News and recent developments from the McStas team

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GREGORY S. TUCKER, ESS DMSC
THOMAS KITTELMANN, ESS DMSC

Advanced computer simulations methods for neutron scattering instruments 2025

Agenda

- 4-slide McStas intro
- V 3.5.x news:
  - mcstas-pygen
  - Easy access to data interpretation
  - New 3D visualisation
  - Test tools
  - mcstas-antlr
  - Conda-forge packaging / shorter release cycle
  - GPU hackathon in FZJ
  - Enriched NeXus, use in ESS data pipeline work
- Thanks / funding

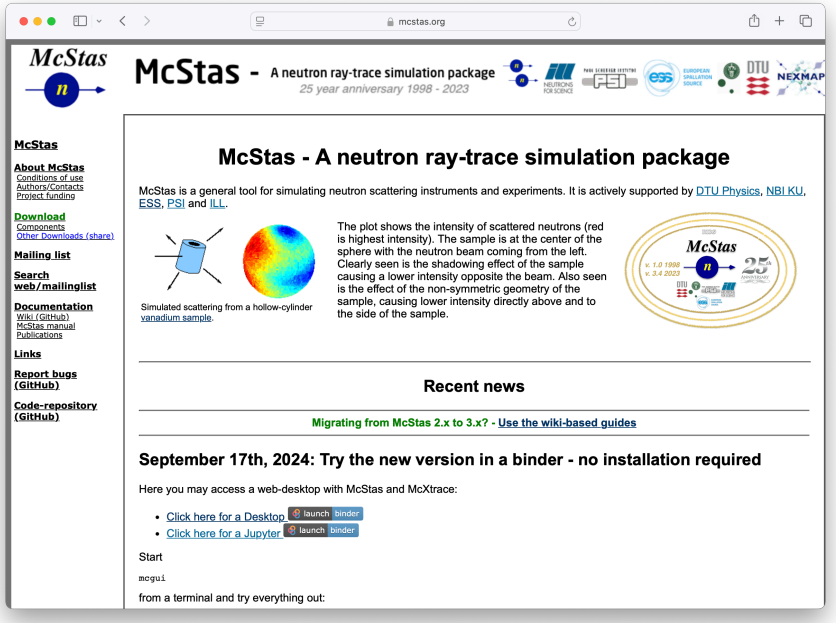
McStas Introduction

- Flexible, general simulation utility for neutron scattering experiments.
- Original design for Monte carlo Simulation of triple axis spectrometers

GNU GPL v3 license

Open Source

- Developed at DTU Physics, ILL, PSI, Uni CPH, ESS DMSC
- V. 1.0 by **K Nielsen** & **K Lefmann** (1998) RISØ
- Currently ~6 people on joint McStas-McXtrace team but only **2 full time**, based at ESS DMSC / DTU

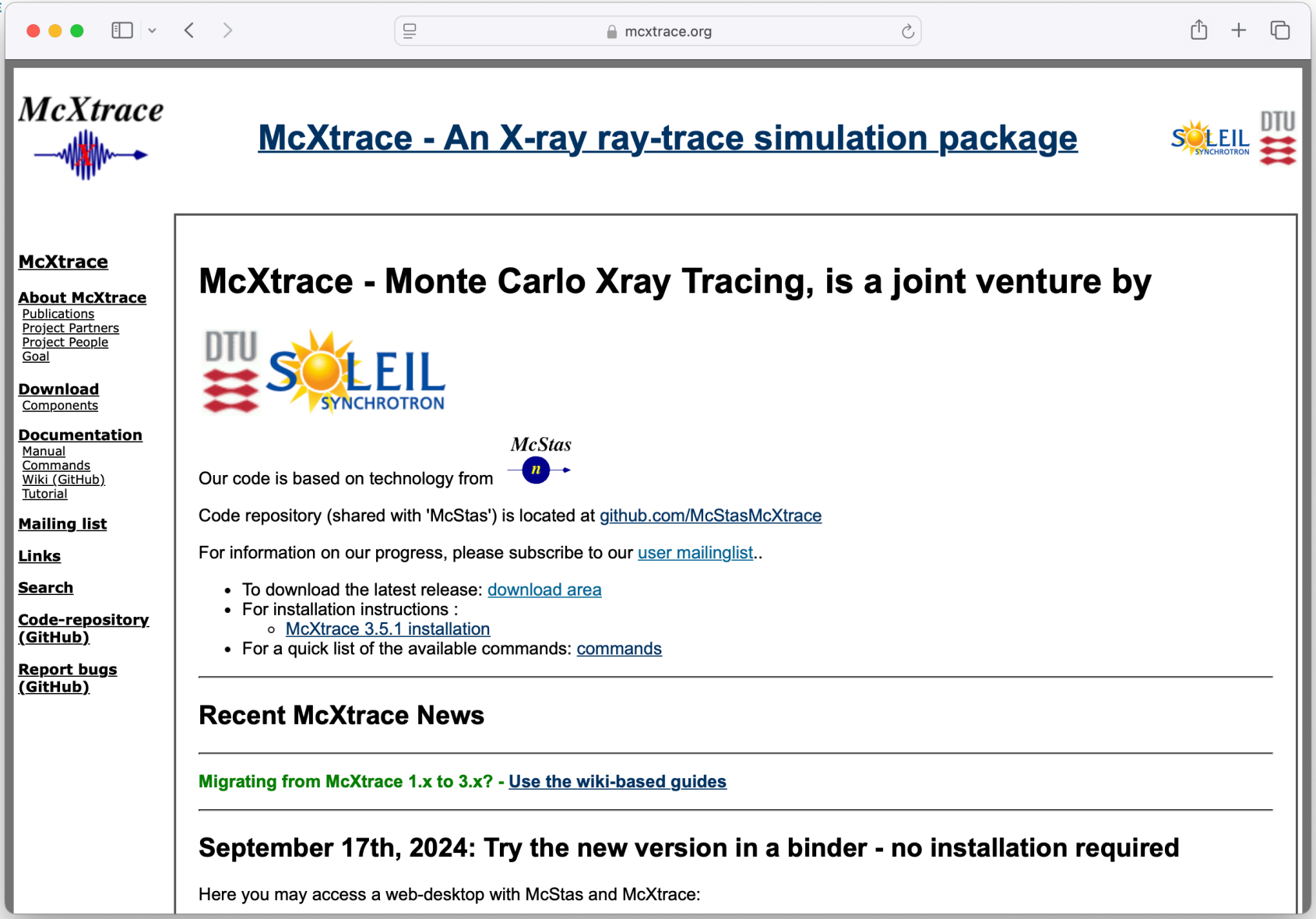


Project website at

http://www.mcstas.org

mcstas-users@mcstas.org mailinglist

McXtrace - since jan 2009 similar for X-rays



mcxtrace-users@mcxtrace.org
mailinglist

Project website at

http://www.mcxtrace.org

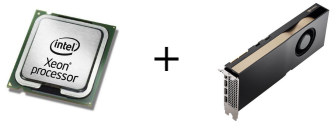
Original consortium

Risø DTU

Funding from NABIIT, DSF and the above parties.

- **Synergy, knowledge transfer, shared infrastructure, repo etc.**

McStas: simulation toolkit for neutron scattering instruments, virtual experiments



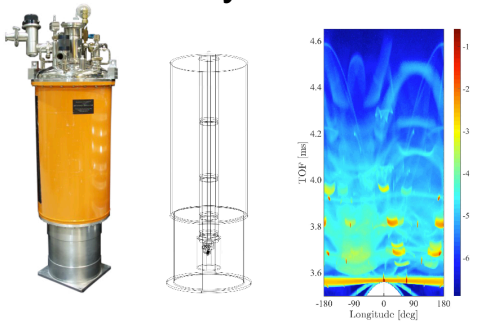
2020: McStas 3.0 with support for MPI and multiple GPUs

McStas + NVIDIA

McStas 3.x acc. on NVIDIA GPUs

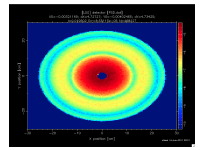
- 2 orders of magnitude speedup. (1x Tesla V100 vs 1 modern Intel Xeon core)

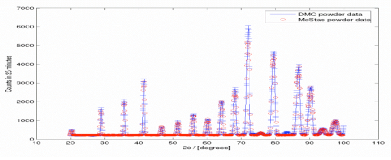
Sample-environments - Union subsystem



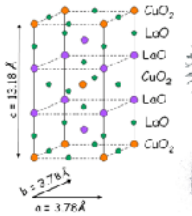
nt at a facility

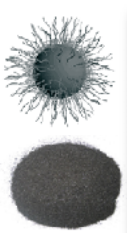
Detectors



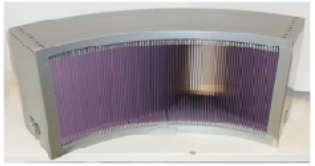


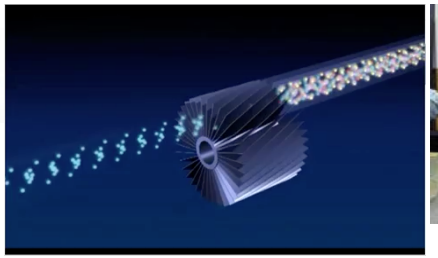
Scientific model-samples

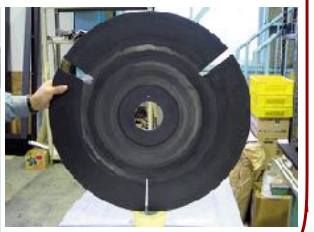




Neutron optics





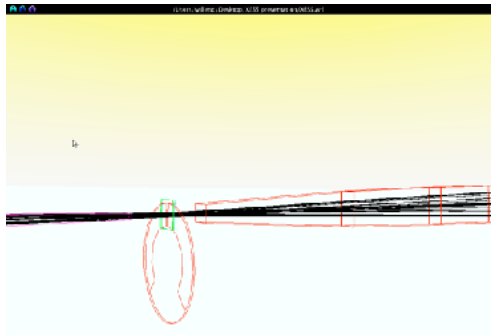


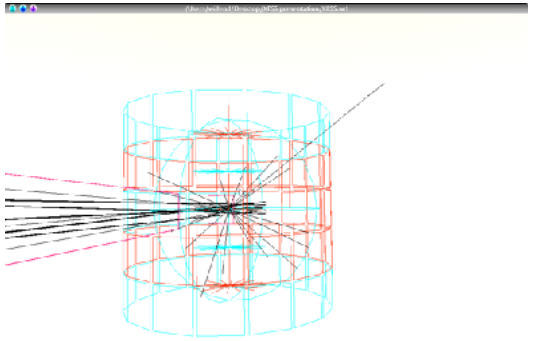
Starts with a source of neutrons, be it a reactor- or spallation source

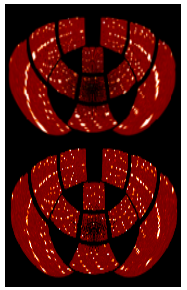
Neutron moderators is where McStas starts

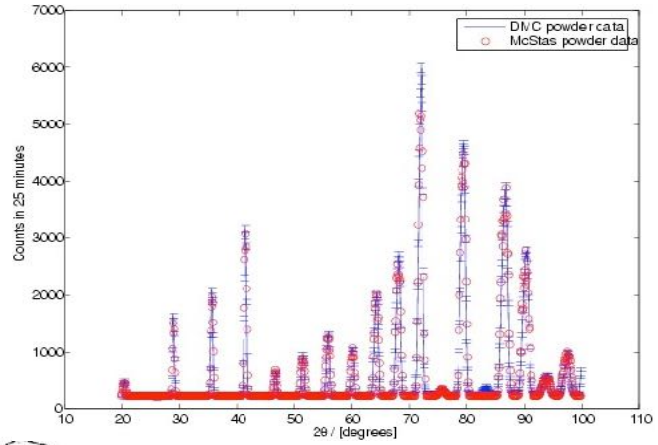
What is McStas used for?

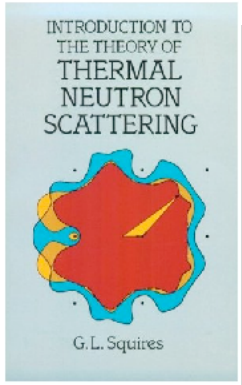
- Instrumentation
- Planning
- Construction
- Virtual experiments
- Data analysis
- Teaching (KU, DTU)

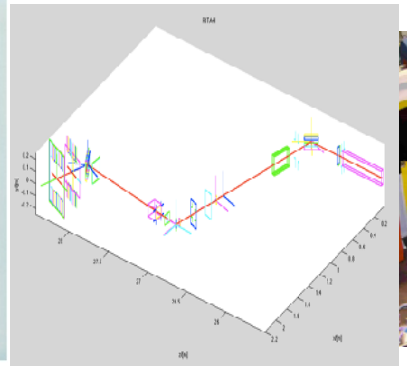


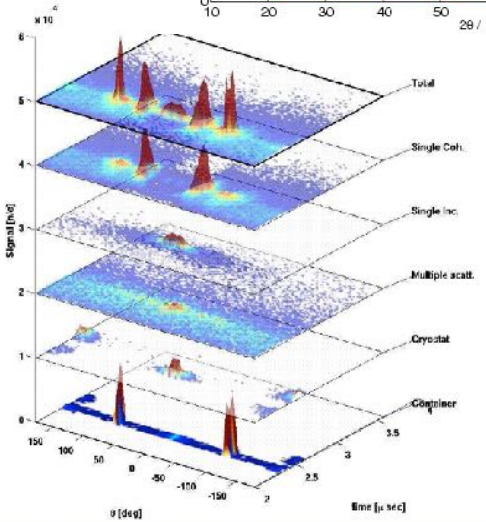






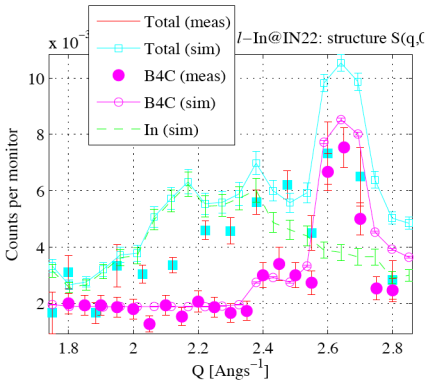




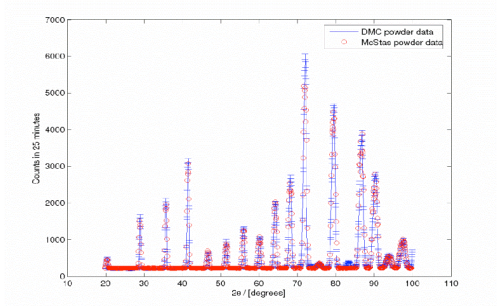


Reliability - cross comparisons

- Much effort has gone into this
- Here: simulations vs. exp. at powder diffract. DMC, PSI
- The bottom line is
- McStas agree very well with other packages (NISP, Vitess, SIMRES, MCViNE)
- Experimental line shapes are within 5%
- Absolute intensities are within 10%
- Common understanding: McStas and similar codes are reliable



E. Farhi, P. Willendrup, from IN22 benchmark exp.



P. Willendrup et al., Physica B, 386, (2006), 1032.

Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment

Volume 1063, June 2024, 169291

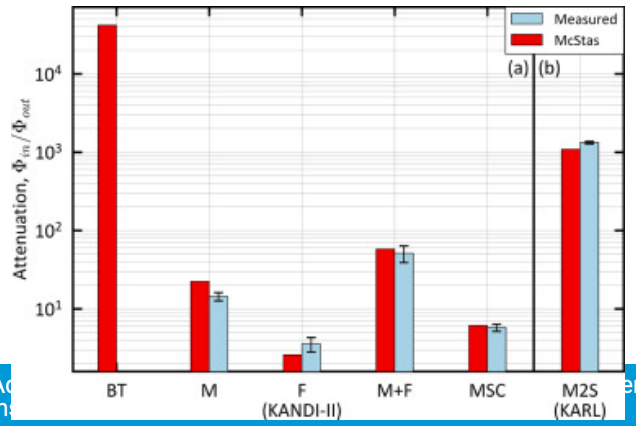
Full Length Article

Verification of the McStas code using two double axis neutron diffractometers

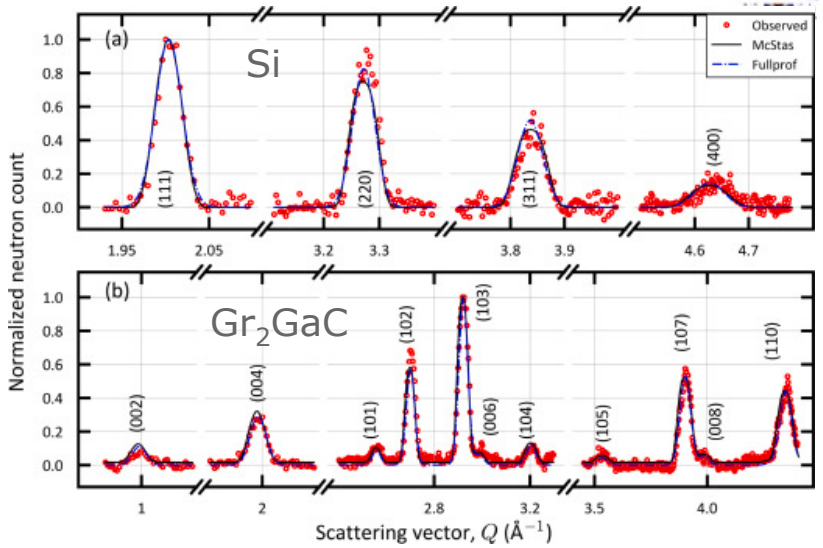
D. Potashnikov [a], A. Pesach [a], O. Rivin [a], O. Ozeri [b], Z. Yungrais [c], M. Bertelsen [d], E.N. Caspi [a]

https://doi.org/10.1016/j.nima.2024.169291

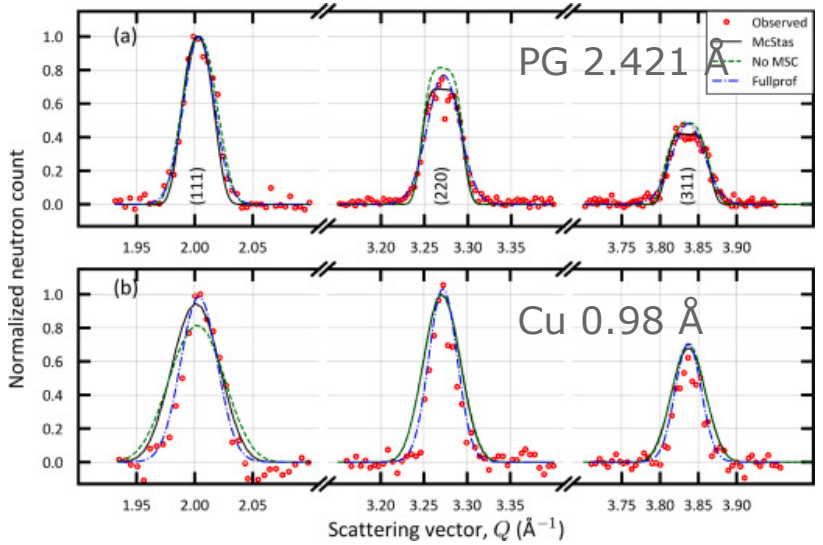
Gold foil intensity measurements



KANDI-II 2.47 Å



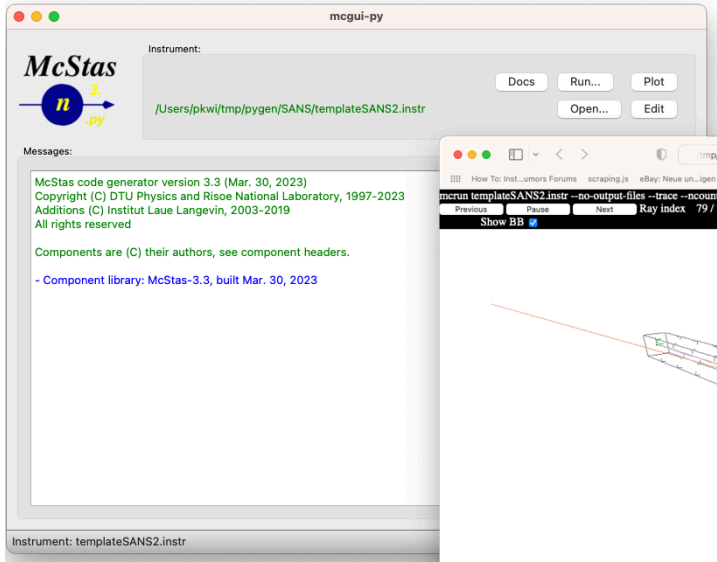
KARL Si sample

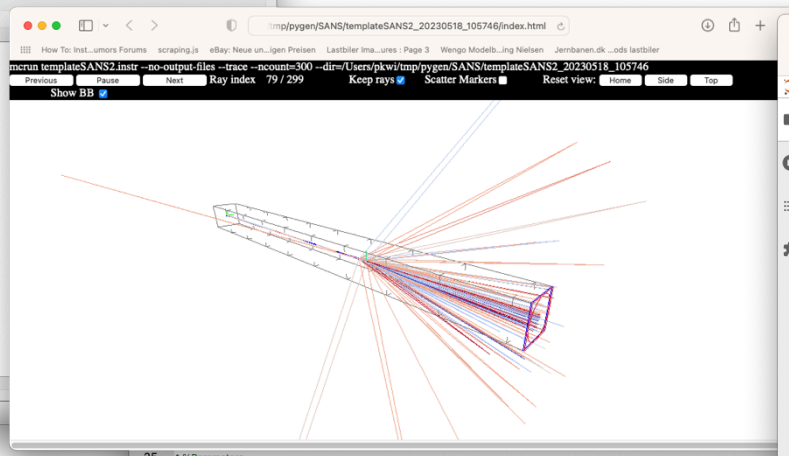


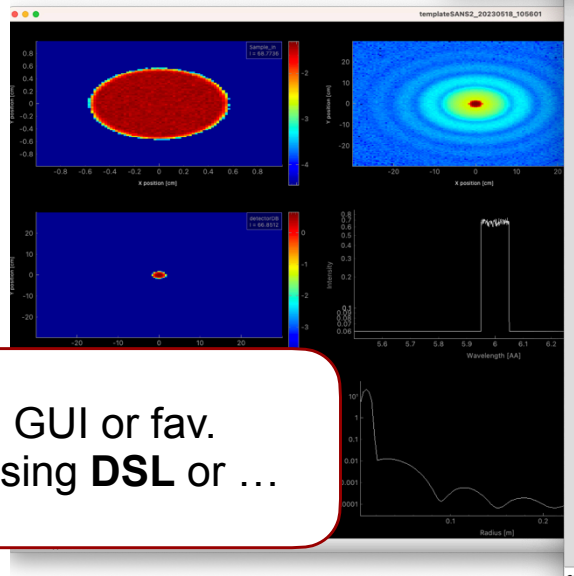
McStas: simulation toolkit for neutron scattering instruments, V.E.

… in .py / Jupyter notebooks using McStasscript

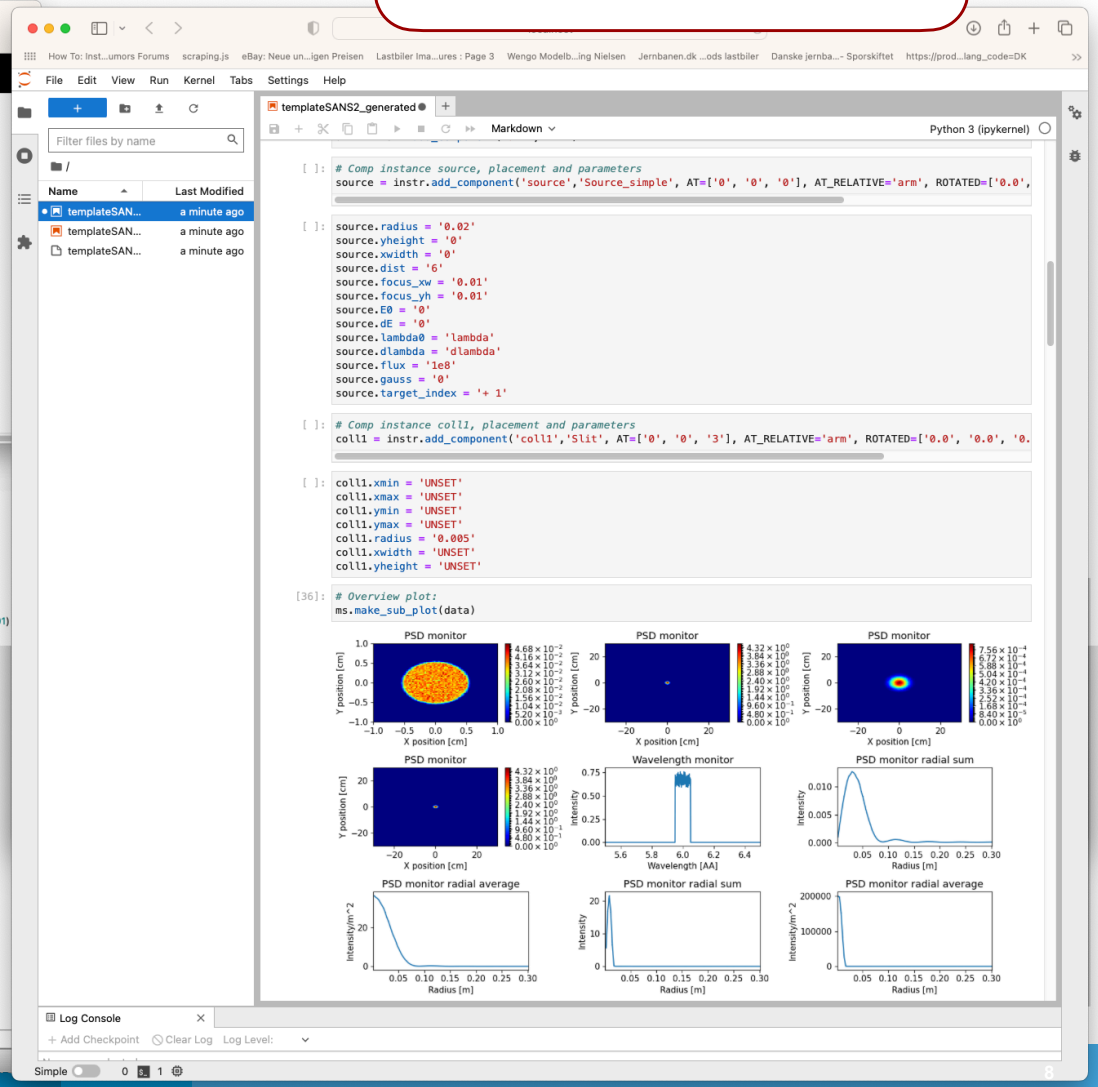
Work in GUI or fav. editor using **DSL** or …





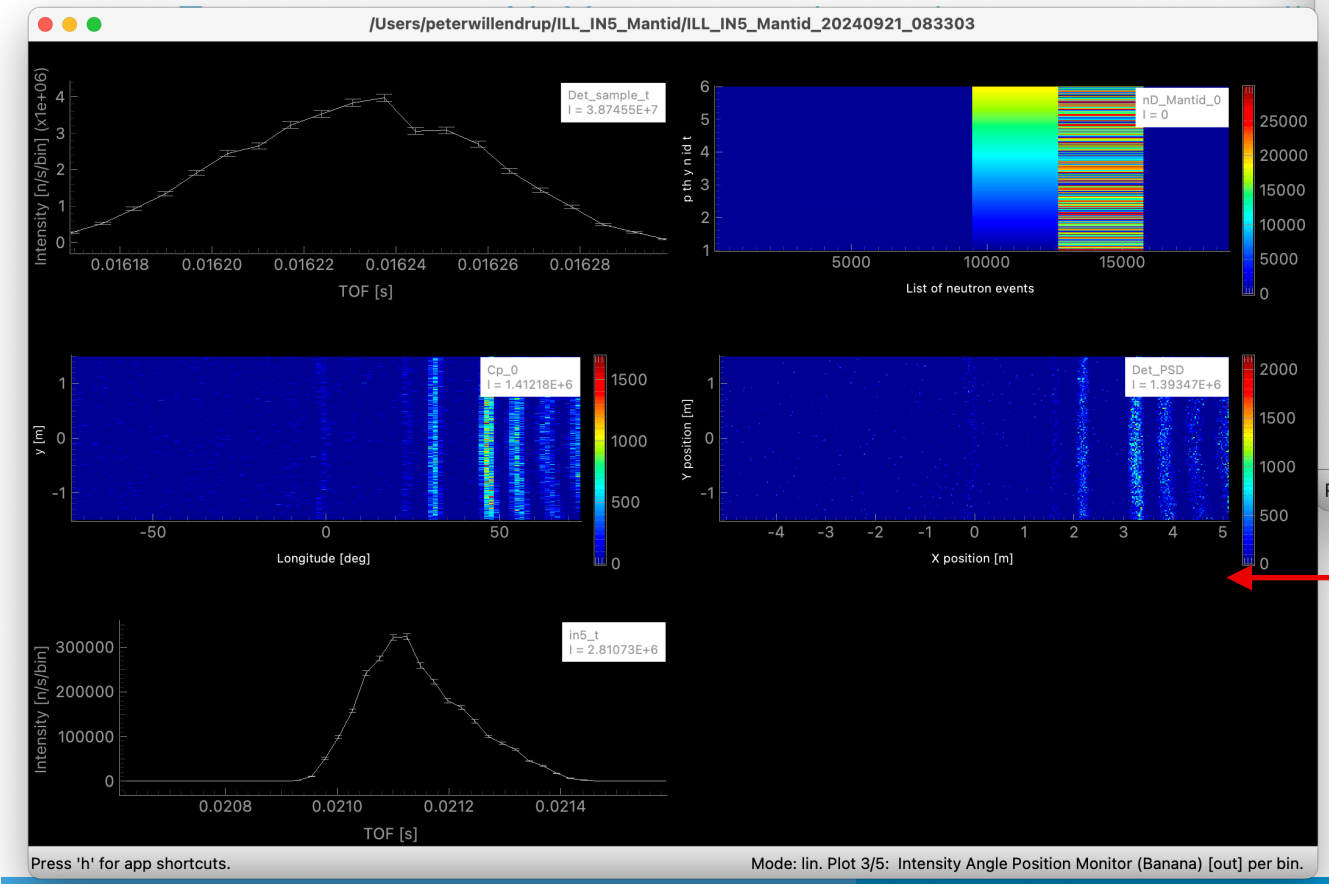


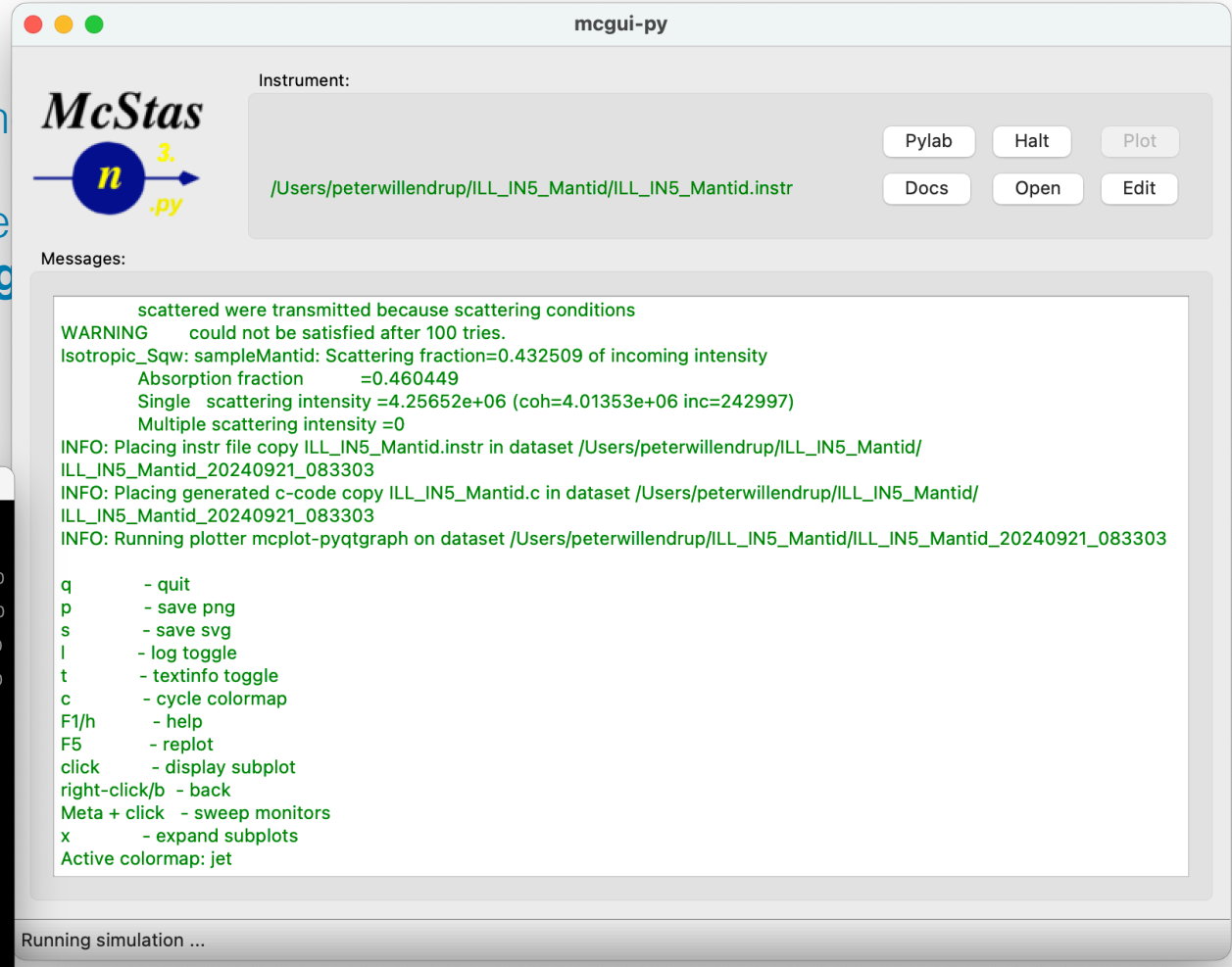
```
* %Parameters
* lambda:      [AA]  Mean wavelength of neutrons
* dlambda:     [AA]  Wavelength spread of neutrons
* r:           [AA]  Radius of scattering hard spheres
* PHI:         [1]   Particle volume fraction
* Delta_Rho: [cm^-2]  Scattering length density
* frac_dir:    [1]   Fraction of statistics for direct beam
* frac_inc:    [1]   Fraction of statistics for incoherent scattering in scattered beam
*
* %Link
*
* %End
*******************************************************************************/
DEFINE INSTRUMENT templateSANS2(lambda=6, dlambda=0.05, r=150, PHI=1e-3, Delta_Rho=6e10, frac_dir=0.03, frac_inc=0.01)

USERVARS %{
  int was_scattered;
%}

TRACE

COMPONENT a1 = Progress_bar()
  AT (0,0,0) ABSOLUTE

COMPONENT arm = Arm()
  AT (0, 0, 0) ABSOLUTE

COMPONENT source = Source_simple(
    radius = 0.02, dist = 6, focus_xw = 0.01, focus_yh = 0.01,
    lambda0 = lambda, dlambda = dlambda, flux = 1e8)
  AT (0, 0, 0) RELATIVE arm

COMPONENT coll1 = Slit(
    radius = 0.005)
  AT (0, 0, 3) RELATIVE arm

COMPONENT coll2 = Slit(
    radius = 0.005)
  AT (0, 0, 6) RELATIVE arm

COMPONENT sample_position = Arm()
AT (0,0,0.2) RELATIVE coll2

COMPONENT Sample_in = PSD_monitor(xwidth=0.02,yheight=0.02, filename="SamplePos",restore_neutron=1)
  AT(0,0,0) RELATIVE PREVIOUS
search...
```



New stuff in series 3.5.x

- Common release and versioning for McStas & McXtrace - n
- **We are now on conda-forge!**
  - Forms support basis for Windows, macOS and non-De
- **Lots of work from SOLEIL toward official Debian packag**
- **CI (GitHub + conda) in place**
- Usability:
  - One-click transfer to McStasScript/Jupyter





Classic McStas/McXtrace data rep. via ‘mcplot’

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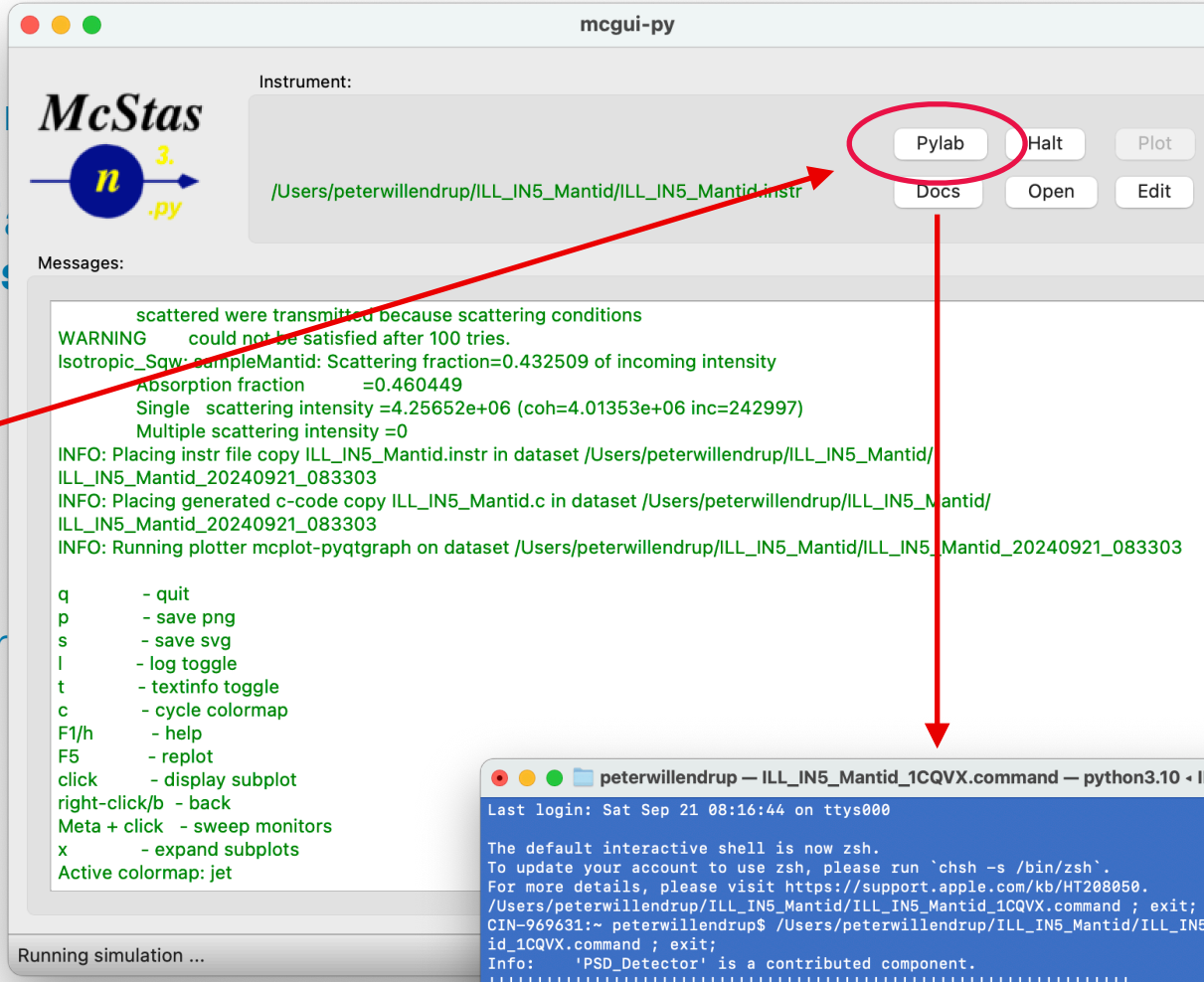
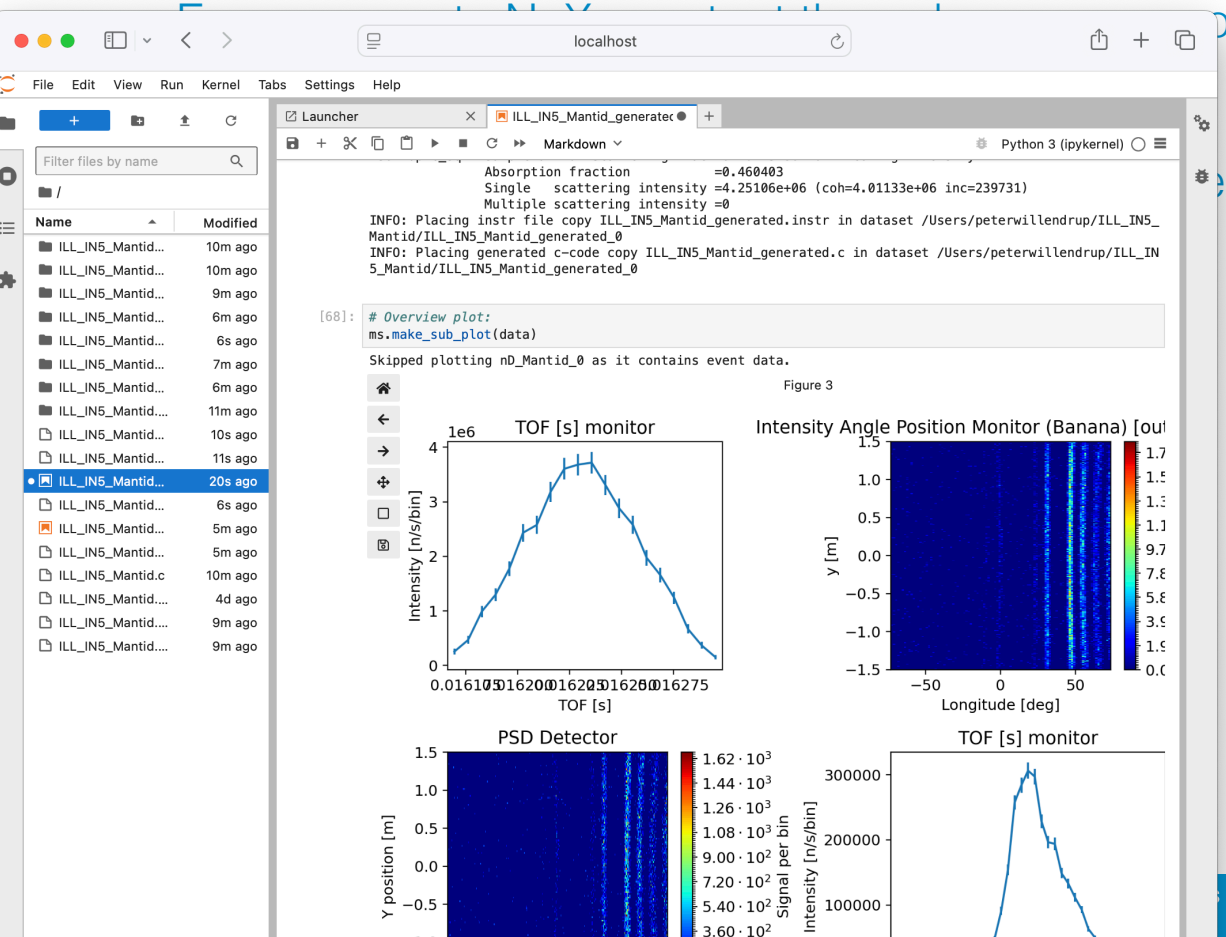
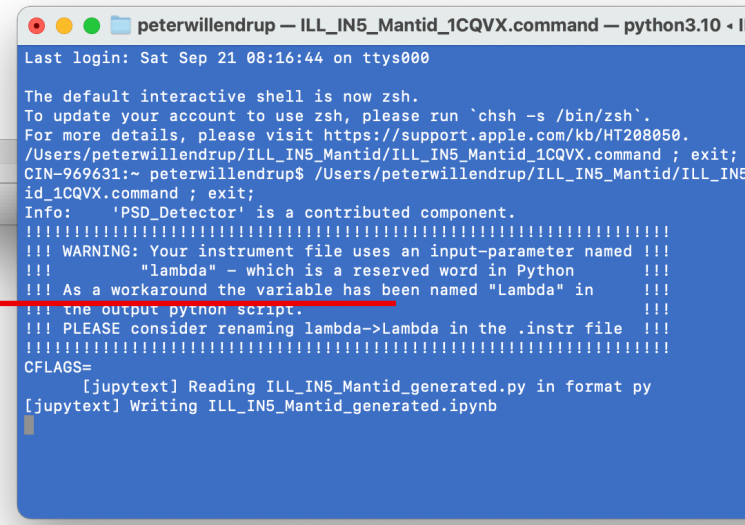
or silx

ed later







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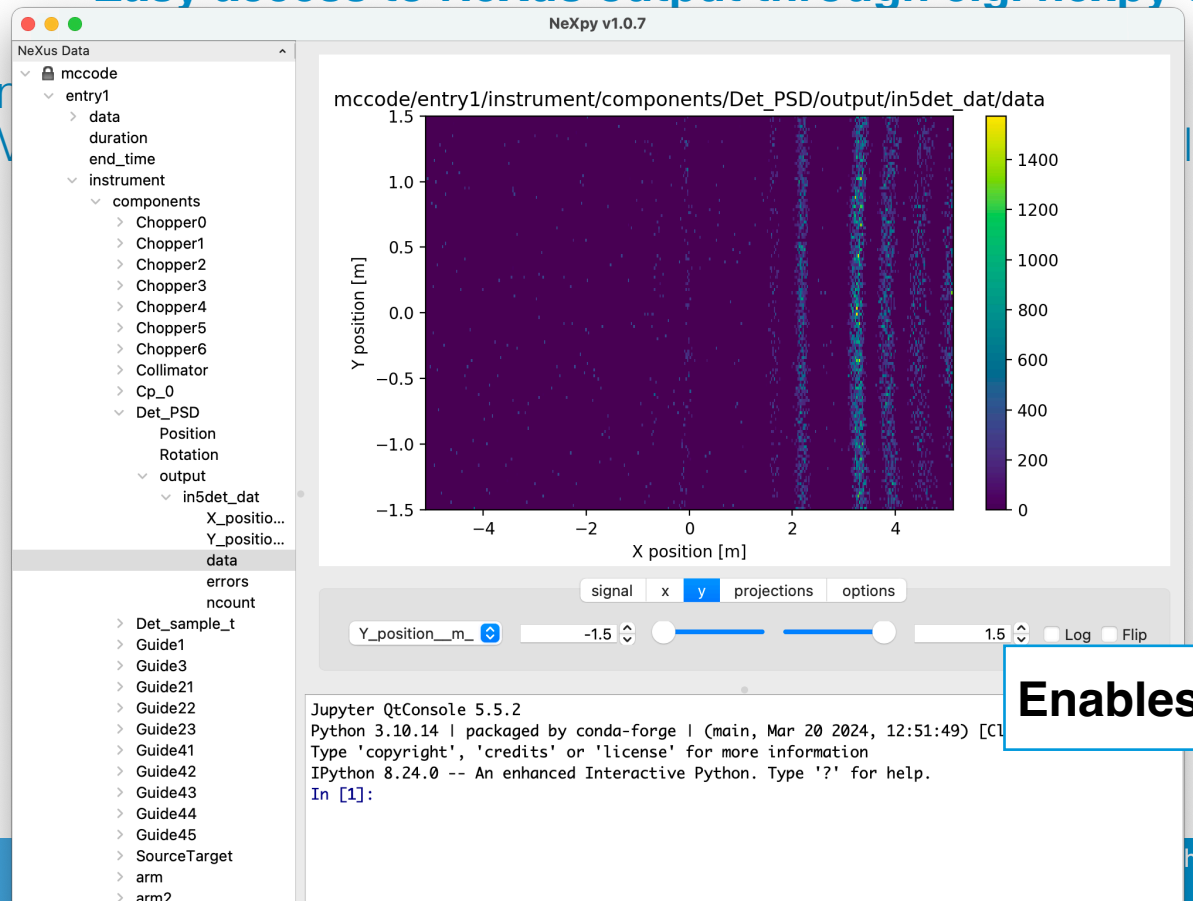
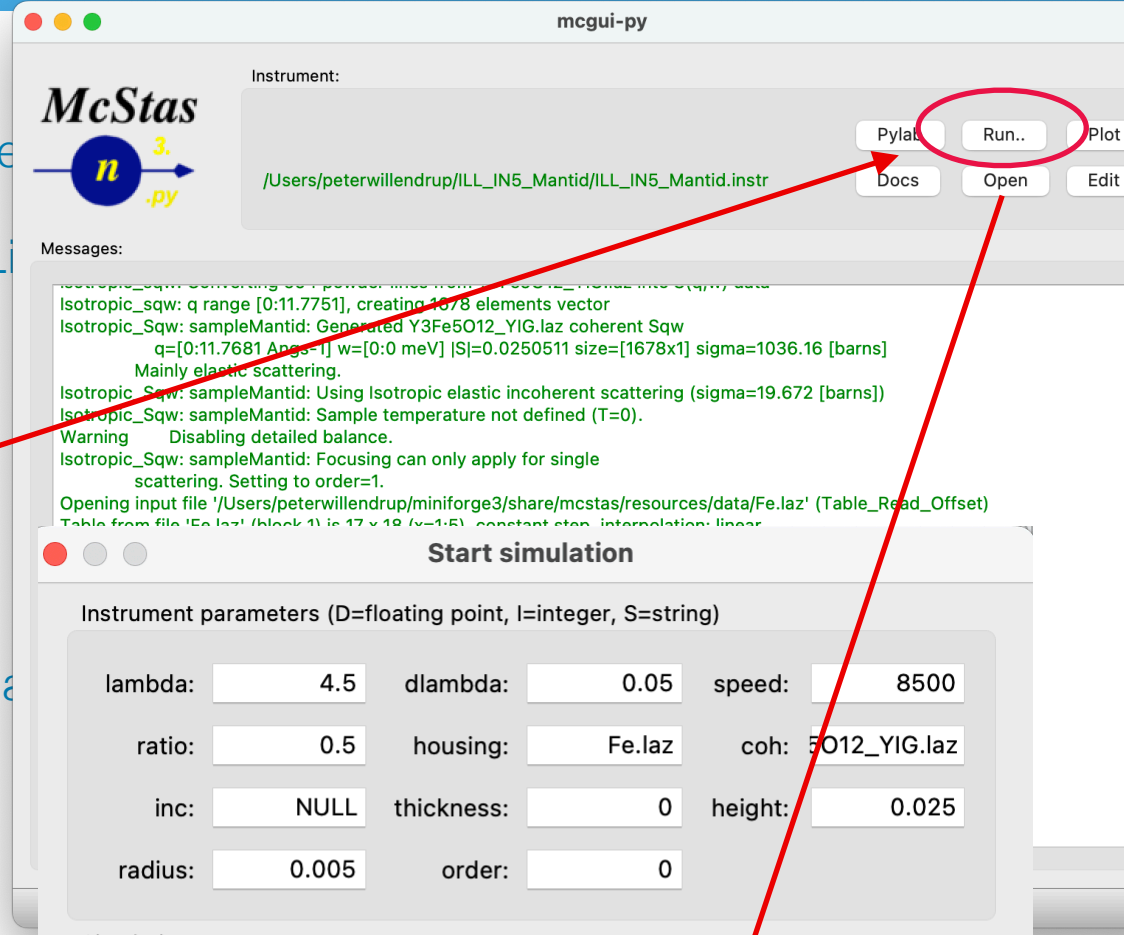
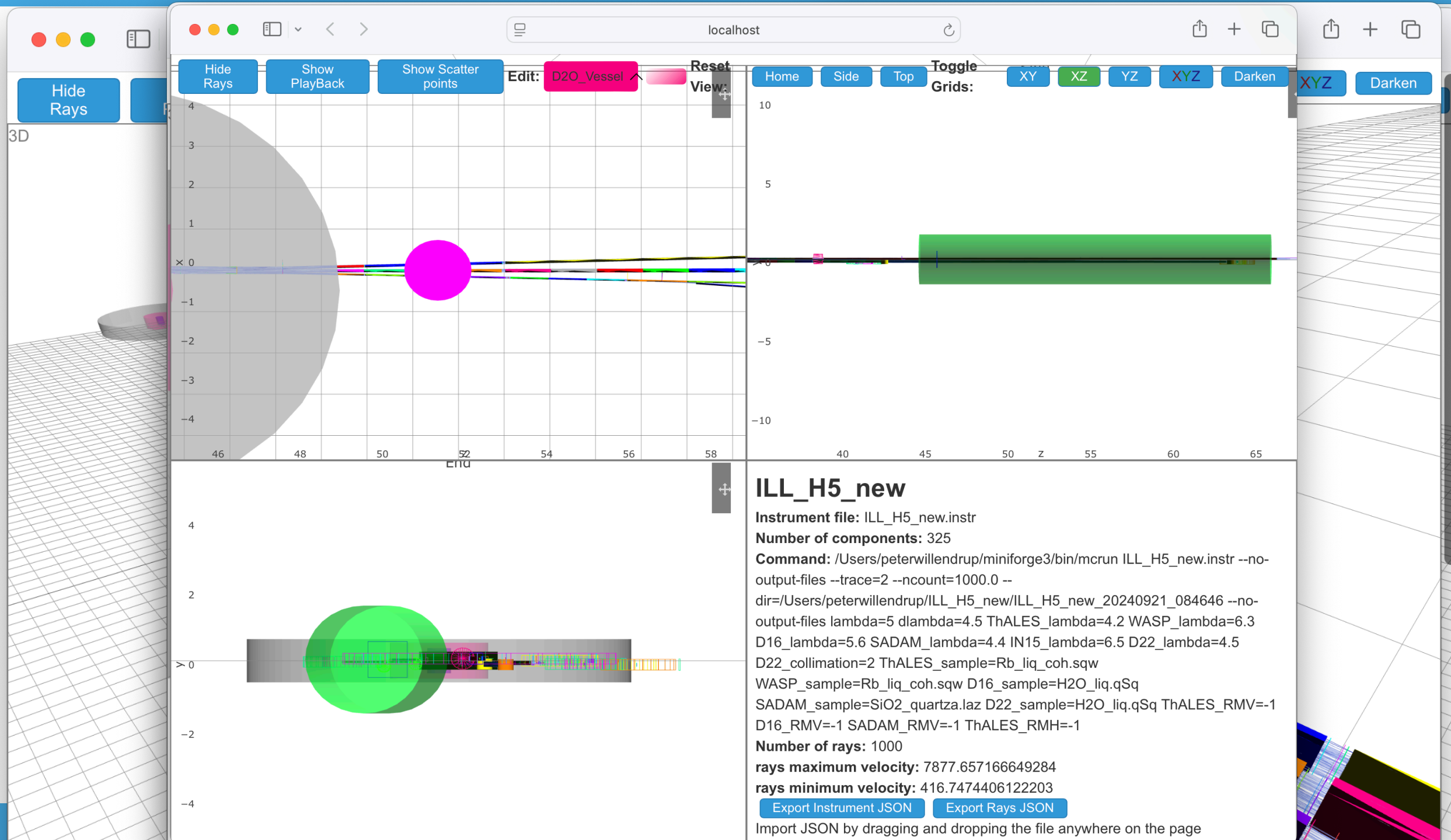
- V later toda





Enables easy access to fitting etc.


localhost
Hide Rays
Show PlayBack
Show Scatter points
Edit:
D2O_Vessel
Reset View:
Home
Side
Top
Toggle Grids:
XY
XZ
YZ
XYZ
Darken
End
ILL_H5_new
Instrument file: ILL_H5_new.instr
Number of components: 325
Command: /Users/peterwillendrup/miniforge3/bin/mcrun ILL_H5_new.instr --no-output-files --trace=2 --ncount=1000.0 --dir=/Users/peterwillendrup/ILL_H5_new/ILL_H5_new_20240921_084646 --no-output-files lambda=5 dlambda=4.5 ThALES_lambda=4.2 WASP_lambda=6.3 D16_lambda=5.6 SADAM_lambda=4.4 IN15_lambda=6.5 D22_lambda=4.5 D22_collimation=2 ThALES_sample=Rb_liq_coh.sqw WASP_sample=Rb_liq_coh.sqw D16_sample=H2O_liq.qSq SADAM_sample=SiO2_quartza.laz D22_sample=H2O_liq.qSq ThALES_RMV=-1 D16_RMV=-1 SADAM_RMV=-1 ThALES_RMH=-1
Number of rays: 1000
rays maximum velocity: 7877.657166649284
rays minimum velocity: 416.7474406122203
Export Instrument JSON
Export Rays JSON
Import JSON by dragging and dropping the file anywhere on the page

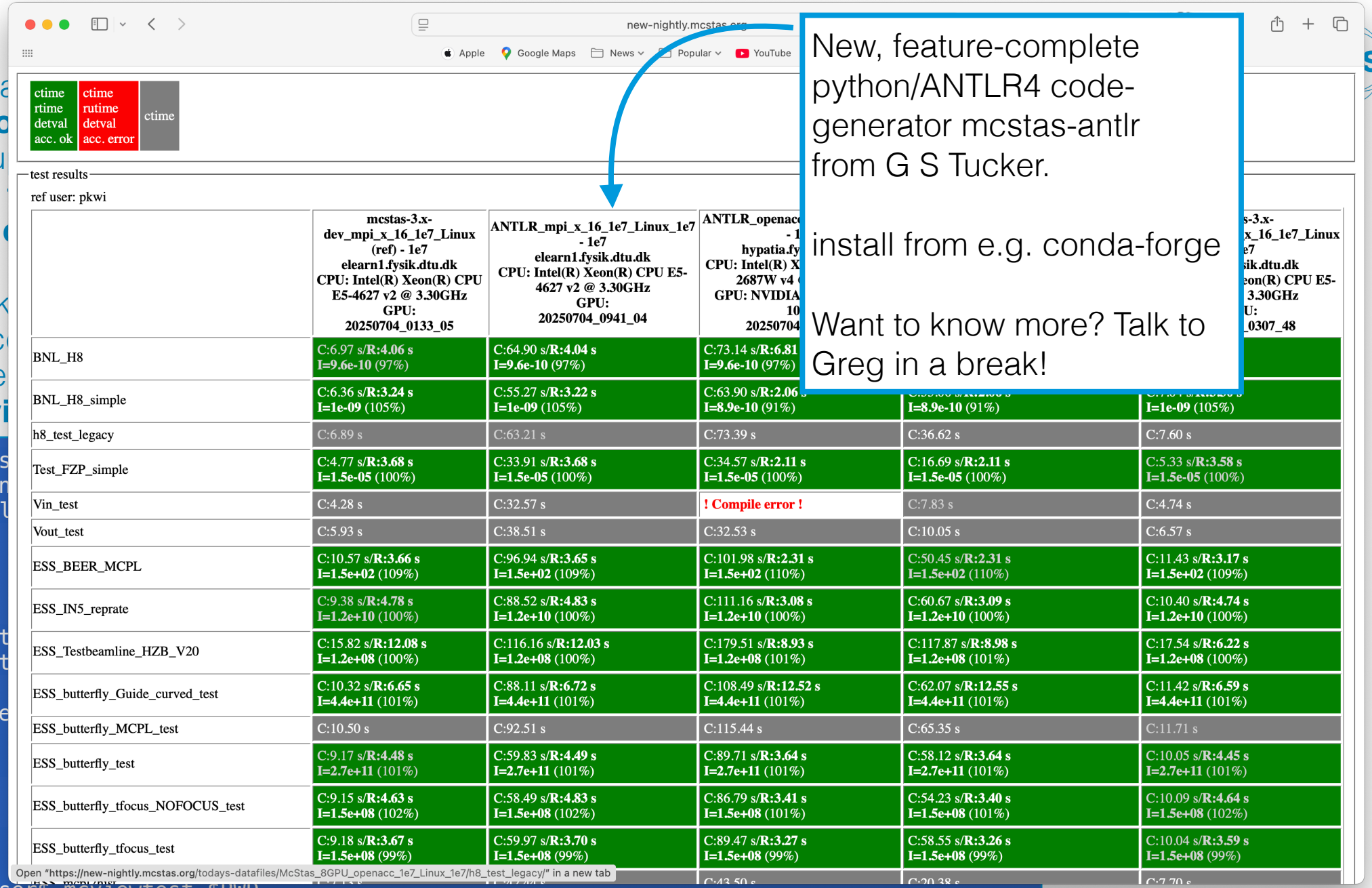
- Common relea
- **We are now c**
  - Forms su
- **Lots of work**
- **CI (GitHub + c**
- Usability:
  - One-click
  - Easy acc
  - 3D rende
- **mctest / mcvi**

```
(base) laptop:~ us
loading system con
Output of test wil
ncount is: 1e7
mpi count is: 10
Testing: 3.5.32

Finding instrument
Copying instrument

Compiling instrume
BNL_H8          :
BNL_H8_simple :

Running tests…
BNL_H8          :
BNL_H8_simple   :
(base) laptop:~ user$ mcviewtest $PWD
```



New, feature-complete python/ANTLR4 code-generator mcstas-antlr from G S Tucker.

install from e.g. conda-forge

Want to know more? Talk to Greg in a break!

New stuff in series 3.5.x

DTU

EUROPEAN SPALLATION SOURCE

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  - One-click transfer to McStasScript/Jupyter
  - Easy access to NeXus output through e.g. nexpy or silx
  - 3D rendering modernised
- mctest / mcviewtest tools
- **Various component / instr contributions, some presented later today in afternoon session!**

debian

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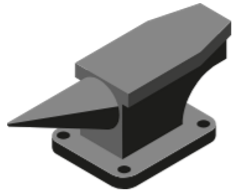
- LOTS of work on many layers + infrastructure -> solid basis for future work:
  - Used for preparing the ESS data pipeline
  - More emphasis on “in-experiment” and data-analysis features
  - Further modernisation

- Project:
  - Historical “yearly release” -> release often, release early mode(conda-forge is the basis)
  - PR-only, “production grade” main branch
  - Plan to extend McStas/McXtrace collaboration
  - Even more emphasis on testing at different levels



Whole stack at conda-forge

Moving towards full Linux/macOS/Windows support

Modelling group

McStas

McXtrace

MCPL

NCrystal

McStasScript

dgcode

simplebuild

Same conda-based deployment strategy for VISA

Community

cif2hkl

mccode-antlr

endf-parserpy

OpenMC

scipp

nexusformat

nexus

nexpy

...

Many community conda pkgs facilitated or maintained by our group

FZJ Hackathon in April

McStas McXtrace

- Got better at profiling
- Overall extra x2 achieved
- New ideas for added parallelism
- New KU-DTU-ESS CS student in spring 26 to continue work

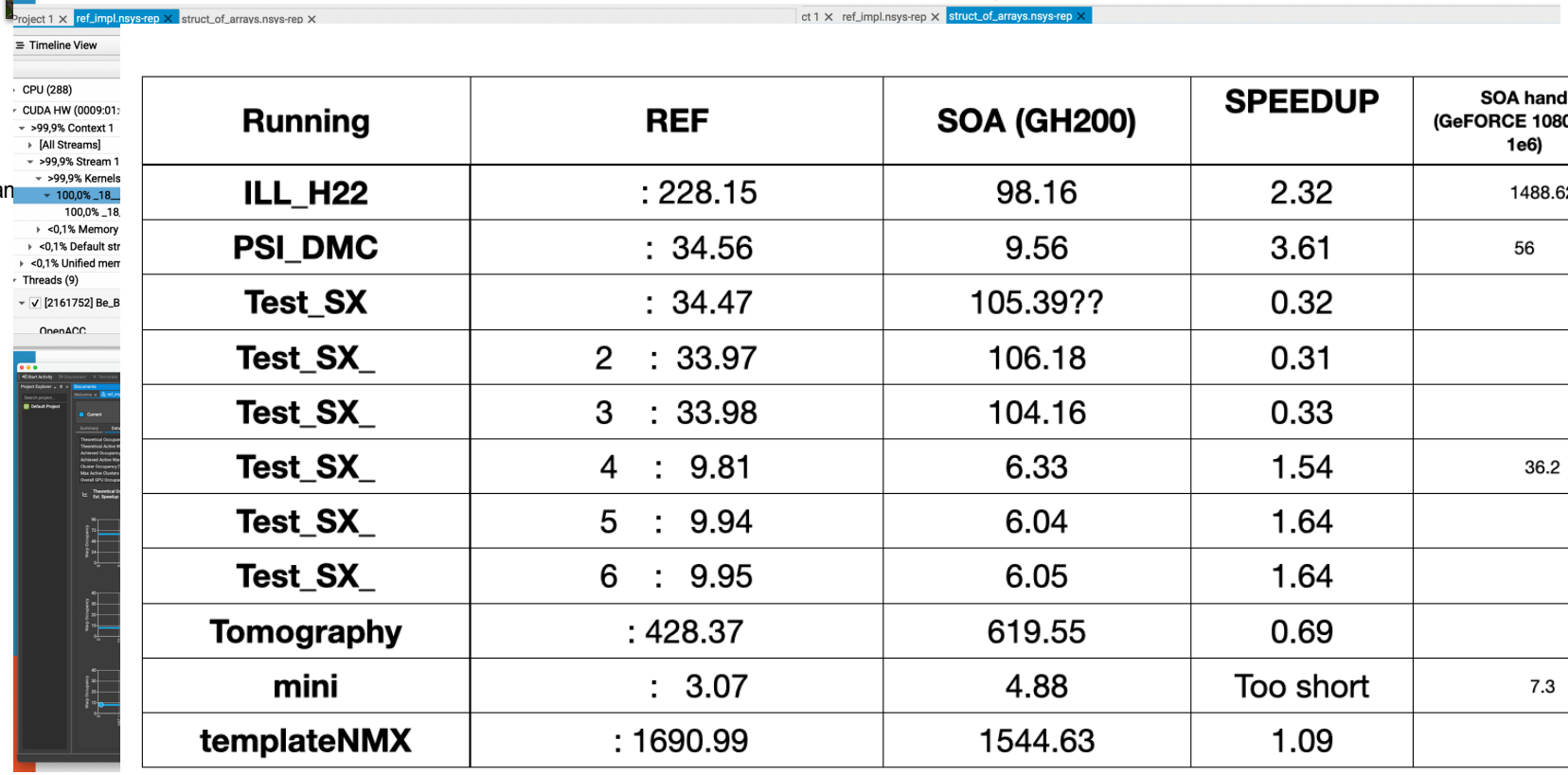
Team

Peter Willendrup
DTU / ESS DMSC

Team

Profiler Output After **restructure** cogen “arrays of struct” -> “struct with arrays”.

“Reference” / monolithic kernel - 1e10 / 5 launches x2e9 “Struct of arrays” / monolithic kernel - 1e10 / 10k launches x1e6



OpenACC OPEN HACKATHONS

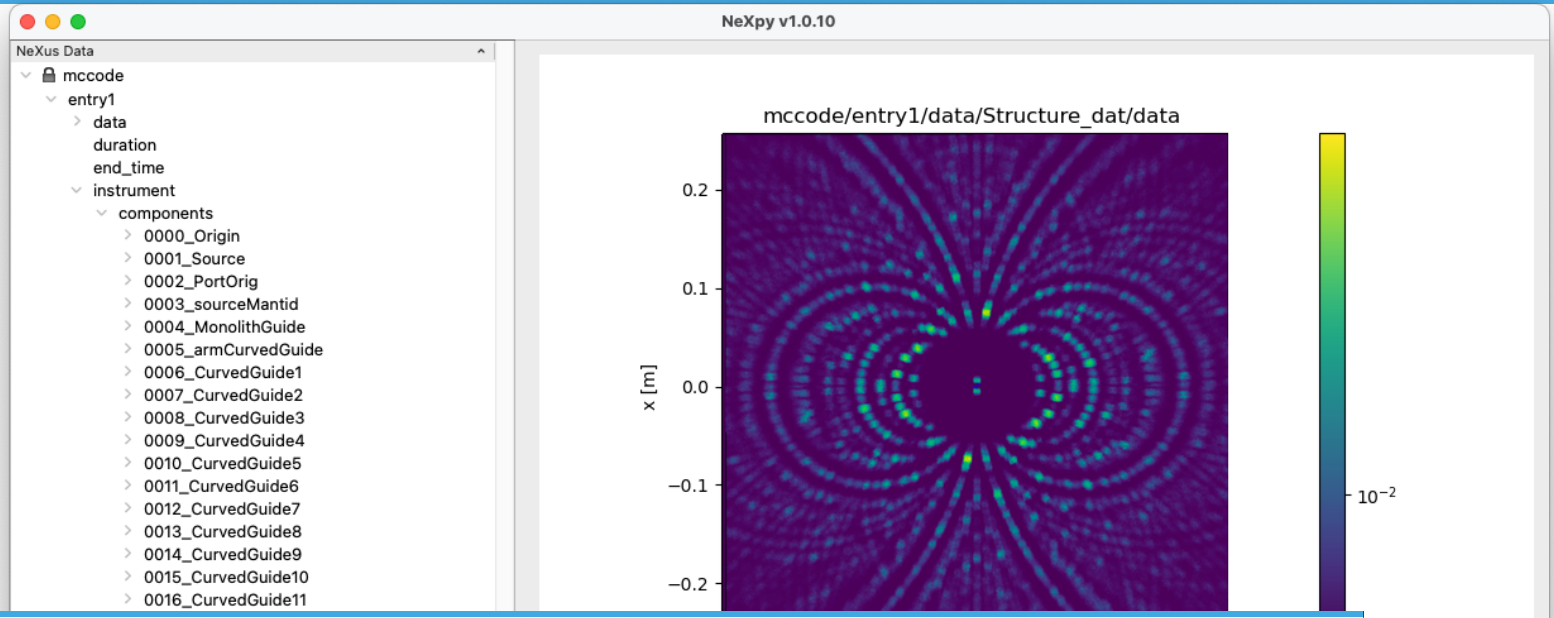
Running	REF	SOA (GH200)	SPEEDUP	SOA handheld (GeFORCE 1080 loop 1e6)	REF (GeFORCE 1080)
ILL_H22	: 228.15	98.16	2.32	1488.62	
PSI_DMC	: 34.56	9.56	3.61	56	
Test_SX	: 34.47	105.39??	0.32		
Test_SX_	2 : 33.97	106.18	0.31		
Test_SX_	3 : 33.98	104.16	0.33		
Test_SX_	4 : 9.81	6.33	1.54	36.2	
Test_SX_	5 : 9.94	6.04	1.64		
Test_SX_	6 : 9.95	6.05	1.64		
Tomography	: 428.37	619.55	0.69		
mini	: 3.07	4.88	Too short	7.3	
templateNMX	: 1690.99	1544.63	1.09		

“Richer NeXus format”

- All component AT / ROTATED data
- All component param=value info
  (currently as text from instr file)
- Monitor_nD geometry data included
- Monitor_nD binning / pixellation arrays

McStasToX

McStas → NeXus → scipp



DTU ESS EUROPEAN SPALLATION SOURCE

“Hooking up to ESS data pipeline”

Peter Willendrup[1,2], Mads Bertelsen[2], Gregory S. Tucker[2]

[1]Technical University of Denmark, Physics Department

[2]European Spallation Source ERIC, Data Management and Software Center

From McStas instrument design to commissioning tool

Preparing to operate the ESS instruments

+ IDS group

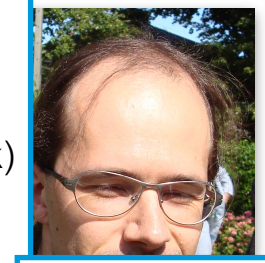
McStas collaboration

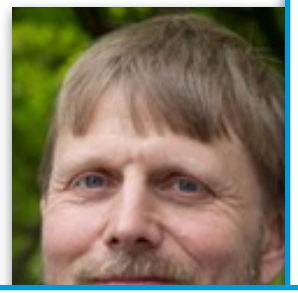
Thanks and acknowledg

Kristian Nielsen

Got input from RISØ physicists, (Incl. Kim & Henrik) architect behind “internals” and LeX-Yacc gram.

Releases 1.0-1.4





Kim Le

Author
compo
“powe
superv
KU stu
secure

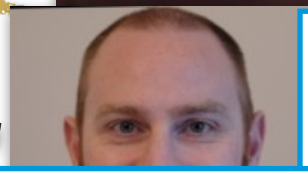
PW:

“Mr. McStas”
2002- ?

Custodian, community caretaker, sustained workforce.

Support for newcomers

Esben Klinkby
Mcnp-hooks, scatter-logger



Torben R. Nielsen:

Contributed solution for connection with “Mantid” data reduction, work on SASmodel integration

Gregory Tucker

ESS event-formation hookup, recent syntax / code-generator additions

Thomas Kittelmann

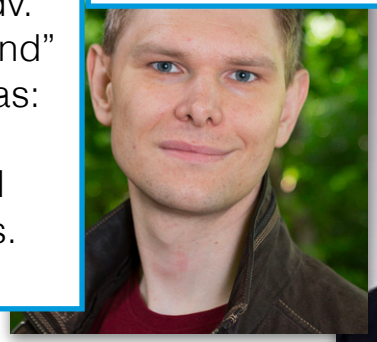
Main developer of MCPL particle list Format and NCrystal structure/ dynamics lib for MC

Plus MANY others among the user community at neutron-facilities, students etc.

Mads Bertelsen

“Next generation”, Phd with KL, contributed adv. systems “around” and “in” McStas:

guide_bot and Union systems.



behind McXtrace.
+ lots more

Left for CPH Atomics in 2022.

Grammar ext.
advanced comps.
+ lots more
Now works mainly on McXtrace.

Johan Brinch
Transfer to CMake
1st round of .py tools

Main McStas Funding sources

During its lifetime, McStas efforts have been supported through several European Union RTD and JRA programmes, plus several instrument development projects for facilities.

Project	Program type	Funding period
XENNI	RTD (EU FP4)	1996 - 2000
Cool Neutrons	RTD (EU FP4)	1998 - 2001
SCANS	RTD (EU FP5)	2000 - 2004
MCNSI	JRA in NMI3 (EU FP6)	2004 - 2006
MCNSI7	JRA in NMI3/FP7 (EU FP7)	2006 - 2008
NMI3-II/FP7 outreach project	JRA in NMI3/FP7 (EU FP7)	2012 - 2016
ISIS TS2 EU project	Infrastructure project in (EU FP6)	2006-2009
Instrument simulations for the ESS design update	Danish in-kind project toward the ESS	2009-2012
Secondment of P Willendrup from DTU for supporting instrument simulations for the ESS	33% part of the ESS DMSC	2014-2022
SINE2020	Part of WP3 and WP8 (EU H2020)	2016 - 2019
PaNOSC	Part of Software and E-learning (EU H2020)	2019 - 2022
HighNESS	Contributions to WPs 6,8,9 (EU H2020)	2020 - 2023
Secondment of P Willendrup from DTU for supporting instrument simulations for the ESS	100% part of the ESS DMSC	2023-2027