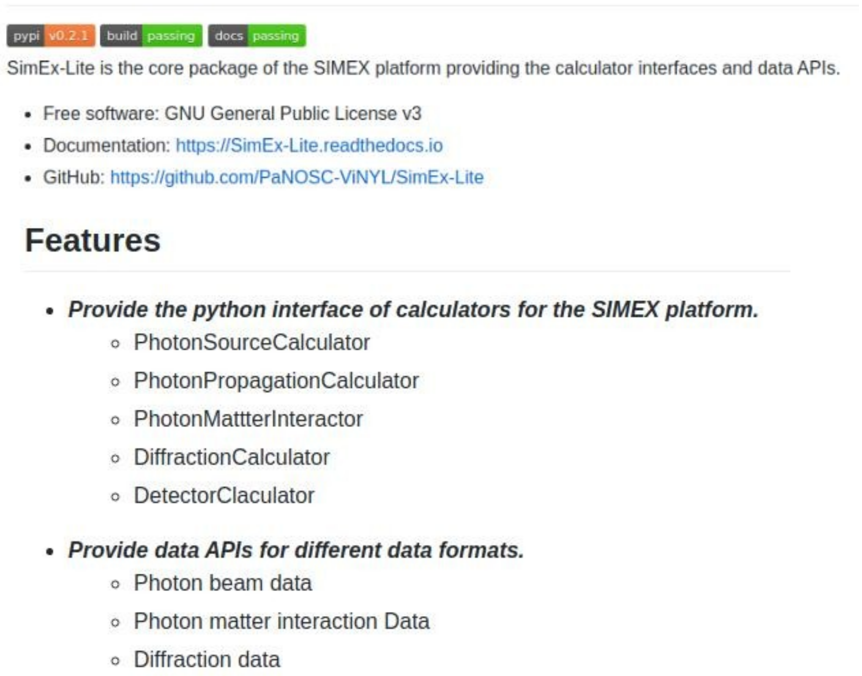
Contributions from European XFEL

Ongoing:

- Export simulation data in NeXus format (https://github.com/panosc-nexus/demo): T5.5, D5.4
- SimEx notebooks repository (https://github.com/PaNOSC-ViNYL/SimEx-notebooks/tree/instrument_test): D5.3
- SimEx-Lite development (https://github.com/PaNOSC-ViNYL/SimEx-Lite): T5.1, M5.3, M5.4,






pypi v0.2.1 build passing docs passing

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

- Free software: GNU General Public License v3
- Documentation: https://SimEx-Lite.readthedocs.io
- GitHub: https://github.com/PaNOSC-ViNYL/SimEx-Lite

Features

- ***Provide the python interface of calculators for the SIMEX platform.***
  - PhotonSourceCalculator
  - PhotonPropagationCalculator
  - PhotonMattterInteractor
  - DiffractionCalculator
  - DetectorClaculator
- ***Provide data APIs for different data formats.***
  - Photon beam data
  - Photon matter interaction Data
  - Diffraction data

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Outlook and Conclusions

- WP5 is on track to complete all Deliverables and Milestones
- Open issues include deployment of services in PaN Portal / VISA and integration in workflow engines with database support
- Thanks to a dedicated distributed team that consistently contributes to site specific solutions as well as to the global simulation infrastructure

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