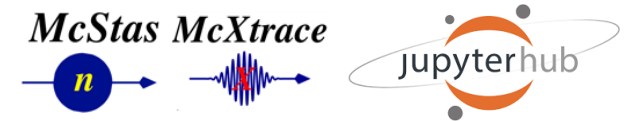


pan-learning.org:

Demo of McStas-McXtrace simulator and
Jupyter-bridge

February 9th, 2021

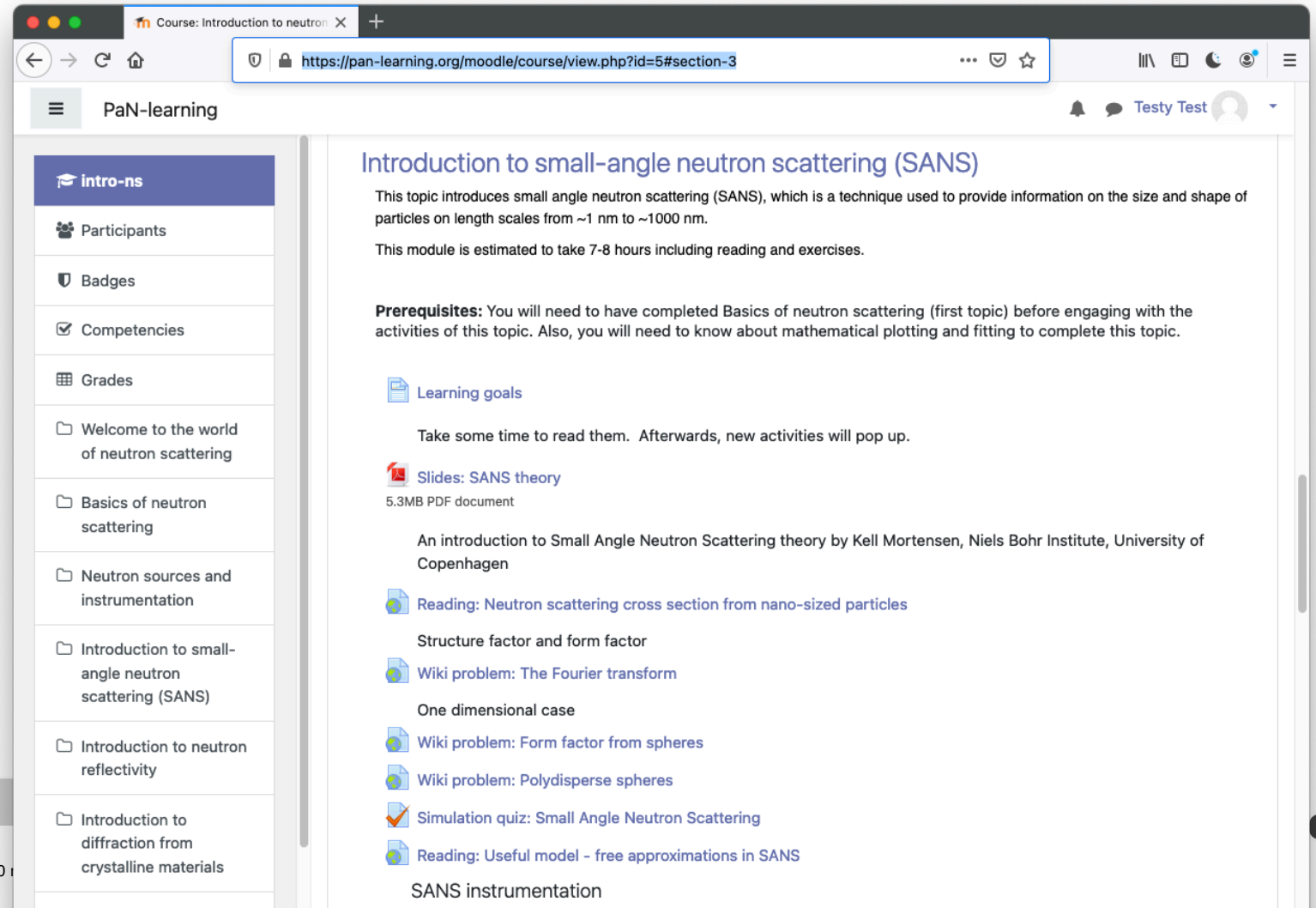
Author: Peter Willendrup, ESS DMSC



1. McStas and McXtrace web-simulator

- Example use case, intro-ns topic

“[Introduction to small-angle neutron scattering \(SANS\)](#)”



The screenshot shows a web browser displaying a Moodle course page. The browser's address bar shows the URL: <https://pan-learning.org/moodle/course/view.php?id=5#section-3>. The page title is "Introduction to small-angle neutron scattering (SANS)". The left sidebar contains a navigation menu with the following items: "intro-ns" (selected), "Participants", "Badges", "Competencies", "Grades", "Welcome to the world of neutron scattering", "Basics of neutron scattering", "Neutron sources and instrumentation", "Introduction to small-angle neutron scattering (SANS)", "Introduction to neutron reflectivity", and "Introduction to diffraction from crystalline materials". The main content area includes the following text and links:

Introduction to small-angle neutron scattering (SANS)

This topic introduces small angle neutron scattering (SANS), which is a technique used to provide information on the size and shape of particles on length scales from ~1 nm to ~1000 nm.

This module is estimated to take 7-8 hours including reading and exercises.

Prerequisites: You will need to have completed Basics of neutron scattering (first topic) before engaging with the activities of this topic. Also, you will need to know about mathematical plotting and fitting to complete this topic.

Learning goals

Take some time to read them. Afterwards, new activities will pop up.

Slides: SANS theory
5.3MB PDF document

An introduction to Small Angle Neutron Scattering theory by Kell Mortensen, Niels Bohr Institute, University of Copenhagen

Reading: Neutron scattering cross section from nano-sized particles

Structure factor and form factor

Wiki problem: The Fourier transform

One dimensional case

Wiki problem: Form factor from spheres

Wiki problem: Polydisperse spheres

Simulation quiz: Small Angle Neutron Scattering

Reading: Useful model - free approximations in SANS

SANS instrumentation

- “[Simulation quiz](#)”



- [Simulation quiz](#): Small Angle Neutron Scattering

The screenshot shows a web browser window displaying a Moodle quiz page. The browser's address bar shows the URL: <https://pan-learning.org/moodle/mod/quiz/view.php?id=98>. The page header includes the site name 'PaN-learning' and a user profile 'Testy Test'. The main content area is titled 'Introduction to neutron scattering' and contains a breadcrumb trail: 'Dashboard / My courses / intro-ns / Introduction to small-angle neutron scattering (SANS) / Simulation quiz: Small Angle Neutron Scattering'. Below this, the quiz title 'Simulation quiz: Small Angle Neutron Scattering' is displayed. The quiz description states: 'In this problem set you will use the live simulation of a small angle neutron scattering (SANS) experiment to investigate scattering data. The virtual instrument you will be using simulates scattering off of either spheres or spherical shells, and you will use your knowledge later on in the course. However, for this particular problem set, you will only consider spheres. After this problem set you should be able to' followed by a bulleted list of learning objectives: 'differentiate between reciprocal and real space variables', 'analyse a SANS experiment using graphs, images and mathematical expressions', 'describe how and why raw SANS data is converted to other representations and', and 'use a simulation to analyse the effect of varying different parameters in a SANS experiment.' Below the list, it says: 'Before you proceed, open the simulation in a new tab or window: <https://sim.e-neutrons.esss.dk/instrument/intro-ns/SANSsimple/>. Log in with your username and password.' The time limit is '7 days' and the grading method is 'Highest grade'. A button labeled 'Attempt quiz now' is at the bottom right. A left-hand sidebar menu shows the course structure, with 'Introduction to small-angle neutron scattering (SANS)' highlighted in blue.

- Click [simulator link](#)



Simulator elements

intro-ns: Simulation quiz: Small Instrument

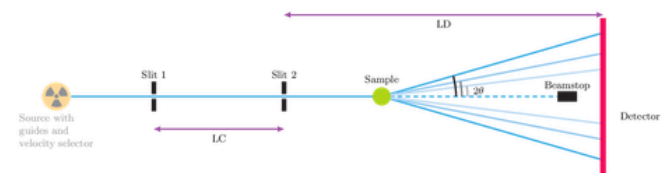
https://sim.e-neutrons.esss.dk/instrument/intro-ns/SANSSimple/

panosc McStas McXtrace

Logged in as testytest (see recent simruns) Logout

Show menu

SANSSimple (click for documentation)



Parameters for SANSSimple

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

Runtime configuration

neutron rays:	<input type="text" value="1000000"/>
simulation steps:	<input type="text" value="1"/>
random seed:	<input type="text" value="0"/>
gravity:	<input type="checkbox"/>

Start simulation run

(ensure recalculation)

A web-based interface for [McStas](#) and [McXtrace](#).



Simulator elements

- Sketch of the instrument

intro-ns: Simulation quiz: Small Instrument

https://sim.e-neutrons.esss.dk/instrument/intro-ns/SANSsimple/

panosc McStas McXtrace

Logged in as testytest (see recent simruns) Logout

Show menu

SANSsimple (click for documentation)

Parameters for SANSsimple

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

Runtime configuration

neutron rays:	<input type="text" value="1000000"/>
simulation steps:	<input type="text" value="1"/>
random seed:	<input type="text" value="0"/>
gravity:	<input type="checkbox"/>

Start simulation run

Launch

(ensure recalculation)

A web-based interface for [McStas](#) and [McXtrace](#).



Simulator elements

- Sketch of the instrument
- Instrument-specific simulation parameters

intro-ns: Simulation quiz: Small Instrument

https://sim.e-neutrons.esss.dk/instrument/intro-ns/SANSsimple/

panosc McStas McXtrace

Logged in as testytest (see recent simruns) Logout

Show menu

SANSsimple (click for documentation)

Source with guides and velocity selector Slit 1 Slit 2 Sample Beamstop Detector

LC LD

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	Volume fraction 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 of spherical shells. (1)
Sigma_a [barn] :	0	Absorption crosssection of the sample (0)

Runtime configuration

neutron rays:	1000000
simulation steps:	1
random seed:	0
gravity:	<input type="checkbox"/>

Start simulation run

Launch

(ensure recalculation)



Simulator elements

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

intro-ns: Simulation quiz: Small Instrument

https://sim.e-neutrons.esss.dk/instrument/intro-ns/SANSsimple/

panosc McStas McXtrace

Logged in as testytest (see recent simruns) Logout

Show menu

SANSsimple (click for documentation)

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)
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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 of spherical shells. (1)
Sigma_a [barn] :	0	Absorption crosssection of the sample (0)

Runtime configuration

neutron rays:	1000000
simulation steps:	1
random seed:	0
gravity:	<input type="checkbox"/>

Start simulation run

Launch

(ensure recalculation)



Simulator elements

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

Access to other instruments

Show menu

SANSsimple ([click for documentation](#))

Logged in as testytest ([see recent simruns](#)) [Logout](#)

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)
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PHI [1] :	0.01	Volume fraction 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 of spherical shells. (1)
Sigma_a [barn] :	0	Absorption crosssection of the sample (0)

Runtime configuration

neutron rays:	1000000
simulation steps:	1
random seed:	0
gravity:	<input type="checkbox"/>

Start simulation run

[Launch](#)
(ensure recalculation)



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 of spherical shells. (1)
Sigma_a [barn] :	0	Absorption crosssection of the sample (0)



Simulator elements

pinhole_rad [m] :	<input type="text" value="0.004"/>	radius of the collimating pinholes (0.004)
LC [m] :	<input type="text" value="3"/>	length of the collimator – distance between pinholes (3)
LC2 [m] :	<input type="text" value="3"/>	distance between the last pinhole slit and detector (3)
Lambda [AA] :	<input type="text" value="6"/>	Average wavelength traced from source (6)
DLambda [AA] :	<input type="text" value="0.6"/>	Wavelength band +/- traced from source (0.6)
R [AA] :	<input type="text" value="400"/>	radius of the hard, monodisperse spheres in the sample (400)
dR [AA] :	<input type="text" value="0"/>	Normal variance of Radius (0)
dbilayer [AA] :	<input type="text" value="35"/>	Thickness of spherical shell, only relevant when SAMPLE==2 (35)
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Delta_Rho [fm/AA^3] :	<input type="text" value="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] :	<input type="text" value="0.3"/>	Maximum scattering vector allowed by geometry to hit the detector area (0.3)
BEAMSTOP [0/1] :	<input type="text" value="1"/>	If set, the beamstop is inserted in front of the detector in order to block the transmitted beam (1)
SAMPLE [0/1/2] :	<input type="text" value="1"/>	When SAMPLE==0, no sample is used, SAMPLE==1 sample is composed of hard spheres, if SAMPLE==2 sample is composed of spherical shells. (1)
Sigma_a [barn] :	<input type="text" value="0"/>	Absorption cross section of the sample (0)

Simulation launch specifics:

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

Runtime configuration

neutron rays:	<input type="text" value="1000000"/>
simulation steps:	<input type="text" value="1"/>
random seed:	<input type="text" value="0"/>
gravity:	<input type="checkbox"/>

Start simulation run

(ensure recalculation)

• 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)

intro-ns: Simulation quiz: Small Instrument Simulation Data

https://sim.e-neutrons.esss.dk/static/data/testy 80%

panOSC McStas McXtrace

SANSsimple

Loaded cache data from 14:26:58, 02/02-2021

[Reconfigure](#)

Simulation

params: pinhole_rad=0.004 LC=3 LD=3 Lambda=6 DLambda=0.6 R=400 dR=0 dbilayer=35 PHI=0.01 Delta_Rho=0.6 Qmax=0.3 BEAMSTOP=1 SAMPLE=1 Sigma_a=0

neutron rays: 1000000

random seed: 0

simulation steps: 1

Data plots [\(click here for lin-scale\)](#)

2D detector map (left) and 1D intensity profiles (right).

Instrument layout [\(click here to view in a new tab\)](#) and [click here for simple 2D view](#)

```
mcrun SANSsimple.instr --no-output-files --trace --ncount=300 --dir=mcdisplay pinhole_rad=0.004 LC=3 LD=3 Lambda=6 DLambda=0.6 R=400 dR=0 dbilayer=35 PHI=0.01 Delta_Rho=0.6 Qmax=0.3 BEAMSTOP=1 SAMPLE=1 Sigma_a=0
```

Previous Pause Next Ray index 80 / 299 Keep rays Scatter Markers Reset view:

Home Side Top Show BB



Example output 2/3

3D visualisation of the experiment

Downloadable outputs

Instrument layout ([click here to view in a new tab](#) and [click here for simple 2D view](#))

```
mcrun SANSsimple.instr --no-output-files --trace --ncount=300 --dir=mcdisplay pinhole_rad=0.004 LC=3 LD=3 Lambda=6  
DLambda=0.6 R=400 dR=0 dbilayer=35 PHI=0.01 Delta_Rho=0.6 Qmax=0.3 BEAMSTOP=1 SAMPLE=1 Sigma_a=0
```

Previous Pause Next Ray index 80 / 299 Keep rays Scatter Markers Reset view:
Home Side Top Show BB

Download output files

[simrun.tar.gz](#) [SANSsimple.instr](#) [stdout](#) [stderr](#) [VRML](#)

A web-based interface for [McStas](#) and [McXtrace](#).



Example output 3/3

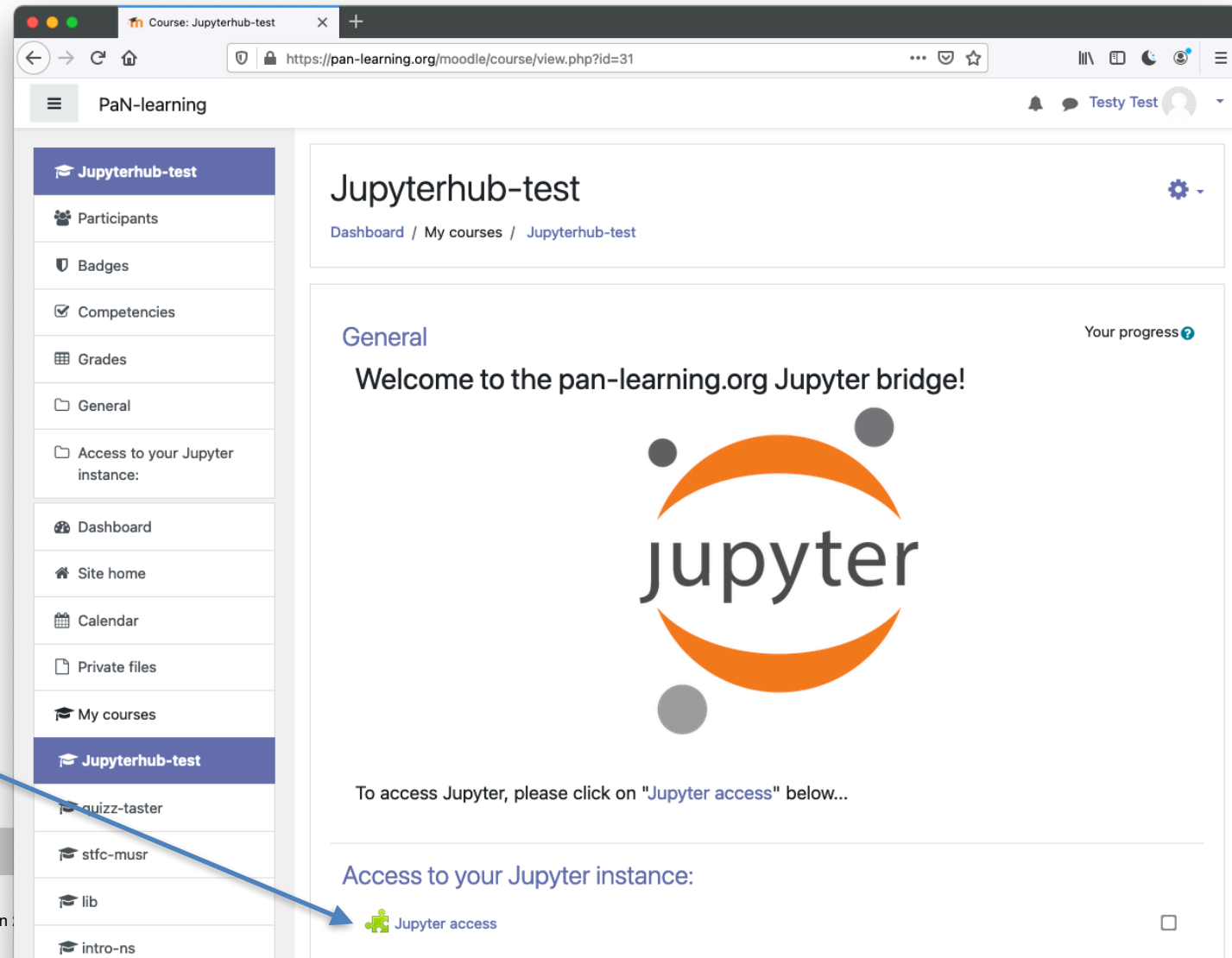
- Clicking a graph brings it forward
- Lin/log by pressing 'l' or link-toggle
- Drag/Zoom-able by mouse

Datafile can be accessed by link

2. Jupyterhub connectivity

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

Next, click the link...



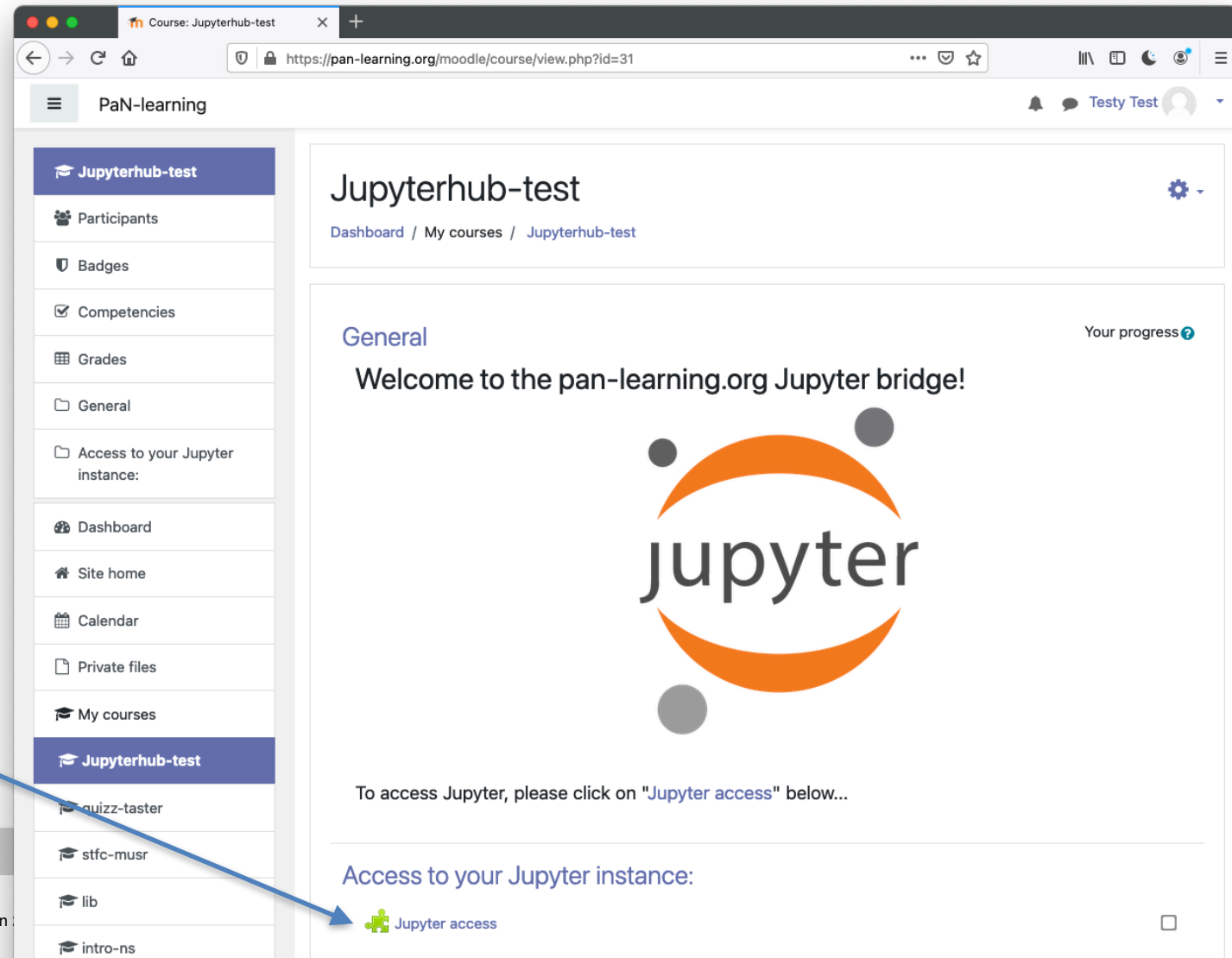
The screenshot shows a web browser window displaying a Moodle course page. The browser's address bar shows the URL <https://pan-learning.org/moodle/course/view.php?id=31>. The page title is "Jupyterhub-test". The left sidebar contains a navigation menu with items like "Participants", "Badges", "Competencies", "Grades", "General", "Access to your Jupyter instance:", "Dashboard", "Site home", "Calendar", "Private files", "My courses", "Jupyterhub-test", "quizz-taster", "stfc-musr", "lib", and "intro-ns". The main content area has a heading "Jupyterhub-test" and a sub-heading "General". Below this, it says "Welcome to the pan-learning.org Jupyter bridge!". A large Jupyter logo is centered on the page. Below the logo, it says "To access Jupyter, please click on 'Jupyter access' below...". At the bottom of the page, there is a section titled "Access to your Jupyter instance:" with a link labeled "Jupyter access" and a small square icon to its right.



2. Jupyterhub connectivity

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

Next, access the course and click the link...



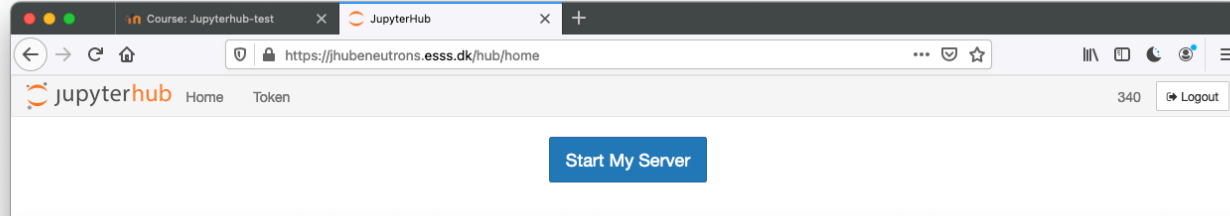
The screenshot shows a web browser window displaying a Moodle course page. The browser's address bar shows the URL <https://pan-learning.org/moodle/course/view.php?id=31>. The page title is "Jupyterhub-test". The left sidebar contains a navigation menu with items like "Participants", "Badges", "Competencies", "Grades", "General", "Access to your Jupyter instance:", "Dashboard", "Site home", "Calendar", "Private files", "My courses", "Jupyterhub-test", "quizz-taster", "stfc-musr", "lib", and "intro-ns". The main content area has a heading "Jupyterhub-test" and a sub-heading "General". Below this, it says "Welcome to the pan-learning.org Jupyter bridge!". A large Jupyter logo is centered on the page. Below the logo, it says "To access Jupyter, please click on 'Jupyter access' below...". At the bottom of the main content area, there is a section titled "Access to your Jupyter instance:" with a link labeled "Jupyter access" and a small square icon to its right.



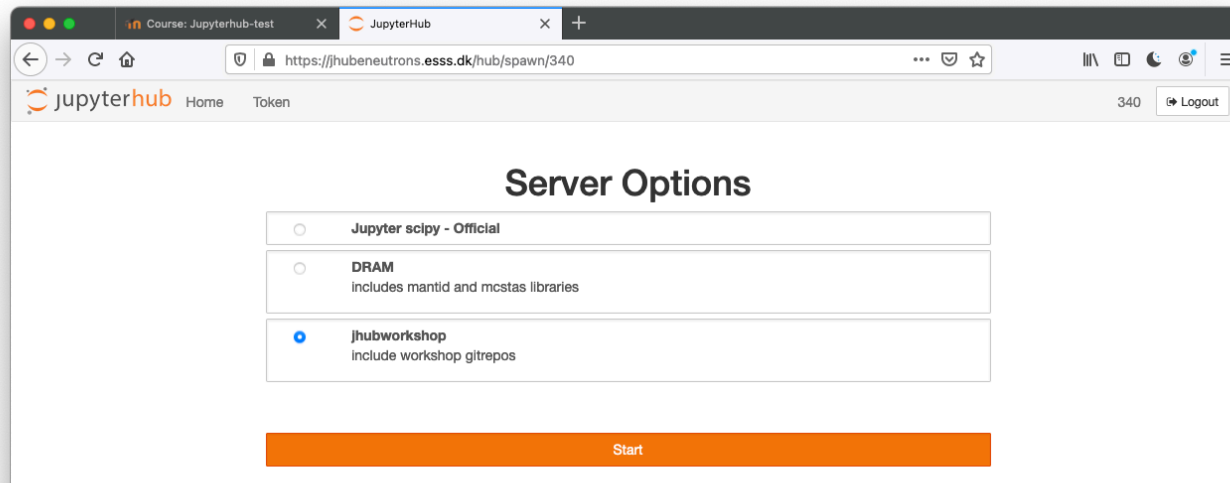
2. Jupyterhub connectivity

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

- start server...

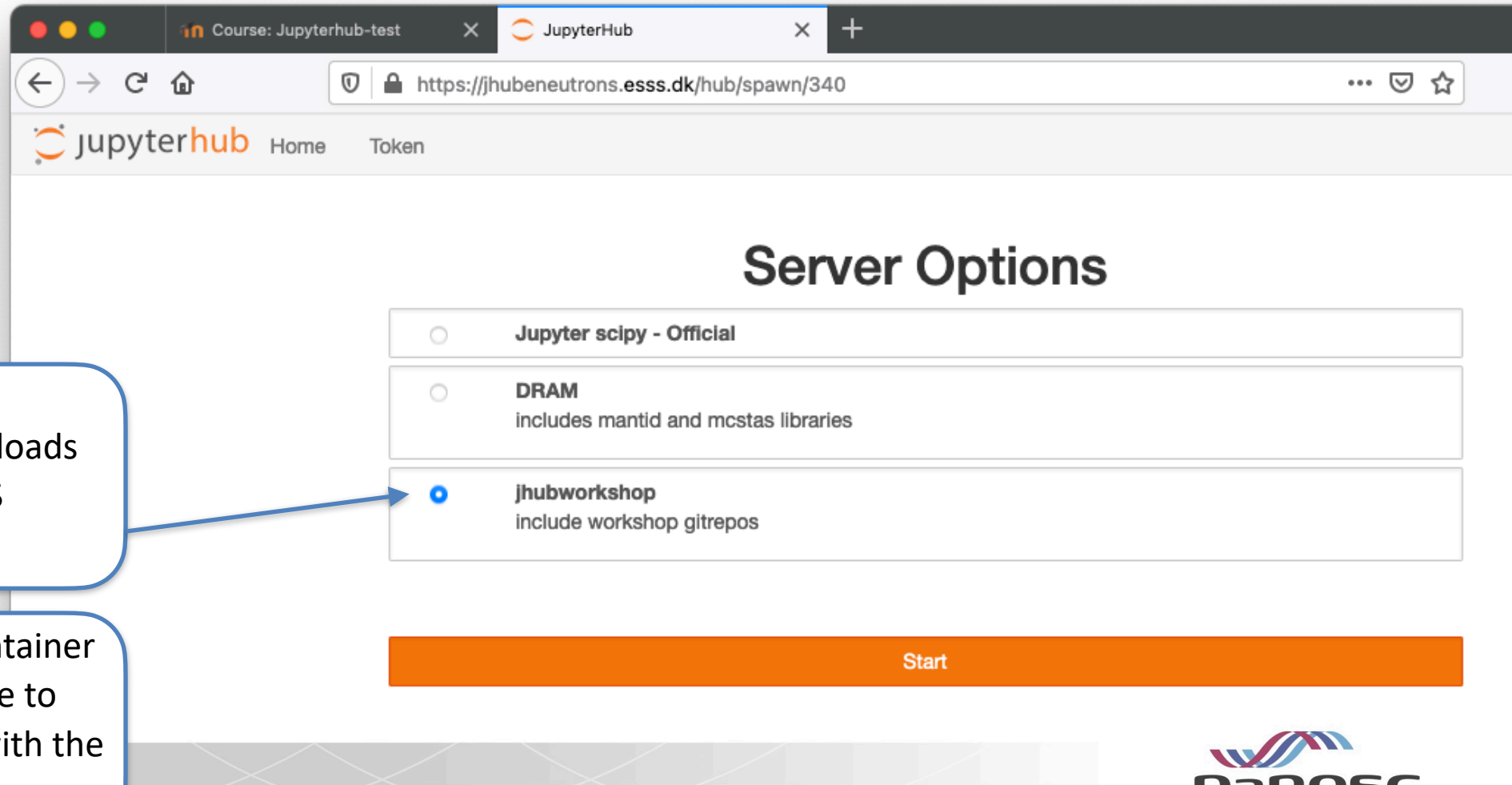


- pick a container...



2. Jupyterhub connectivity

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



The screenshot shows a web browser window with two tabs: 'Course: Jupyterhub-test' and 'JupyterHub'. The address bar displays 'https://jhubeneutrons.esss.dk/hub/spawn/340'. The page header includes the JupyterHub logo, 'Home', and 'Token'. The main content area is titled 'Server Options' and lists three choices:

- Jupyter scipy - Official
- DRAM
includes mantid and mcstas libraries
- jhubworkshop
include workshop gitrepos

Below the options is a large orange 'Start' button.

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.

2. Jupyterhub connectivity

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

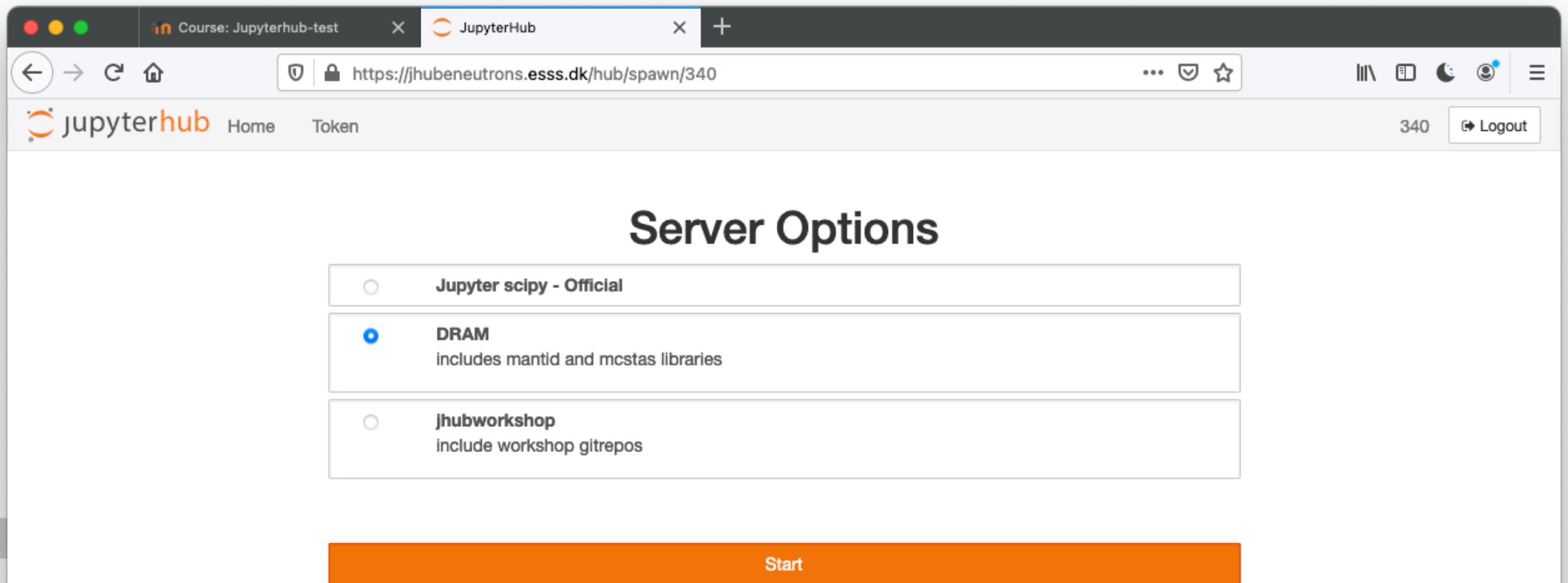
The image shows two overlapping browser windows. The background window displays the JupyterHub 'Server Options' page for a user with token 340. It lists three container options: 'Jupyter scipy - Official', 'DRAM (includes mantid and mcstas libraries)', and 'jhubworkshop (include workshop gitrepos)'. The 'jhubworkshop' option is selected with a blue radio button, and a blue arrow points from it to the right. Below the options is a large orange 'Start' button. The foreground window shows a file browser interface for the user's notebooks, listing folders like '1_jupyter_basics', '2_python_basics', '3_using_external_libraries', '4_molecular_visualization', and '5_extras'.

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.

2. Jupyterhub connectivity

- To access, please self-enrol to the course [Jupyterhub-test](#)
- The DRAM container contains McStasScript (you need to manually add/upload a notebook, e.g. [this one](#))



The screenshot shows a web browser window with two tabs: "Course: Jupyterhub-test" and "JupyterHub". The address bar displays "https://jhubeneutrons.esss.dk/hub/spawn/340". The page header includes the JupyterHub logo, "Home", "Token", and a "Logout" button. The main content area is titled "Server Options" and features three radio button options:

- Jupyter scipy - Official
- DRAM
includes mantid and mcstas libraries
- jhubworkshop
include workshop gitrepos

At the bottom of the options list is a large orange "Start" button.



Thank you

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