pan-learning.org:
Demo of McStas-McXtrace simulator and Jupyter-bridge

February 9th, 2021

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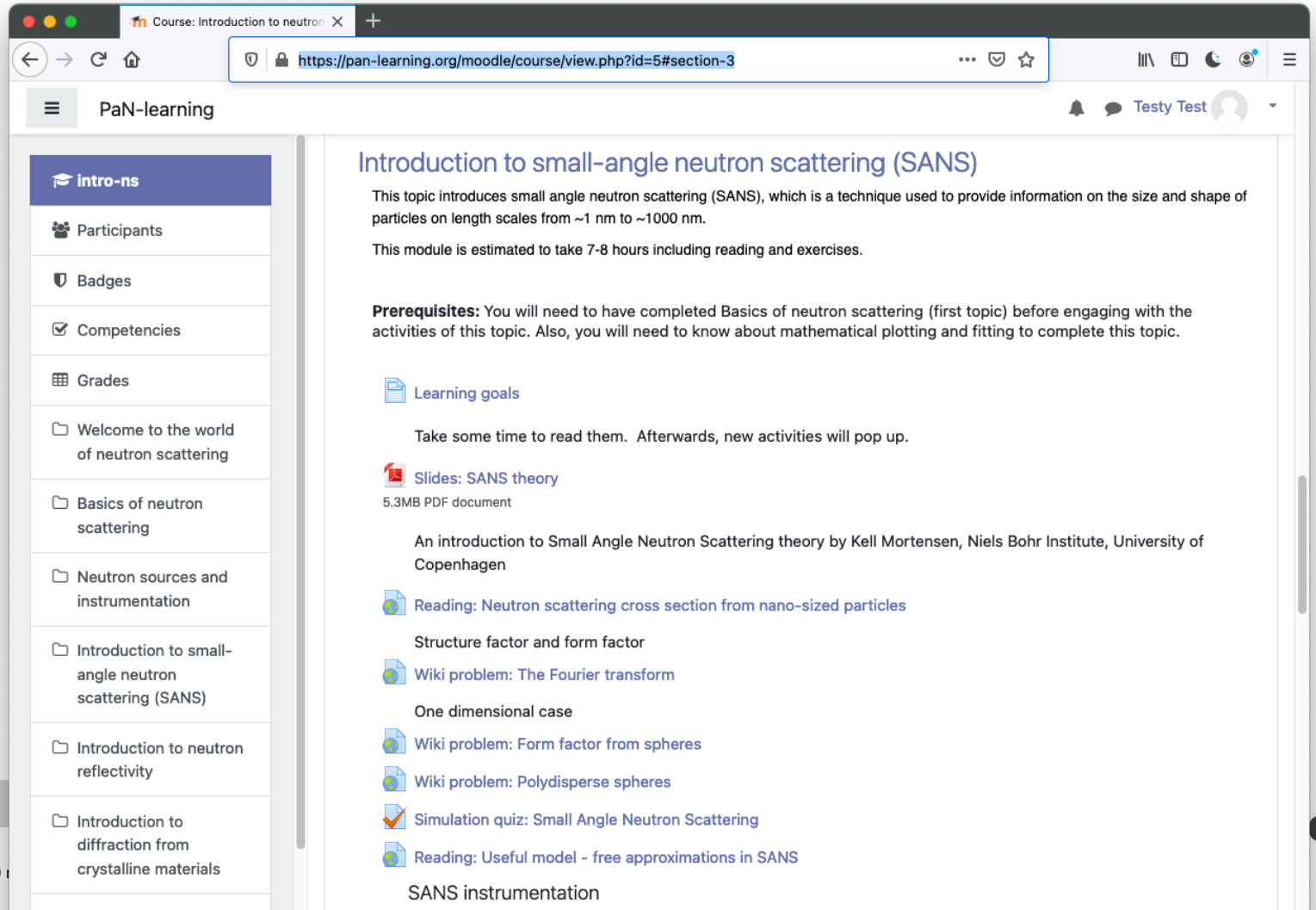
This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 823852

1. McStas and McXtrace web-simulator

- Example use case, intro-ns topic
  "Introduction to small-angle neutron scattering (SANS)"



- "Simulation quiz"

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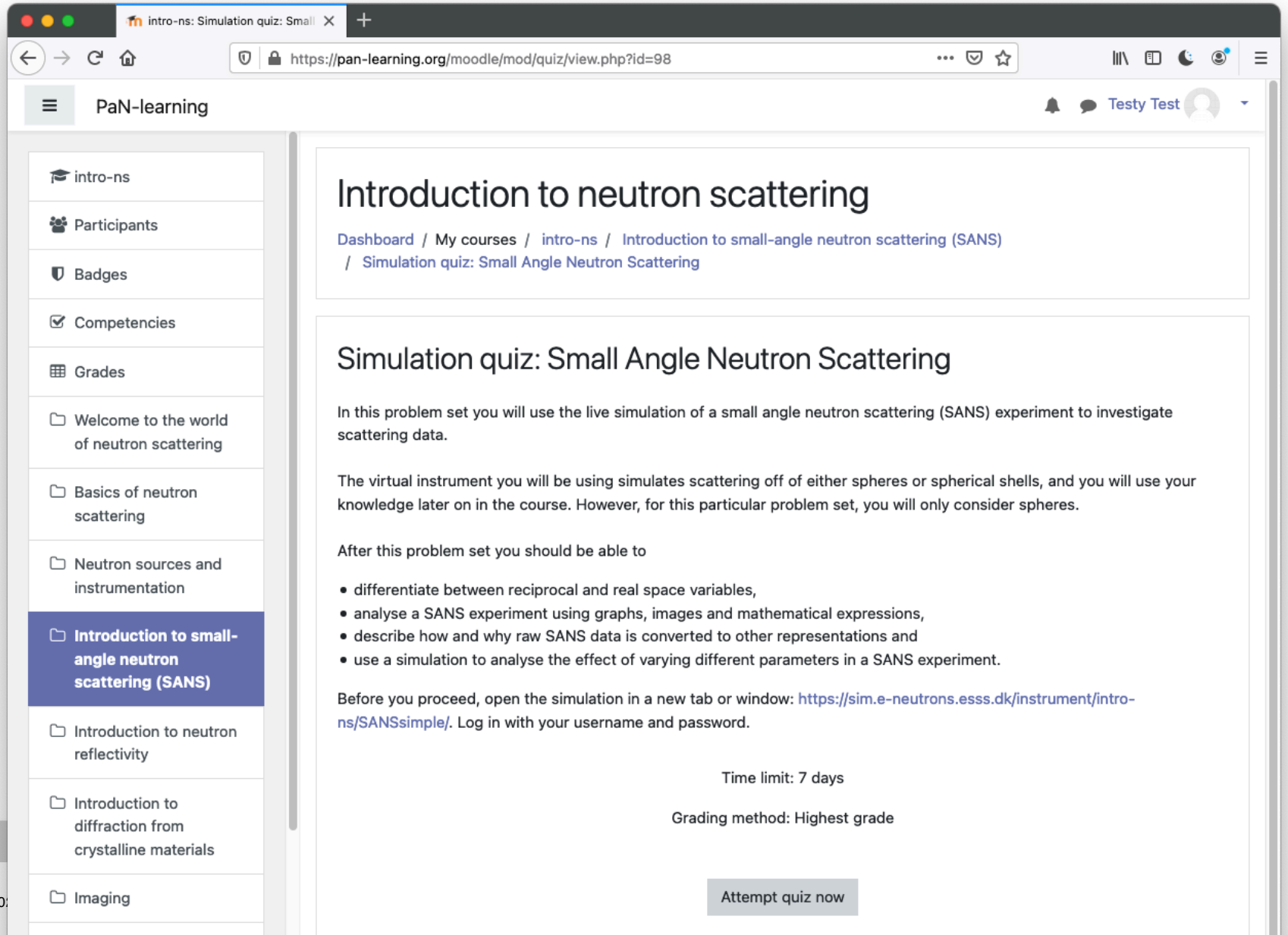
- **Simulation quiz**: Small Angle Neutron Scattering



- Click **simulator link**

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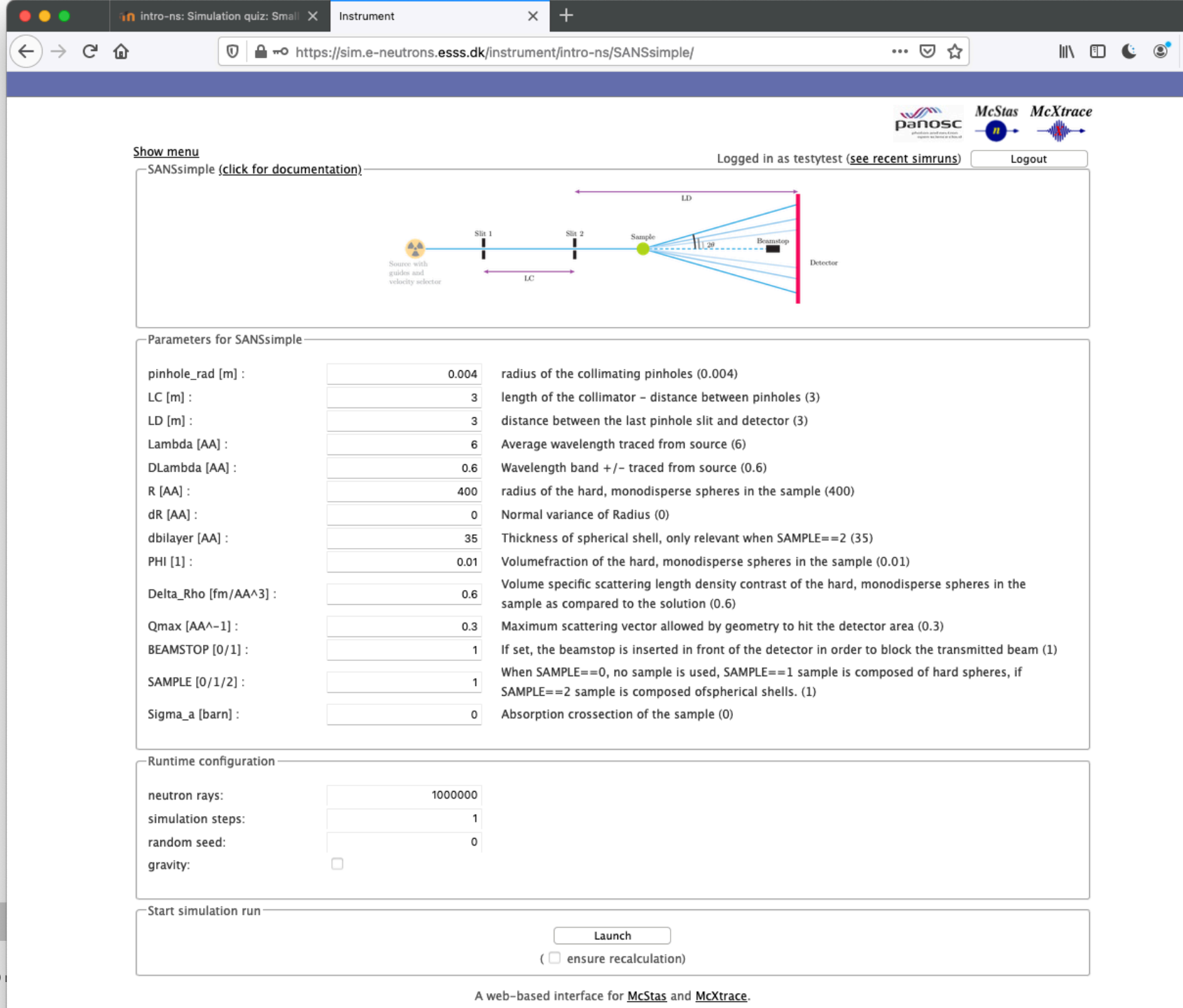
Simulator elements



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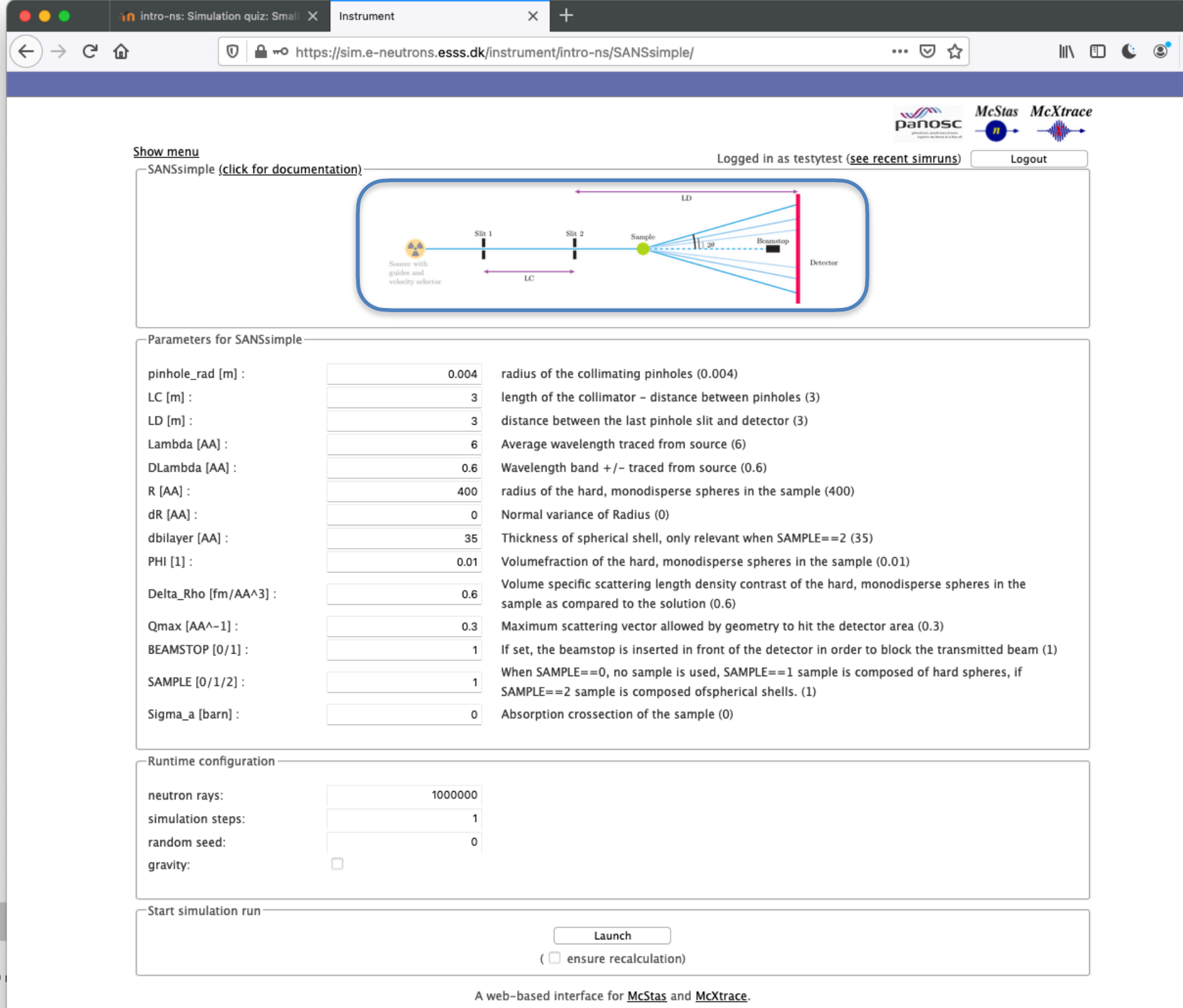
Simulator elements

- Sketch of the instrument



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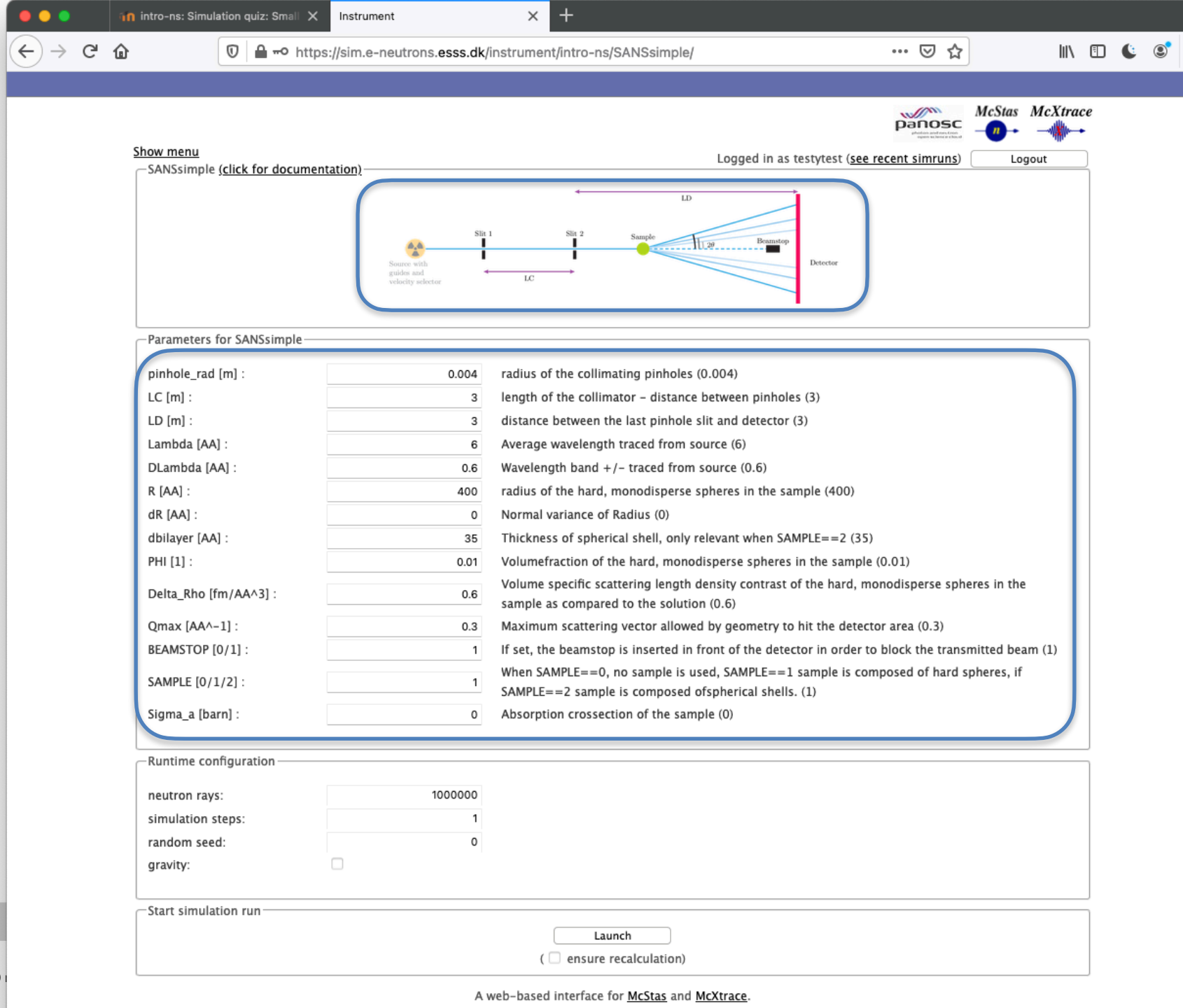
Simulator elements

- Sketch of the instrument
- Instrument-specific simulation parameters



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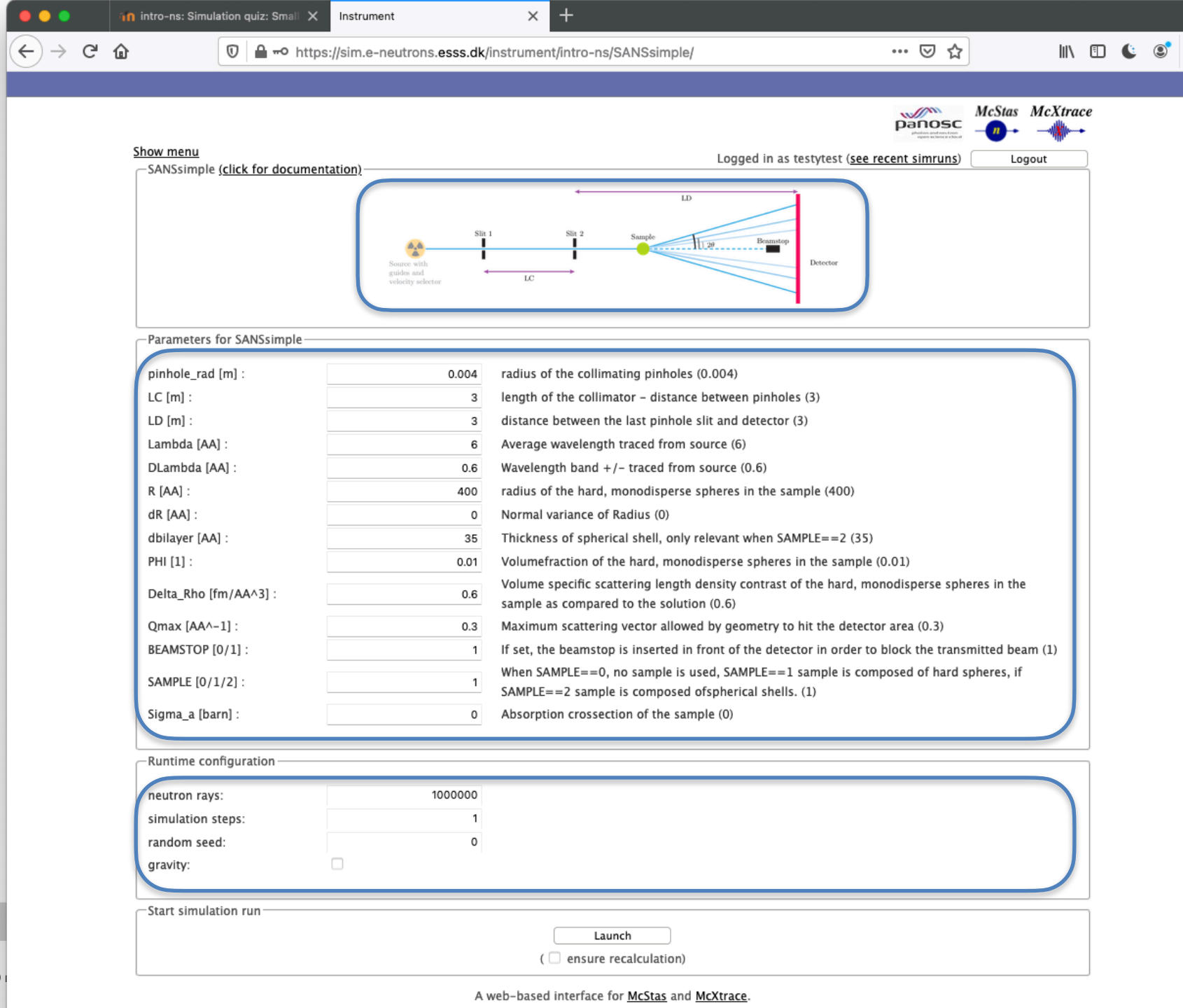
Simulator elements

- Sketch of the instrument
- Instrument-specific simulation parameters
- Generic simulation parameters



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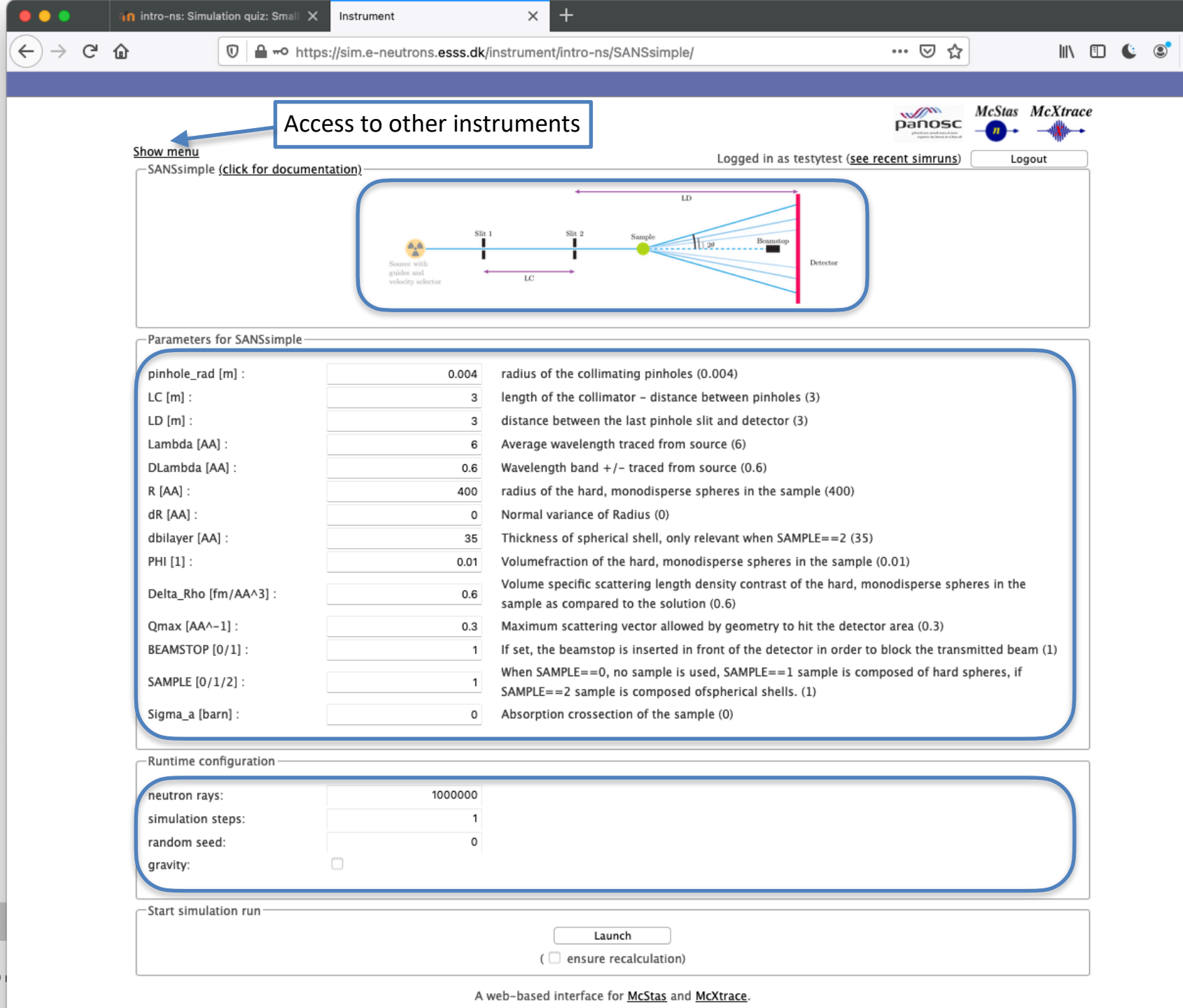
Simulator elements

- Sketch of the instrument
- Instrument-specific simulation parameters
- Generic simulation parameters



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Simulator elements

- **Simulation scenario: SANS experiment, monodisperse, hard spheres in thin solution**

Instrument setup: collimation, simulated wavelength etc.

Sample parameters, physical constants etc.

Detection specifics

Parameters for SANSsimple

pinhole_rad [m] :	0.004	radius of the collimating pinholes (0.004)
LC [m] :	3	length of the collimator – distance between pinholes (3)
LD [m] :	3	distance between the last pinhole slit and detector (3)
Lambda [AA] :	6	Average wavelength traced from source (6)
DLambda [AA] :	0.6	Wavelength band +/- traced from source (0.6)
R [AA] :	400	radius of the hard, monodisperse spheres in the sample (400)
dR [AA] :	0	Normal variance of Radius (0)
dbilayer [AA] :	35	Thickness of spherical shell, only relevant when SAMPLE==2 (35)
PHI [1] :	0.01	Volumefraction of the hard, monodisperse spheres in the sample (0.01)
Delta_Rho [fm/AA^3] :	0.6	Volume specific scattering length density contrast of the hard, monodisperse spheres in the sample as compared to the solution (0.6)
Qmax [AA^-1] :	0.3	Maximum scattering vector allowed by geometry to hit the detector area (0.3)
BEAMSTOP [0/1] :	1	If set, the beamstop is inserted in front of the detector in order to block the transmitted beam (1)
SAMPLE [0/1/2] :	1	When SAMPLE==0, no sample is used, SAMPLE==1 sample is composed of hard spheres, if SAMPLE==2 sample is composed ofspherical shells. (1)
Sigma_a [barn] :	0	Absorption crossection of the sample (0)

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Simulator elements

Parameters for SANSsimple

pinhole_rad [m] :	0.004	radius of the collimating pinholes (0.004)
LC [m] :	3	length of the collimator – distance between pinholes (3)
SD [m] :	3	distance between the last pinhole slit and detector (3)
Lambda [AA] :	6	Average wavelength traced from source (6)
DLambda [AA] :	0.6	Wavelength band +/- traced from source (0.6)
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Runtime configuration

neutron rays:	1000000
simulation steps:	1
random seed:	0
gravity:	☐

Start simulation run

Launch

(☐ ensure recalculation)

A web-based interface for McStas and McXtrace.

Simulation launch specifics:

- Statistics
- # steps in a “scan” (combine with e.g. R=100,400)
- RNG seed
- Gravitation - for neutrons

- Start by hitting ‘launch’
- x in ensure recalculation enables to “force simulating” - i.e. that result to be shown is generated and not read from an earlier simulation…

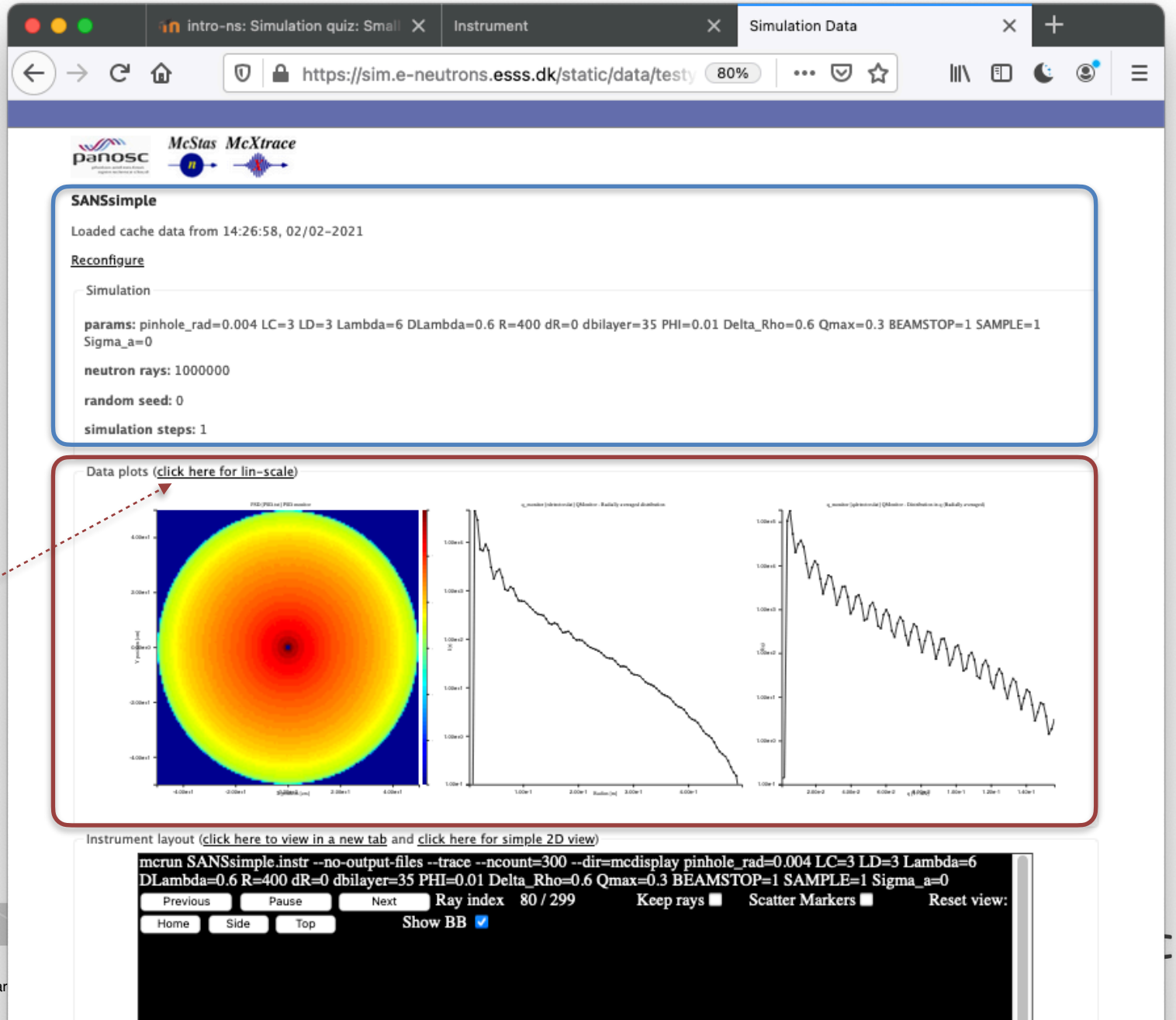
This project has received

Example output 1/3 (from default parameters)

Simulation info, stats etc.

Clickable, interactive detector outputs.

(use ‘l’ or link to google lin/log scale)



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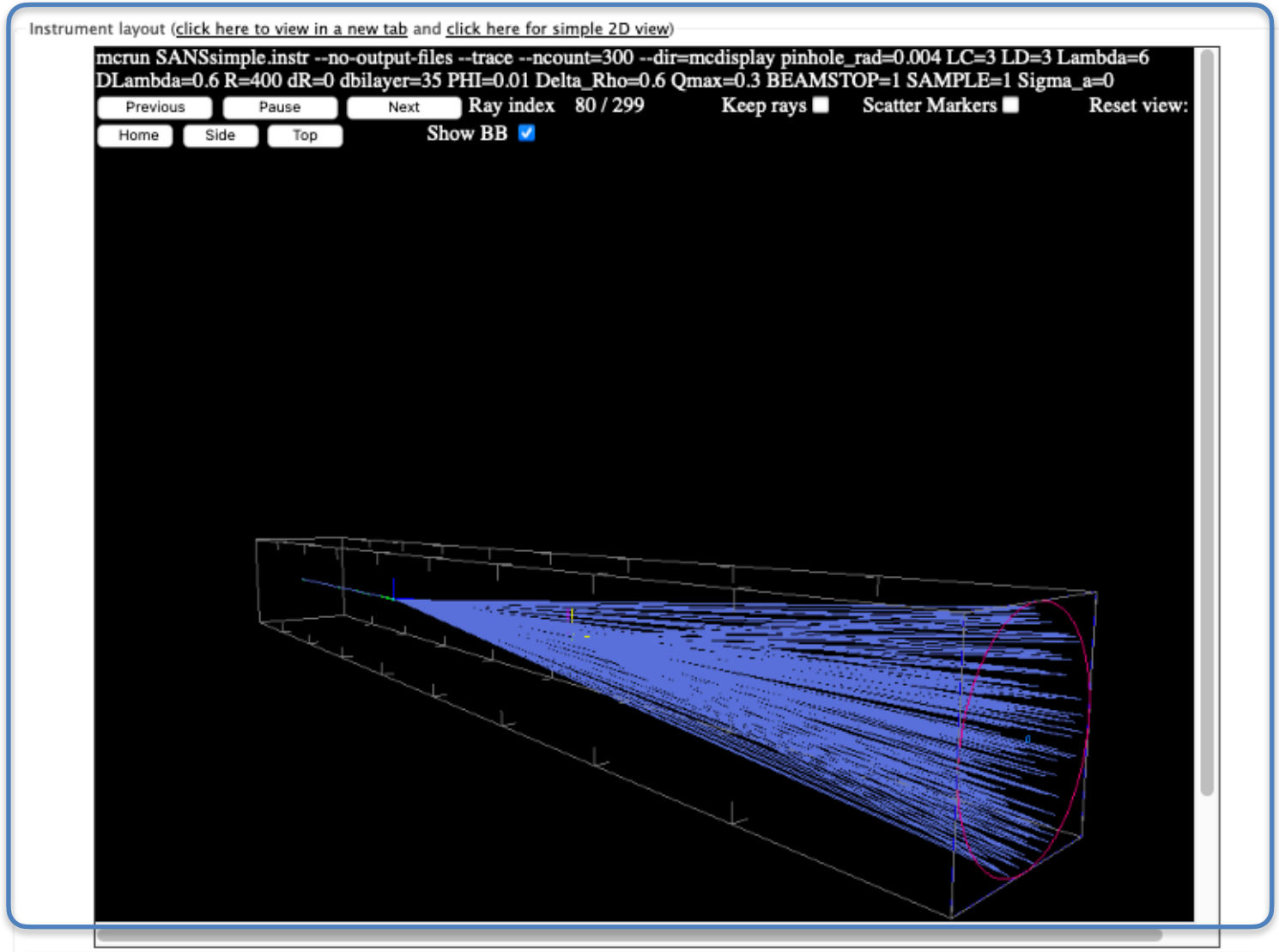
Example output 2/3

3D visualisation of the experiment

Downloadable outputs



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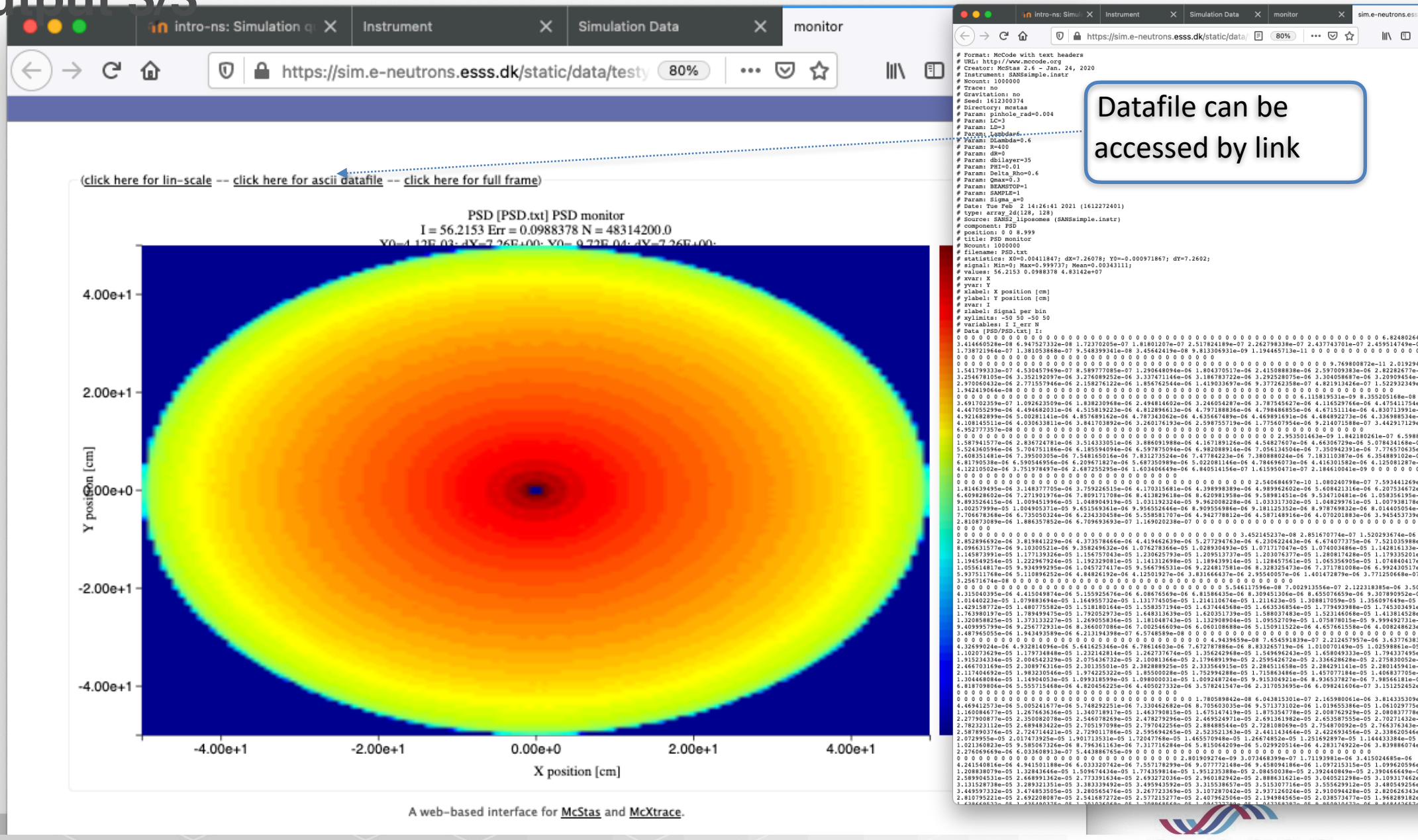
Example output 3/3

- Clicking a graph brings it forward
- Lin/log by pressing ‘l’ or link-toggle
- Drag/Zoom-able by mouse



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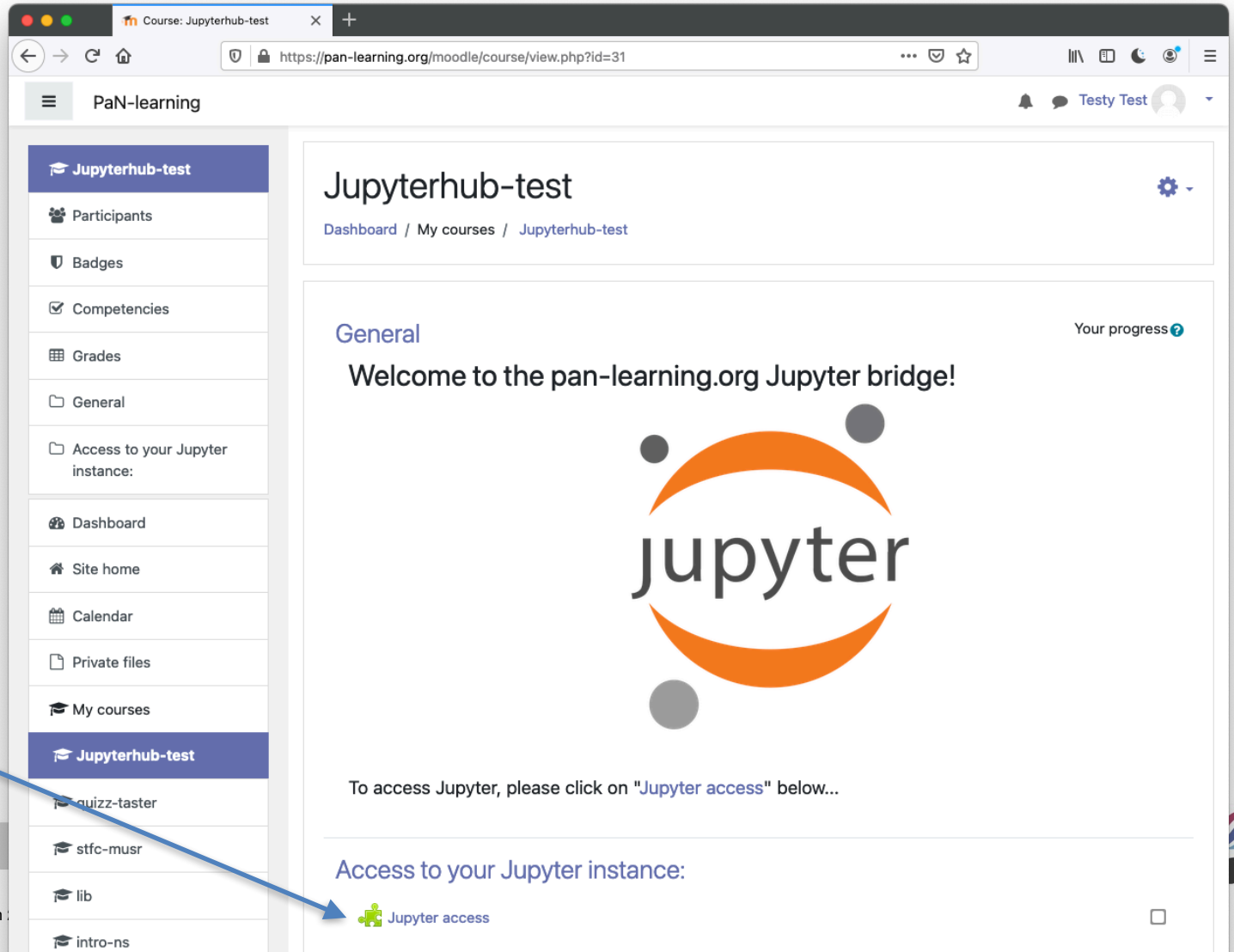
2. Jupyterhub connectivity

- To access, please self-enrol to the course [Jupyterhub-test]



Next, click the link…

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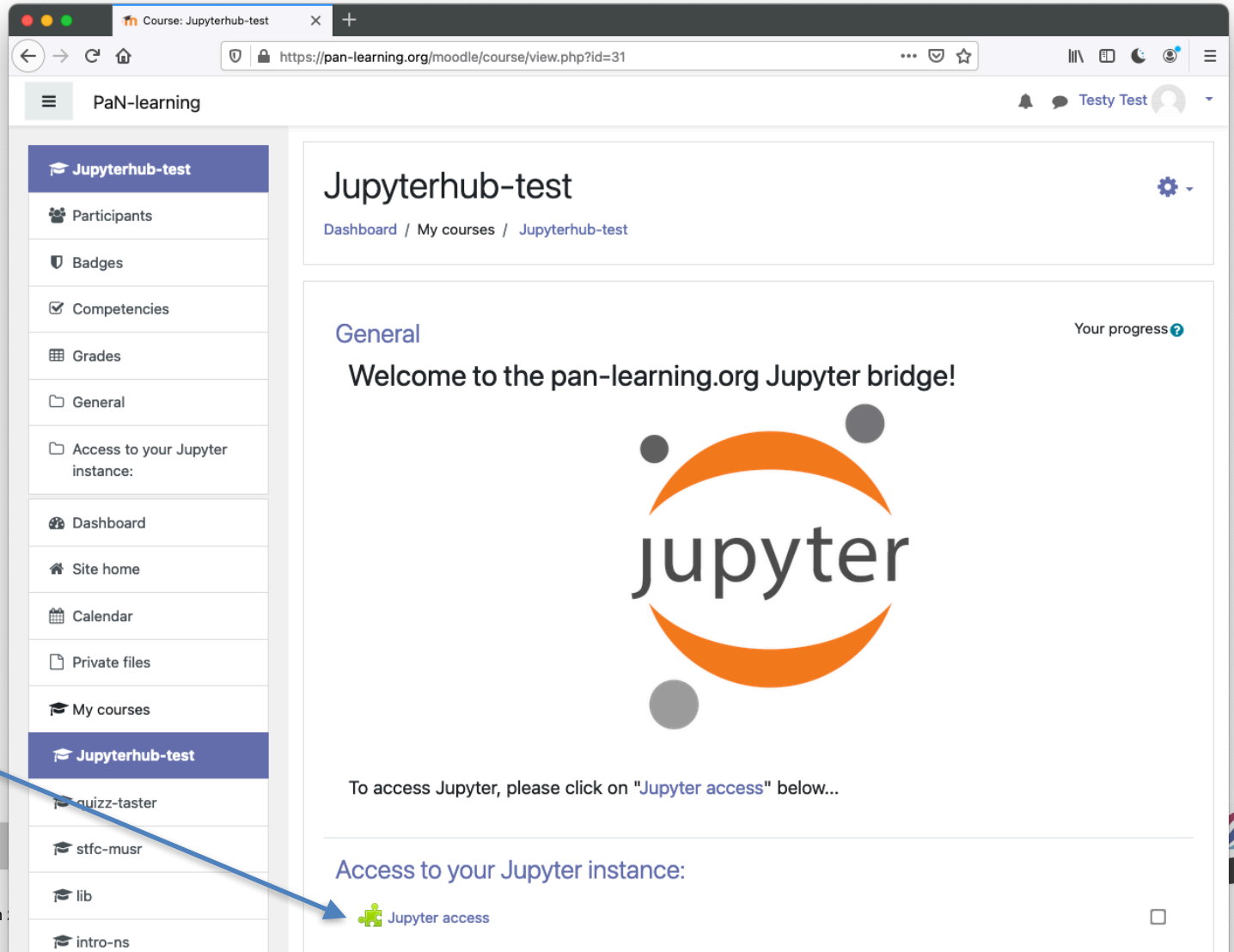
Next, access the course and click the link…



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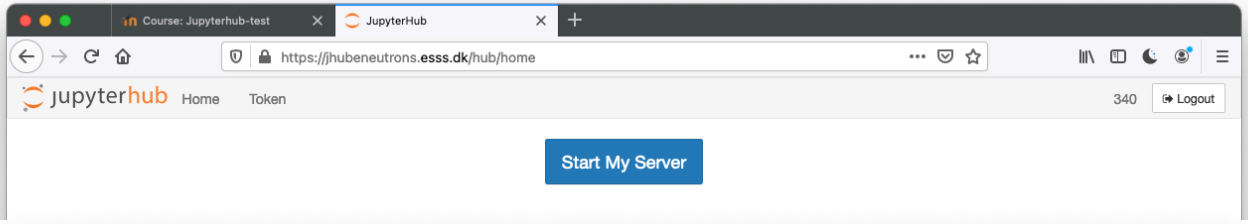
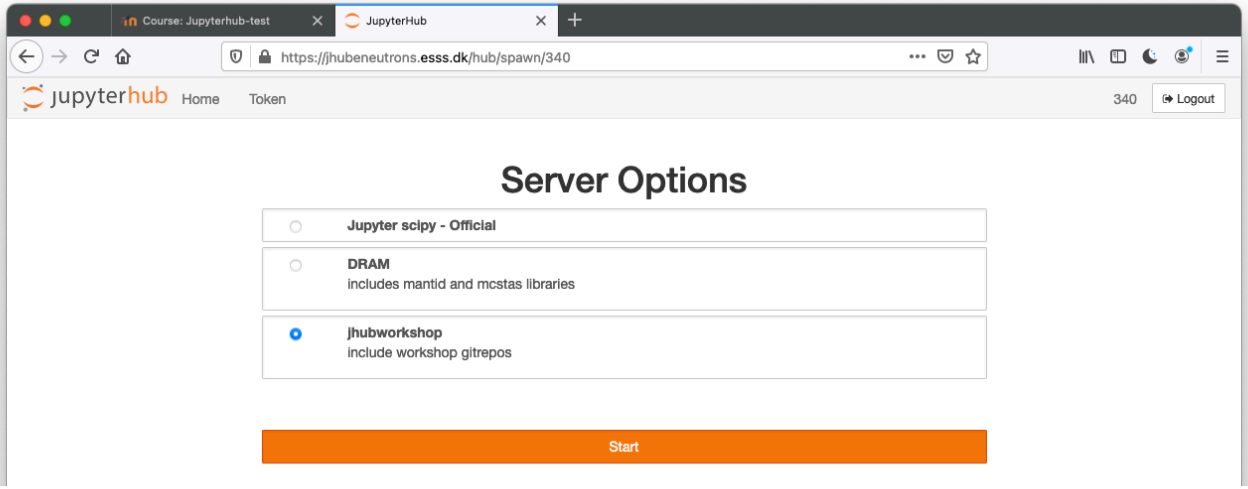
- start server…



- pick a container…



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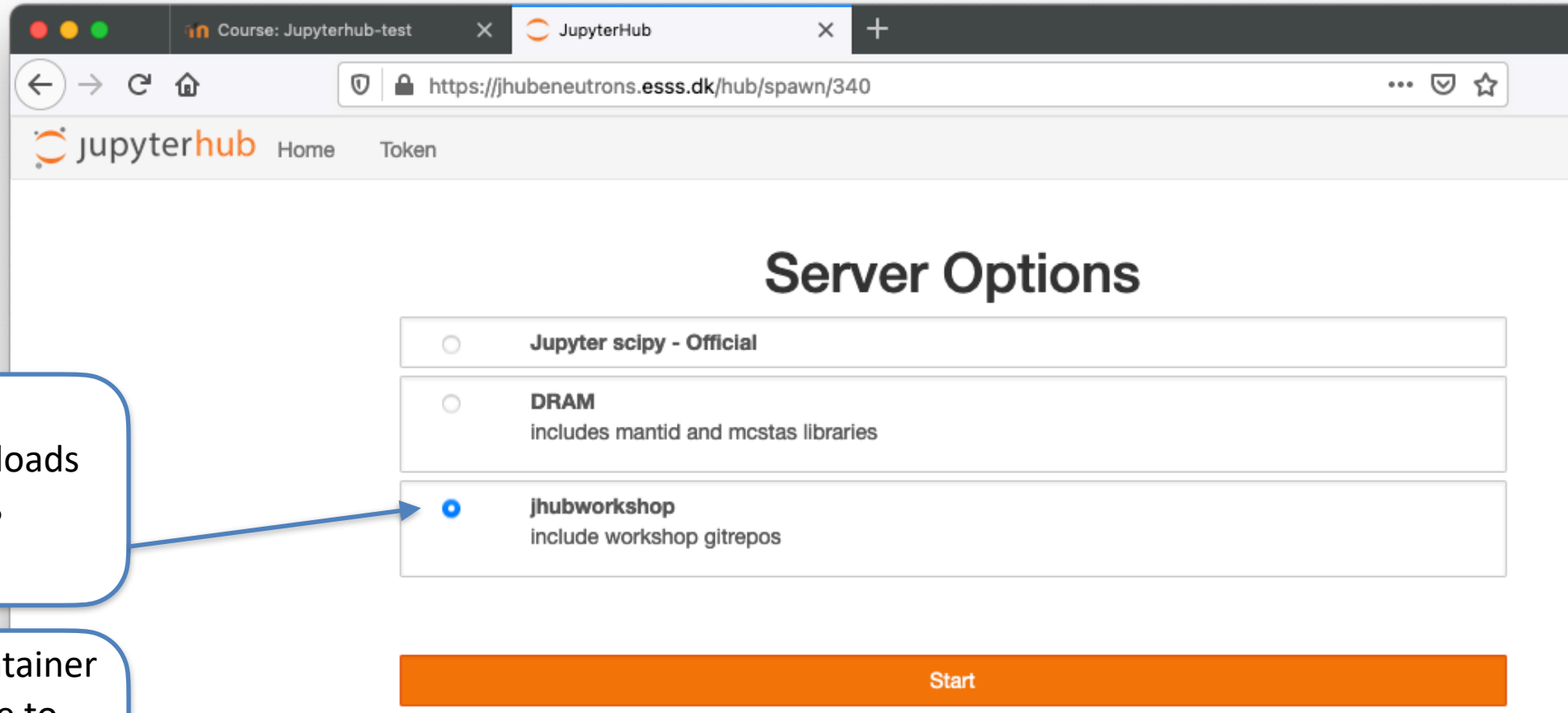

Best starting-point is the 'jhubworkshop' container that loads various files from an earlier ESS Python/Jupyter workshop.

To later try e.g. the DRAM container with McStasScript, you will have to shut down server and restart with the other container.

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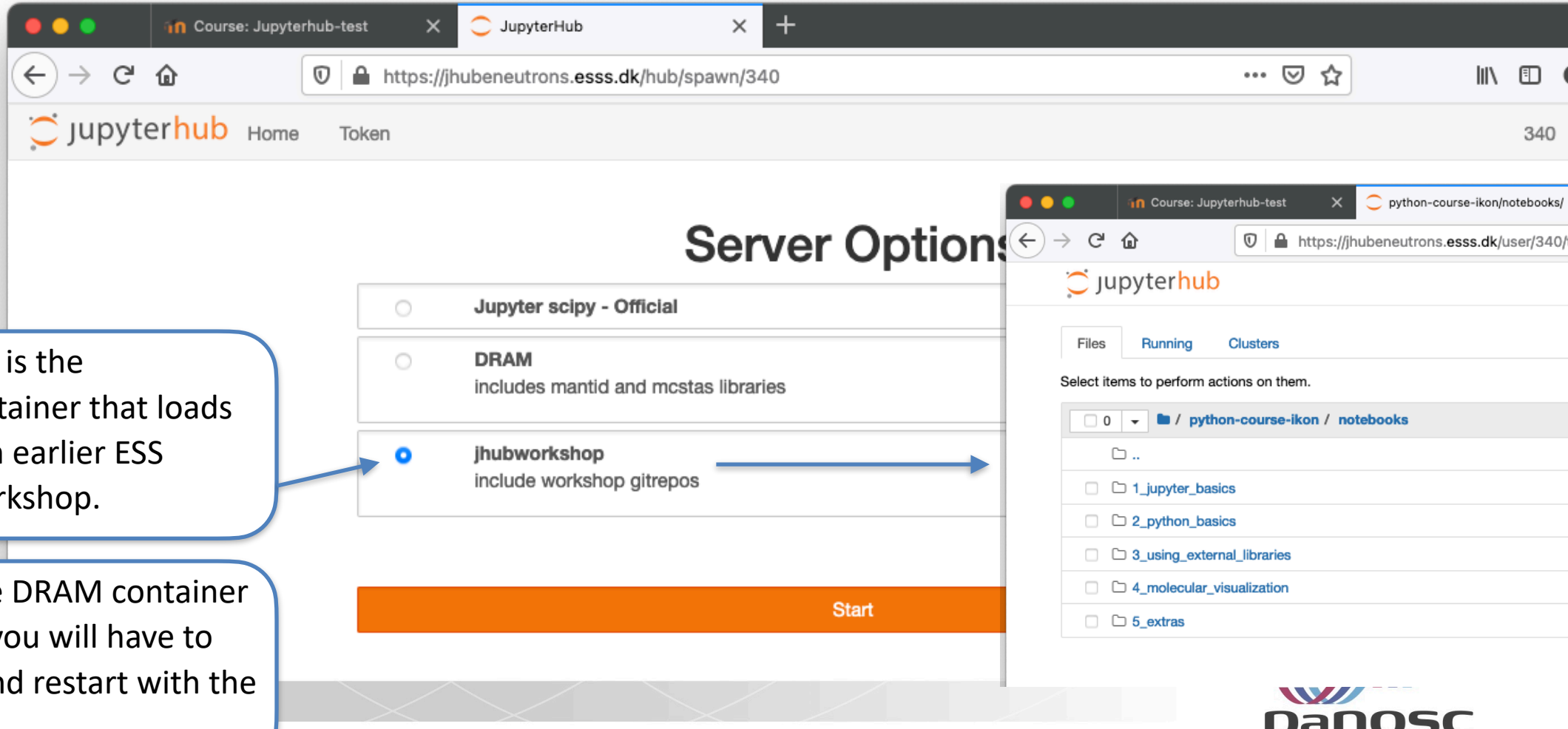

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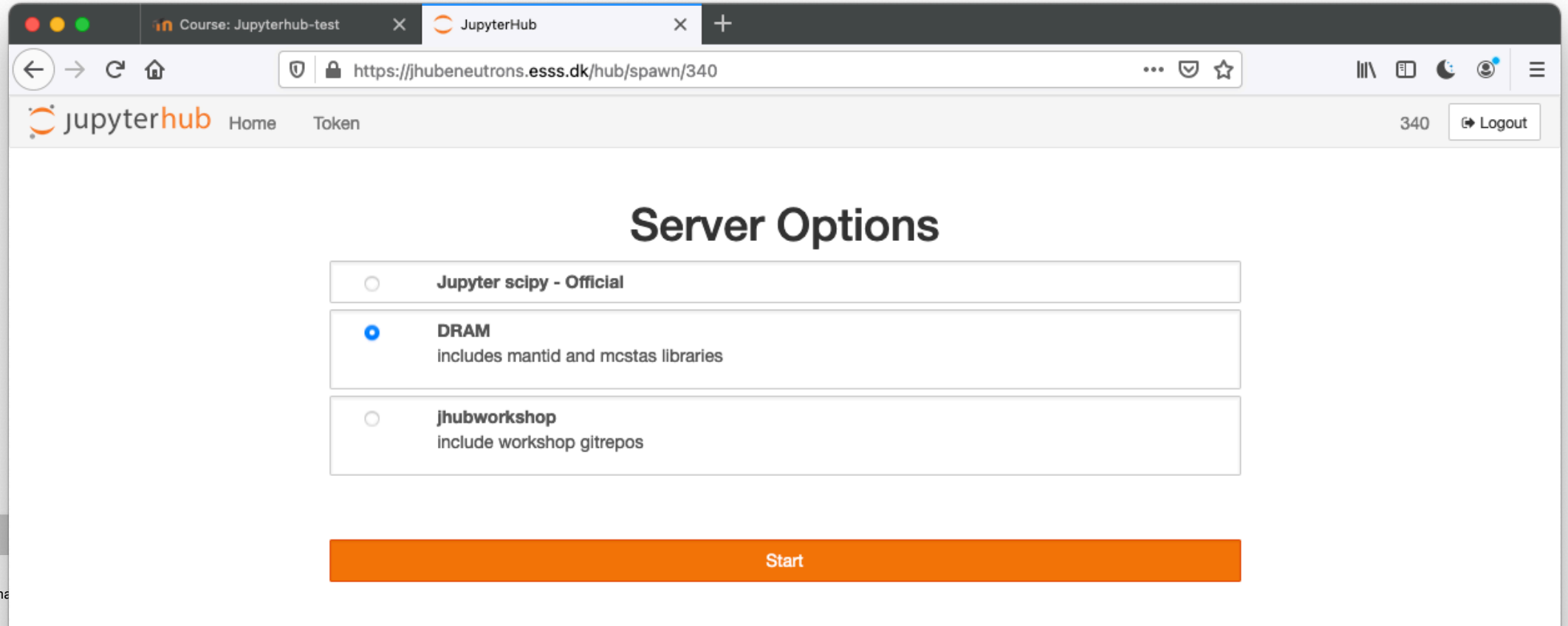
- The DRAM container contains McStasScript (you need to manually add/upload a notebook, e.g. this one



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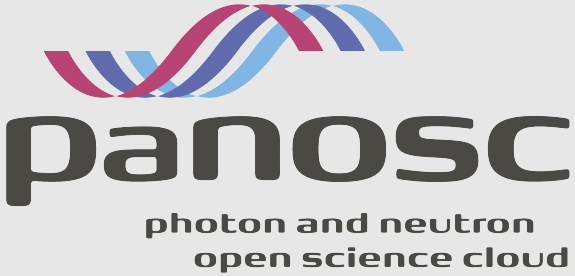

Thank you

peter.willendrup@ess.eu

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