ESS Workpackage 5 update

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European Spallation Source

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

Quick introduction

- Mads Bertelsen here!
- Employed at the European Spallation Source
- Part of the McStas development team, neutron ray-tracing software
- Involved mainly in PaNOSC WP5, but also WP8 (e-learning)

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Overview

- My shifting work assignment
- McStasScript still exists!
  - Will combine with ViNYL harmonized interface during this workshop
- Latest news on McStas
- openPMD extension combined with beamphysics
- openPMD needs to be supported in McStas
- pan-learning.com is running, we will soon get requests
- Wish to have server at ESS with latest ViNYL build for demos

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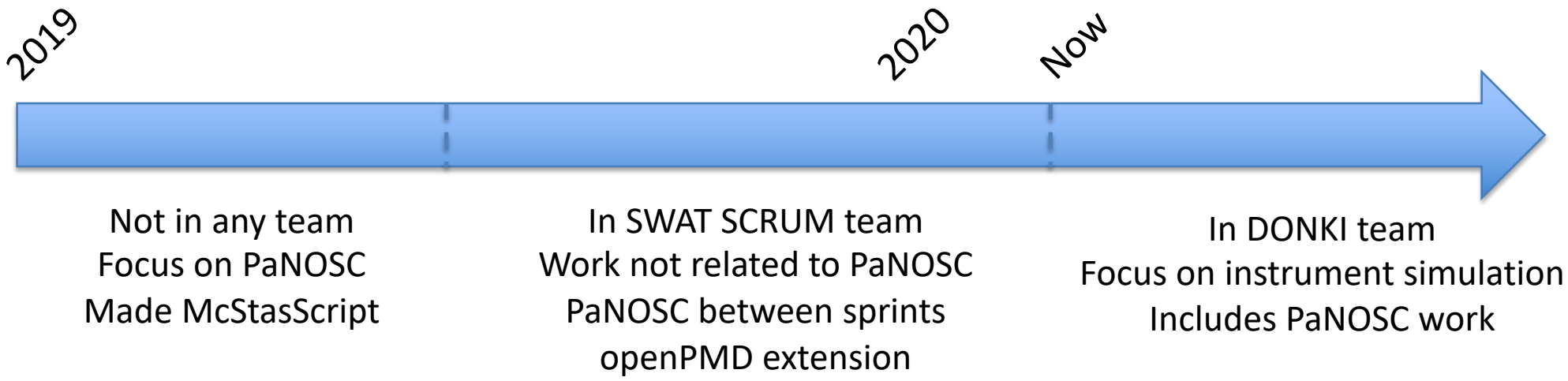
My shifting work assignments

- Had period with less time for PaNOSC
- Counts hours, so no PaNOSC funding used for other tasks
- Was recently reassigned to a team with more focus on simulation and PaNOSC



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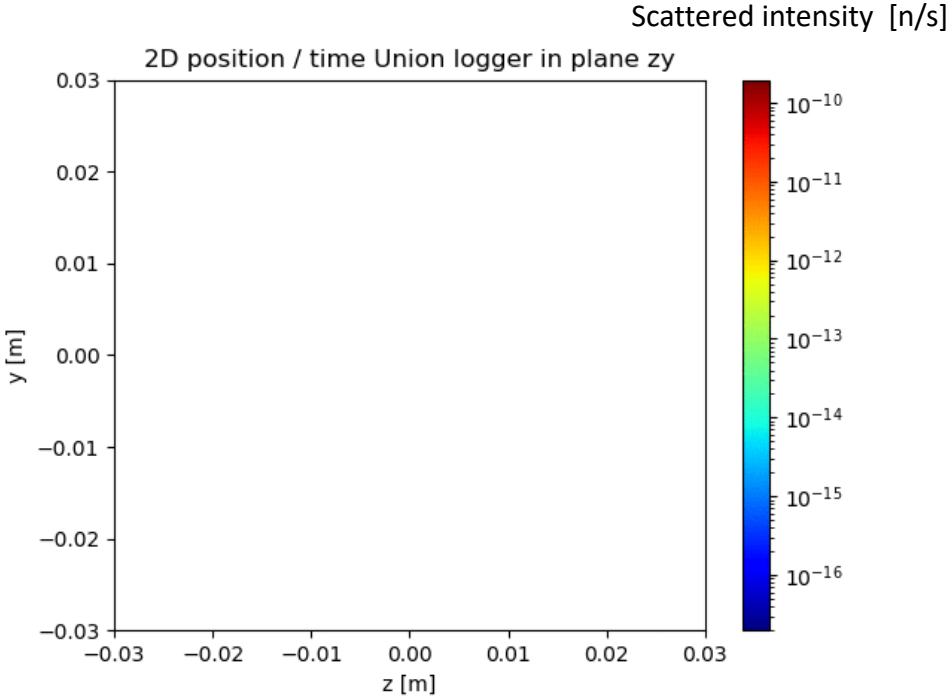
McStasScript status

- **Python API for McStas, installed seperately**
- **Some small updates since November,**
  - Used the software on beamtime, very flexible
  - Travis runs unittests on github commit
  - Started work on interacting with clusters directly
  - Still lacks an internal review
  - Interface is largly compatible with ViNYL
- **Believe it is an appropriate API for our purpose**

Diamond anvil cell



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McStas status

- **McStas 3.0 beta ready (with subset of components)**
  - Move to functions instead of defines
  - Some changes in how components are written, loose backward compatability
  - Faster compile time, better compiler optimization

- **nVidia GPU support beta (with smaller subset of components)**
  - Possible in 3.0 due to new structure
  - openACC used for porting to GPU
  - See wide range of speedups depending on usecase
  - Best case speedup: one GPU using 250 W doing work eqvivalent to ~200 CPU cores

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openPMD situation

- Extension for neutron/photon particle data
- Beamphysics extentsion was appropriate, necessary changes made
- openPMD needs to be implemented in McStas as input/output components

- Currently either ASCII or MCPL is used to transfer/save neutron states
- Interest from ESS in MCPL / openPMD conversion tool

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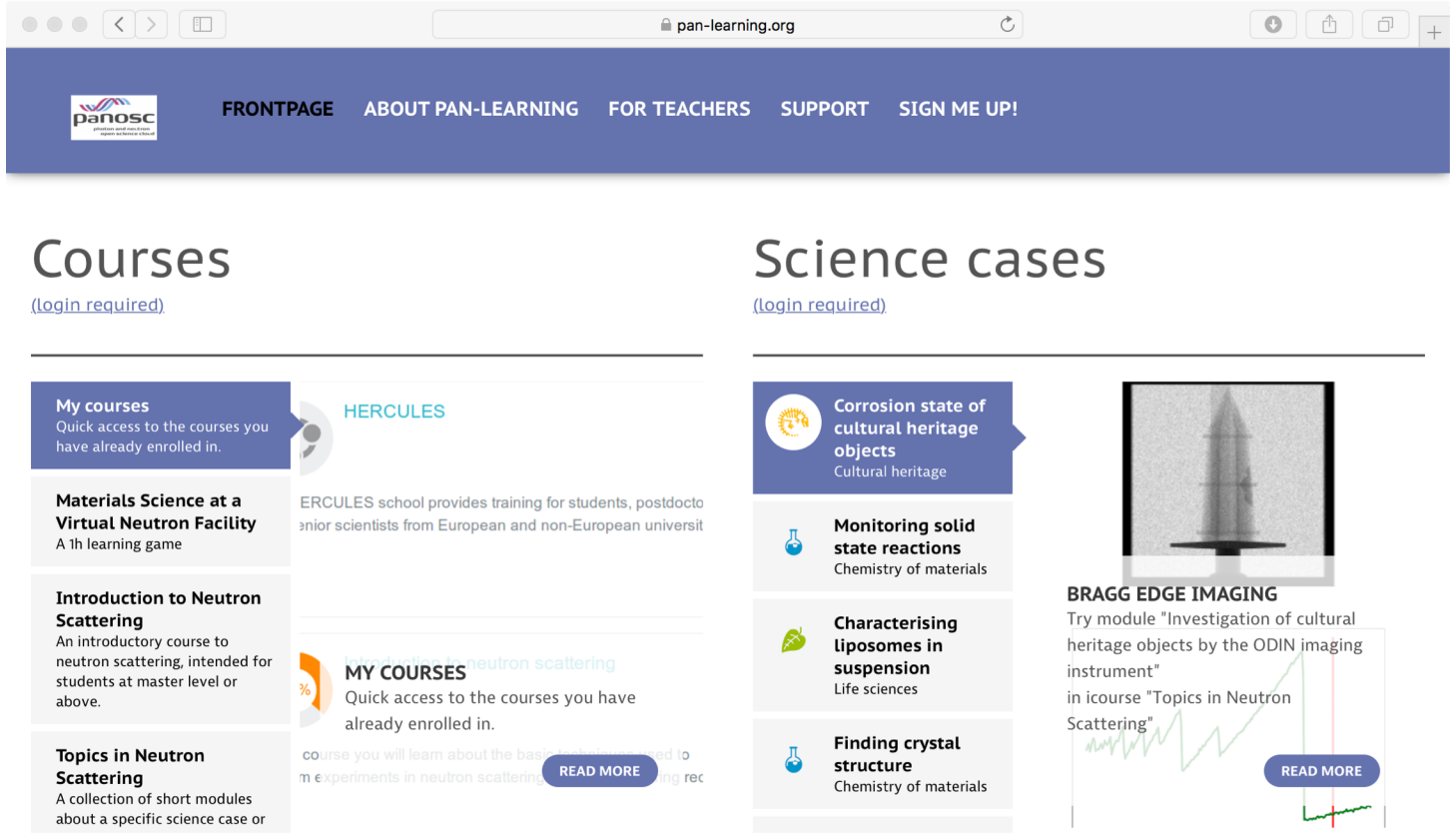
WP8 e-learning

- **Weekly WP5-8 internal meetings**

- **Pan-learning.com**
  - Migration to ESS server almost complete
  - Has simple McStas simulation interface, but parametric
  - Will probably soon request simulation interfaces
  - Will primarily run simulations through jupyter notebooks



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ViNYL wishlist from ESS

- Wish to have server with latest ViNYL software at ESS for demos
- Emphasis on continous integration
- Simple and documented install procedure

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Thanks for your attention

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