

McStas do's and don'ts

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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!

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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...

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)
- 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 → E. Knudsen

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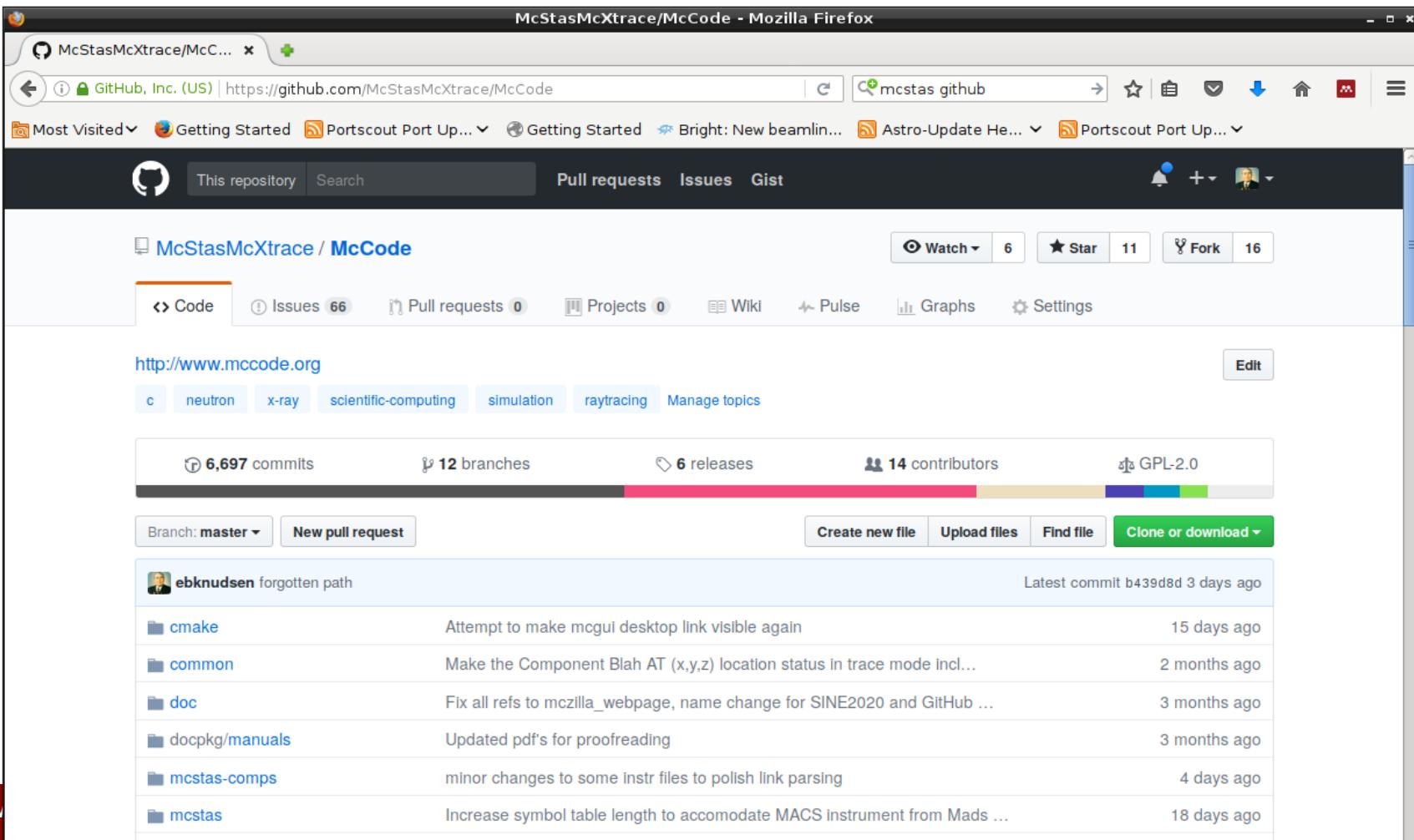
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源

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



McStasMcXtrace/McCode - Mozilla Firefox

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

This repository Search Pull requests Issues Gist

Watch 6 Star 11 Fork 16

McStasMcXtrace / McCode

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

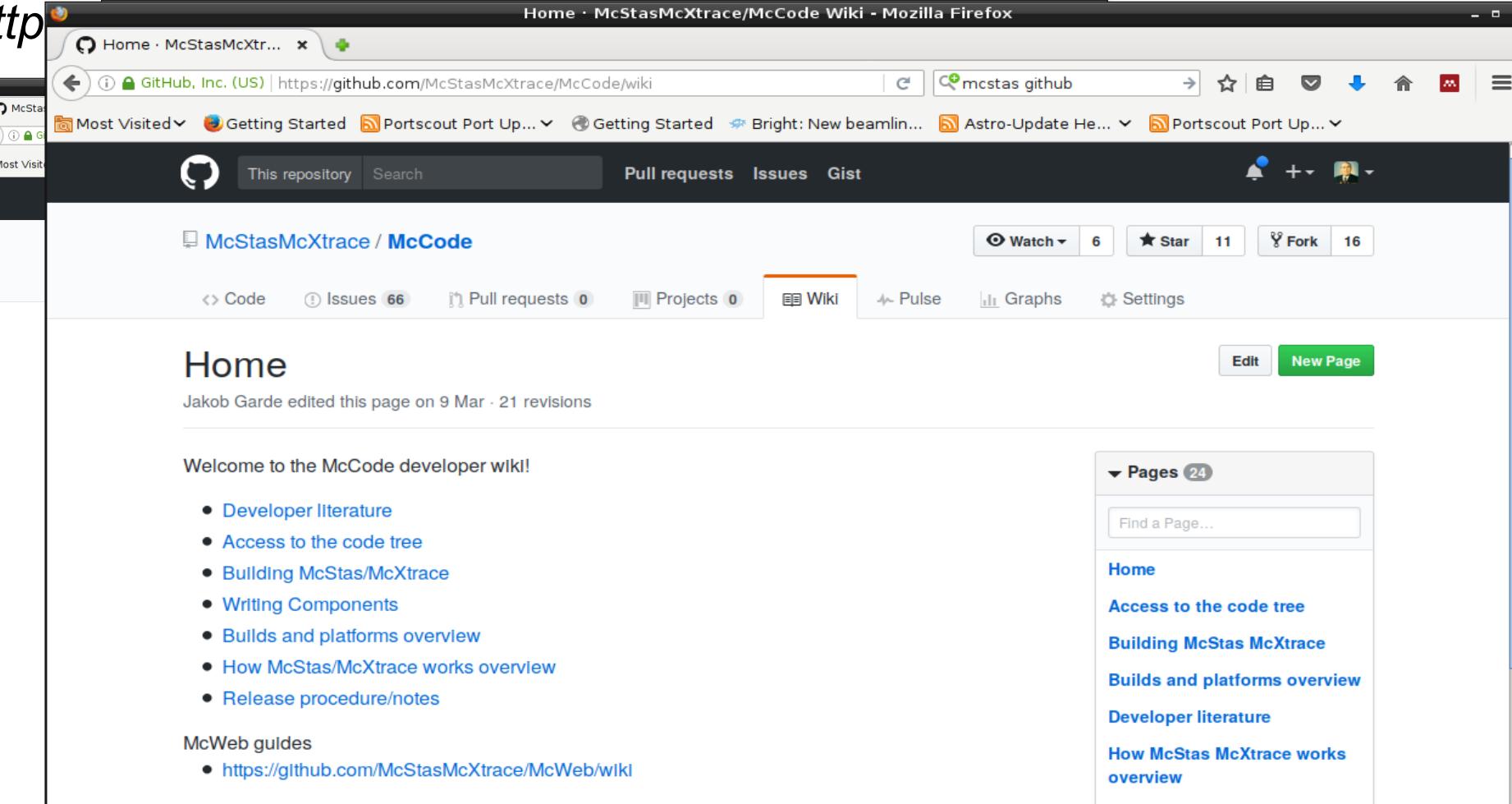
docpkg/manuals Updated pdf's for proofreading 3 months ago

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

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

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

Pages 24

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

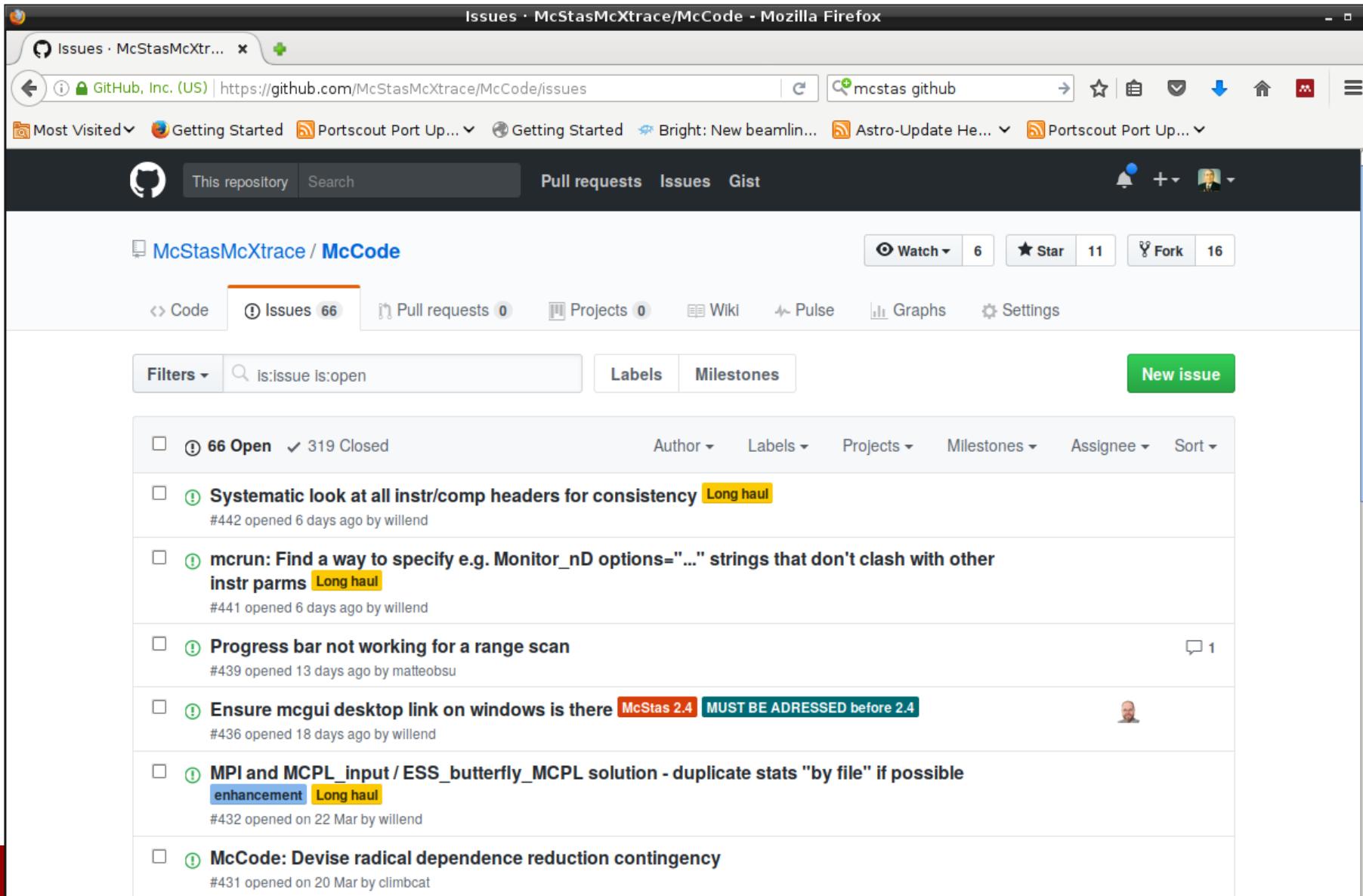
GitHub.com: Issue Tracker



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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

McStas homepage - Mozilla Firefox

mcdoc.pl: Search result f... | McStas homepage | +

|   www.mcstas.org/list/ |  Search |      

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

McStas



McStas - A neutron ray-trace simulation package



mcstas-users mailing list

To subscribe to mcstas-users, fill in your email address and press subscribe:

To access the mailing list interface, go to <http://mailman.mcstas.org/cgi-bin/mailman/listinfo/mcstas-users>

To access archived messages, go to <http://mailman.mcstas.org/pipermail/mcstas-users>.

New: Search capability has now been [added](#) to the website!

[Printable version](#)

Last Modified: [Printable version](#)

Last Modified: Thursday, 12-Jun-2008 12:57:22 CEST

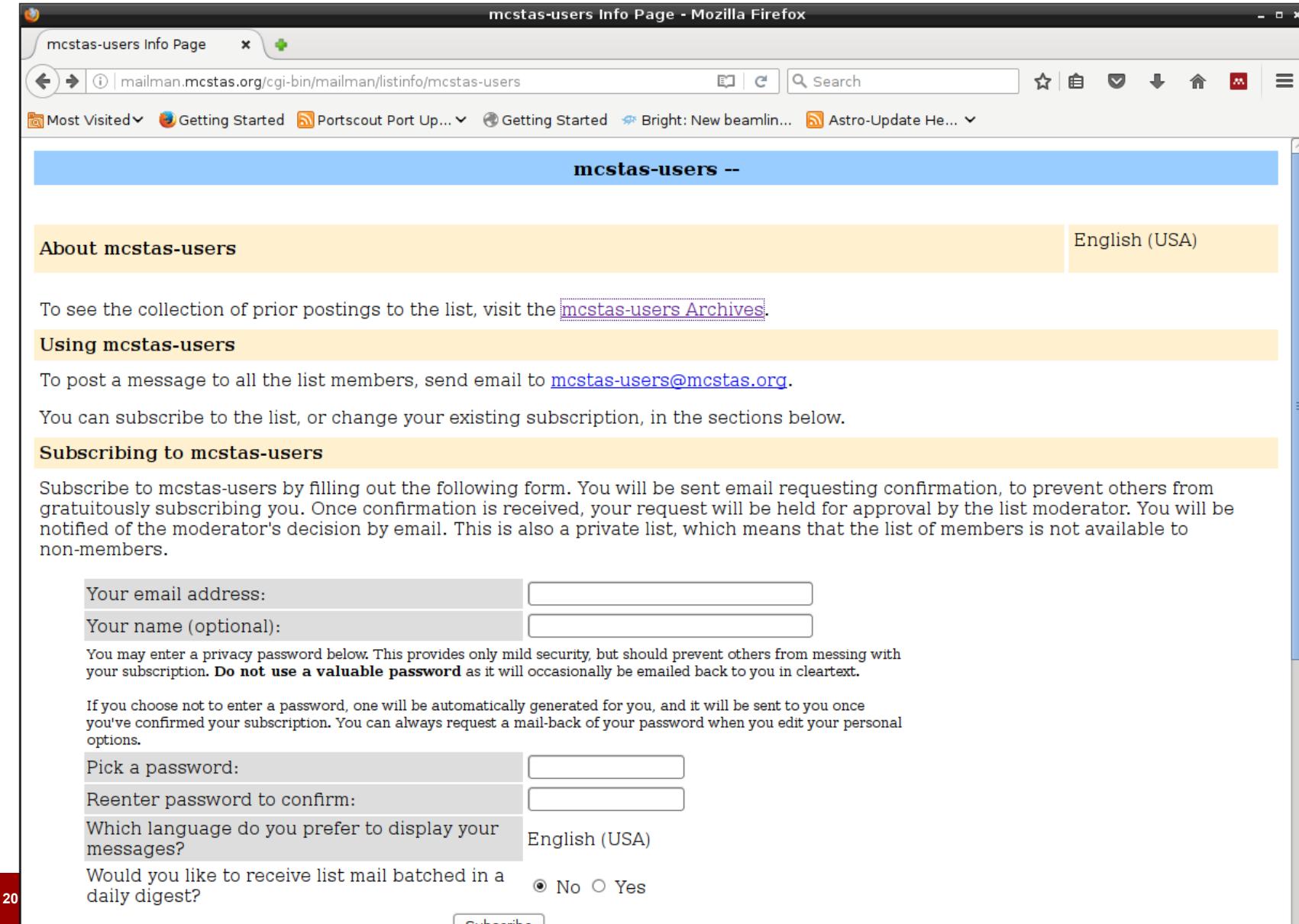
Mailing List



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

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mcstas-users --

About mcstas-users

To see the collection of prior postings to the list, visit the [mcstas-users Archives](#).

Using mcstas-users

To post a message to all the list members, send email to mcstas-users@mcstas.org.

You can subscribe to the list, or change your existing subscription, in the sections below.

Subscribing to mcstas-users

Subscribe to mcstas-users by filling out the following form. You will be sent email requesting confirmation, to prevent others from gratuitously subscribing you. Once confirmation is received, your request will be held for approval by the list moderator. You will be notified of the moderator's decision by email. This is also a private list, which means that the list of members is not available to non-members.

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)

Would you like to receive list mail batched in a daily digest? No Yes

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The mcstas-users Archives

You can get [more information about this list](#).

Archive	View by:	Downloadable version
Second quarter 2017:	[Thread] [Subject] [Author] [Date]	[Gzip'd Text 481 bytes]
First quarter 2017:	[Thread] [Subject] [Author] [Date]	[Gzip'd Text 4 KB]
Fourth quarter 2016:	[Thread] [Subject] [Author] [Date]	[Gzip'd Text 7 KB]
Third quarter 2016:	[Thread] [Subject] [Author] [Date]	[Gzip'd Text 6 KB]
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]

User forum and help since 1997!!

Spirit of the mailinglist:

- Very friendly and open!
- There is **no such thing** as a stupid question!
- Often answers are given from McStas users rather than the developers, especially in areas that include very specific domain science.
- contact: mcstas-users@mcstas.org

<http://csns2019.mcstas.org>



CSNS 2019 (March) McStas link page!

McStas

$n \rightarrow$ DTU ess
EUROPEAN SPALLATION SOURCE

SNS

中国散裂中子源
China Spallation Neutron Source



通知			
序号	日期/时间	会议地点	会议名称
01	3月25日 09:00	104	McStas Training School
02	3月25日 14:00	316	讨论会
03	3月25日 15:00	102	面试

2019年03月25日 星期一 16时25分19秒

Links for the 2019 CSNS McStas school

- Presentations and Exercise instructions from the school are [available through GitHub](#) <---

OVF based virtual machine can be downloaded [here](#)

Agenda

(bigger view by [clicking here](#))

Useful links below....



<http://csns2019.mcstas.org>

Get the code, report bugs etc.

- [McStas website](#)
- [McStas mailinglist subscription](#) (Please enrol!)
- [McStas Facebook page](#) (Please follow us!)
- [McStas downloads](#)
- [McStas+McXtrace GitHub](#)
- [McStas+McXtrace issues + bug reporting](#)

Neutron scattering + McStas e-learning

- [e-neutrons](#) website (free enrolment)

Tutorials, howto's, docs

- [How McStas works - in 2 minutes](#)
- [Tutorial: Build a SANS](#)
- [McStas user manual](#) - Better use `mcdoch -m` in the terminal!
- [McStas component manual](#) - Better use `mcdoch -c` in the terminal!
- [McStas component docs](#) - Better use `mcdoch` in the terminal!
- [McStas sample model functionality matrix](#) (not fully up to date)
- [McStas and McXtrace GitHub wiki](#) - tutorials, guides and more
- [User documentation for the 2017- Python tool set](#)
- [mcrun variants - table overview](#)
- [mcplot variants - table overview](#)
- [mcdisplay variants - table overview](#)

ESS specific McStas docs

- [McStas space on ESS confluence](#)
- [Running McStas on the ESS DMSC cluster](#) - plus general DMSC cluster info
- [MCPL input to describe the ESS source](#)
- ['Benchmarking' website for the ESS butterfly component](#)

Material from earlier schools

- [Dropbox with material from 2-day workshop event at ORNL, October 2018](#)
- [Dropbox with materials from the 5-day MDANSE2018 workshop event in Puerto de la Cruz, Tenerife, Spain](#)
- [Material from ESS DMSC McStas workshop June 2018](#)
- [Website and materials from a 3-day STFC event \(including public Dropbox link to presentations etc.\)](#)
- [Website and materials from a 3-day ESS event \(including public Dropbox link to presentations etc.\)](#)
- [Website and materials from a 2-day NOBUGS event \(including public Dropbox link to presentations etc.\)](#)
- [Dropbox with materials from a 5-day event in Bariloche, Argentina](#)

Useful links below....

(Older schools currently
DropBox, will transport
these to GitHub soon!)



You are of course also very welcome to contact us directly:

Mads Bertelsen: mads.bertelsen@esss.se

Erik B Knudsen: erkn@fysik.dtu.dk

Peter K Willendrup: pkwi@fysik.dtu.dk