10-11 November 2020

PaNOSC & ExPaNDS Annual Meeting

Update on PaNOSC WP 5: Simulations. Virtual Neutron and X-ray Laboratory

10th November, 2020

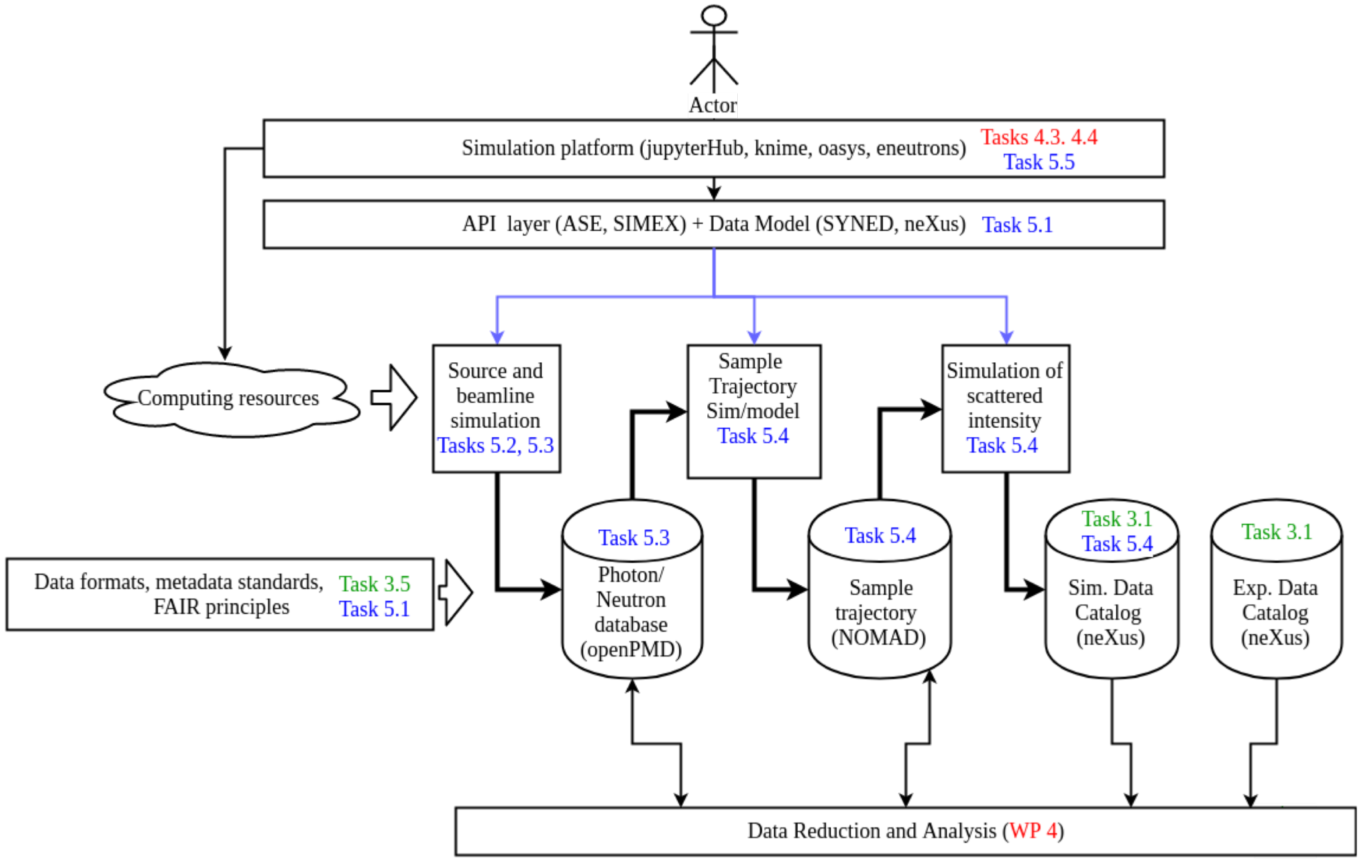
Author: Mads Bertelsen, European Spallation Source

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.

Introduction

Aim of work package 5

- Provide popular simulation tools as online services
- Ensure data and meta data satisfy FAIR principles



Published paper on the concept!

J. C. E, A. Hafner, T. Kluyver, M. Bertelsen, M. Upadhyay Kahaly, Z. Lecz, S. Nourbakhsh, A. P. Mancuso, and 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

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Introduction

Neutrons	• <u>Mads Bertelsen</u>, European Spallation Source	*McStas*
	• Shervin Nourbakhsh, Institute Laue Langevin	
X-rays	• **Carsten Fortman-Grote**, European XFEL GmbH	*SIMEX*
	• Juncheng E, European XFEL GmbH	
	• Aljoša Hafner, CERIC-ERIC	*OASYS*
Materials	• Mousumi Upadhyay Kahaly, ELI-ALPS	
	• Zsolt Lécz, ELI-ALPS	
Cloud	• Daniel Webster, CERIC-ERIC / Cloudbusting	

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Introduction

- Codes we directly contribute to
  - McStas: Neutron instrument simulation, 1999
  - SIMEX: X-ray simulation, text based, 2015
  - OASYS: X-ray simulations with GUI, 2017
  - openPMD: Hierarchical data format, 2017
- Codes used
  - ASE: Molecular dynamics simulation

SIMEX

ASE

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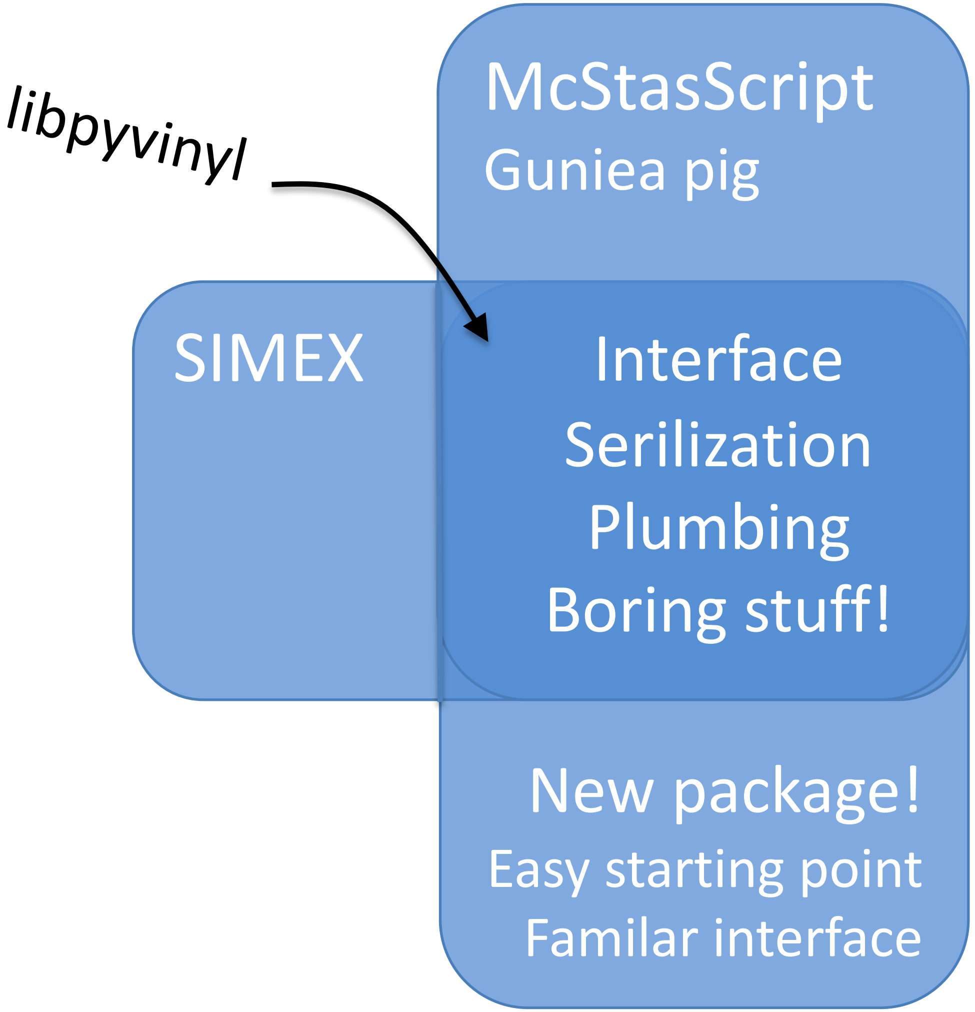
Introduction

- libpyvinyl, python base classes
- SIMEX structure generalized
- Harmonization of interface, easier for users
- McStasScript prototype runs with libpyvinyl
- New packages have a starting point



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Introduction

- Jupyter Notebooks as interface
- Jupyter Hubs should be easily deployed
- Simulation packages deployed using docker containers
- libpyvinyl base classes
  - Parameter / Backengine objects
  - Serialization for dumping / loading

```
In [ ]: myparams = IonMatterInteractor(ion_name='proton')
        myparams.xsec_file = 'D_D_-_3He_n.txt'

In [ ]: mysource = TNSAIonMatterIteractor(parameters=myparams,
                                          input_path='Data/0010.sdf'
                                          output_path='Data/Neutron.h5')

In [ ]: mysource.backengine()

In [ ]: mysource.saveH5()
```

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How we work

- Work separately with weekly meetings
- Had two sprints this year with closer collaboration

1st Sprint 17/4 – 30/4
Team 1: Neutrons
openPMD, pyvinyl McStasScript prototype
Team 2: Materials
ASE DFT results used as McStas sample
Team 3: X-ray
OASYS virtual experiment, GAPD into SimEx

2nd Sprint 14/9 – 28/9
Releases of each package (McStas, SIMEX, Wiser)
Create or prepare docker images
Run each package on online service
Create libpyvinyl repository and pypi
Milestone report
Make master repository

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Status of deliverables and milestones

	Description	Deadline	Status
Milestone 5.1	Simulation codes in PaNData software catalog	M6	Accepted
Deliverable 5.1	Prototype simulation data formats	M12	Accepted
Deliverable 5.2	Documented simulation APIs	M24	Submitted
Milestone 5.2	Demonstration of simulation services	M24	Submitted
Deliverable 5.3	Documented simulation tasks executable	M42	In progress
Milestone 5.3	VINYL software release	M42	
Deliverable 5.4	Software tested and release including interactive simulation and analysis workflow	M48	
Milestone 5.4	Validation of simulation services	M48	

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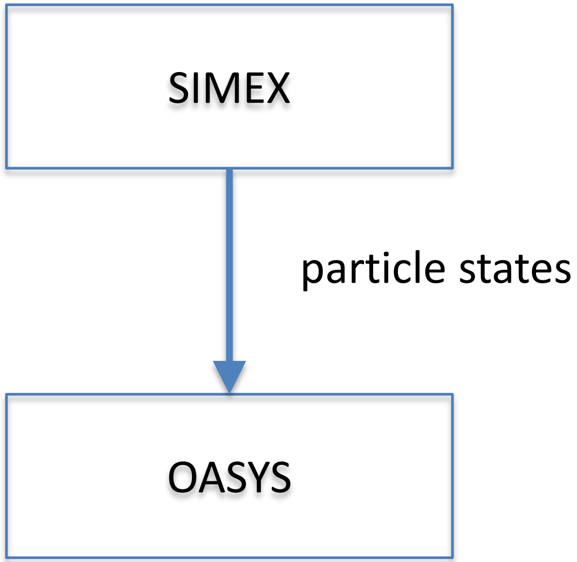
openPMD

Data standard

- Chosen openPMD to transfer ray-tracing / molecular dynamic data between packages
- Contributed extensions to central repository
- C++ McStas read / write component
- Incorporated as a widget in OASYS



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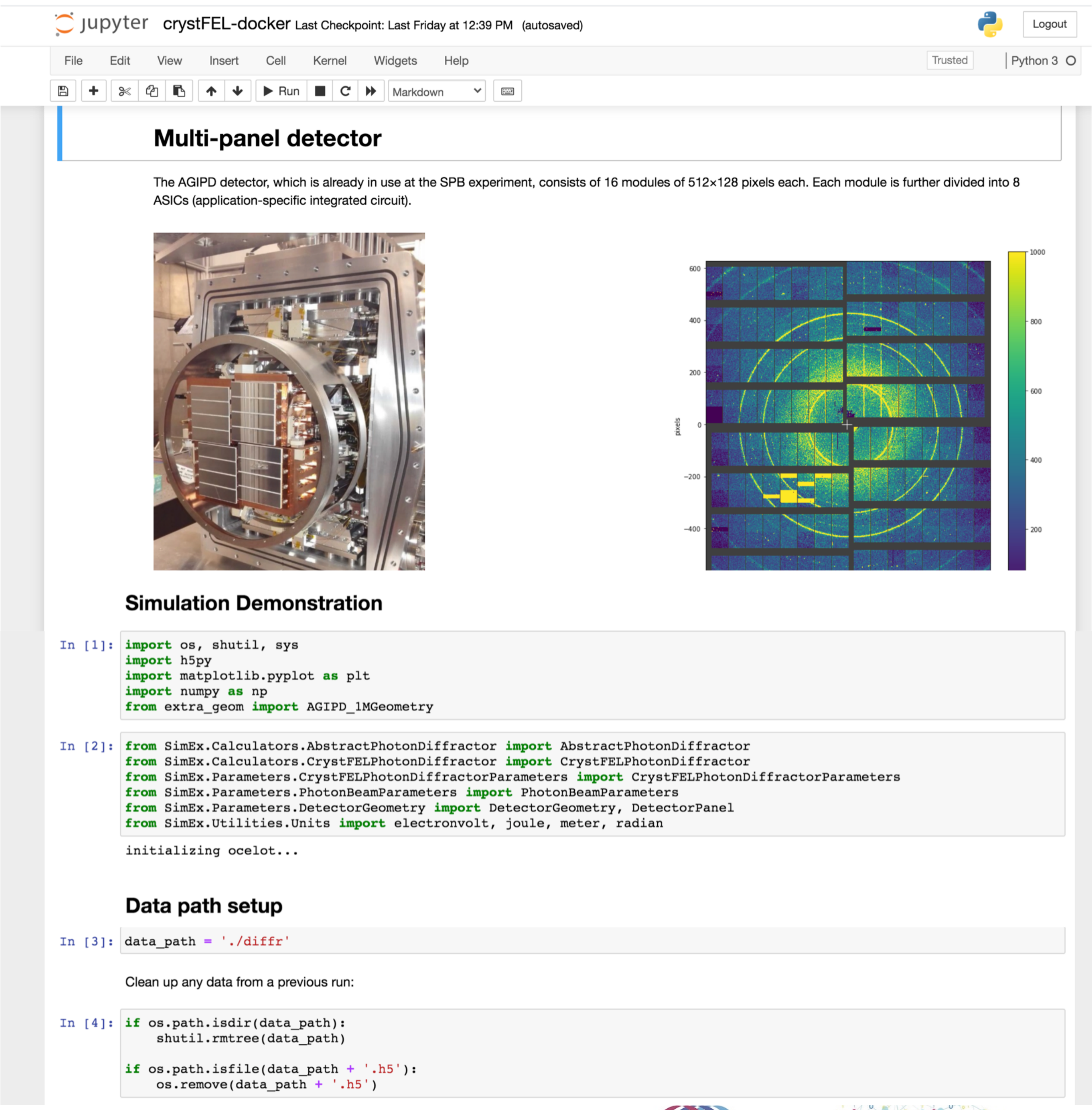
Progress in the last year

SIMEX - Overview

- Improved code distribution
  - Conda installation
  - Docker image
- Being deployed in Jupyter Hubs
- SimEx being used in research
- Integration of GAPD



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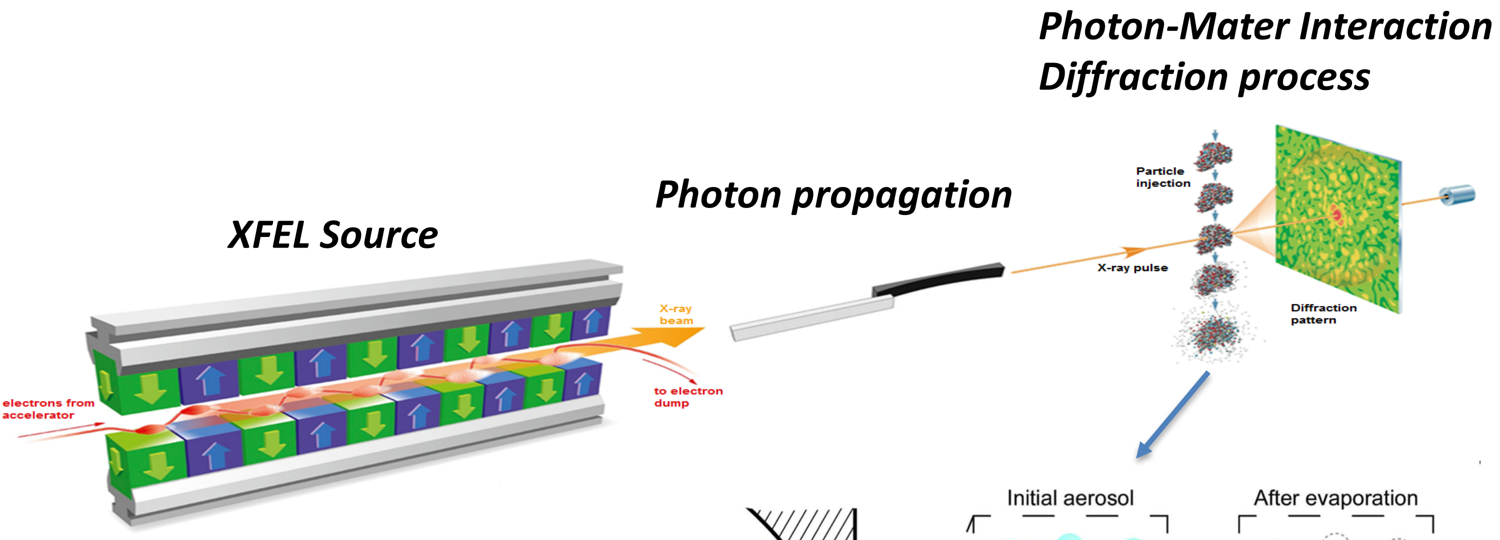
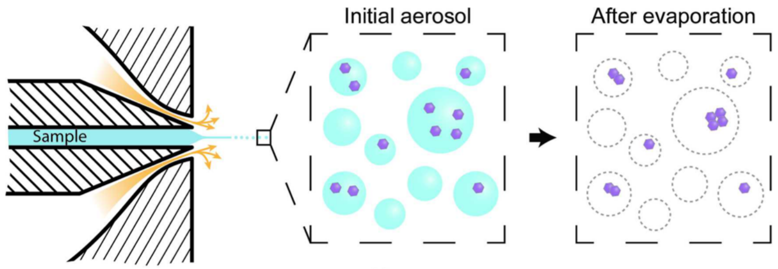
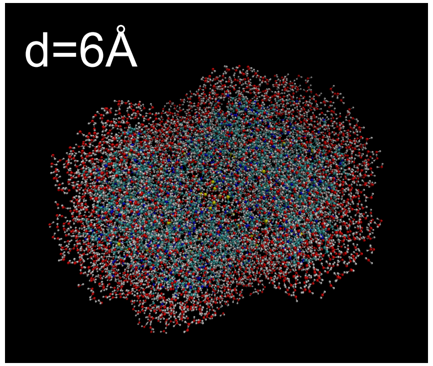
Progress in the last year

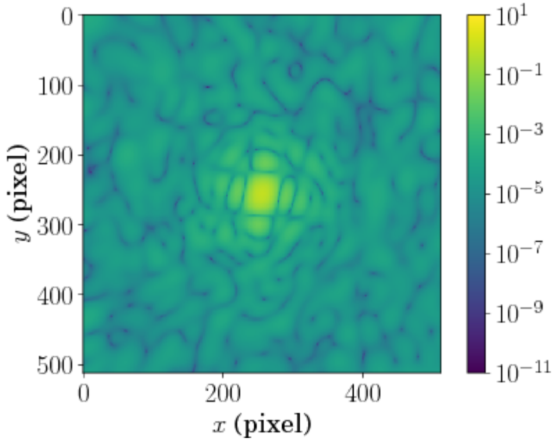
SIMEX - Hydrated protein diffraction simulation



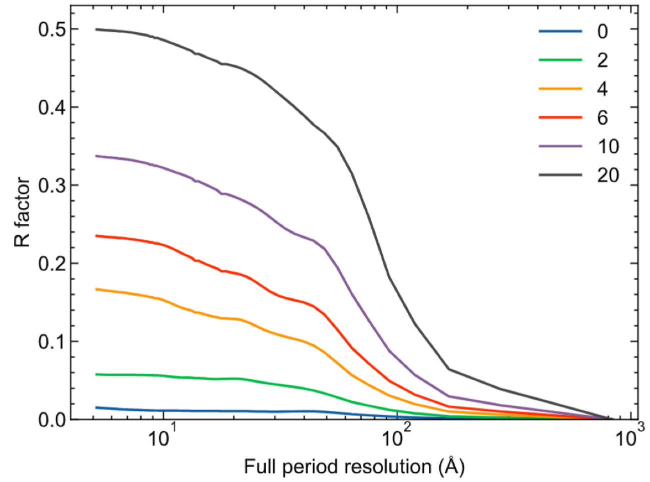


Daurer et al., IUCrJ **4**, 251 (2017)





Ionized hydrated protein + water layer



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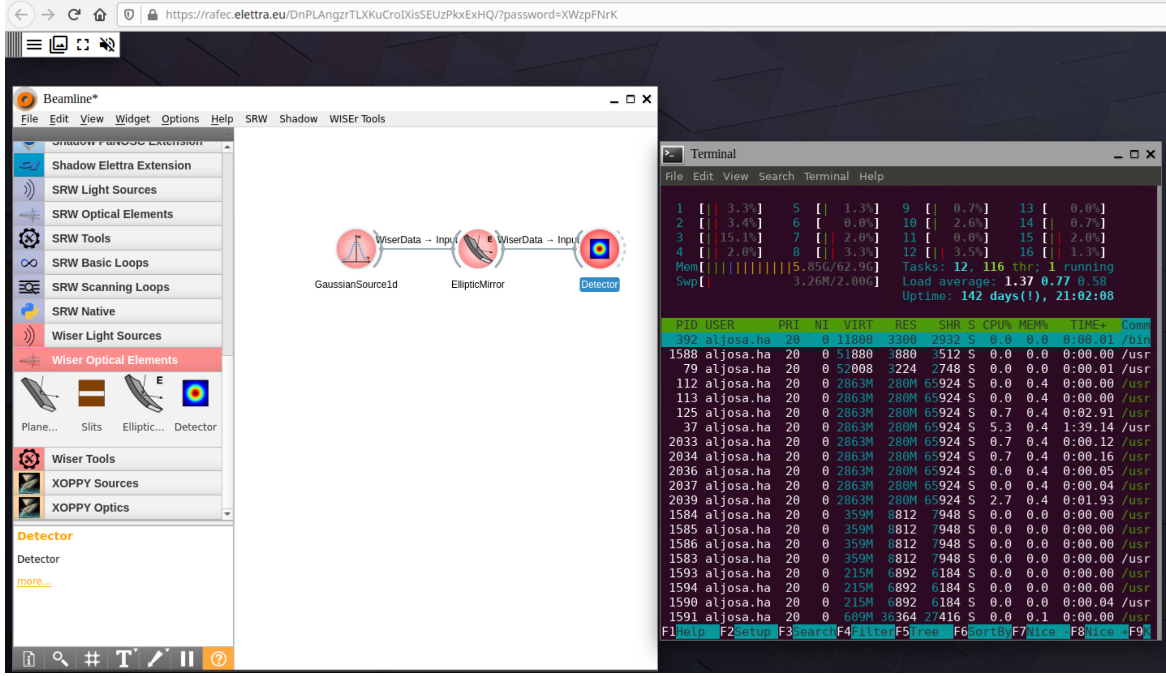
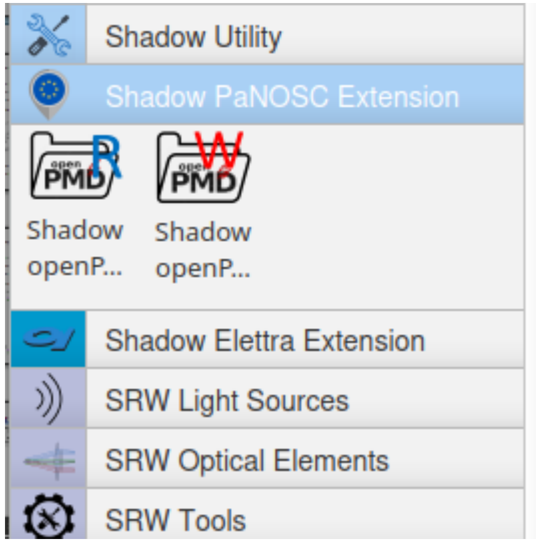
Progress in the last year

OASYS

- Release of **Wiser**, numerical integration code for X-ray propagation
- Demonstration in RAFEC (remote framework)
- Widget suite for OASYS
- openPMD read / write capability
- Access to remote workspaces





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Progress in the last year

McStas and McStasScript

- McStasScript python API for McStas
- McStas / McStasScript tutorial in notebooks
- Review of McStasScript in progress
- McStas expanded to simulate detectors
- Available on internal Jupyter Hub

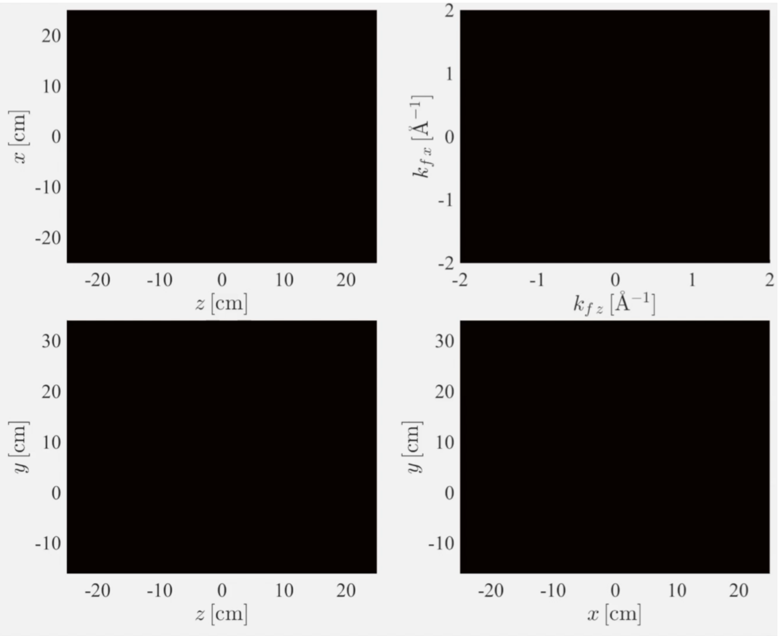
```
In [4]: demo.add_parameter("wavelength", value=4.0, comment="[AA] Wavelength simulated")
        demo.show_parameters()

 wavelength  =  4.0  // [AA] Wavelength simulated

In [5]: src = demo.add_component("source", "Source_simple")
        src.xwidth = 0.11
        src.yheight = 0.11
        src.focus_xw = 0.05
        src.focus_yh = 0.05
        src.dist = 2.0
        src.lambda0 = "wavelength"
        src.dlambda = "0.1*wavelength"
        src.flux = 1E13

In [7]: monochromator_Q = 1.8734
        demo.add_declare_var("double", "mono_Q", value=monochromator_Q)
        demo.add_declare_var("double", "wavevector")
        demo.append_initialize("wavevector = 2*PI/wavelength;")

        demo.add_declare_var("double", "mono_rotation")
        demo.append_initialize("mono_rotation = asin(mono_Q/(2.0*wavevector))*RAD2DEG;")
```



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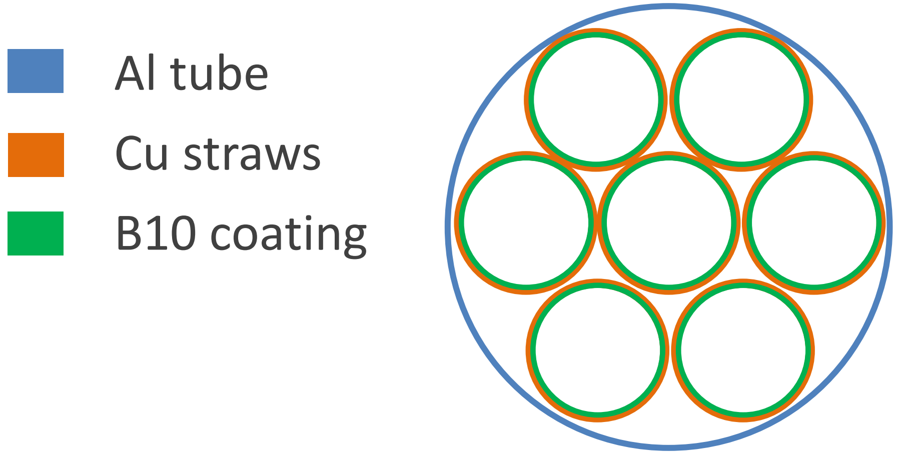
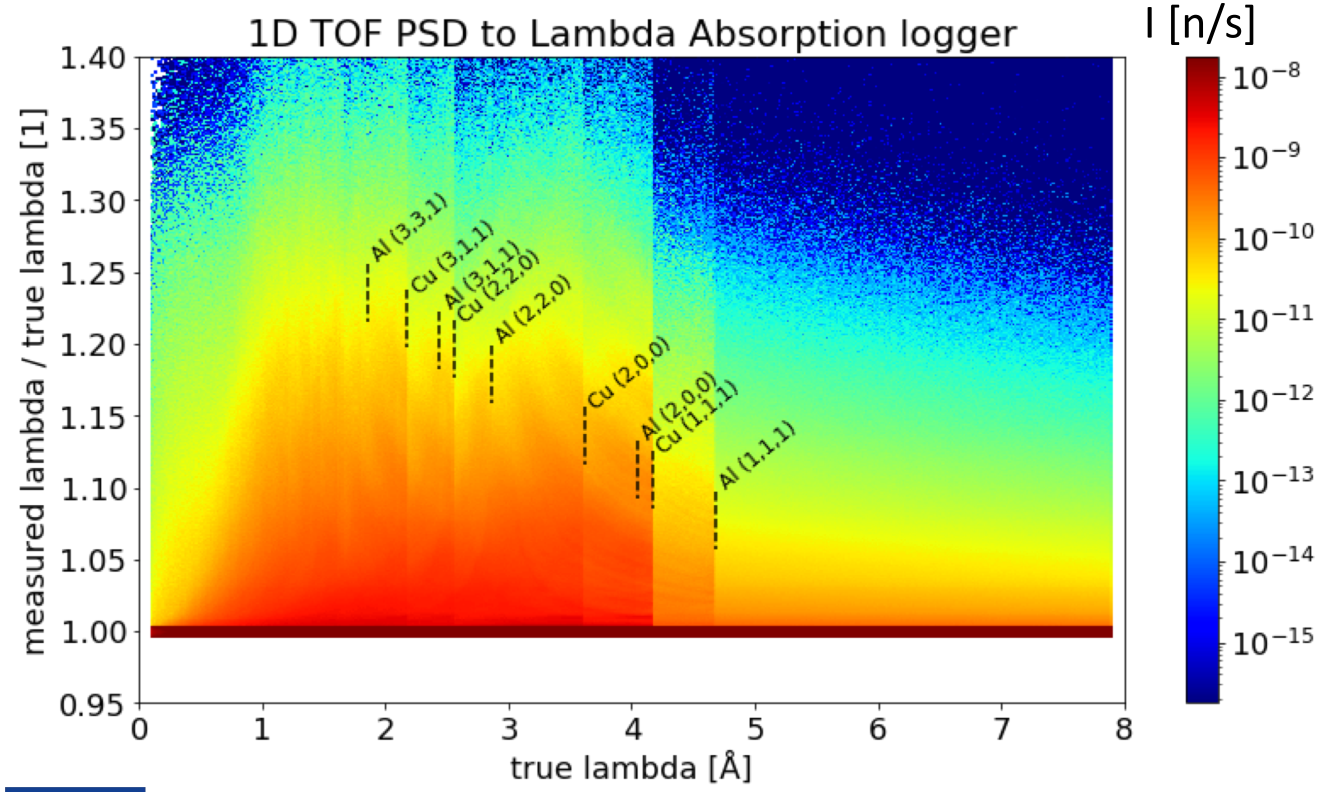
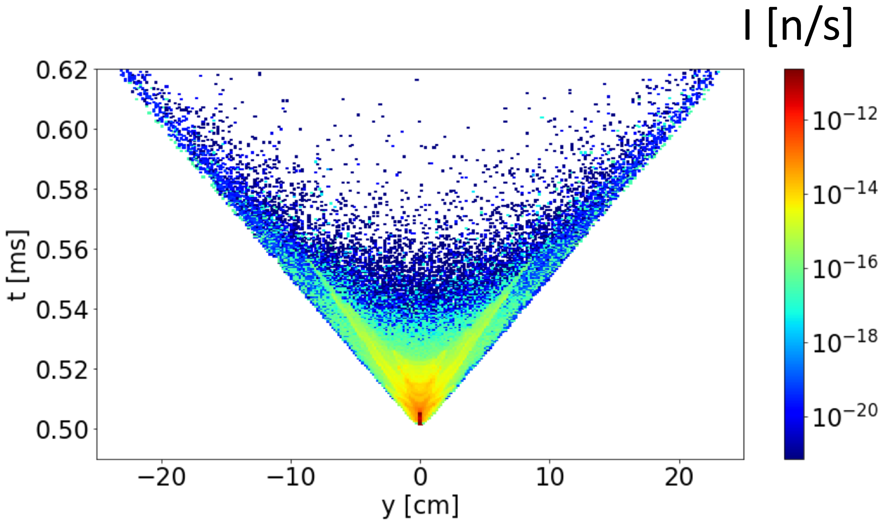
Progress in the last year

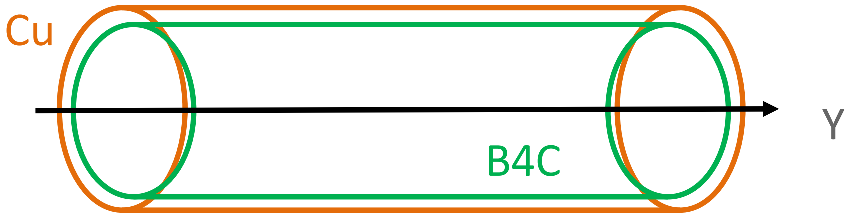
McStas and McStasScript

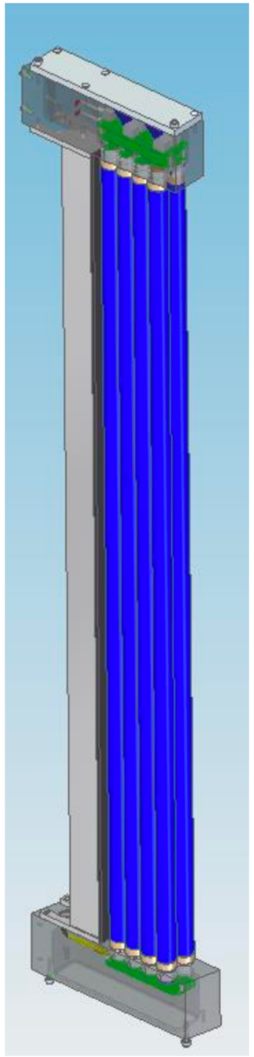
- Simulation of detector tube











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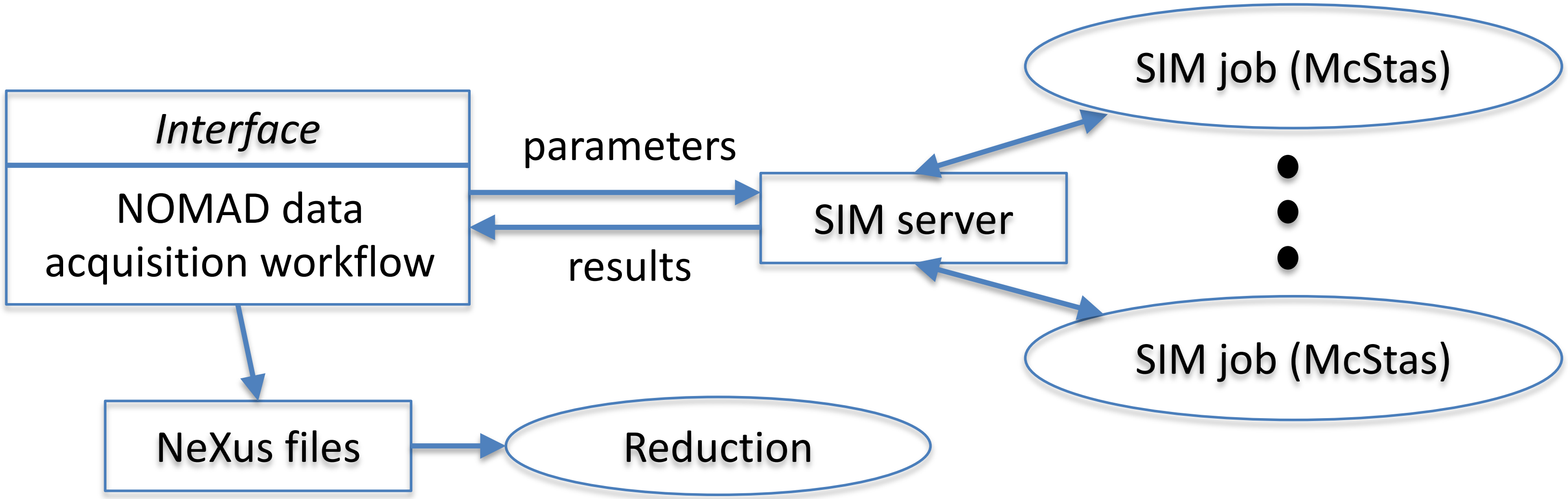
Progress in the last year

Simulation server at ILL



- SIM server (C++):
  - Receives simulation request from users
  - Launches job (local or cluster), caching, and returns results
  - openPMD data in MongoDB for caching
- Users can request simulations while performing their experiment

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Progress in the last year

Material simulations

- Ran structural relaxation using energy/force minimization with DFT or TDDFT in ASE
- Devised workflow that splits input, raw data and analyzed data
- Used DFT output as McStas sample

Download here one CIF file

In [5]:
```
CIF_file = '1527603.cif'
print('Downloading CIF file '+CIF_file+' from crystallography.net')
os.system("wget -c https://www.crystallography.net/cod/"+CIF_file)
```

```
Downloading CIF file 1527603.cif from crystallography.net
```

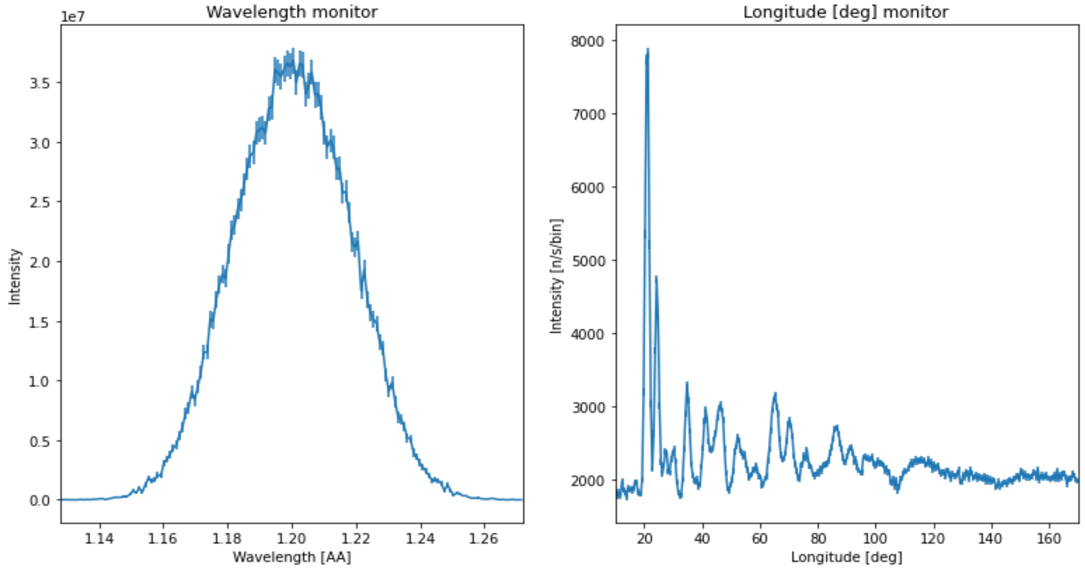
Out[5]: 0

Download the pseudo potential for Nitrogen:

In [6]:
```
pseudopotfile = 'N.pbe-n-kjpaw_psl.1.0.0.UPF'
pseudo_dir = tmpdir+"/pseudo/"
os.makedirs(pseudo_dir,exist_ok=True)
os.chdir(pseudo_dir)
os.system("wget -c https://www.quantum-espresso.org/upf_files/"+pseudopotfile)
os.system("wget -c https://raw.githubusercontent.com/PaNOSC-ViNYL/workshop2020/team2/demo/team2/
e-n-radius_5.UPF")
os.chdir(tmpdir)
pseudopotfile = 'N.pbe-n-radius_5.UPF'
```

In [32]:
```
plotter.make_sub_plot(data)
```

```
number of elements in data list = 2
Plotting data with name L_mon
Plotting data with name monitor
```



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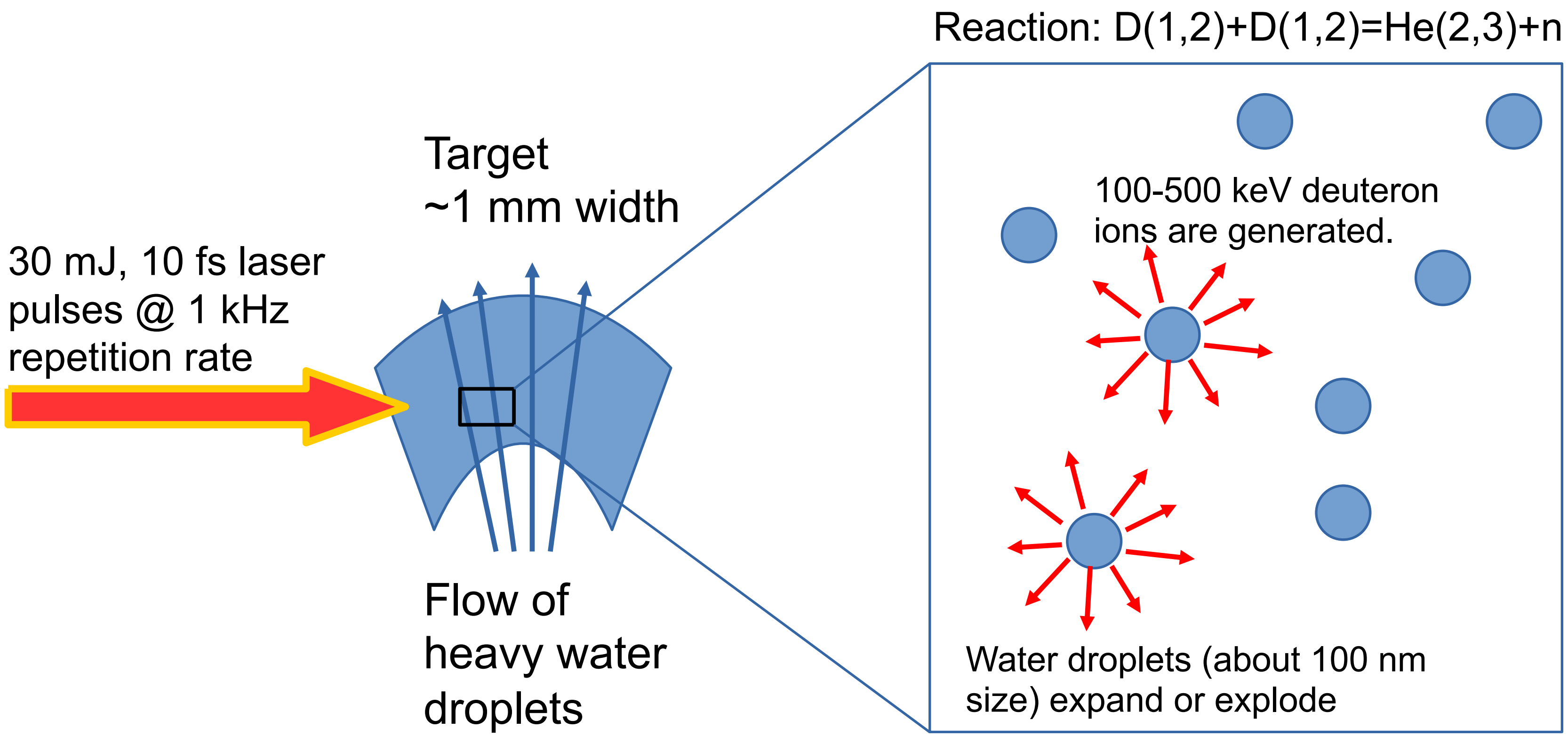
Progress in the last year

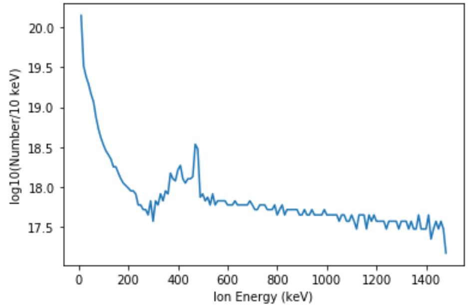
Neutrons from laser

- 10^{10} n/s -> openPMD -> Instrument concept simulation



In [15]:
```python
fig = plt.figure()
ax = plt.axes()

ax.plot(np.divide(mysource.binedges, 1000), np.log10(mysource.counts))
plt.xlabel("Ion Energy (keV)")
plt.ylabel("log10(Number/10 keV)")
plt.show()
```

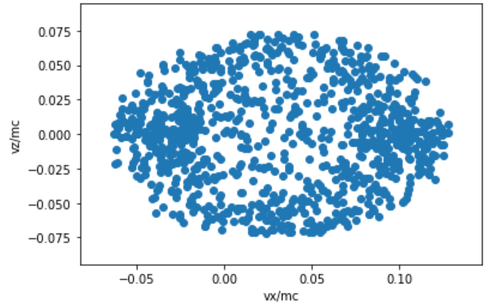


Ion energy spectrum

Check the result by plotting the Neutron distribution in velocity space:

In [16]:
```python
fig1 = plt.figure()
ax1 = plt.axes()

ax1.scatter(mysource.data[3]/3.e8, mysource.data[5]/3.e8)
plt.xlabel("vx/mc")
plt.ylabel("vz/mc")
plt.show()
```



Generated neutron velocities

In [8]:
```python
mysource.saveH5()
```

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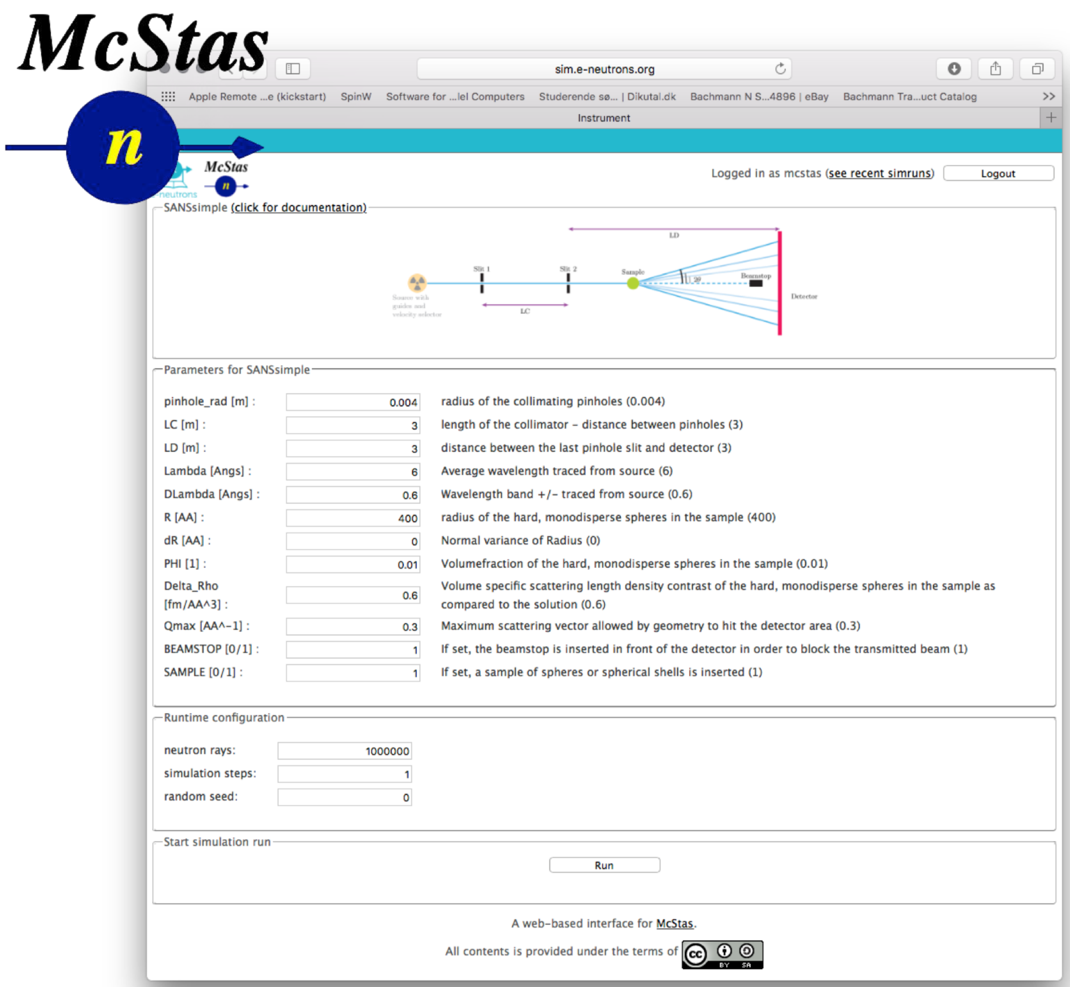
Connections to other work packages

Connection to WP8: e-learning

- Depend on WP8 to teach users about the simulation packages
- WP8 depends on us for simulation packages to be used in exercises
- Can run McStasScript in Jupyter Notebooks launched from e-learning



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Conclusion

- Simulation packages making transition to online services
- Most in Jupyter Notebooks from hubs, OASYS with GUI via remote desktop
- Providing base classes in libpyvinyl to streamline process for other/new packages

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Thank you

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photon and neutron open science cloud

European Open Science Cloud Photon and Neutron Data Services