

# McStas advanced language features

## - and other important, not so well known details

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# McStas



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# What is really the information content...?

- ◆ McStas sources generally provide “intensity” in units of neutrons/s (into a chosen solid angle)
- ◆ That intensity is carried through the instrument on a discrete set of “neutron rays”

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## Onto efficiency...

- ◆ Apply focusing techniques
  - ◆ At the source (spatially, temporally, in wavelength...)
  - ◆ At the sample, if possible
- ◆ (carefully!) Apply SPLIT - but only if immediately followed by Monte Carlo choices, e.g. in sample
- ◆ Alternatively use MCPL o/i which allows repetition - beware of biases!

## Onto efficiency...

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*All of this can be considered "variance reduction" or biasing*

## Onto efficiency...

- ◆ Use MPI parallelisation - included in macOS install from 2.4, easy to get on Linux...
- ◆ The Intel C compiler is known to give ~factor of 2 wrt. gcc in most cases
- ◆ - Still consider if you are asking the right question if runtimes reach days/weeks...

# Advanced language features

- Macros and tricks for your instrument...

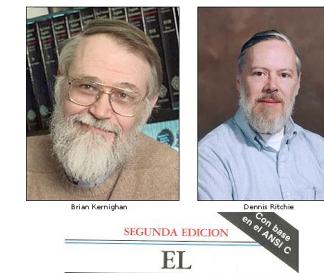


# DECLARE / INITIALIZE

- Use the DECLARE section define user variables and functions.
  - `DECLARE %{`
  - `double myvar;`
  - `%}`
- Use INITIALIZE for initialization of user variables and calculations.
  - `INITIALIZE %{`
  - `myvar = sqrt(PI*input_var)*rand01();`
  - `%}`
- - Both use normal c-syntax.
- BEWARE: (example) What you do in the c-style areas is c-standard, e.g. trigonometric functions from `math.h` use radians! - McStas placement specifiers work in degrees, etc...



K & R



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Dennis Ritchie

SEGUNDA EDICION  
en base  
a la ANSI C

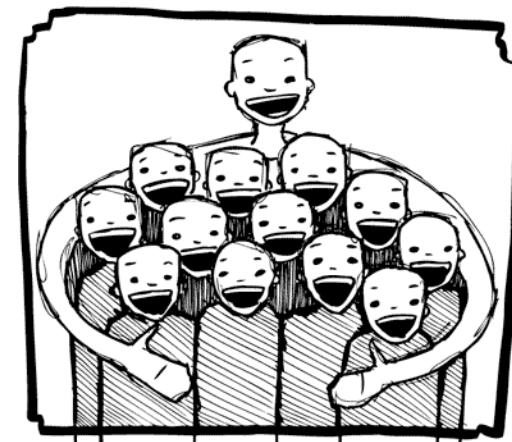
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 PROGRAMACION



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Prentice Hall  
Educational Publishers

## %include

- Instrumentfiles can include external c-code or other instrumentfiles... See the examples:
- ILL\_H15\_IN6.instr:%include "monitor\_nd-lib"
- ILL\_H16\_IN5.instr:%include "ILL\_H16.instr"
- ILL\_H25\_IN22.instr:%include "ILL\_H25.instr"
- ILL\_H25\_IN22.instr:%include "templateTAS.instr"
- Used in the DECLARE section



# Syntax in one, complex view...

```
{SPLIT} COMPONENT name = comp(parameters) {WHEN condition}  
AT (...) [RELATIVE [reference|PREVIOUS] | ABSOLUTE]  
{ROTATED {RELATIVE [reference|PREVIOUS] | ABSOLUTE} }  
{GROUP group_name}  
{EXTEND C_code}  
{JUMP [reference|PREVIOUS|MYSELF|NEXT] [ITERATE number_of_times | WHEN condition] }
```

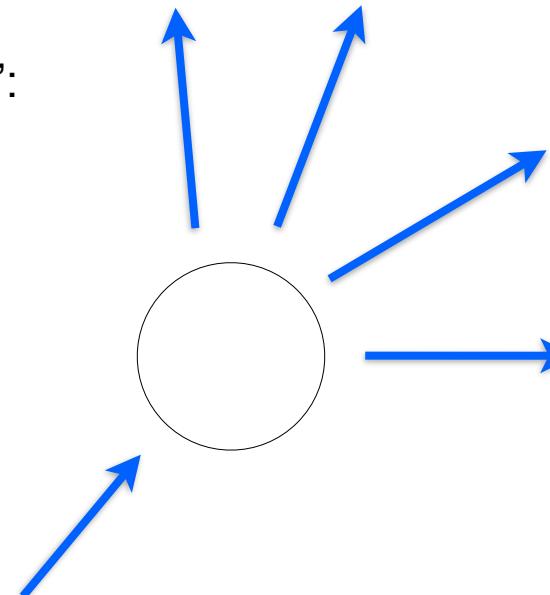
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# SPLIT

- Increase statistics beyond this point in the instrumentfile
- SPLIT n MyArm = Arm()
- AT somewhere
- will “formulate an if-statement”:
  - for j=1:n
  - comp1
  - comp2
  - comp3
  - ...
  - end (of instrument)
- ONLY meaningful in case of Monte Carlo choices after SPLIT point...



*slight sidetrack....*

# Problem: McStas Single\_crystal.comp “slow” for large unit cell diffraction studies

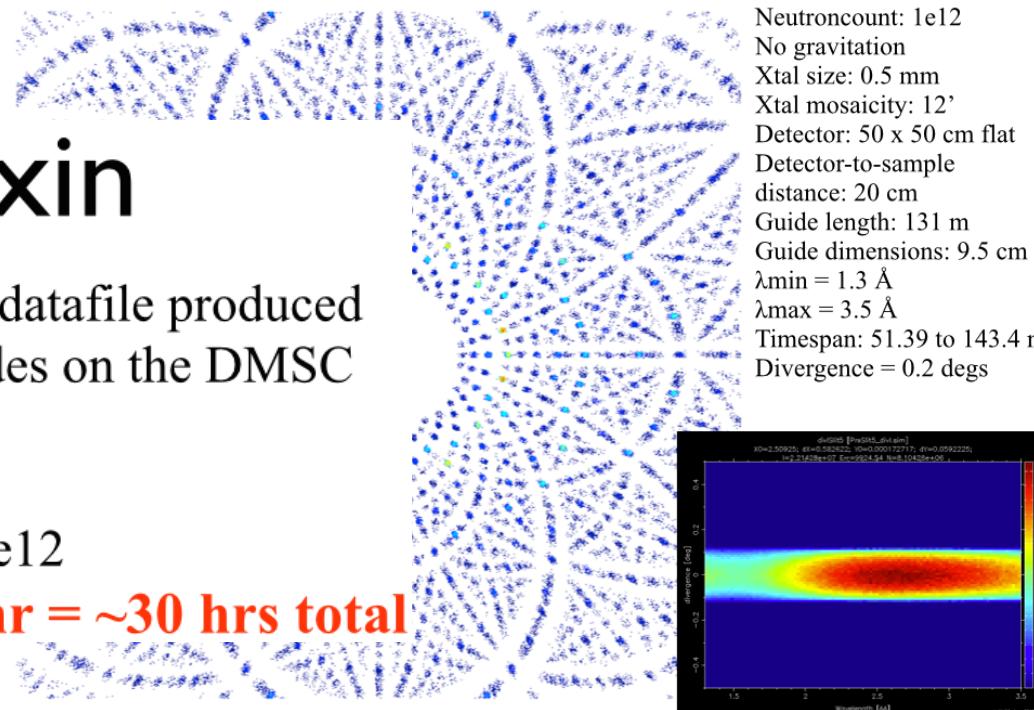
- Example: Rubredoxin

1 timebin, 1000 x,y-bins

## Rubredoxin

Images created from simulated datafile produced August 20th 2012 using 25 nodes on the DMSC cluster.

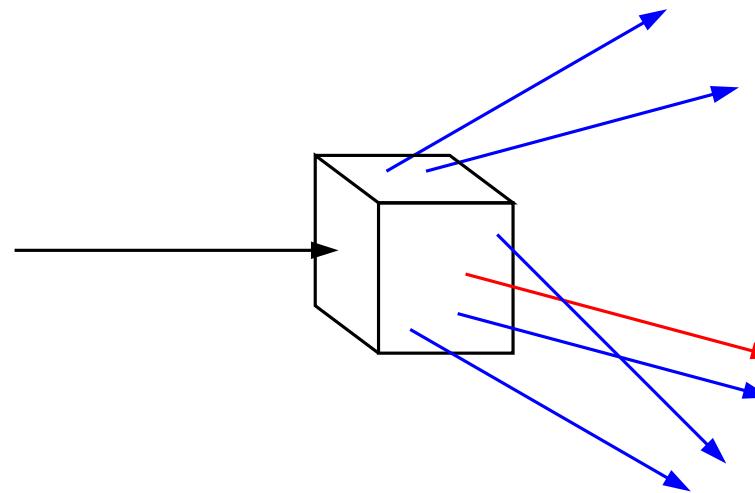
Neutron count: 1e12

**Simulation time: ~10 + ~20 hr = ~30 hrs total**

slight sidetrack....

# Algorithm improvement: Use incoming neutrons more efficiently - scatter each one on all possible reflections

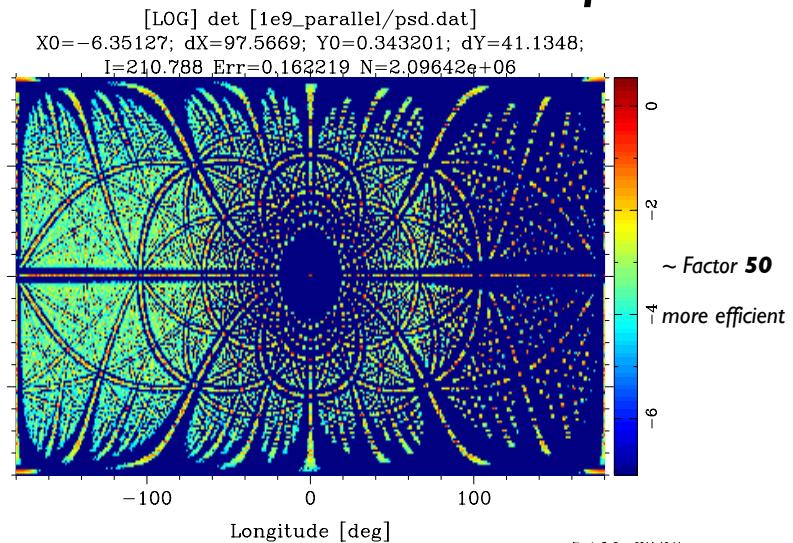
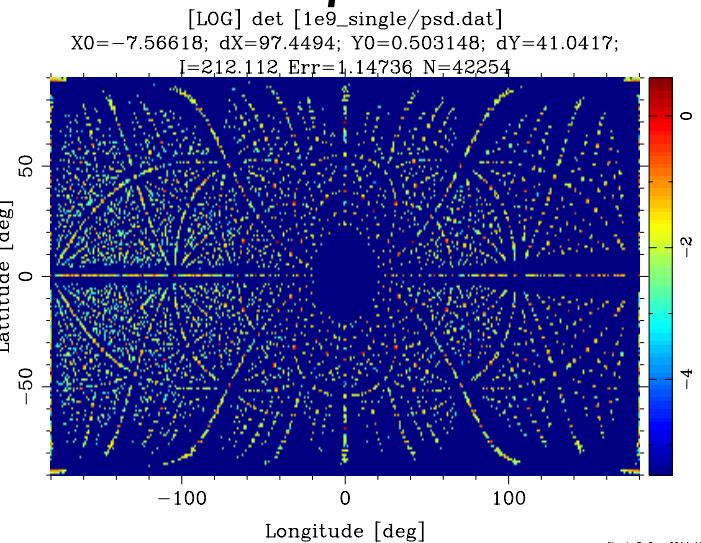
- **Red:** Original algorithm, one incoming neutron used only once
- **Blue:** Improved algorithm, each incoming neutron scattered (via SPLIT keyword) all possible times
- Component makes **estimate on average number of “active” diffraction spots** - in the case Rubredoxin this is around **50!**



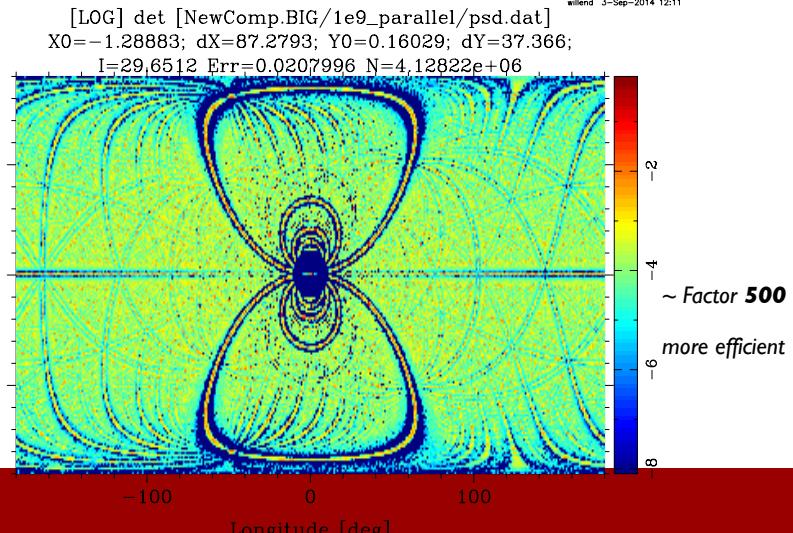
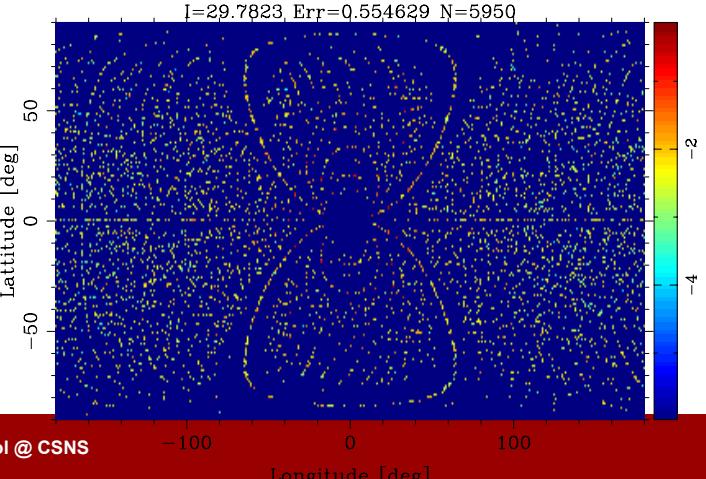
# Sim data speak for themselves - 1e9 rays

## Old comp      New comp

Rubedoxin  
124K reflections



Predeuterated  
pyrophosphatase  
1.7M reflections



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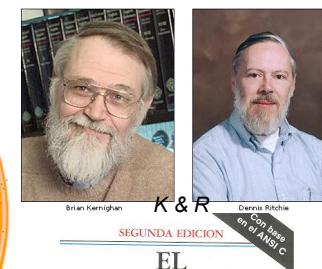
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# WHEN

- Syntax:
- COMPONENT Mine = Yours(blah, blah)
- WHEN (c-expression) AT (....)
- Is very powerful when combined with EXTEND and user variables, or as a method to let input parameters select if certain components are active.
- Example: Use EXTEND to flag if neutron was scattered on one monochromator blade or another. Then later use WHEN to only show contribution from blade N at sample position?
- COMPONENT Mon = PSD\_monitor(...)
- WHEN (myvar==1) AT (0,0,0) RELATIVE Sample



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# GROUP - components working in parallel

AT (0,0, -LMM) RELATIVE Cradle ROTATED (0,A1/2,0) RELATIVE Cradle  
GROUP IN6Monoks

AT (0,0, 0) RELATIVE Cradle ROTATED (0,A2/2,0) RELATIVE Cradle  
GROUP IN6Monoks

- One comp after the other is “tried” in sequential order until the neutron was SCATTERED.

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# EXTEND

- Enrich component behaviour using EXTEND:

- COMPONENT Mono1 = Monochromator\_curved(...)

- AT (0,0, -LMM) RELATIVE Cradle ROTATED (0,A1/2,0) RELATIVE Cradle

- GROUP IN6Monoks

- EXTEND

- %{

- if (SCATTERED) { myvar = 1; }

- %}

- ...

- COMPONENT Mono2 = Monochromator\_curved(...)

- AT (0,0, 0) RELATIVE Cradle ROTATED (0,A2/2,0) RELATIVE Cradle

- GROUP IN6Monoks

- %{

- if (SCATTERED) { myvar = 2 ; }

- %}



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Dennis Ritchie

SEGUNDA EDICION

en la base

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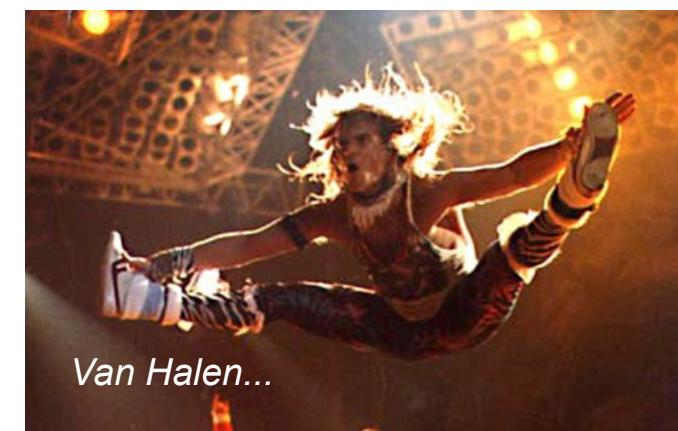
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# JUMP

- A goto. Be careful. Can be used in two situations:
- JUMP to myself
- JUMP to an Arm
- No coordinate transformations are applied... (Meaning that if the Arms you JUMP between do not coincide you will “move” / “reorient” the neutrons...)
- Syntaxes:
- COMPONENT a=b(...)
- WHEN (expr) AT (...) JUMP somewhere
- COMPONENT a=b(...)
- WHEN (expr) AT (...) JUMP myself



# JUMP

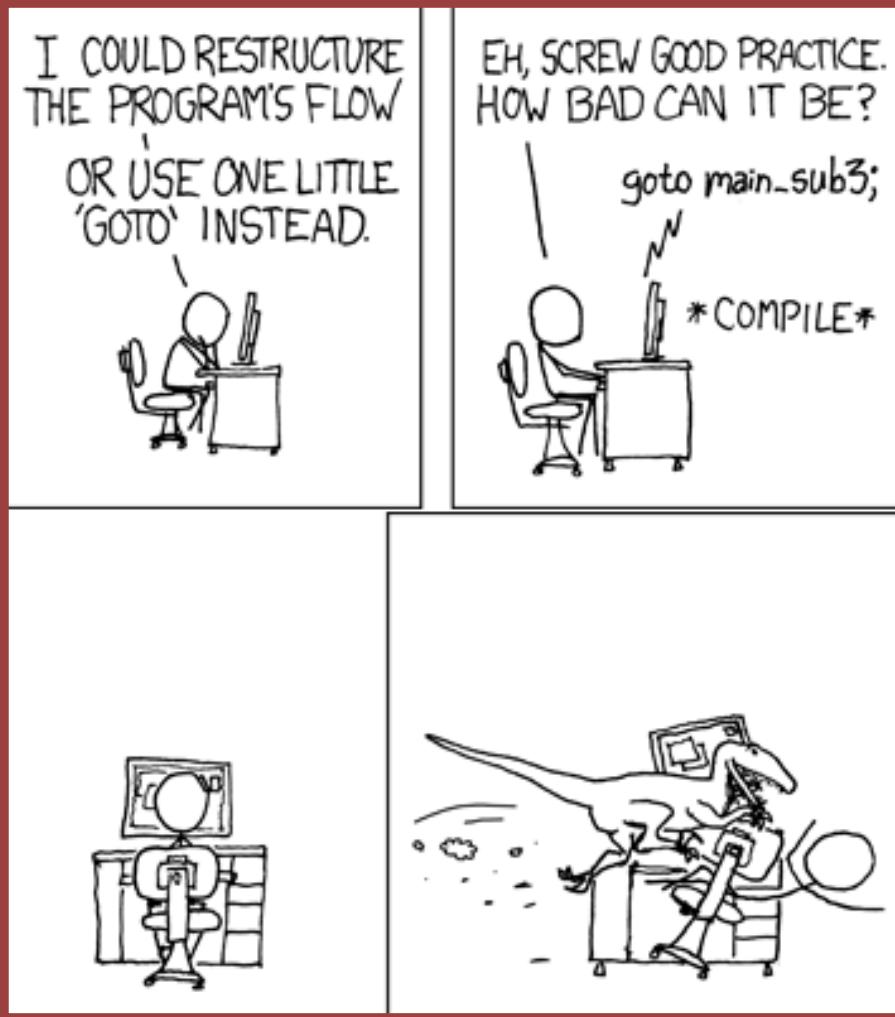
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- Syntaxes:
- COMPONENT a=b(...)
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**BEWARE - This IS a**



# JUMP

- A goto. Better?
- JUMP to me
- JUMP to a
- No coordination between d
- Syntaxes:
- COMPONENT
- WHEN (example)
- COMPONENT
- WHEN (example)



**BEWARE - This IS a**

that if the Arms you JUMP  
the neutrons...)



'alen...

# COPY- inside instruments

- In instruments: (see ILL\_H25.instr)
  - COMPONENT H25\_1 = Guide\_gravity(
    - w1=0.03, h1=0.2, w2=0.03, h2=0.2, l=L\_H25\_1,
    - R0=gR0, Qc=gQc, alpha=gAlpha, m=m, W=gW)
    - AT (0,0,AI\_Thickness+gGap) RELATIVE PREVIOUS
    - ROTATED (0,Rh\_H25\_1,0) RELATIVE PREVIOUS
  - COMPONENT COPY(H25\_1) = COPY(H25\_1)
    - AT (0,0,L\_H25\_1+gGap) RELATIVE PREVIOUS
    - ROTATED (0,Rh\_H25\_1,0) RELATIVE PREVIOUS
  - COMPONENT COPY(H25\_1) = COPY(H25\_1)(W=2\*gW)
    - AT (0,0,L\_H25\_1+gGap) RELATIVE PREVIOUS
    - ROTATED (0,Rh\_H25\_1,0) RELATIVE PREVIOUS



## 6 McStas various utils

- Hidden gems and useful little things...
- + Disclaimers and tips for the next couple of days...

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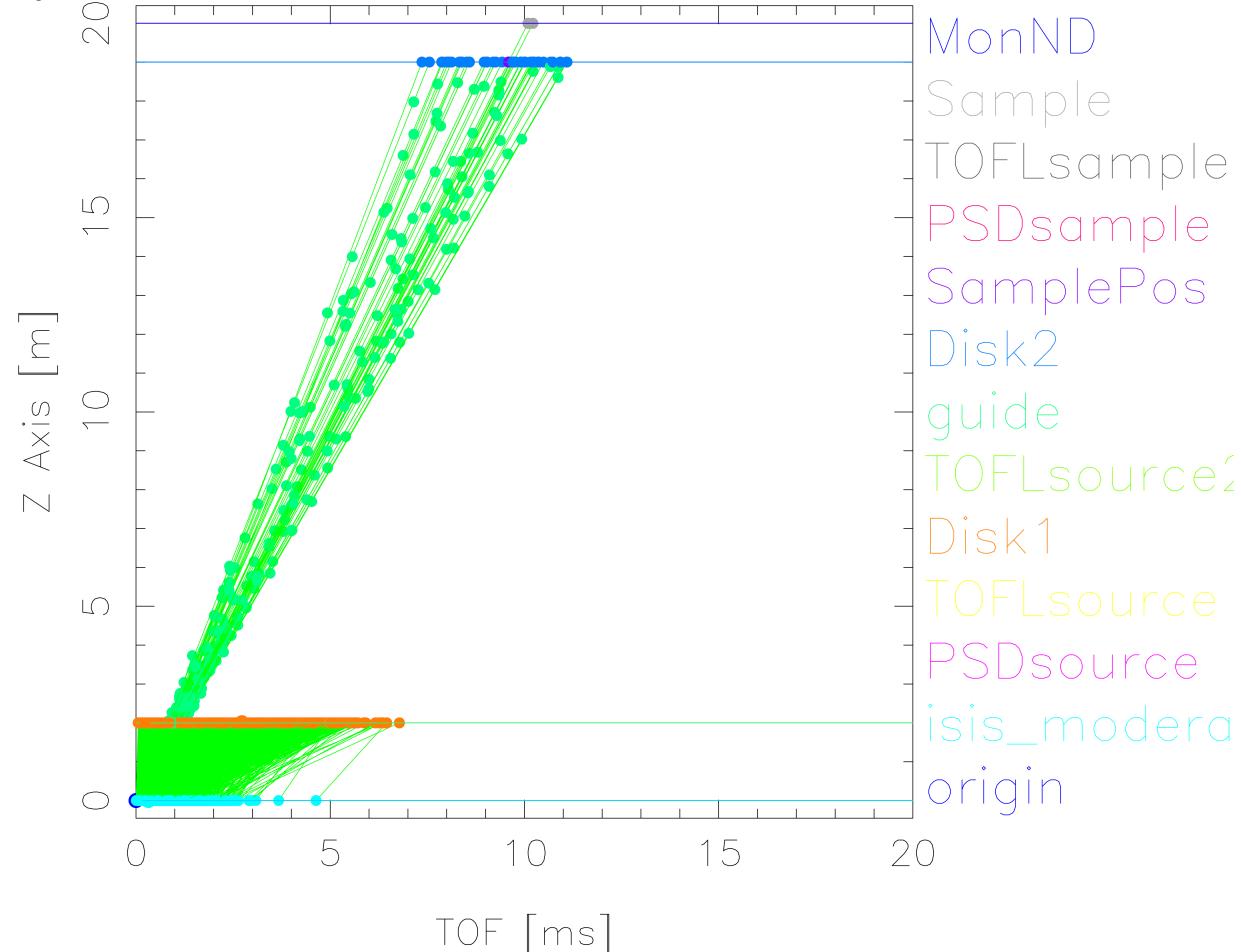
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# TOF diagram util based on mcdisplay

TOF diagram: STEP3.out

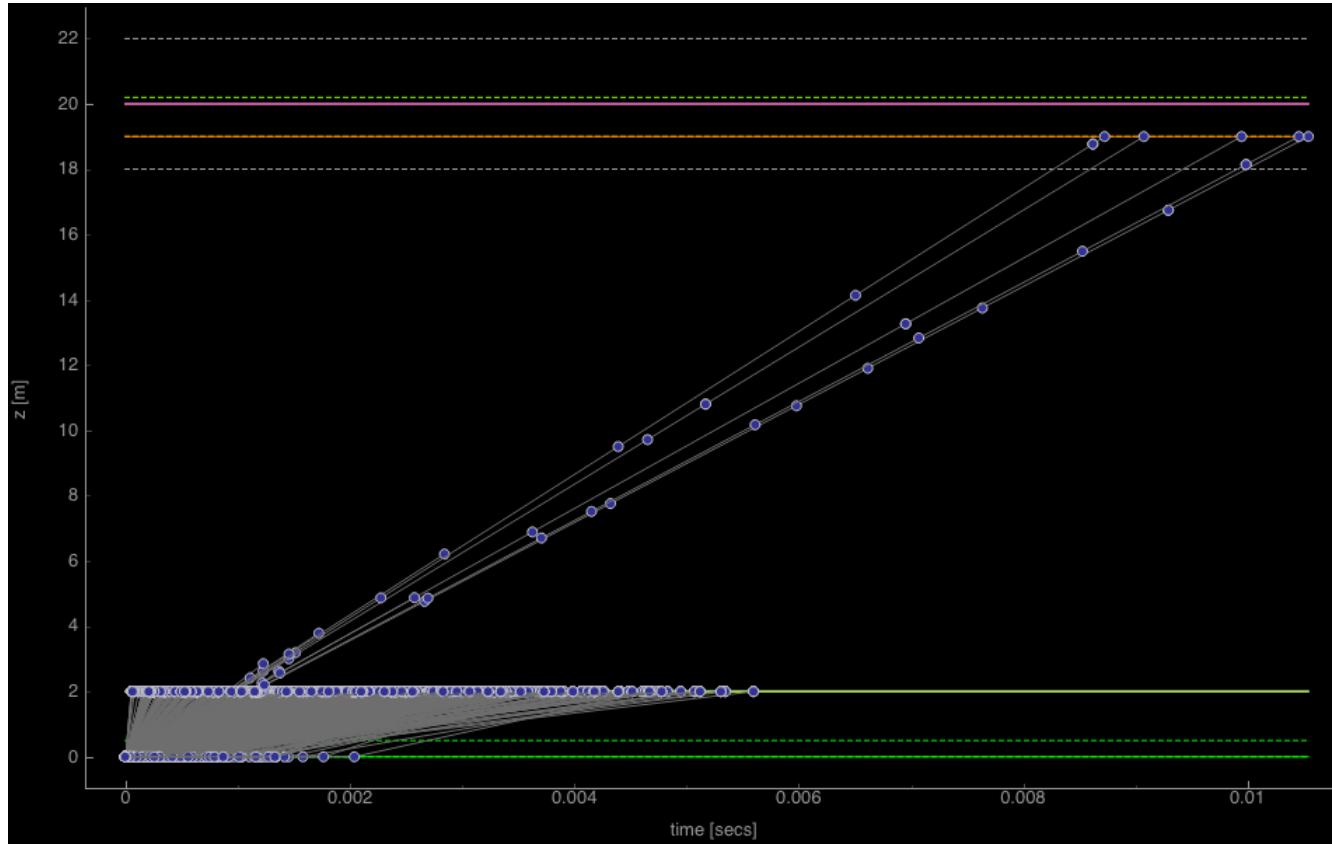
• `mcdisplay.pl --TOF --tmax=20 instrument...`





# TOF diagram util based on mcdisplay

- mcdisplay-pyqtgraph --TOF instr



# Cluster utility scripts

```
./mcsub_slurm.pl
Usage: ./mcsub_slurm.pl [options] [mcrun params]
-h      --help          Show this help
-rN     --runtime=N     Specify maximum runtime (hours) [default 1]
-qQNAME --queue=QNAME  Specify wanted SLURM queue [default 'express']
-e<mail> --email=<mail> Specify address to notify in reg. sim status [default none]
--nodes=NUM        Specify wanted number of nodes [default 1]
--name=NAME        Specify slurm job name [default "McSub_<USERNAME>_<TIMESTAMP>"]

After running ./mcsub_slurm.pl NAME.batch is ready for submission using the sbatch command
```

- Takes a “mcrun commandline”
- Writes batch file “template” for use with PBS or slurm cluster queue systems
- <https://github.com/McStasMcXtrace/McCode/tree/master/tools/cluster-scripts>

# Vitess - compatibility

- Utility script for converting Vitess reflectivity files for use with McStas ([https://github.com/McStasMcXtrace/McCode/blob/master/tools/other/Refl\\_Vitess2McStas.sh](https://github.com/McStasMcXtrace/McCode/blob/master/tools/other/Refl_Vitess2McStas.sh))
- mcstas2vitess generates Vitess module + tcl snippet from McStas component (poor docs, will improve)

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- *Simple grep* →
  - 370 examples of *Monitor\_nD*
  - 51 examples of *Source\_gen*
  - 10 examples of *ISIS\_moderator*
  - 10 examples of *Single\_crystal*

- *Simple grep →*
  - 370 examples of Monitor nD

*They have an author name!*

*For instance:*

*ISIS\_CRISP → R. Dalgliesh*

*SE\_example → me (E. Knudsen)*

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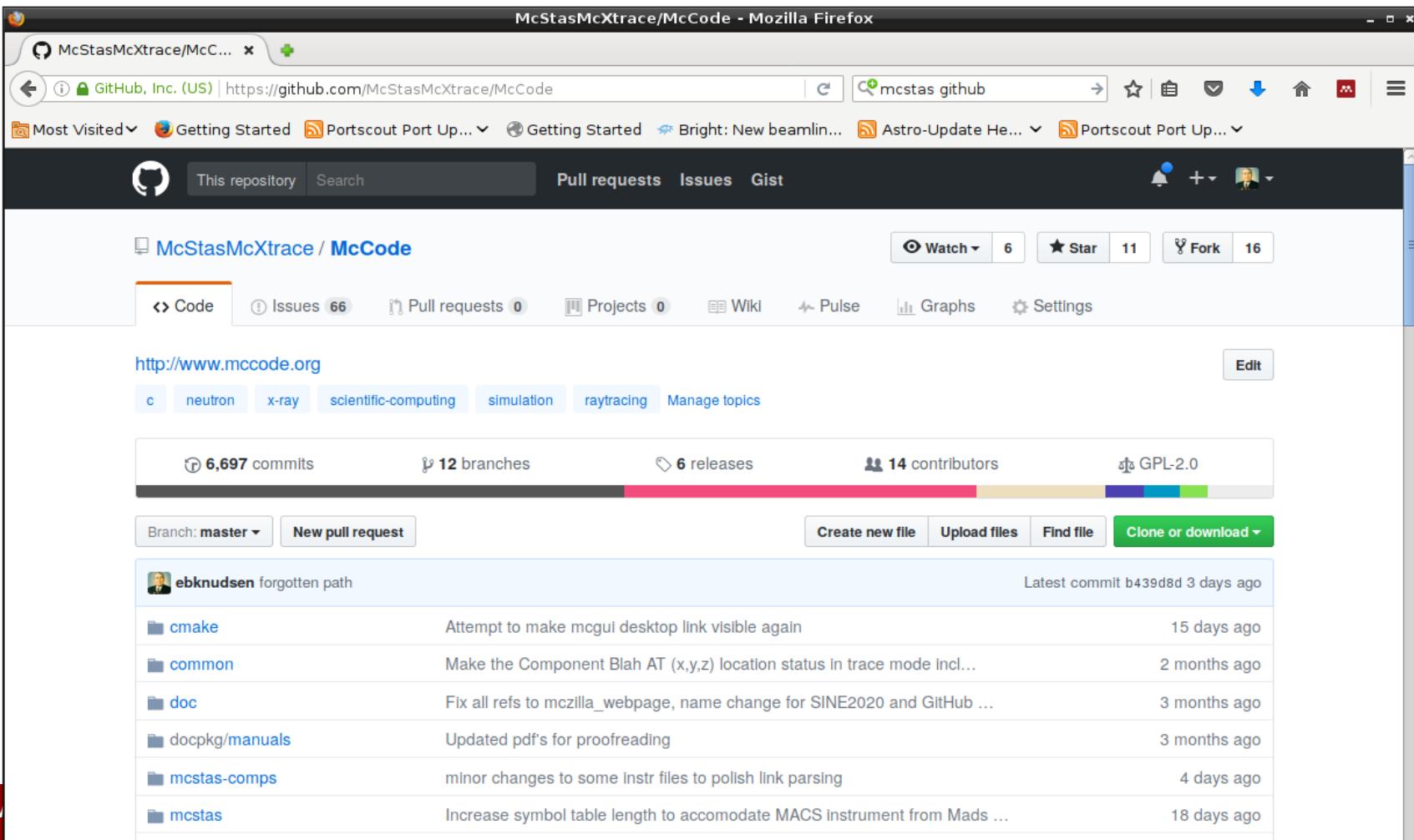
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<https://github.com/McStasMcXtrace/McCode>



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GitHub, Inc. (US) | https://github.com/McStasMcXtrace/McCode

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Code Issues 66 Pull requests 0 Projects 0 Wiki Pulse Graphs Settings

http://www.mccode.org Edit

c neutron x-ray scientific-computing simulation raytracing Manage topics

6,697 commits 12 branches 6 releases 14 contributors GPL-2.0

Branch: master New pull request Create new file Upload files Find file Clone or download

ebknudsen forgotten path Latest commit b439dad 3 days ago

cmake Attempt to make mcgui desktop link visible again 15 days ago

common Make the Component Blah AT (x,y,z) location status in trace mode incl... 2 months ago

doc Fix all refs to mczilla\_webpage, name change for SINE2020 and GitHub ... 3 months ago

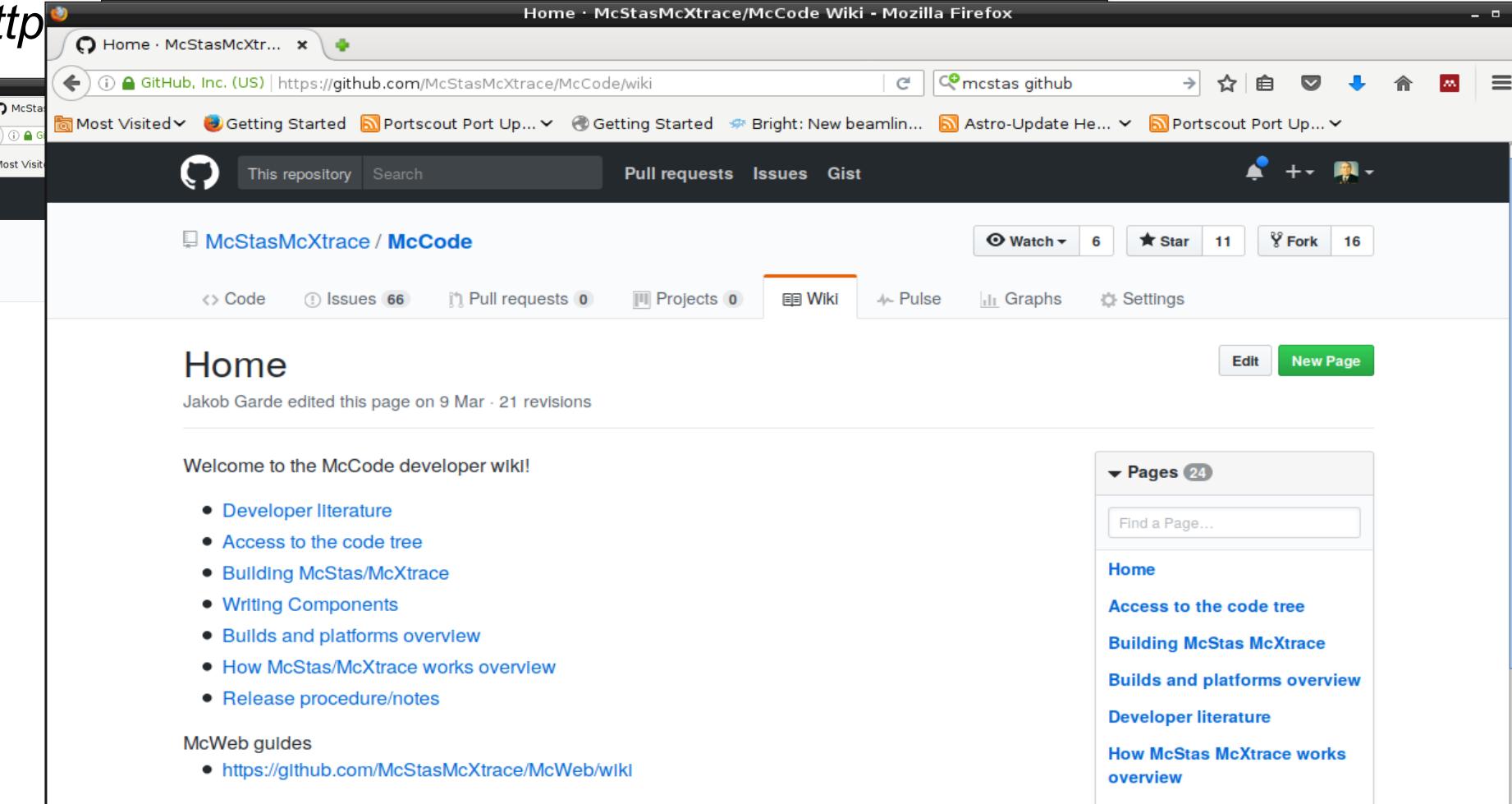
docpkg/manuals Updated pdf's for proofreading 3 months ago

mcstas-comps minor changes to some instr files to polish link parsing 4 days ago

mcstas Increase symbol table length to accomodate MACS instrument from Mads ... 18 days ago

*Mostly developer oriented docs so far*

http://



Home · McStasMcXtrace/McCode Wiki - Mozilla Firefox

GitHub, Inc. (US) | https://github.com/McStasMcXtrace/McCode/wiki

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Home Jakob Garde edited this page on 9 Mar · 21 revisions

Welcome to the McCode developer wiki!

- Developer literature
- Access to the code tree
- Building McStas/McXtrace
- Writing Components
- Builds and platforms overview
- How McStas/McXtrace works overview
- Release procedure/notes

McWeb guides

- <https://github.com/McStasMcXtrace/McWeb/wiki>

Other useful pieces of information

- Single crystal - and generating its Input
- McStas and Mantid

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Find a Page...

Home

Access to the code tree

Building McStas McXtrace

Builds and platforms overview

Developer literature

How McStas McXtrace works overview

How to use Eclipse with PyDev

mcdisplay pyqtgraph

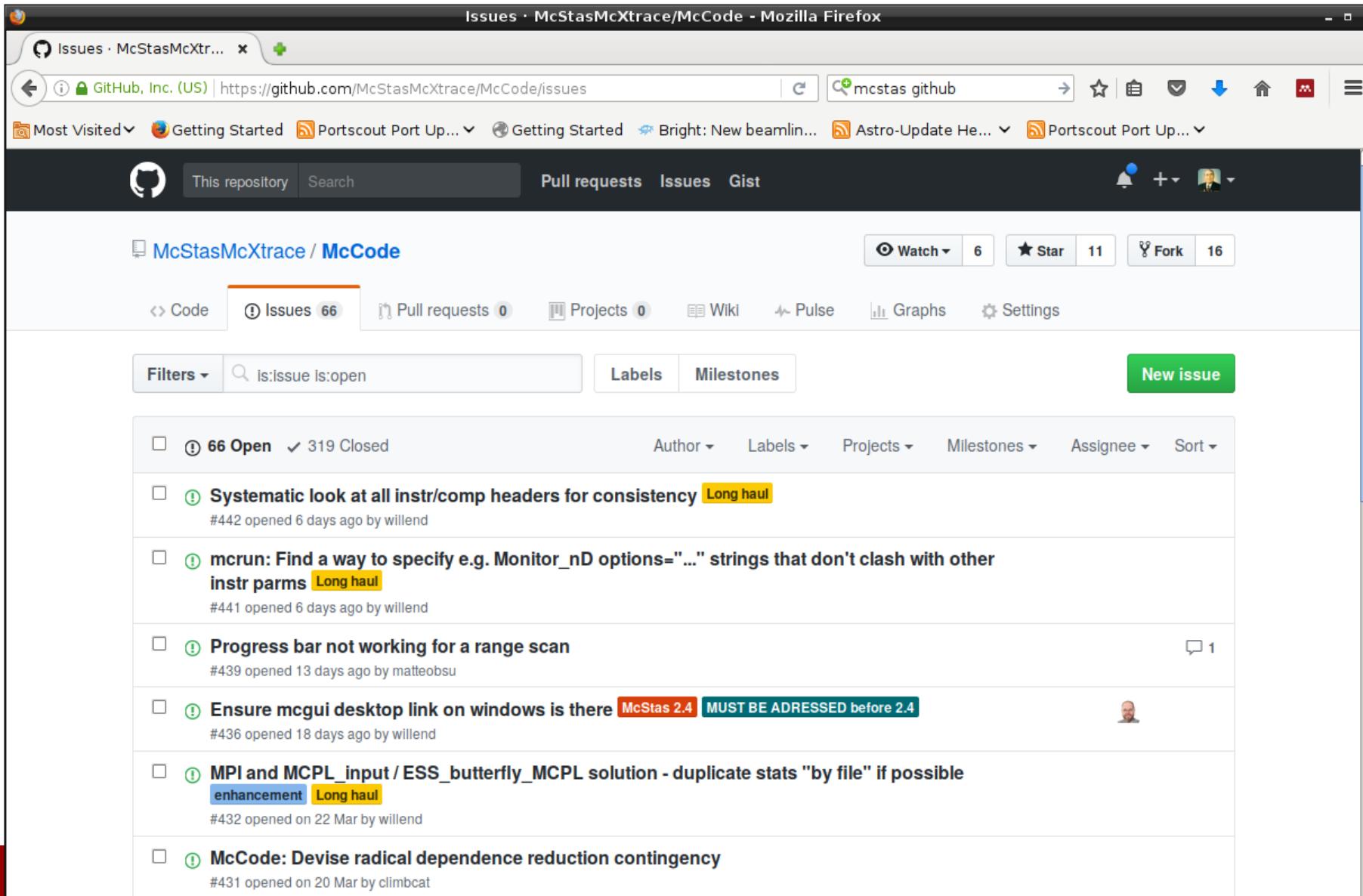
## GitHub.com: Issue Tracker



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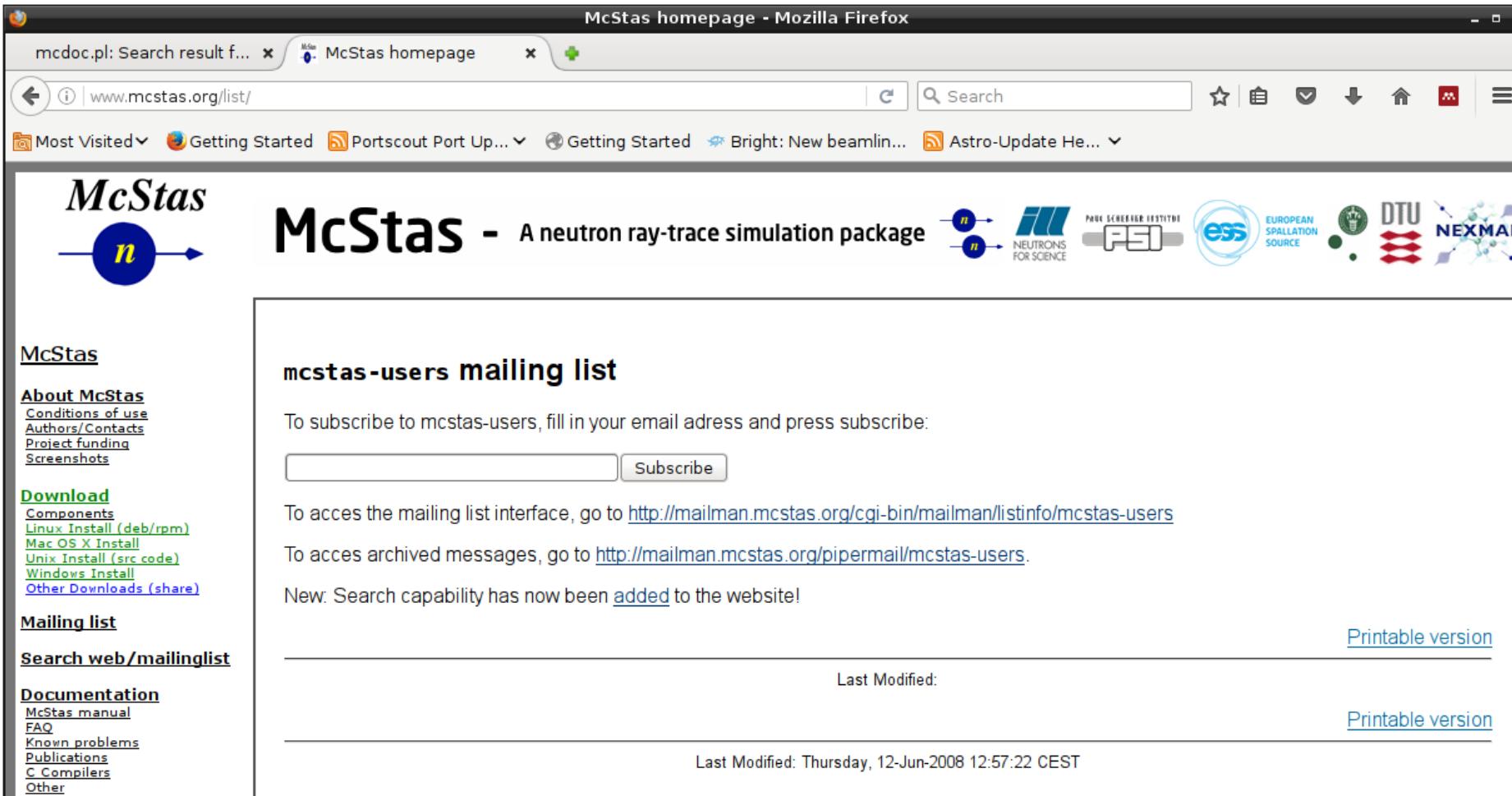
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The screenshot shows the GitHub Issues page for the McStasMcXtrace/McCode repository. The page displays 66 open issues. The first few issues listed are:

- Systematic look at all instr/comp headers for consistency **Long haul** #442 opened 6 days ago by willend
- mcrun: Find a way to specify e.g. Monitor\_nD options="..." strings that don't clash with other instr parms **Long haul** #441 opened 6 days ago by willend
- Progress bar not working for a range scan #439 opened 13 days ago by matteobsu
- Ensure mcgui desktop link on windows is there **McStas 2.4 MUST BE ADRESSED before 2.4** #436 opened 18 days ago by willend
- MPI and MCPL\_input / ESS\_butterfly\_MCPL solution - duplicate stats "by file" if possible enhancement **Long haul** #432 opened on 22 Mar by willend
- McCode: Devise radical dependence reduction contingency #431 opened on 20 Mar by climbcat



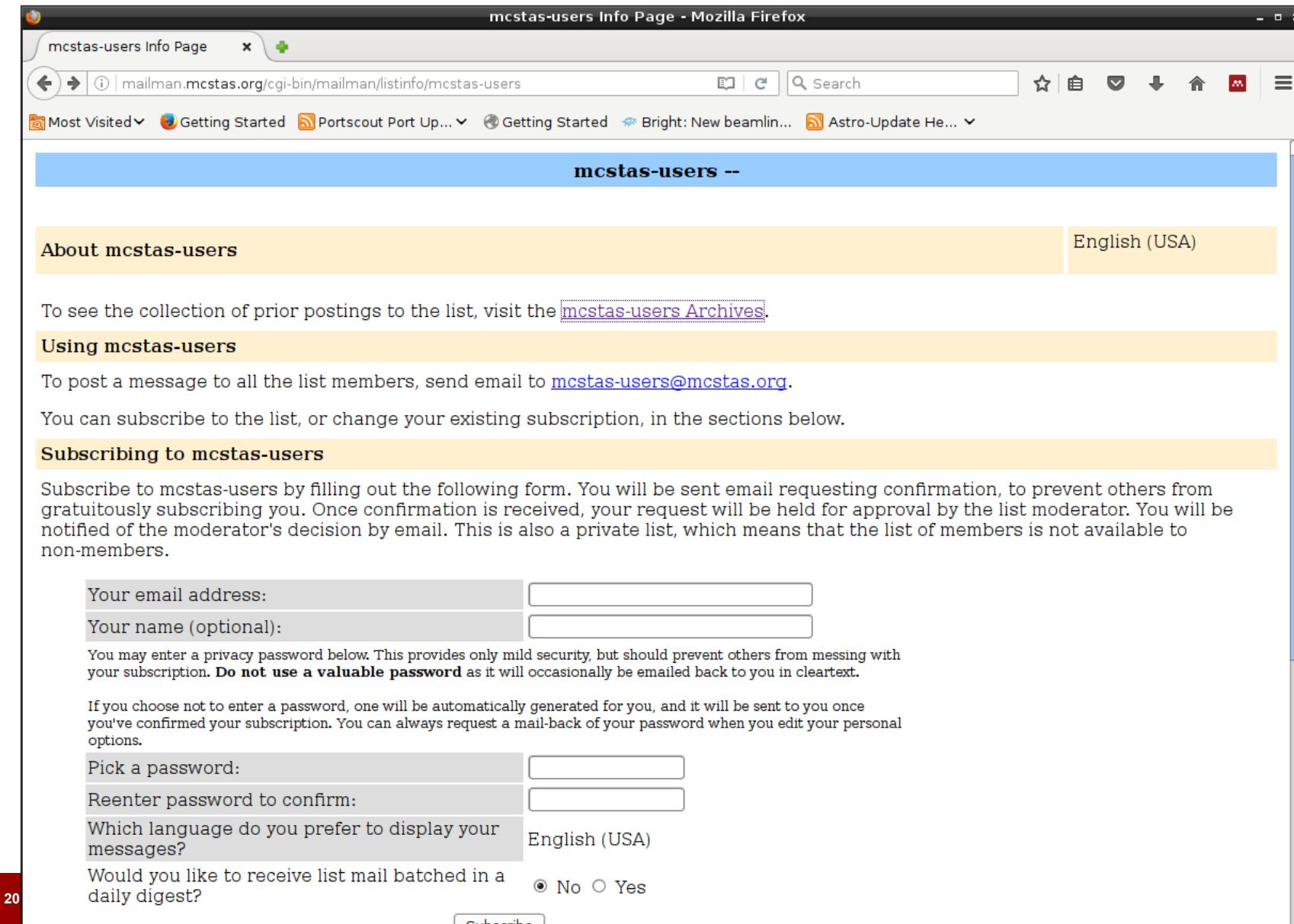
## Mailing List



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mcstas-users Info Page - Mozilla Firefox

mcstas-users Info Page | mailman.mcstas.org/cgi-bin/mailman/listinfo/mcstas-users

Most Visited Getting Started Portscout Port Up... Getting Started Bright: New beamlin... Astro-Update He...

### mcstas-users --

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Your email address:

Your name (optional):

You may enter a privacy password below. This provides only mild security, but should prevent others from messing with your subscription. **Do not use a valuable password** as it will occasionally be emailed back to you in cleartext.

If you choose not to enter a password, one will be automatically generated for you, and it will be sent to you once you've confirmed your subscription. You can always request a mail-back of your password when you edit your personal options.

Pick a password:

Reenter password to confirm:

Which language do you prefer to display your messages? English (USA)

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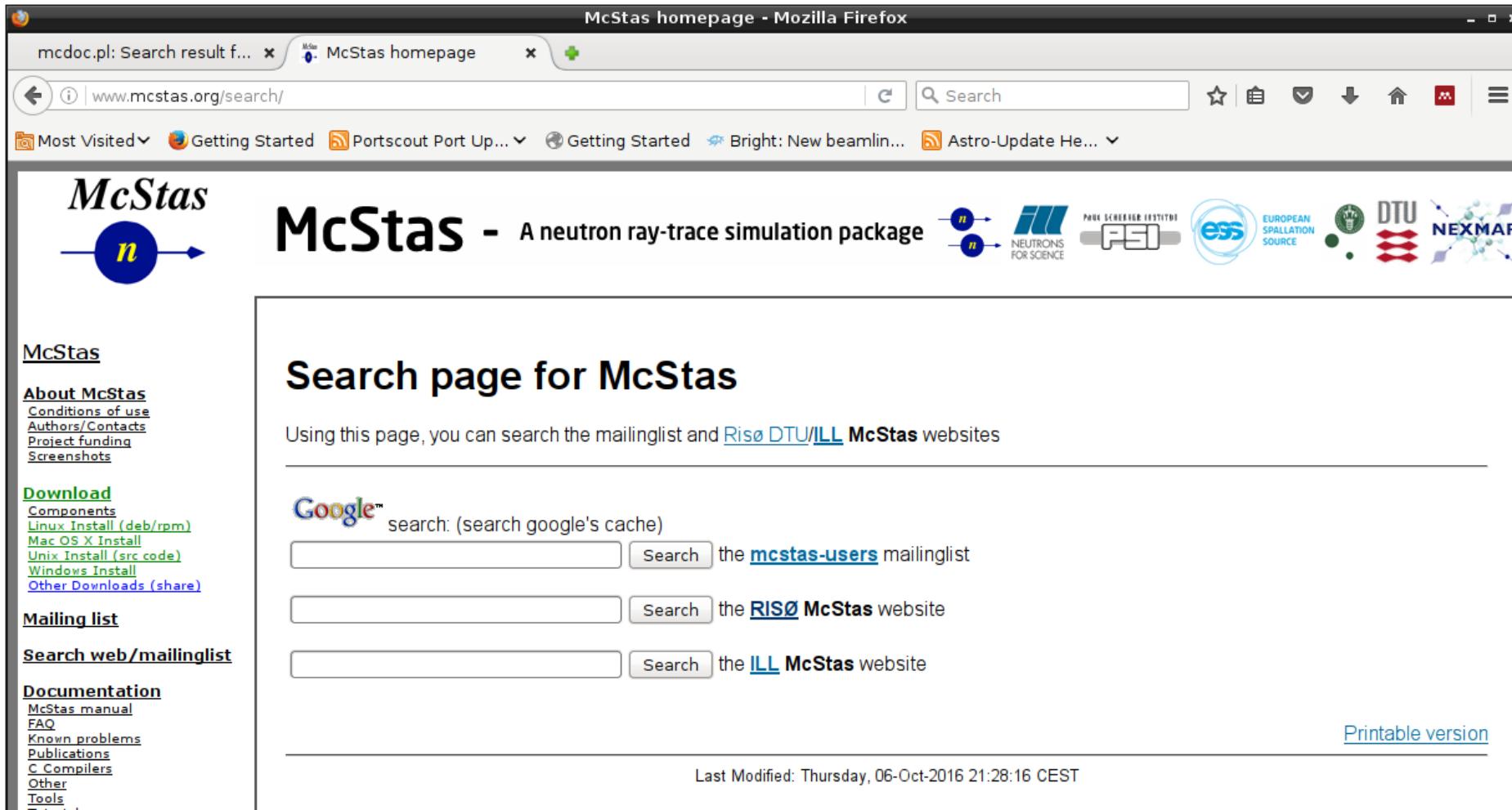
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Archive	View by:	Downloadable version
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First quarter 2017:	[ Thread ] [ Subject ] [ Author ] [ Date ]	[ Gzip'd Text 4 KB ]
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Second quarter 2016:	[ Thread ] [ Subject ] [ Author ] [ Date ]	[ Gzip'd Text 4 KB ]
First quarter 2016:	[ Thread ] [ Subject ] [ Author ] [ Date ]	[ Gzip'd Text 5 KB ]
Fourth quarter 2015:	[ Thread ] [ Subject ] [ Author ] [ Date ]	[ Gzip'd Text 12 KB ]
Third quarter 2015:	[ Thread ] [ Subject ] [ Author ] [ Date ]	[ Gzip'd Text 5 KB ]
Second quarter 2015:	[ Thread ] [ Subject ] [ Author ] [ Date ]	[ Gzip'd Text 14 KB ]
First quarter 2015:	[ Thread ] [ Subject ] [ Author ] [ Date ]	[ Gzip'd Text 13 KB ]
Fourth quarter 2014:	[ Thread ] [ Subject ] [ Author ] [ Date ]	[ Gzip'd Text 12 KB ]
Third quarter 2014:	[ Thread ] [ Subject ] [ Author ] [ Date ]	[ Gzip'd Text 13 KB ]
Second quarter 2014:	[ Thread ] [ Subject ] [ Author ] [ Date ]	[ Gzip'd Text 5 KB ]
First quarter 2014:	[ Thread ] [ Subject ] [ Author ] [ Date ]	[ Gzip'd Text 9 KB ]
Fourth quarter 2013:	[ Thread ] [ Subject ] [ Author ] [ Date ]	[ Gzip'd Text 5 KB ]
Third quarter 2013:	[ Thread ] [ Subject ] [ Author ] [ Date ]	[ Gzip'd Text 59 KB ]
Second quarter 2013:	[ Thread ] [ Subject ] [ Author ] [ Date ]	[ Gzip'd Text 12 KB ]
First quarter 2013:	[ Thread ] [ Subject ] [ Author ] [ Date ]	[ Gzip'd Text 15 KB ]
Fourth quarter 2012:	[ Thread ] [ Subject ] [ Author ] [ Date ]	[ Gzip'd Text 15 KB ]
Third quarter 2012:	[ Thread ] [ Subject ] [ Author ] [ Date ]	[ Gzip'd Text 3 KB ]
Second quarter 2012:	[ Thread ] [ Subject ] [ Author ] [ Date ]	[ Gzip'd Text 7 KB ]



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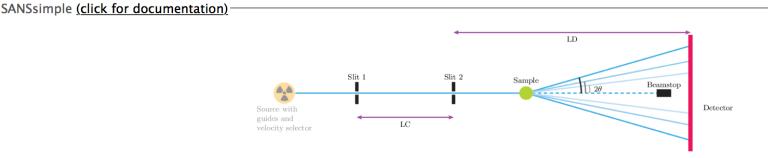


# Web interface @ e-neutrons.org

sim.e-neutrons.org

Instrument

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 [Angs]	6	Average wavelength traced from source (6)
DLambda [Angs]	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)
PHI [1]	0.01	Volumefraction of the hard, monodisperse spheres in the sample (0.01)
Delta_Rho	0.6	Volume specific scattering length density contrast of the hard, monodisperse spheres in the sample as compared to the solution (0.6)
[fm/AA^3]		
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]	1	If set, a sample of spheres or spherical shells is inserted (1)

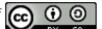
Runtime configuration

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

Start simulation run

Run

A web-based interface for **McStas**.

All contents is provided under the terms of 

sim.e-neutrons.org

SANSsimple

Completed 15:57:50, 16/12/2015

Reconfigure

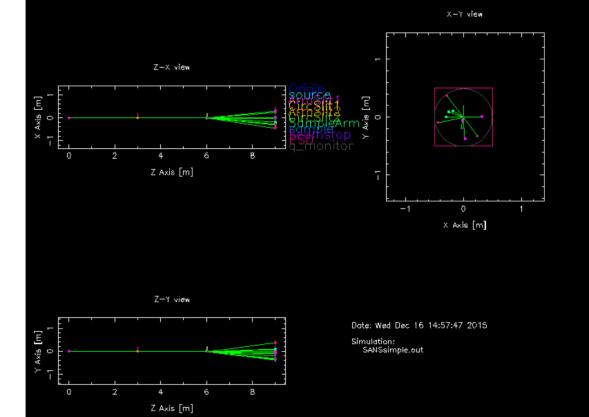
Simulation

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

neutron rays: 10000000

random seed: 0

Instrument layout



Z-X view

Z-Y view

X-Y view

Date: Wed Dec 16 14:57:47 2015

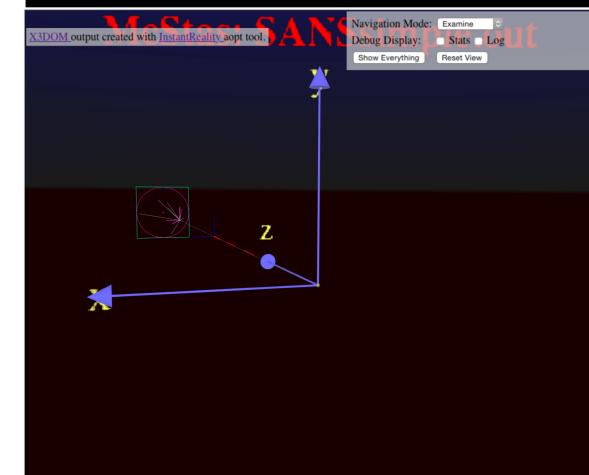
Simulation: SANSsimple.out

Navigation Mode: Examine

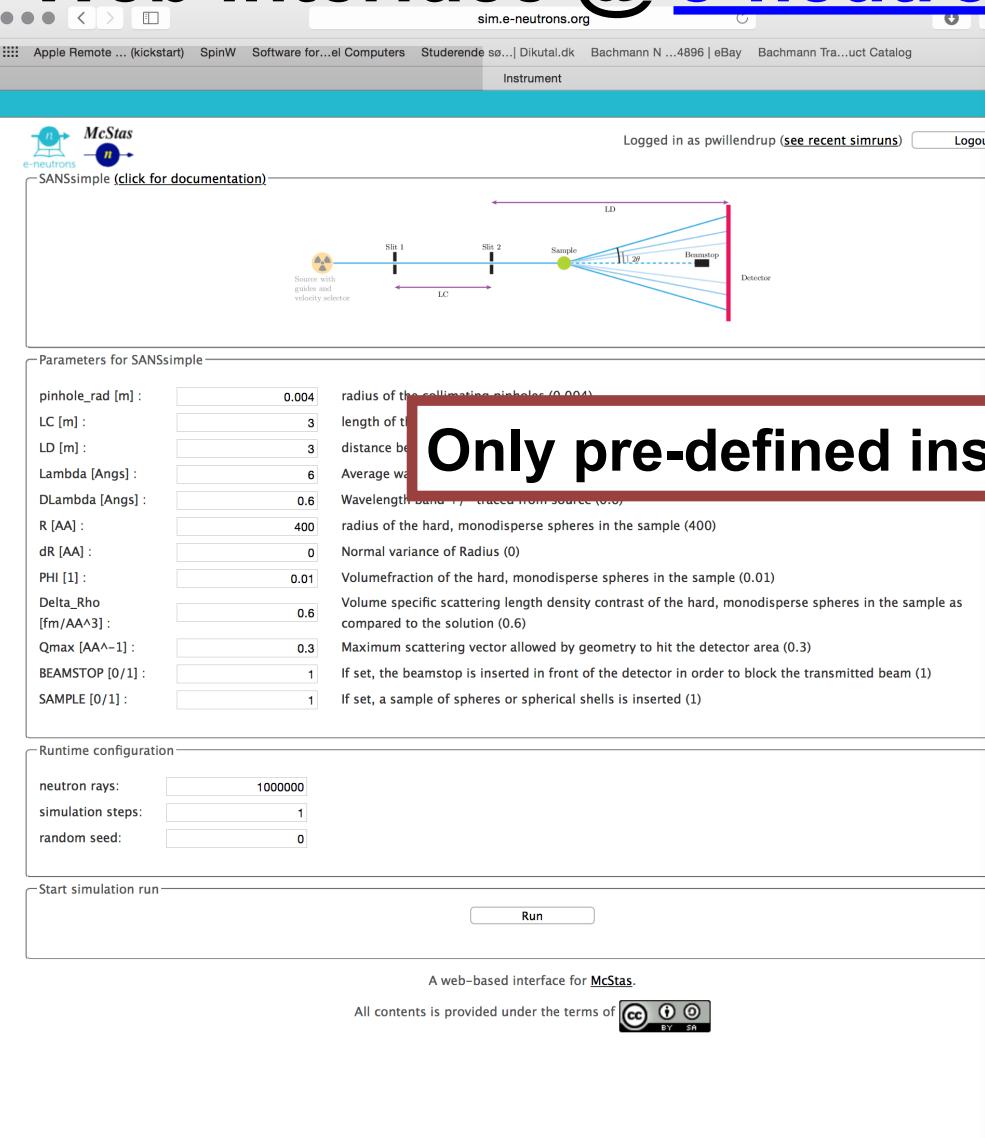
Debug Display: Stats Log

Show Everything Reset View

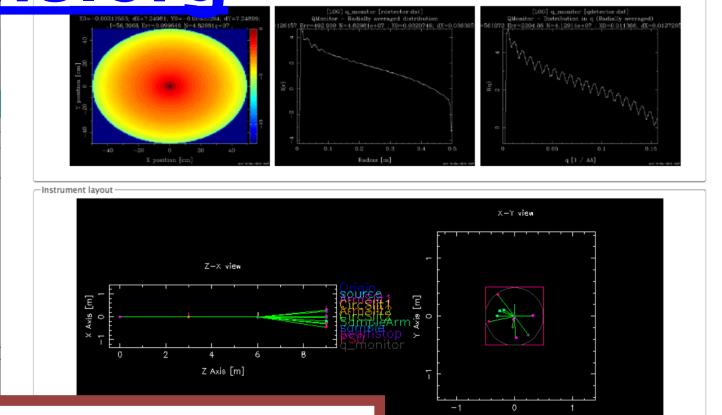
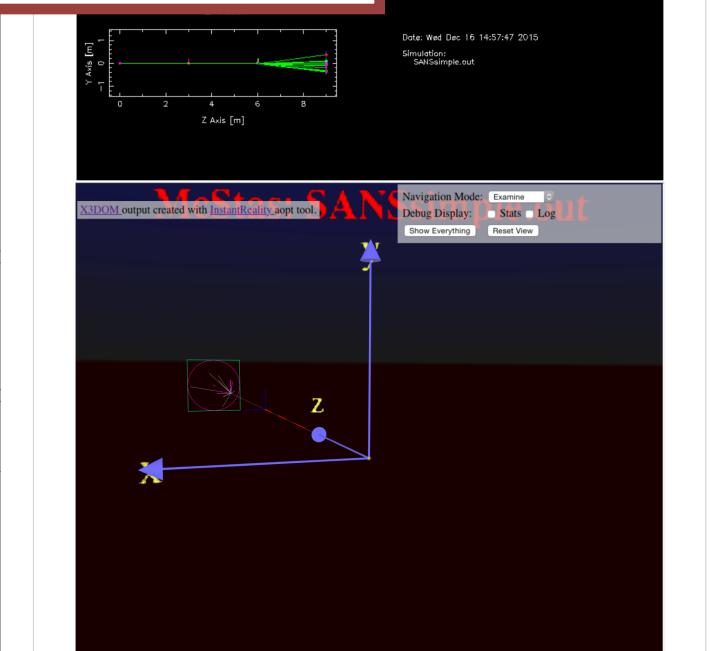
McStas SANS output



# Web interface @ e-neutrons.org



**Only pre-defined instruments!!!**

# Web i

[e-neutrons.org](https://e-neutrons.org)

FRONTPAGE ABOUT E-NEUTRONS FOR TEACHERS GET AN ACCOUNT

Username: pwillendru Password: ..... Login

## Courses

- Introduction to Neutron Scattering** High-guidance self study
- Introduction to Neutron Scattering** Open course for blended learning
- Muon Spin Spectroscopy** A course on a complementary technique to neutron scattering

**INTRODUCTION TO NEUTRON SCATTERING - SELF STUDY**  
 This course contains 10 high-guidance modules on master-level physics.  
 Each module takes approximately 10-20h to complete.

[READ MORE](#)

## Science cases

- Finding crystal structure** Chemistry of materials
- Characterising liposomes in suspension** Life sciences
- Characterising magnetic order** Magnetic and electronic phenomena

**CRYSTAL STRUCTURE**  
 Try module "Diffraction from crystalline materials" in course "Introduction to Neutron Scattering"

[READ MORE](#)

## Exercise taster

**FOURIER TRANSFORM**  
 Do you know what the scattering intensity is from a string of particles?  
 Test yourself here!

[READ MORE](#)

## Quiz taster

**NEUTRON PROPERTIES**  
 Do you know what neutrons are good for and why? Test yourself here ...

[READ MORE](#)

## Simulation taster

**SMALL ANGLE SCATTERING**  
 Do you know what the scattering pattern looks like from small particles in solution?  
 Test yourself here...

[READ MORE](#)

## 2019 CSNS McStas School

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# Web i

[e-neutrons.org](https://e-neutrons.org)

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Username: pwillendru Password: ..... Login

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- Finding crystal structure** Chemistry of materials
- Characterising liposomes in suspension**

**CRYSTAL STRUCTURE**

**Online-course on neutron scattering available!**

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**READ MORE**

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**READ MORE**

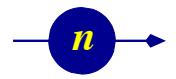
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Do you know what the scattering pattern looks like from small particles in solution?  
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**READ MORE**

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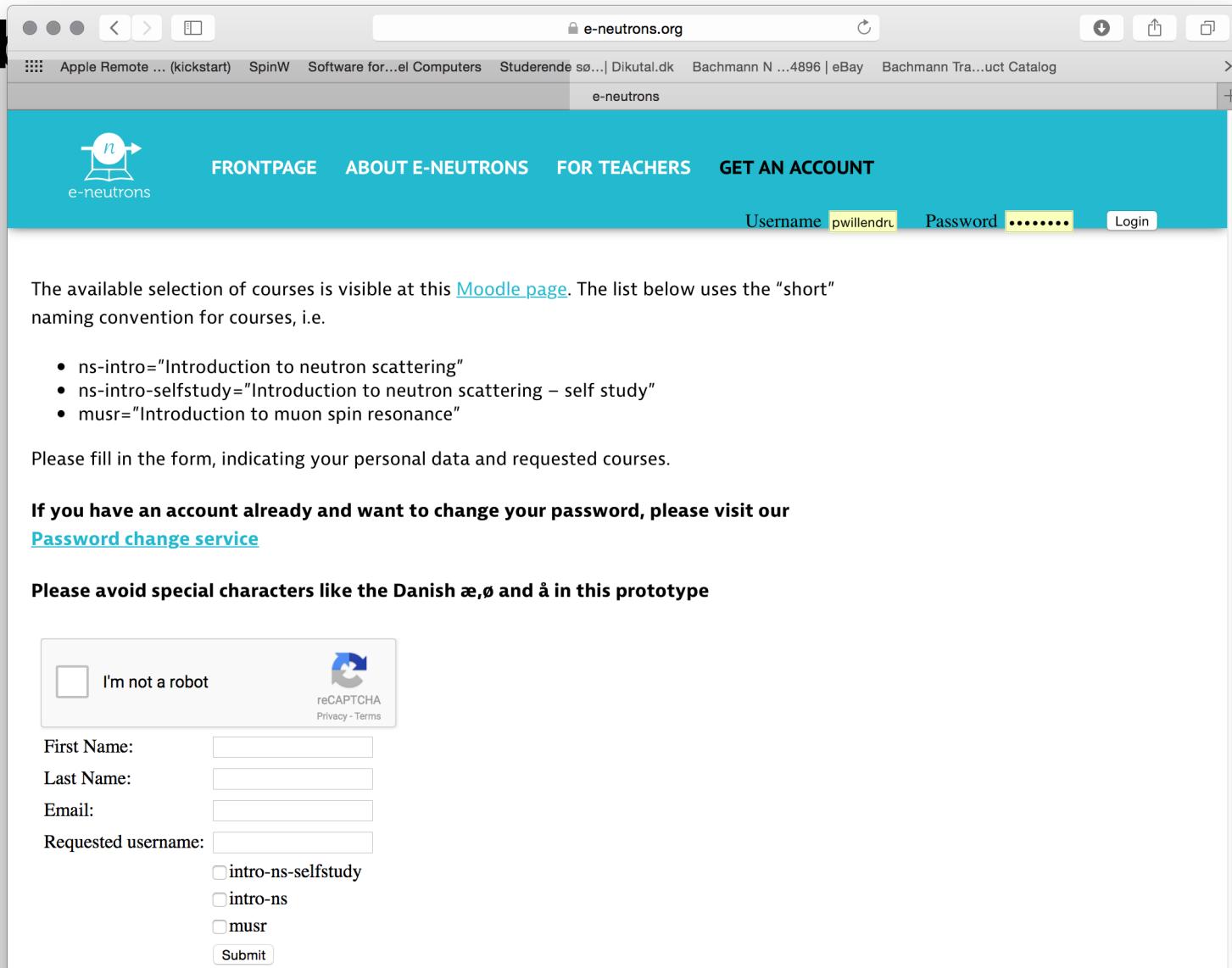

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2019 CSNS  
McStas  
School

McStas  




Welcome



The screenshot shows a web browser window for [e-neutrons.org](https://e-neutrons.org). The header includes the ESS logo and navigation links: FRONTPAGE, ABOUT E-NEUTRONS, FOR TEACHERS, and GET AN ACCOUNT. A login form is present with fields for Username (pwillendorf) and Password (redacted), and a Login button. The main content area contains text about available courses, a list of course names, and instructions for filling out a form. It also includes a reCAPTCHA and a note about avoiding Danish characters.

The available selection of courses is visible at this [Moodle page](#). The list below uses the "short" naming convention for courses, i.e.

- ns-intro="Introduction to neutron scattering"
- ns-intro-selfstudy="Introduction to neutron scattering – self study"
- musr="Introduction to muon spin resonance"

Please fill in the form, indicating your personal data and requested courses.

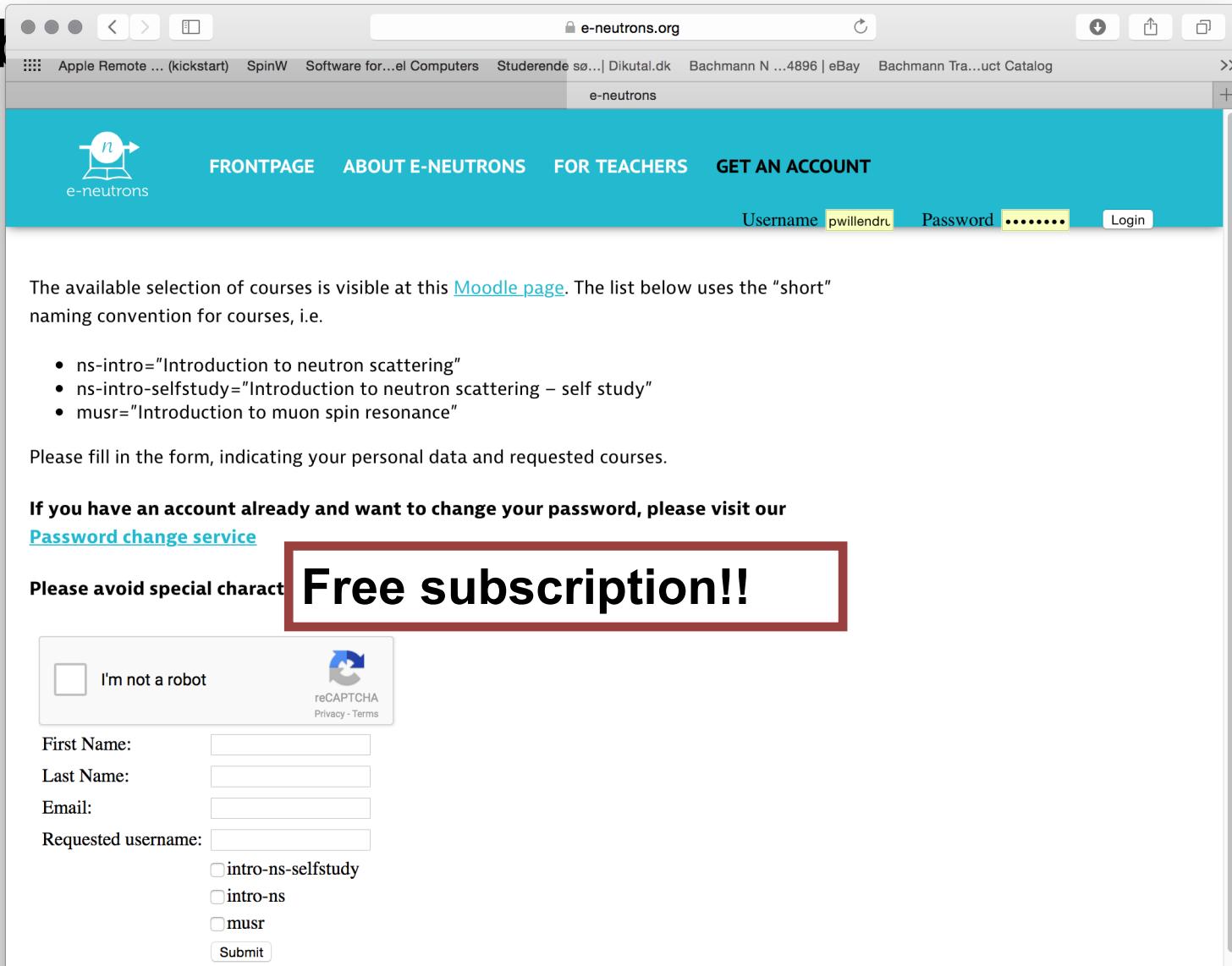
If you have an account already and want to change your password, please visit our [Password change service](#)

Please avoid special characters like the Danish æ,ø and å in this prototype

I'm not a robot  reCAPTCHA Privacy - Terms

First Name:   
Last Name:   
Email:   
Requested username:   
 intro-ns-selfstudy  
 intro-ns  
 musr

Welcome



The screenshot shows a web browser window for [e-neutrons.org](https://e-neutrons.org). The header includes the ESS logo and navigation links for FRONTPAGE, ABOUT E-NEUTRONS, FOR TEACHERS, and GET AN ACCOUNT. A login form is present with fields for Username (pwillendr) and Password (redacted), and a Login button. The main content area contains text about available courses via a Moodle page and a list of course names:

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- ns-intro-selfstudy="Introduction to neutron scattering – self study"
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It also instructs users to fill in a form for personal data and requested courses, and provides a link to a password change service. A large red box highlights the text "Please avoid special characters" and "Free subscription!!". A reCAPTCHA verification box is at the bottom left.

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Please avoid special characters

**Free subscription!!**

I'm not a robot  reCAPTCHA  
Privacy - Terms

First Name:

Last Name:

Email:

Requested username:

intro-ns-selfstudy

intro-ns

musr