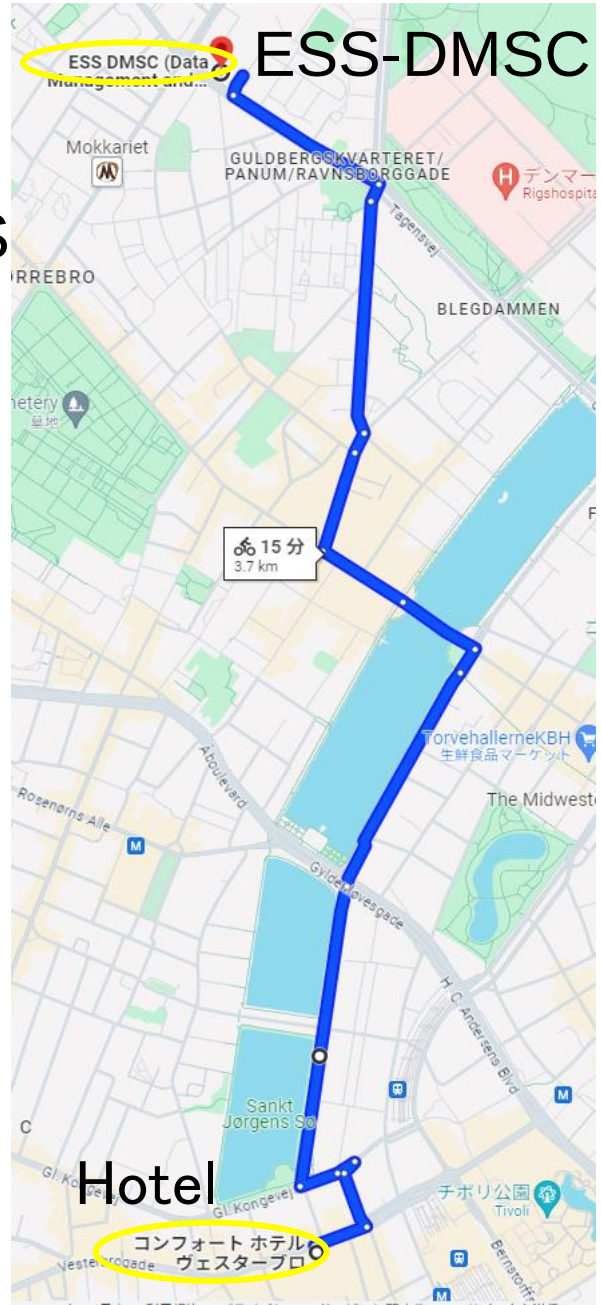
ESS-DMSC(Data Management Software Center)

Midterm (08/10/2023-31) visit report

J-PARC Center, JAEA

Kazuyoshi TATSUMI

Destination：ESS-DMSC



Reached Denmark through Bering Strait and Swiss.

Broad lane for small bike, bicycle,

Data analysis software development in DMSC, lectured by Piotr

✓ Remote data analyses via virtual machines

This service will start at the beginning of the user operation

✓ GUI for easily extracting materials info from data

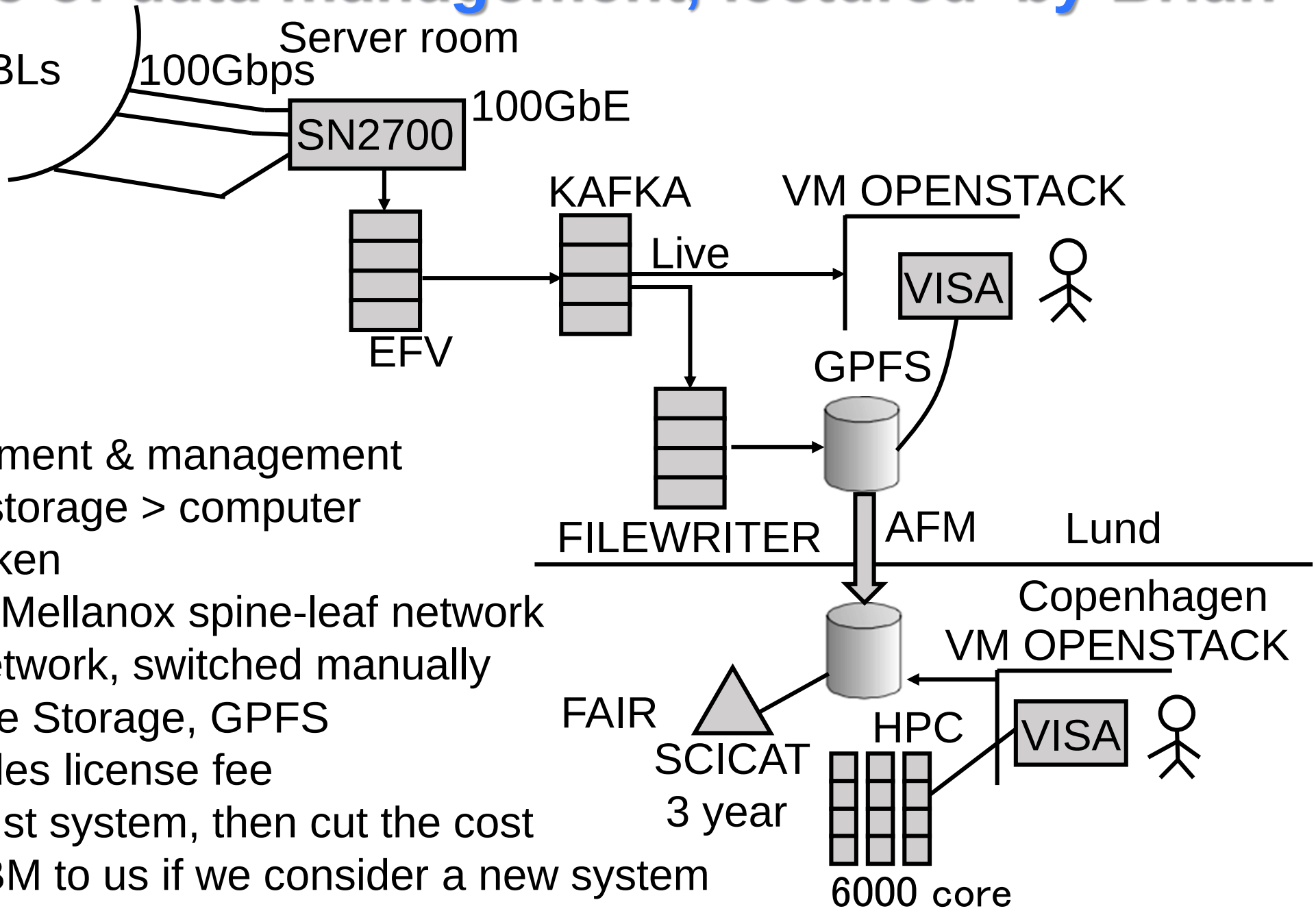
Easyxxxx (xxxx=diffraction, reflectometry)

Analysis engine: open sources from other groups in the world
(I found Bayesian inference in diffraction analysis engine)

✓ VISA (Virtual Infrastructure for Scientific Analysis)

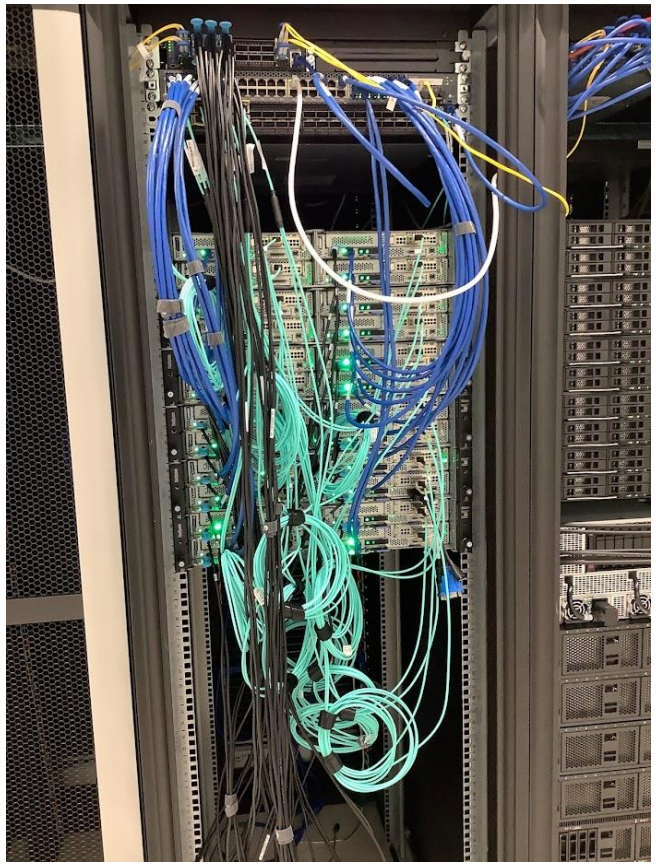
Remote data analysis platform originally developed in ILL
Easyxxxx can be operated on this platform
HPC & VM promote PaNOSC/ExPaNDS to open science

Infrastructure of data management, lectured by Brian



- ✓ 5 staffs for development & management
- ✓ Priority : network > storage > computer
- ✓ Switch is rarely broken
  infini band (nvidia) Mellanox spine-leaf network
- ✓ Redundant Main network, switched manually
- ✓ IBM Spectrum Scale Storage, GPFS
  Product price includes license fee
- ✓ Pay money for robust system, then cut the cost
- ✓ He can introduce IBM to us if we consider a new system

Server room on underground floor in DMSC

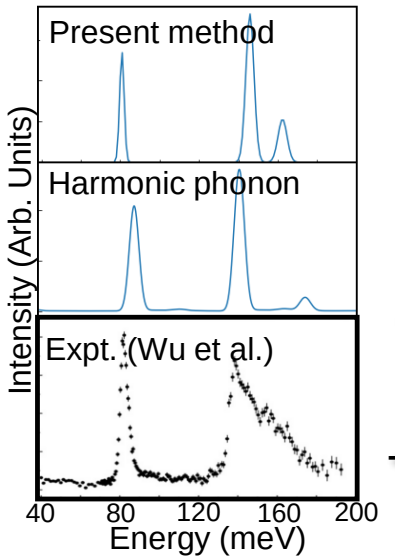


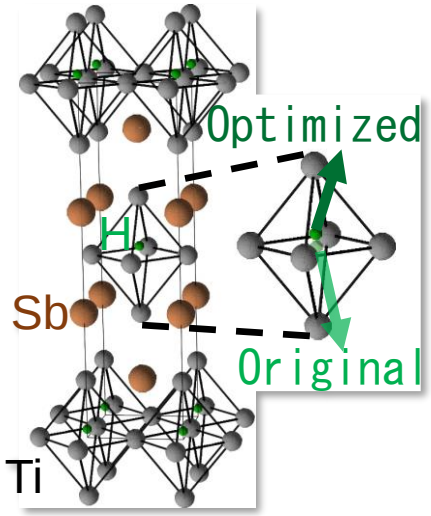
Switches

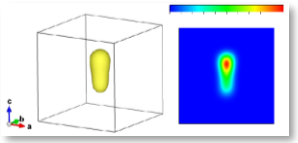
Efficient cooling within racks by
a large scale water cooling system

Research Meeting (I)

- Hydrogen INS calculation







Greg & Piotr

- How much is the shift of H position?
- Is the peak intensities in the high energy side due to dispersion?
- How were the defect model constructed?
- Future experimental intensity map in ***q*** space

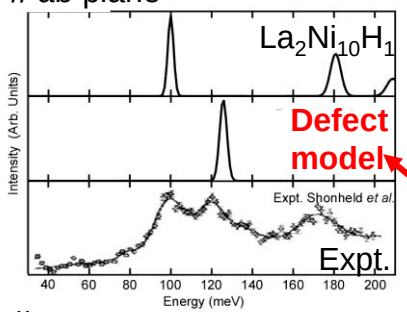
  Possible BLs:

  SNS(ARCS, SEQUOIA)

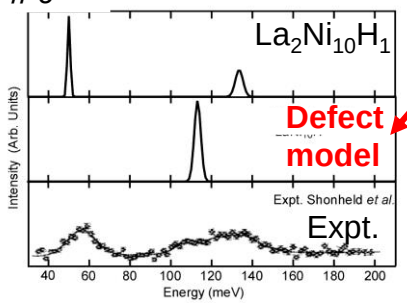
  ISIS(MAPS, MERLIN)

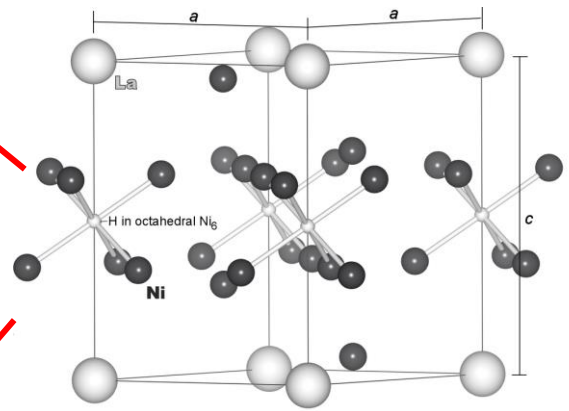
  (ESS(T-REX))

q // *ab* plane



q // *c*





J. Phys.: Condensed Matter., accepted.

Research Meeting (II)

- S(q, w) based on MD with machine learning interatomic potentials (on line)


Chalmers TU
J-PARC/ESS

Paul, Eric
Tatsumi, PD / Piotr

Dynasor developpers

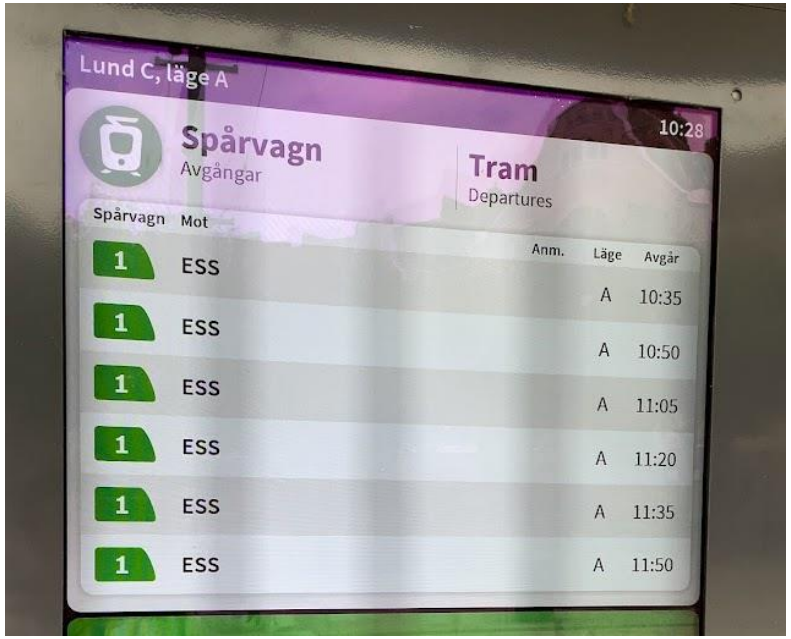
MD atom trajectories→S(q,w) calculation code

Check computational conditions for accurate S(q,w)

They also develop NN-ML potentials
Active Training can be done by their code

On our road map in computational science,
we extend our ability to calculate accurate theoretical S(q,w) of atomic motions.
We will accumulate our experiences on the calculations and collaborate with
Chalmers TU & ESS, in the near future

Seminar in ESS & tour in experimental halls



Seminar

- QENS denoising by KDE

  Poor counts 0 or 1 in high energy region
  →Not use such region for analysis!

- Denoising by supervised learning

  How about large clutters?

Alex Holms

- Bayesian inference determined by priors?

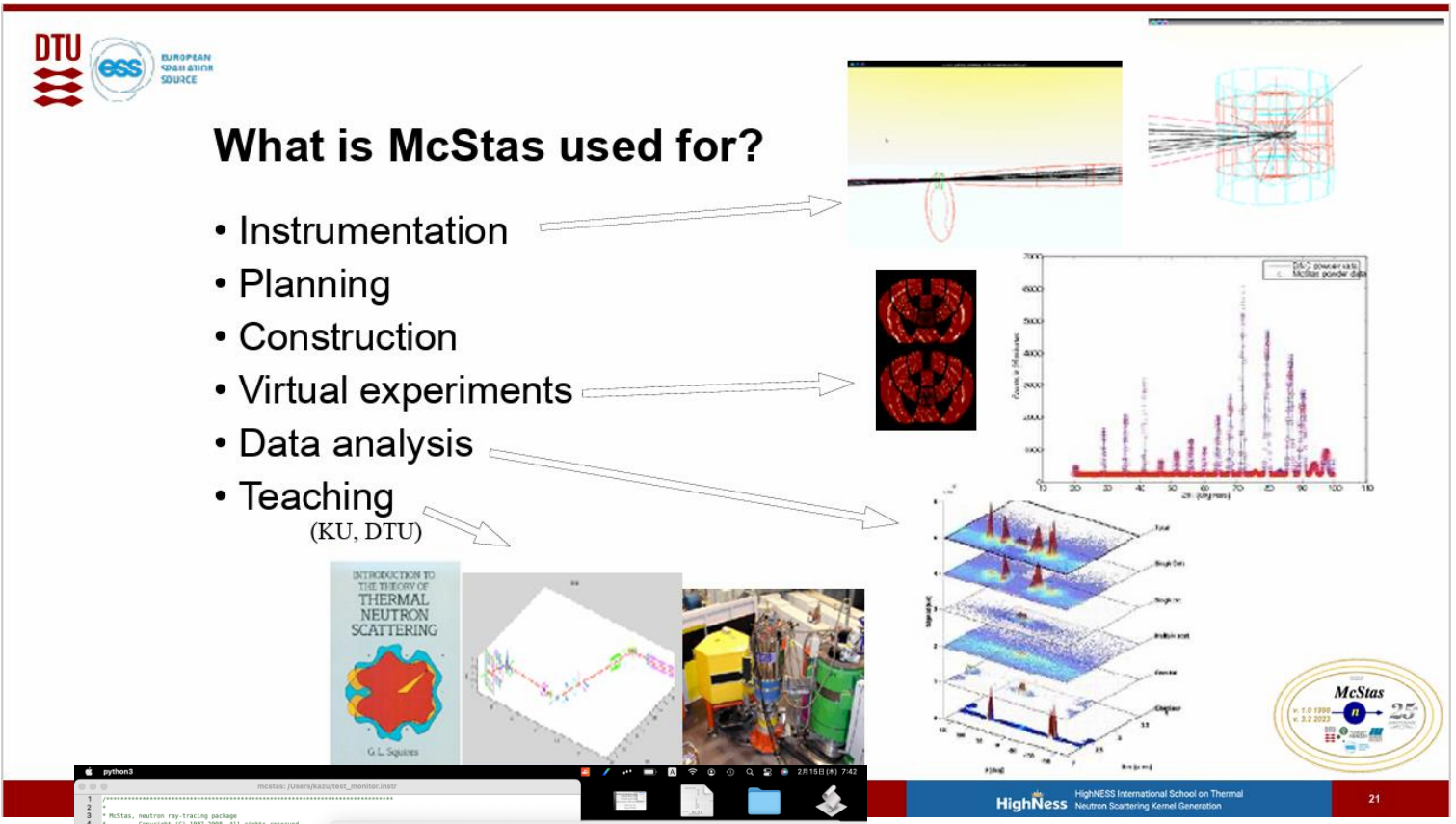
  Published Bayesian inference on SANS as his hobby.

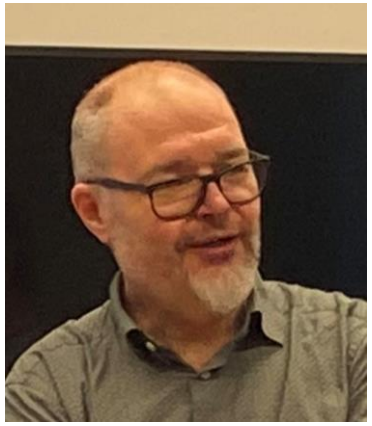
Tour

- Vast several halls, suggesting very accurate TOF spectra
- Covering all sciences by neutrons

Better cafeteria than in DMSC

McStas Lecture & Hands on

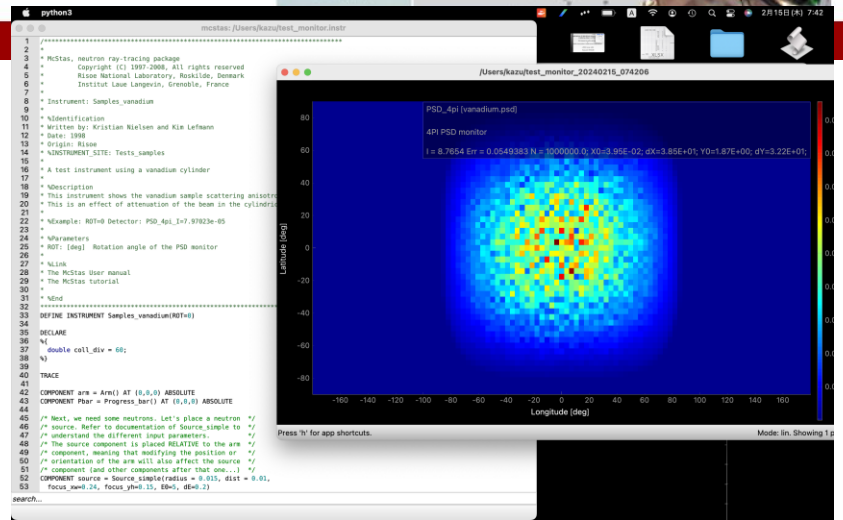




Peter & Mads

I asked them for descriptions on McStas, because I suppose simulated data for machine learning.

Presently, DMSC does not touch to machine learning as their task



- Collaborations in machine learning with university labs
- Easy computations on Mac
- Seems difficult to input accurate BL devices geometries
- Workshop can be served for J-PARC, if needed

Visit results and outlook

- Collaborations on informatics and computation science with ESS-DMSC may require more time, because presently they do not orient to this field

- Simulated data by McStas for machine learning can appear in near future by fast computation with GPU

- I obtained a connection with experts for data storing system
- I obtained an indirect connection with the Chalmers TU group
- Hydrogen INS calculation study was published after this visit

Additional things

Bag in supermarket Irma
Popular in Japan
But Irma stores were gradually closed
I could not find it.

Railroad “anonymous” card
I can give it someone

Peter gave me an umbrella
& sweets of Irma

Too much salty snacks were a result of my misunderstanding the content.