McXtrace

FAQ, advanced grammar, tips and tricks

Peter Willendrup (pkwi@fysik.dtu.dk)

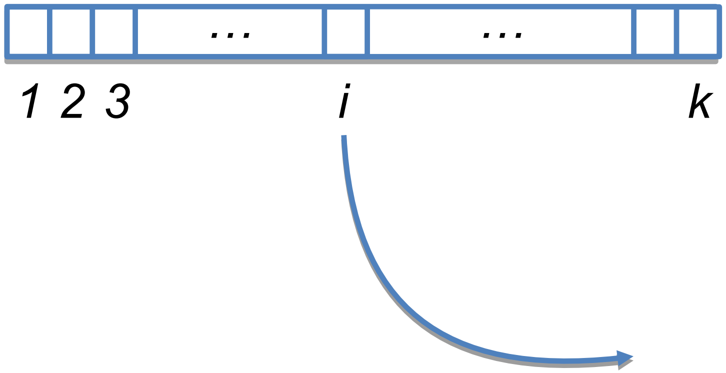
What is really the information content…?

- McXtrace sources generally provide “intensity” in units of photons/s (into a chosen solid angle)

- That intensity is carried through the instrument on a discrete set of “X-ray rays”

In a histogram sense

- Imagine a histogram, e.g. I(λ)



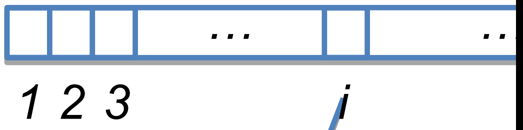
In bin i, N events each carrying a fractional intensity p_j so that

$$I = \sum_N p_j$$

- The RMS variance over that set becomes our statistical error bar *E*

In a histogram sense

Imagine a histogram, e.g. I(



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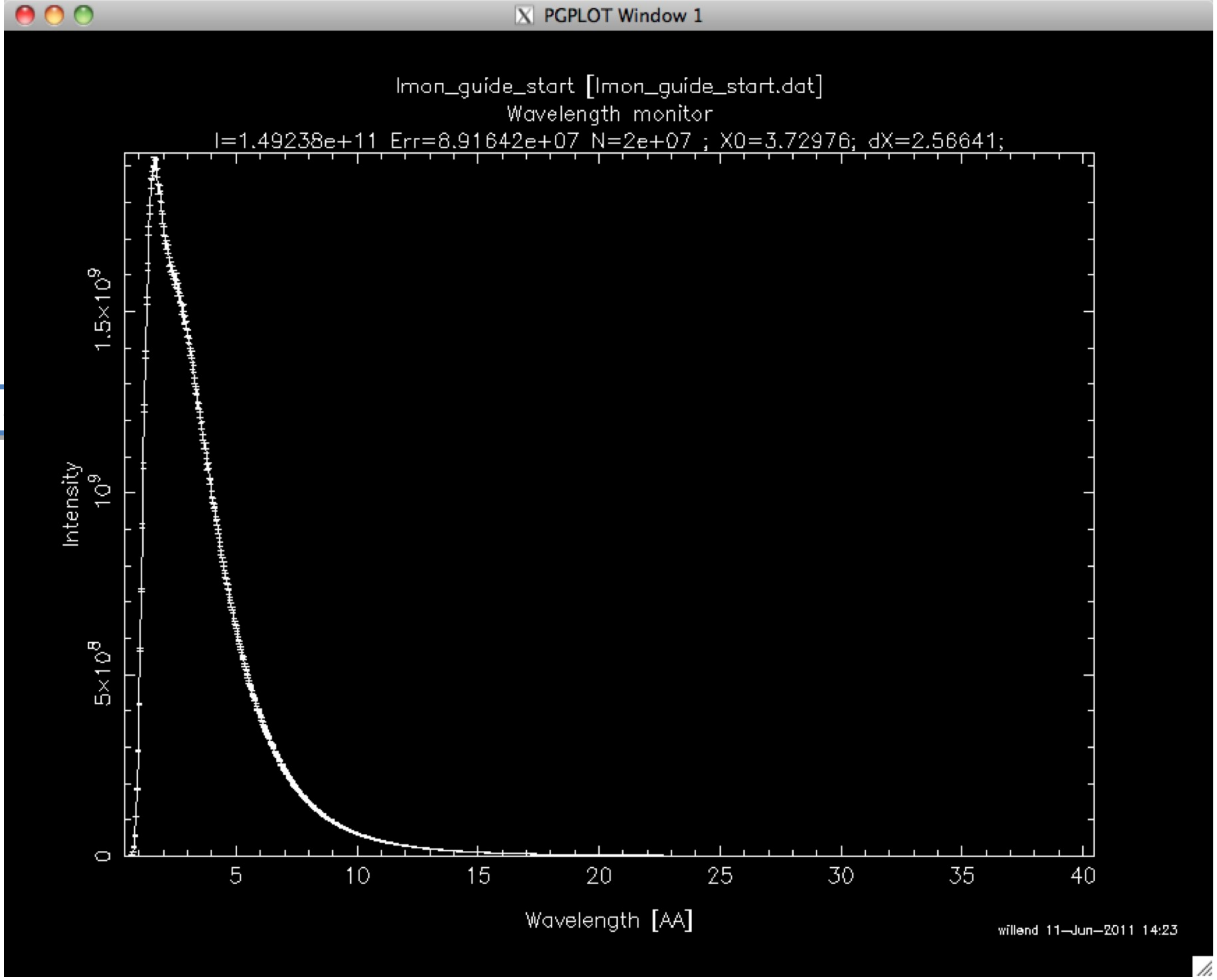
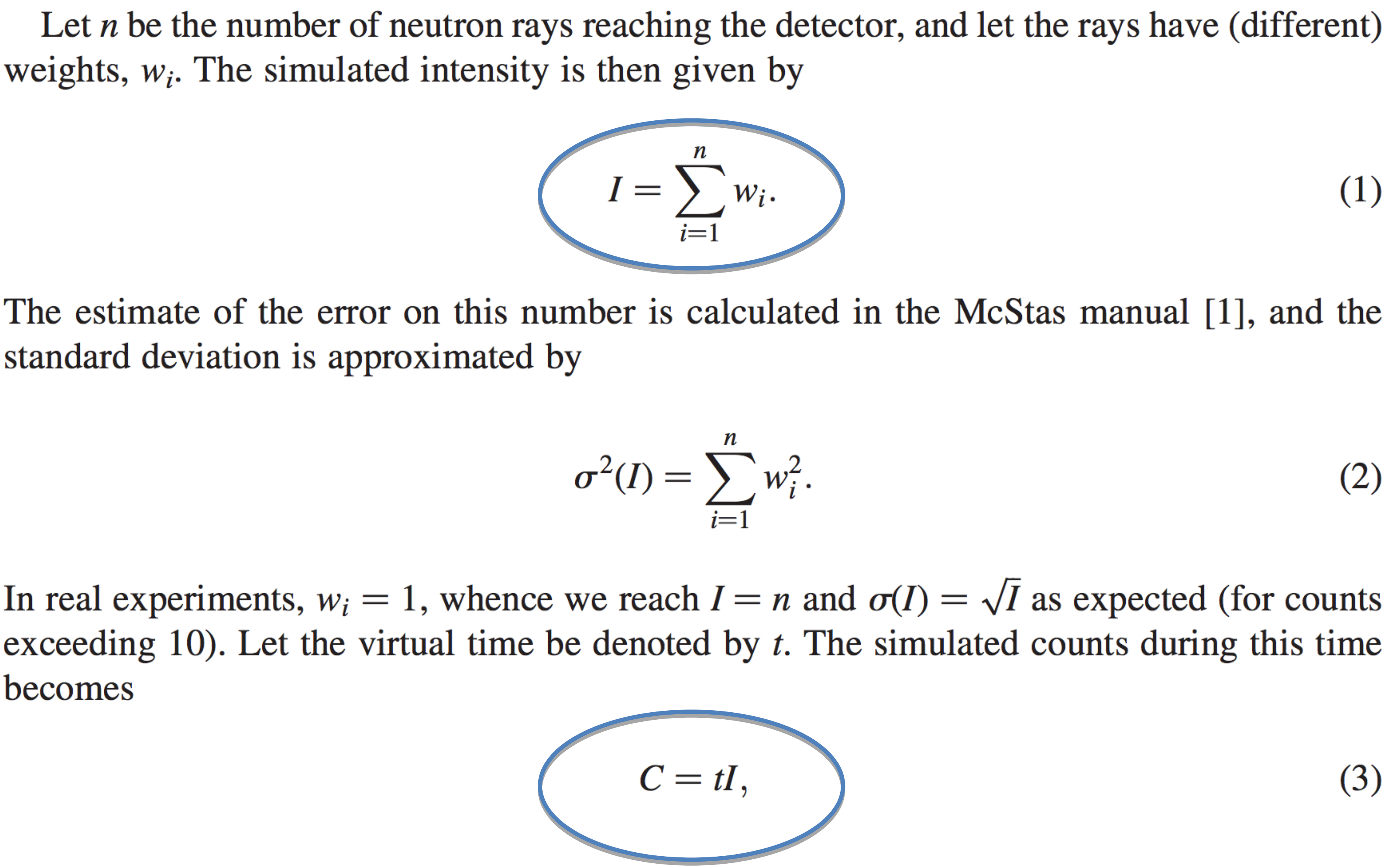


PGPLOT Window 1

Imon_guide_start [Imon_guide_start.dat]
Wavelength monitor
I=1.49238e+11 Err=8.91642e+07 N=2e+07 ; X0=3.72976; dX=2.56641;

The RMS variance over that set becomes our statistical error bar *E*

From "Virtual experiments - the ultimate aim of neutron ray-tracing simulations", K. Lefmann et al., Journal of Neutron Research 16, 97-111 (2008)



Let n be the number of neutron rays reaching the detector, and let the rays have (different) weights, w_i. The simulated intensity is then given by

$$\boxed{I = \sum_{i=1}^{n} w_i.} \tag{1}$$

The estimate of the error on this number is calculated in the McStas manual [1], and the standard deviation is approximated by

$$\sigma^2(I) = \sum_{i=1}^{n} w_i^2. \tag{2}$$

In real experiments, $w_i = 1$, whence we reach $I = n$ and $\sigma(I) = \sqrt{I}$ as expected (for counts exceeding 10). Let the virtual time be denoted by t. The simulated counts during this time becomes

$$\boxed{C = tI,} \tag{3}$$

From "Virtual experiments - the ultimate aim of neutron ray-tracing simulations", K. Lefmann et al., Journal of Neutron Research 16, 97-111 (2008)

and its error bar estimate is

$$\sigma^2(C) = t^2\sigma^2(I). \tag{4}$$

However, to simulate a realistic counting statistics, we must fulfill

$$\sigma_{\mathrm{VE}}(C_{\mathrm{VE}}) = \sqrt{C_{\mathrm{VE}}}. \tag{5}$$

This is obtained by adding to (3) a Gaussian noise $E(\Sigma)$ of mean value zero and standard deviation Σ:

$$C_{\mathrm{VE}} = tI + E(\Sigma). \tag{6}$$

The standard deviation for the VE becomes

$$\sigma^2_{\mathrm{VE}}(C) = t^2\sigma^2(I) + \Sigma^2. \tag{7}$$

Now, the requirement (5) allows us to determine Σ:

$$\Sigma^2 = tI - t^2\sigma^2(I). \tag{8}$$

Since Σ^2 must remain positive, we reach an upper limit on t

$$\boxed{t_{\max} = \frac{I}{\sigma^2(I)}.} \tag{9}$$

Sketch of an algorithm…

1. On a given McXtrace histogram

2. For the non-zero bins, calculate $$t_{\max} = \frac{I}{\sigma^2(I)}.$$

3. The *smallest* $t_{\mathtt{max}}$ defines the “maximal counting time” allowed by your statistics

4. Preferably a “background” should be added - use a “known experimental value” or an estimate…

Important points to remember

1. Your simulation will only contain elements you provided / defined

2. … to the precision you defined

3. Answers the questions you posed

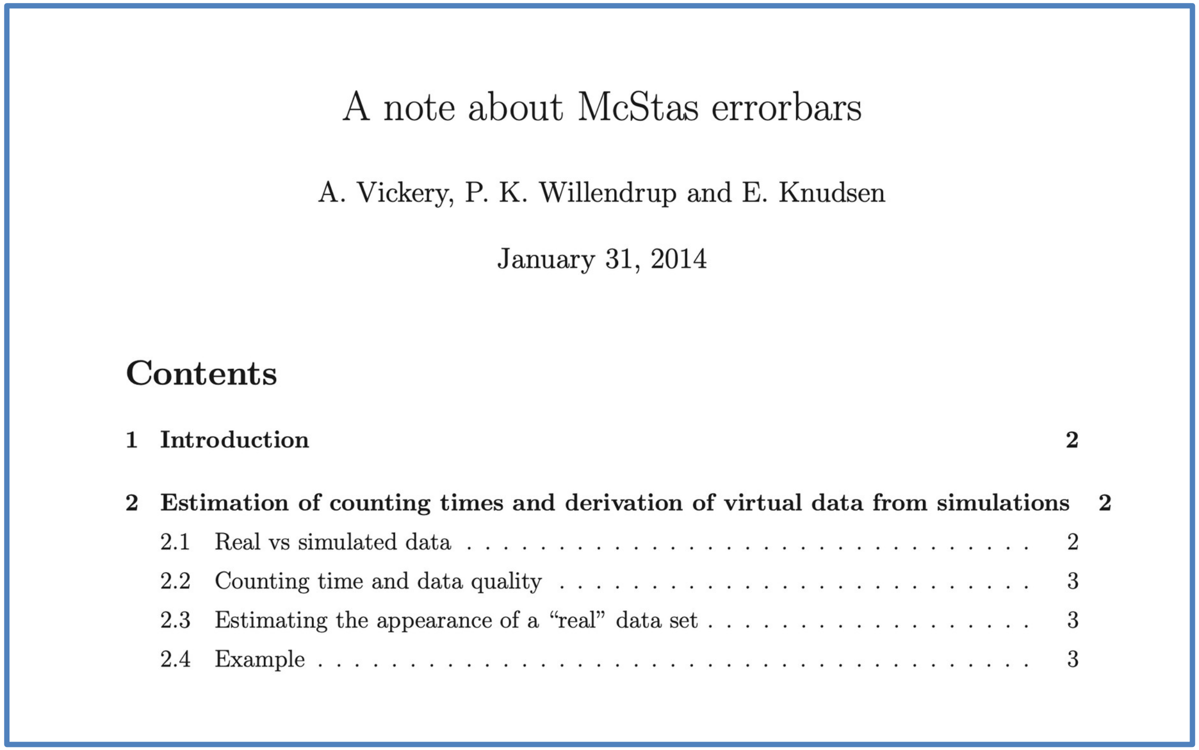
4. Background essentially only from “sample”, or sample-near objects

Errorbars → maximum “integration time”

McXtrace

Lefmann, K., Willendrup, P. K., Udby, L., Lebech, B., Mortensen, K., Birk, J. O., ... Farhi, E. (2008). *Virtual experiments: the ultimate aim of neutron ray-tracing simulations.* Journal of Neutron Research, 16(4-4), 97. https://doi.org/10.1080/10238160902819684

Plus the attached note from Annette Vickery (also true for photons):



A note about McStas errorbars

A. Vickery, P. K. Willendrup and E. Knudsen

January 31, 2014

Contents

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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- Alternatively use MCPL o/i which allows repetition - beware of biases!

All of this can be considered "variance reduction"

or biasing

Onto efficiency…

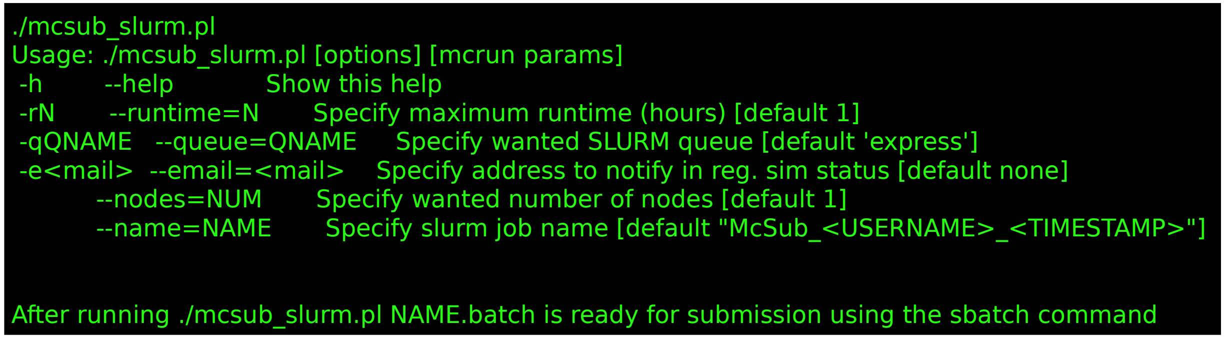
- Use MPI parallelisation - included in macOS install, easy to get on Linux…

- 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 cluster 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 “mxrun commandline”

- Writes batch file “template” for use with PBS or slurm cluster queue systems

- https://github.com/McStasMcXtrace/McCode/tree/master/tools/cluster-scripts

Examples Directory

- *Simple grep →*
  - *25 examples of Monitor_nD*
  - *4 examples of Source_lab*
  - *4 examples of Undulator*
  - *5 examples of PowderN*

Unix/Linux:

*grep Monitor_nD /usr/share/mcxtrace/1.7/examples/**

Examples Directory

- *Simple grep →*

They have an author name!

For instance:

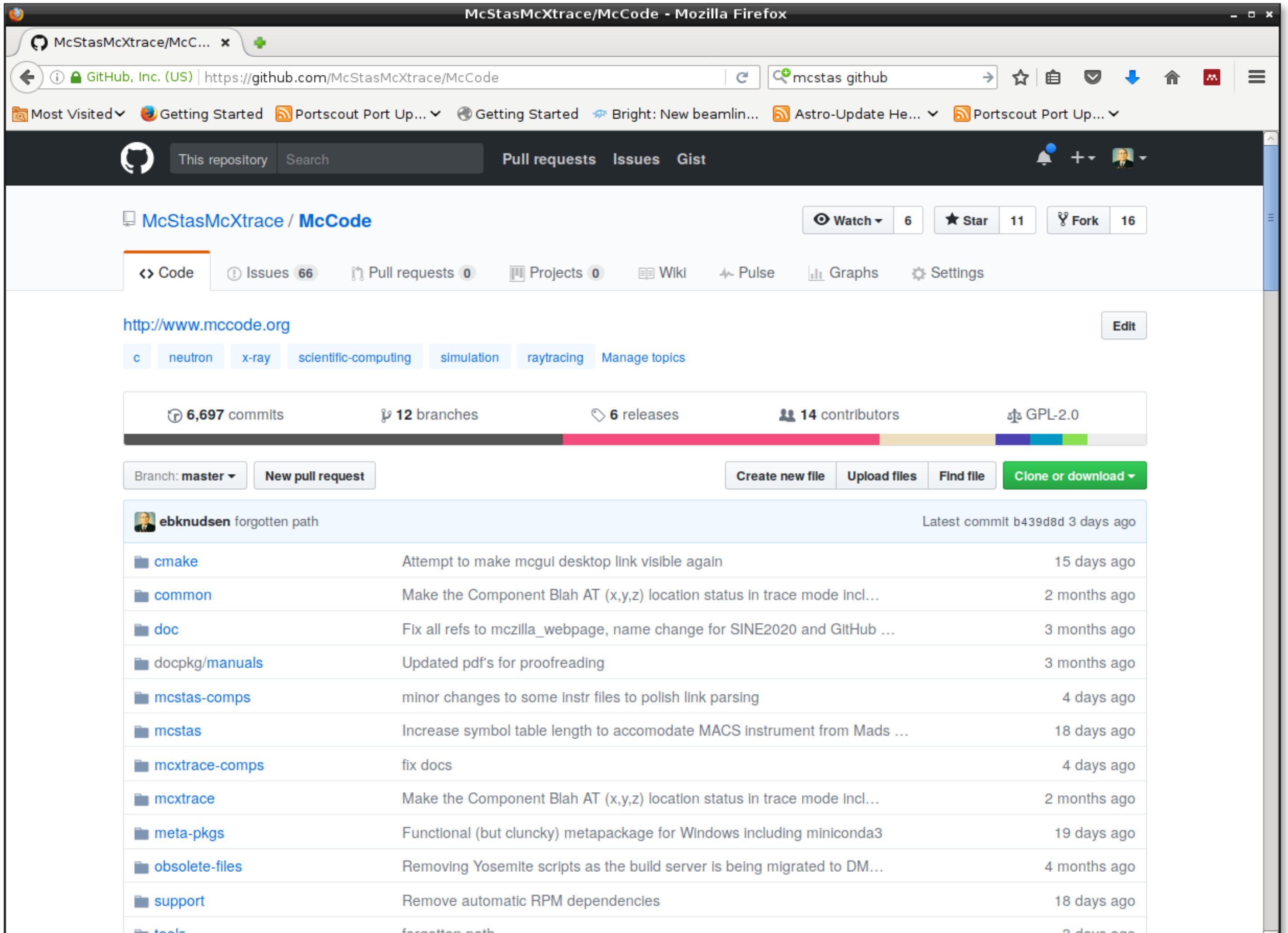
DBD_IBM_Si_analyzer → Marcus H. Mendenhall

Test_SX → E. Farhi

Pump_probe → E. Knudsen

GitHub.com

https://github.com/McStasMcXtrace/McCode



McStasMcXtrace / **McCode**

http://www.mccode.org

c · neutron · x-ray · scientific-computing · simulation · raytracing

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

ebknudsen forgotten path — Latest commit b439d8d 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
mcxtrace-comps	fix docs	4 days ago
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meta-pkgs	Functional (but cluncky) metapackage for Windows including miniconda3	19 days ago
obsolete-files	Removing Yosemite scripts as the build server is being migrated to DM…	4 months ago
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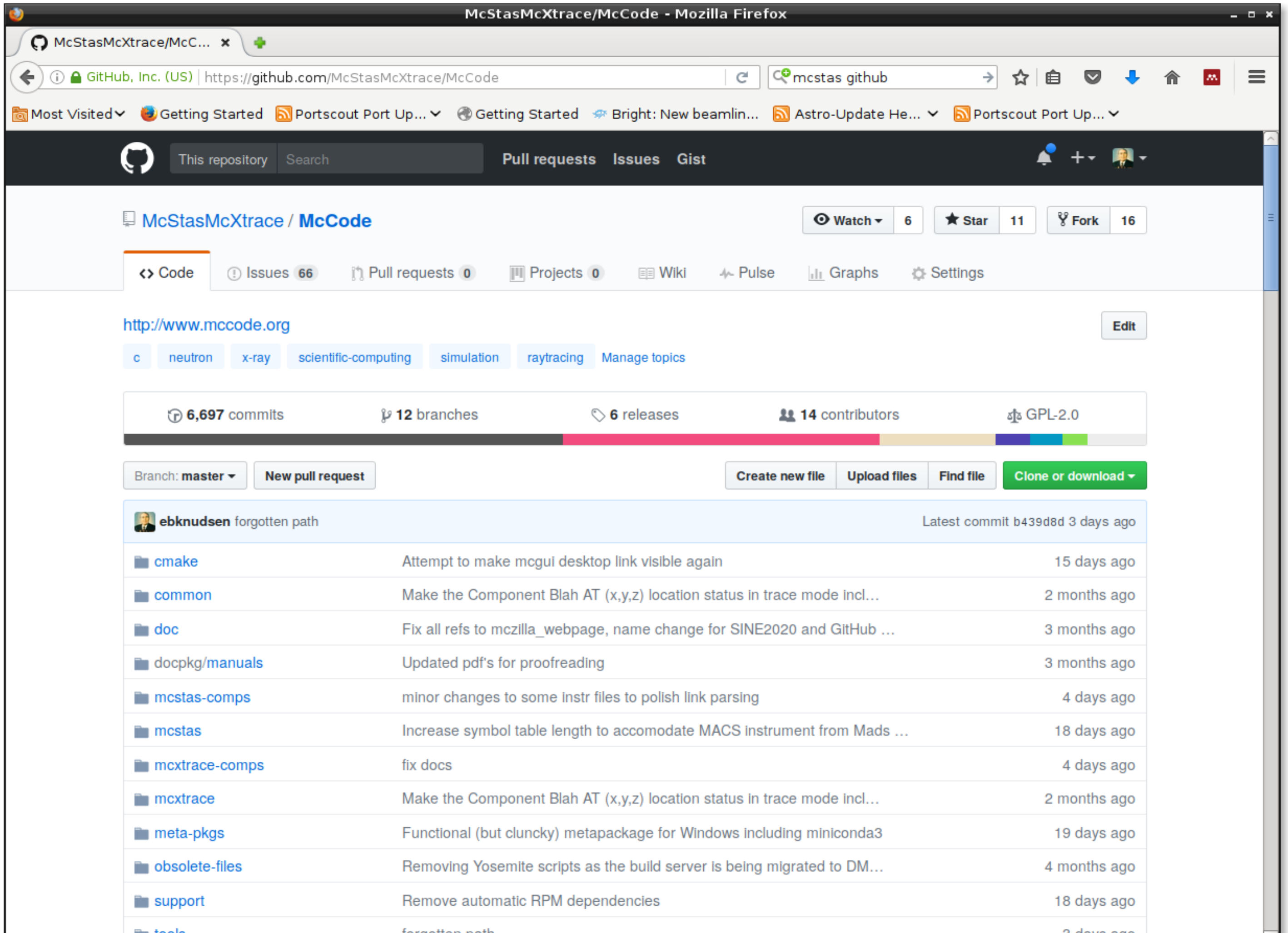
GitHub.com

https://github.com/McStasMcXtrace/McCode



McStasMcXtrace / **McCode**

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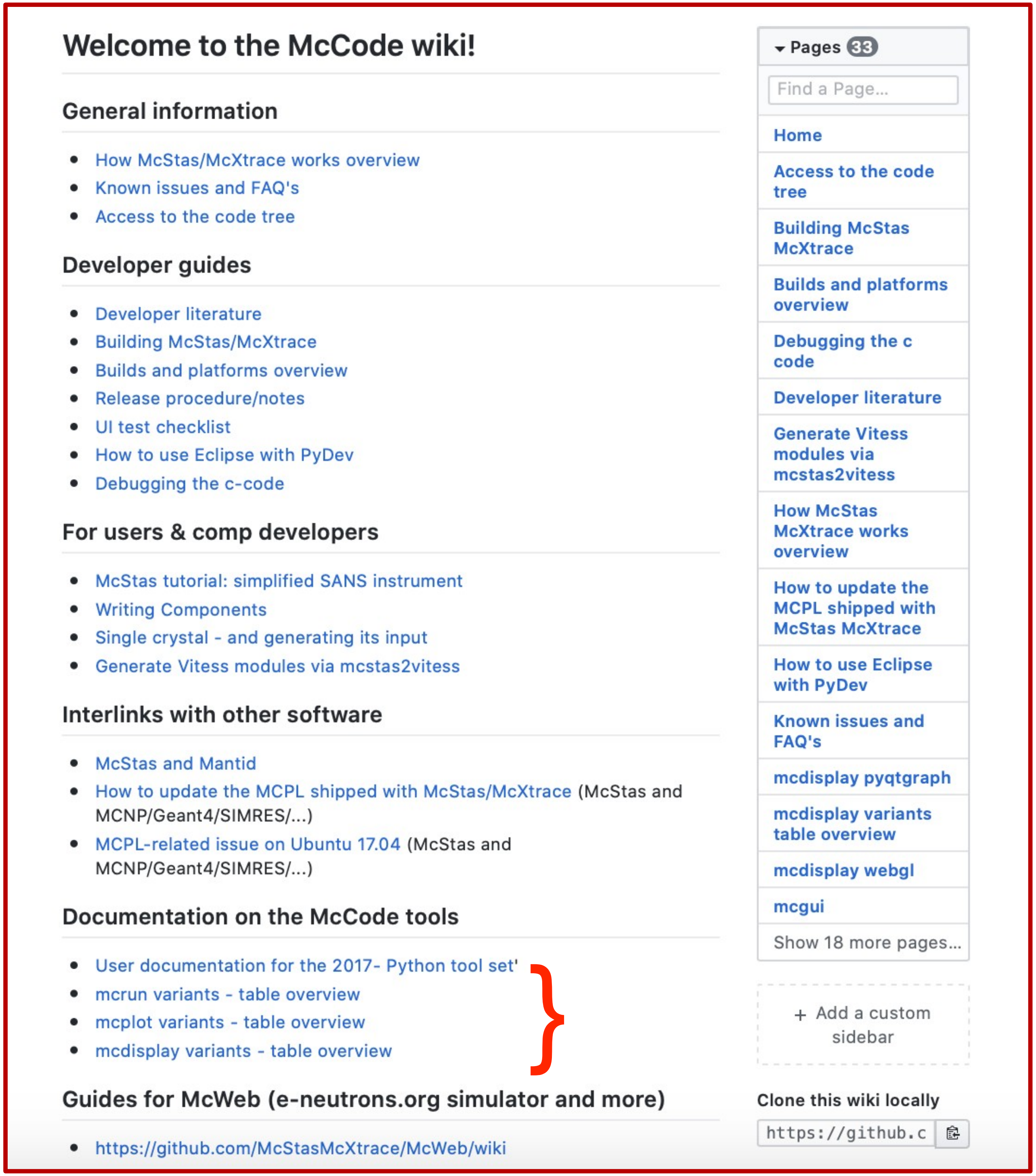
GitHub.com: wiki   User- and developer docs



Welcome to the McCode wiki!

General information

- How McStas/McXtrace works overview
- Known issues and FAQ's
- Access to the code tree

Developer guides

- Developer literature
- Building McStas/McXtrace
- Builds and platforms overview
- Release procedure/notes
- UI test checklist
- How to use Eclipse with PyDev
- Debugging the c-code

For users & comp developers

- McStas tutorial: simplified SANS instrument
- Writing Components
- Single crystal - and generating its input
- Generate Vitess modules via mcstas2vitess

Interlinks with other software

- McStas and Mantid
- How to update the MCPL shipped with McStas/McXtrace (McStas and MCNP/Geant4/SIMRES/...)
- MCPL-related issue on Ubuntu 17.04 (McStas and MCNP/Geant4/SIMRES/...)

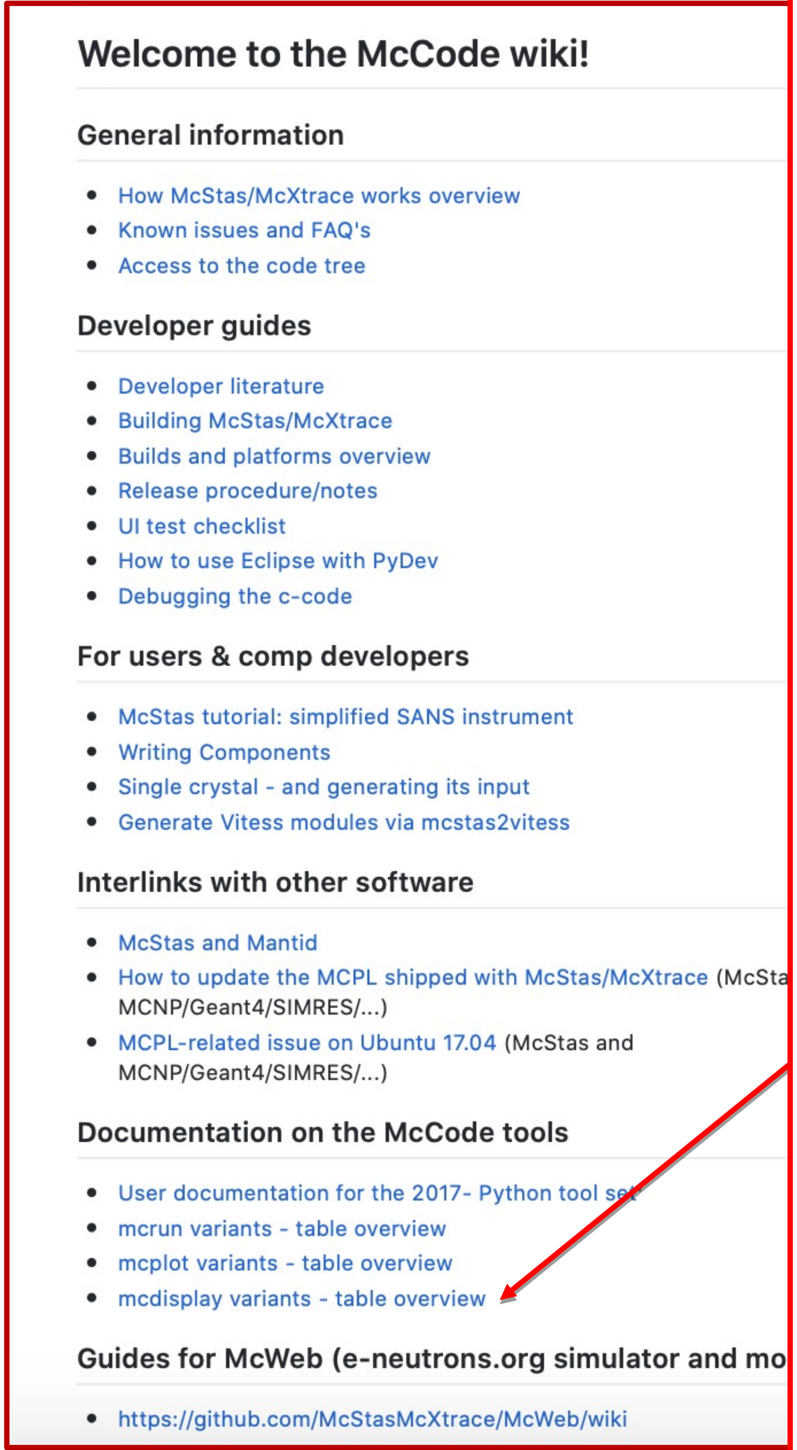
Documentation on the McCode tools

- User documentation for the 2017- Python tool set'
- mcrun variants - table overview
- mcplot variants - table overview
- mcdisplay variants - table overview

Guides for McWeb (e-neutrons.org simulator and more)

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

GitHub.com: wi



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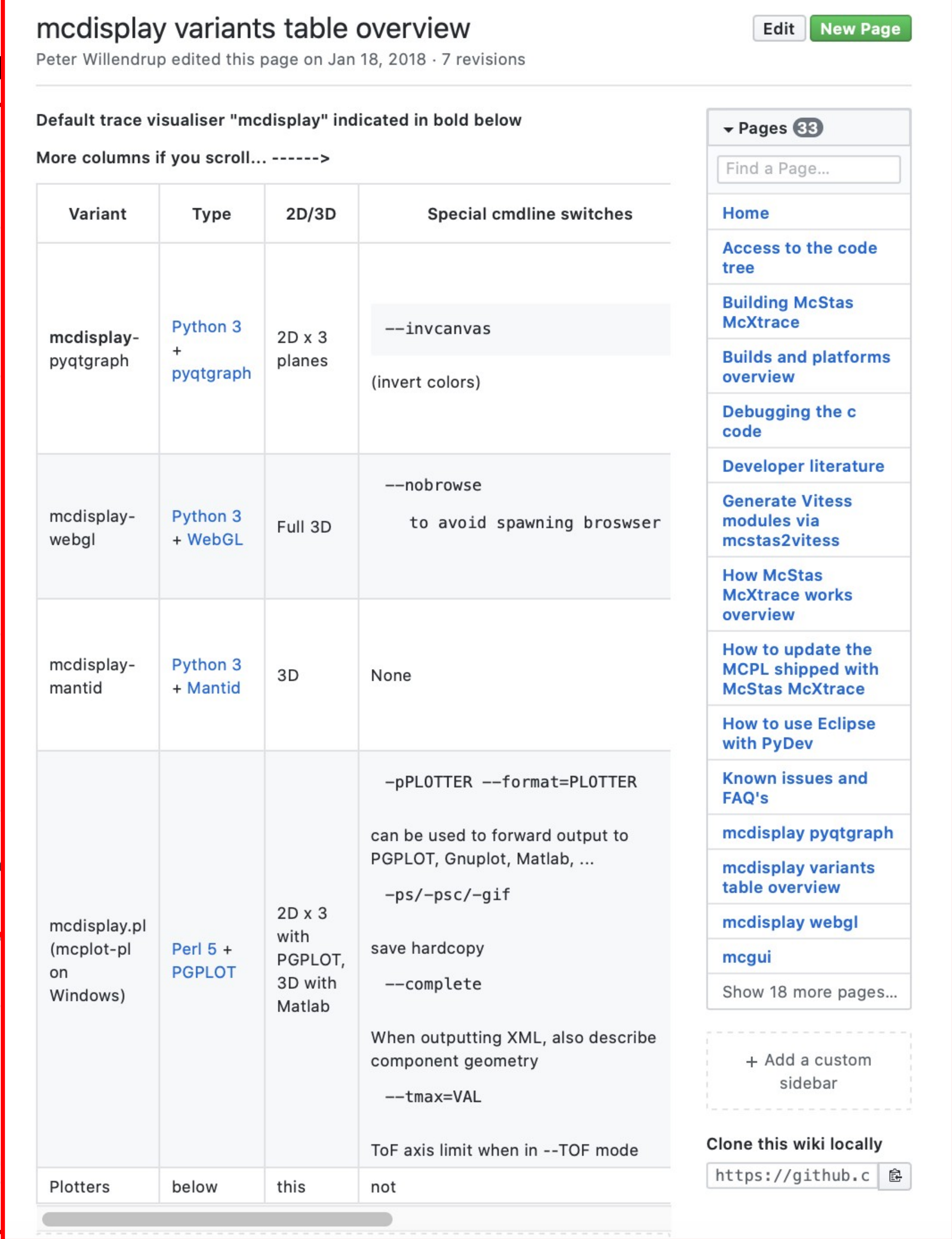

mcdisplay variants table overview

Peter Willendrup edited this page on Jan 18, 2018 · 7 revisions

Default trace visualiser "mcdisplay" indicated in bold below

More columns if you scroll... ------>

Variant	Type	2D/3D	Special cmdline switches
mcdisplay-pyqtgraph	Python 3 + pyqtgraph	2D x 3 planes	`--invcanvas` (invert colors)

mcdisplay-webgl	Python 3 + WebGL	Full 3D	`--nobrowse`
			`to avoid spawning broswser`

mcdisplay-mantid	Python 3 + Mantid	3D	None

mcdisplay.pl (mcplot-pl on Windows)	Perl 5 + PGPLOT	2D x 3 with PGPLOT, 3D with Matlab	`-pPLOTTER --format=PLOTTER`
			can be used to forward output to PGPLOT, Gnuplot, Matlab, ...
			`-ps/-psc/-gif`
			save hardcopy
			`--complete`
			When outputting XML, also describe component geometry
			`--tmax=VAL`
			ToF axis limit when in --TOF mode

Plotters	below	this	not

- Home
- Access to the code tree
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- mcdisplay pyqtgraph
- mcdisplay variants table overview
- mcdisplay webgl
- mcgui
- Show 18 more pages...

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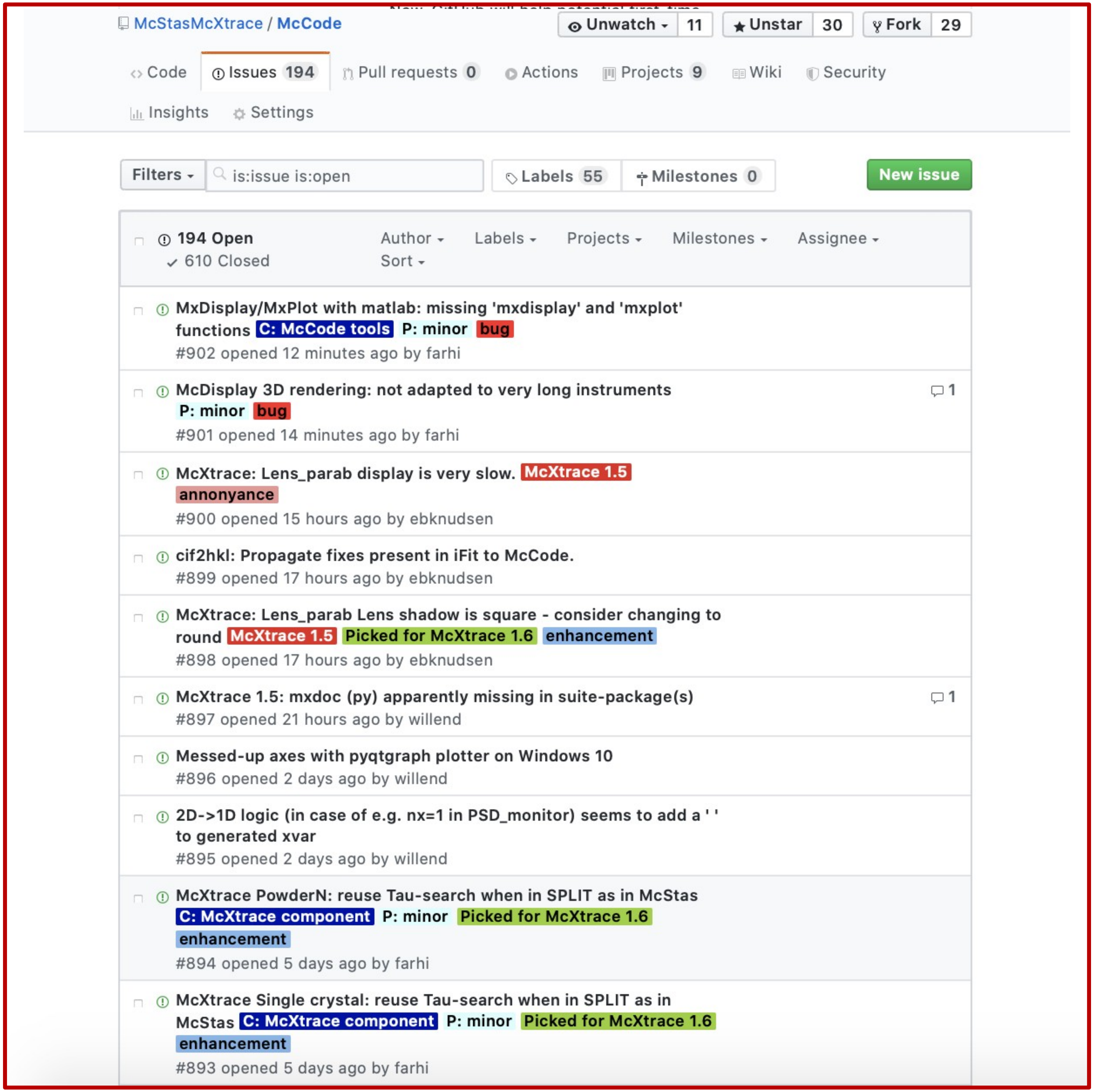
https://github.c

GitHub.com: Issue Tracker



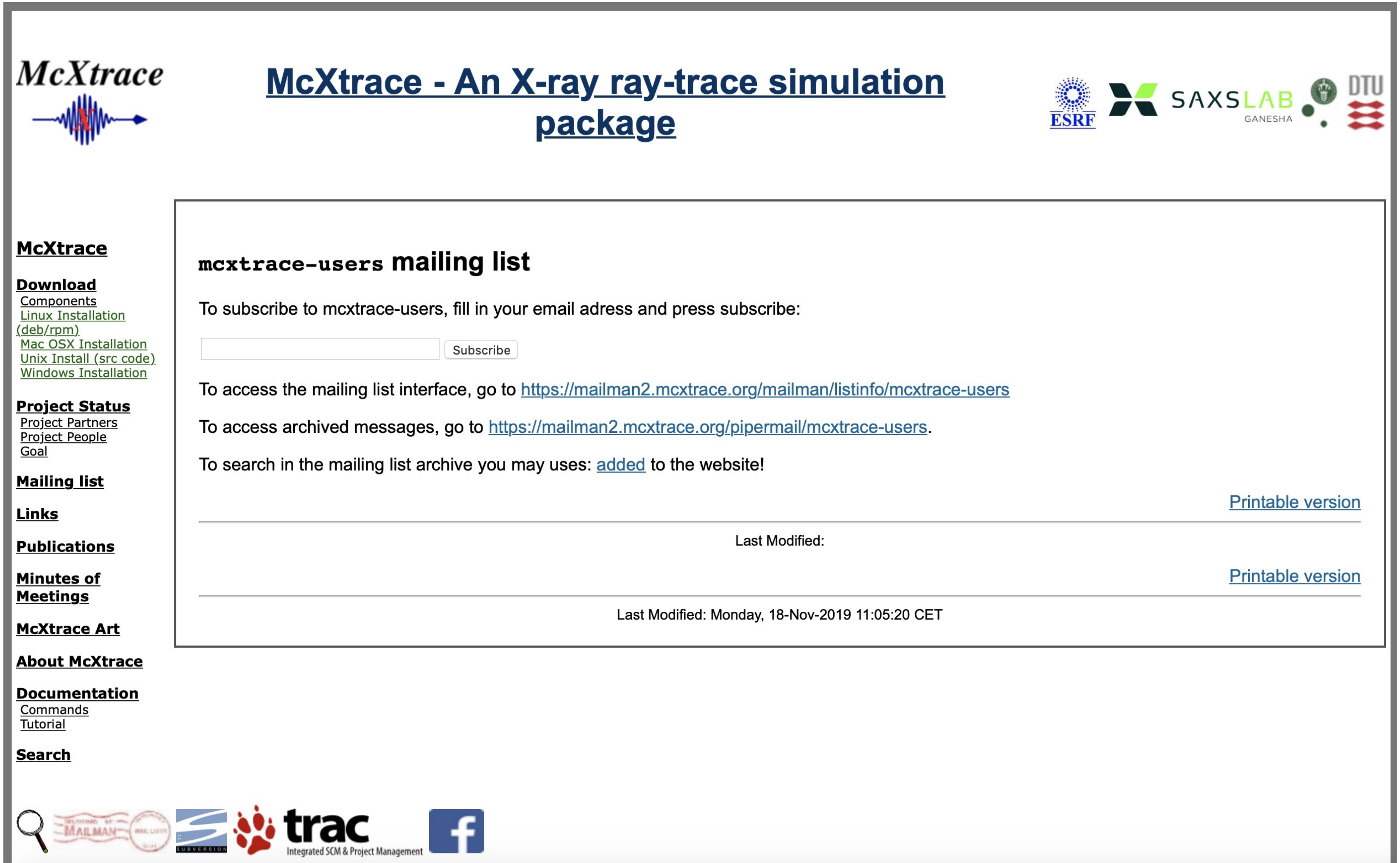
is:issue is:open

194 Open

✓ 610 Closed

- MxDisplay/MxPlot with matlab: missing 'mxdisplay' and 'mxplot' functions C: McCode tools P: minor bug
  #902 opened 12 minutes ago by farhi
- McDisplay 3D rendering: not adapted to very long instruments P: minor bug — 1
  #901 opened 14 minutes ago by farhi
- McXtrace: Lens_parab display is very slow. McXtrace 1.5 annonyance
  #900 opened 15 hours ago by ebknudsen
- cif2hkl: Propagate fixes present in iFit to McCode.
  #899 opened 17 hours ago by ebknudsen
- McXtrace: Lens_parab Lens shadow is square - consider changing to round McXtrace 1.5 Picked for McXtrace 1.6 enhancement
  #898 opened 17 hours ago by ebknudsen
- McXtrace 1.5: mxdoc (py) apparently missing in suite-package(s) — 1
  #897 opened 21 hours ago by willend
- Messed-up axes with pyqtgraph plotter on Windows 10
  #896 opened 2 days ago by willend
- 2D->1D logic (in case of e.g. nx=1 in PSD_monitor) seems to add a ' ' to generated xvar
  #895 opened 2 days ago by willend
- McXtrace PowderN: reuse Tau-search when in SPLIT as in McStas C: McXtrace component P: minor Picked for McXtrace 1.6 enhancement
  #894 opened 5 days ago by farhi
- McXtrace Single crystal: reuse Tau-search when in SPLIT as in McStas C: McXtrace component P: minor Picked for McXtrace 1.6 enhancement
  #893 opened 5 days ago by farhi

Mailing List



McXtrace - An X-ray ray-trace simulation package

`mcxtrace-users` mailing list

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To access archived messages, go to https://mailman2.mcxtrace.org/pipermail/mcxtrace-users.

To search in the mailing list archive you may uses: added to the website!

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Last Modified:

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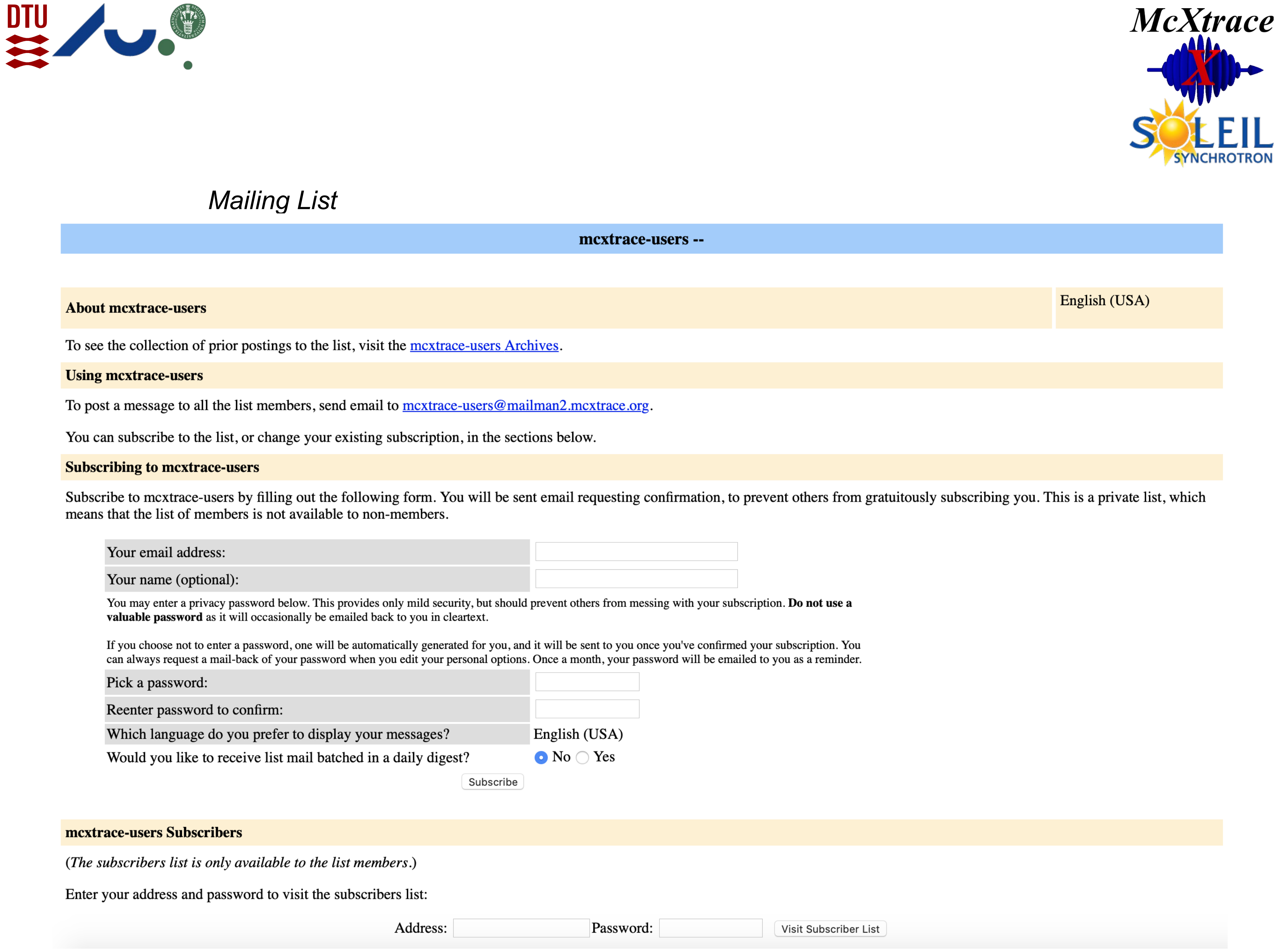

DTU

McXtrace

SOLEIL SYNCHROTRON

Mailing List

mcxtrace-users --

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English (USA)

To see the collection of prior postings to the list, visit the mcxtrace-users Archives.

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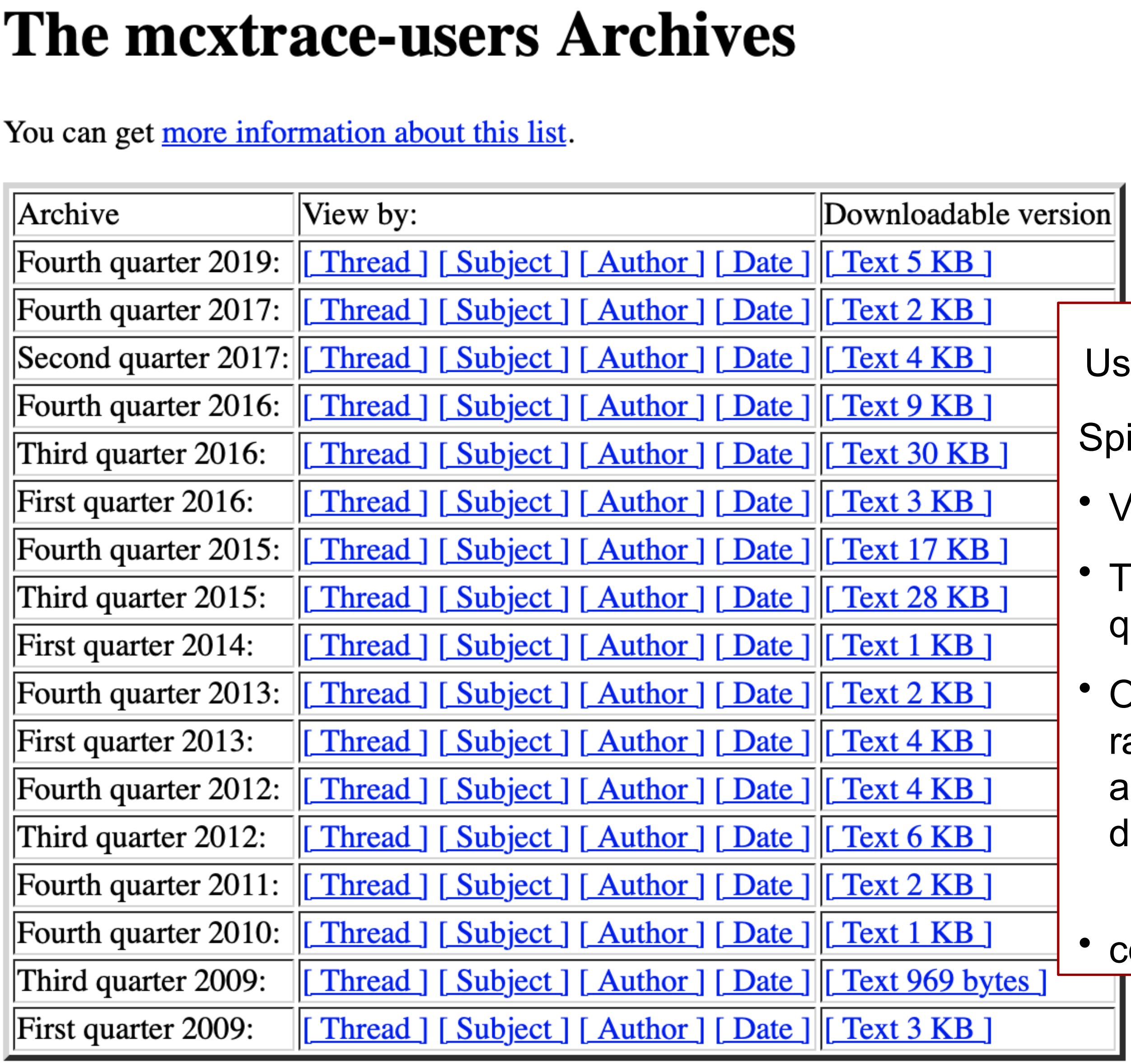

The mcxtrace-users Archives

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Archive	View by:	Downloadable version
Fourth quarter 2019:	[Thread] [Subject] [Author] [Date]	[Text 5 KB]
Fourth quarter 2017:	[Thread] [Subject] [Author] [Date]	[Text 2 KB]
Second quarter 2017:	[Thread] [Subject] [Author] [Date]	[Text 4 KB]
Fourth quarter 2016:	[Thread] [Subject] [Author] [Date]	[Text 9 KB]
Third quarter 2016:	[Thread] [Subject] [Author] [Date]	[Text 30 KB]
First quarter 2016:	[Thread] [Subject] [Author] [Date]	[Text 3 KB]
Fourth quarter 2015:	[Thread] [Subject] [Author] [Date]	[Text 17 KB]
Third quarter 2015:	[Thread] [Subject] [Author] [Date]	[Text 28 KB]
First quarter 2014:	[Thread] [Subject] [Author] [Date]	[Text 1 KB]
Fourth quarter 2013:	[Thread] [Subject] [Author] [Date]	[Text 2 KB]
First quarter 2013:	[Thread] [Subject] [Author] [Date]	[Text 4 KB]
Fourth quarter 2012:	[Thread] [Subject] [Author] [Date]	[Text 4 KB]
Third quarter 2012:	[Thread] [Subject] [Author] [Date]	[Text 6 KB]
Fourth quarter 2011:	[Thread] [Subject] [Author] [Date]	[Text 2 KB]
Fourth quarter 2010:	[Thread] [Subject] [Author] [Date]	[Text 1 KB]
Third quarter 2009:	[Thread] [Subject] [Author] [Date]	[Text 969 bytes]
First quarter 2009:	[Thread] [Subject] [Author] [Date]	[Text 3 KB]

User forum and help since 2009!!

Spirit of the mailinglist:

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

- contact: mcxtrace-users@mcxtrace.org

SPLIT, EXTEND, WHEN, COPY & GROUP

(… and the dangerous JUMP)

- Advanced language features:

Tips and tricks for your instrument

Syntax in one, complex view...

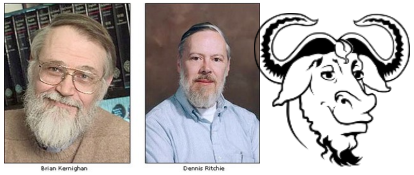
```
{SPLIT} COMPONENT name = comp(parameters) {WHEN condition}
  AT (...) [RELATIVE [reference|PREVIOUS] | ABSOLUTE]
  {ROTATED {RELATIVE [reference|PREVIOUS] | ABSOLUTE} }
  {GROUP group_name}
  {EXTEND C_code}
  {JUMP [reference|PREVIOUS|MYSELF|NEXT] [ITERATE number_of_times
| WHEN condition] }
```

DECLARE / INITIALIZE

- Use the DECLARE section define user variables and functions.

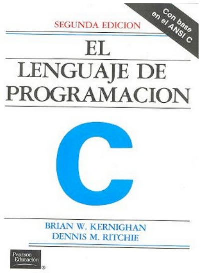
```
DECLARE %{
  double myvar;
%}
```

K & R. / GNU



- Use INITIALIZE for initialization of user variables and calculations.

```
INITIALIZE %{
  myvar = sqrt(PI*input_var)*rand01();
%}
```



SEGUNDA EDICION

Con base en el ANSI C

EL LENGUAJE DE PROGRAMACION

C

BRIAN W. KERNIGHAN
DENNIS M. RITCHIE

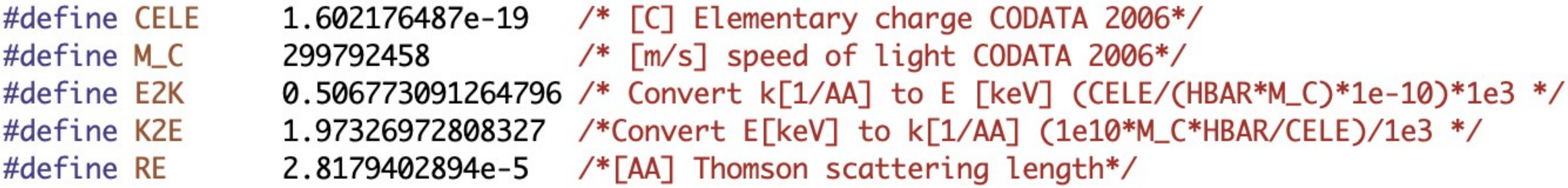
Pearson Educación

- - 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! - McXtrace placement specifiers work in degrees, etc...

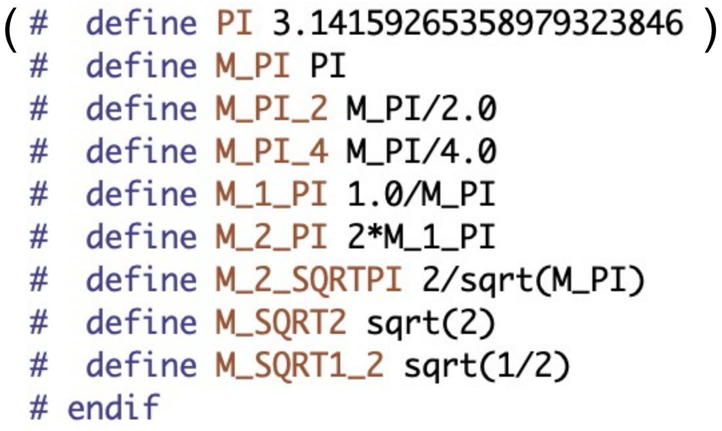
DECLARE / INITIALIZE

Useful physics constants:



```
#define CELE      1.602176487e-19    /* [C] Elementary charge CODATA 2006*/
#define M_C       299792458          /* [m/s] speed of light CODATA 2006*/
#define E2K       0.506773091264796  /* Convert k[1/AA] to E [keV] (CELE/(HBAR*M_C)*1e-10)*1e3 */
#define K2E       1.97326972808327   /*Convert E[keV] to k[1/AA] (1e10*M_C*HBAR/CELE)/1e3 */
#define RE        2.8179402894e-5    /*[AA] Thomson scattering length*/
```

plus e.g. DEG2RAD, RAD2DEG, and these math constants



```
( #  define PI 3.14159265358979323846 )
  #  define M_PI PI
  #  define M_PI_2 M_PI/2.0
  #  define M_PI_4 M_PI/4.0
  #  define M_1_PI 1.0/M_PI
  #  define M_2_PI 2*M_1_PI
  #  define M_2_SQRTPI 2/sqrt(M_PI)
  #  define M_SQRT2 sqrt(2)
  #  define M_SQRT1_2 sqrt(1/2)
  # endif
```

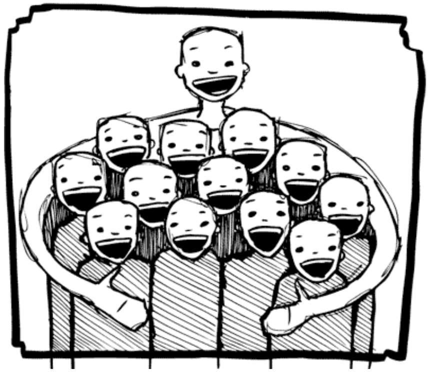
plus anything you can imagine in terms of trigonometric functions from C <math.h>
(beware, these take radians as input - as opposed to our ROTATED statements)

%include

- Instrumentfiles can include external c-code or other instrumentfiles... (These are examples from McStas)

- 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



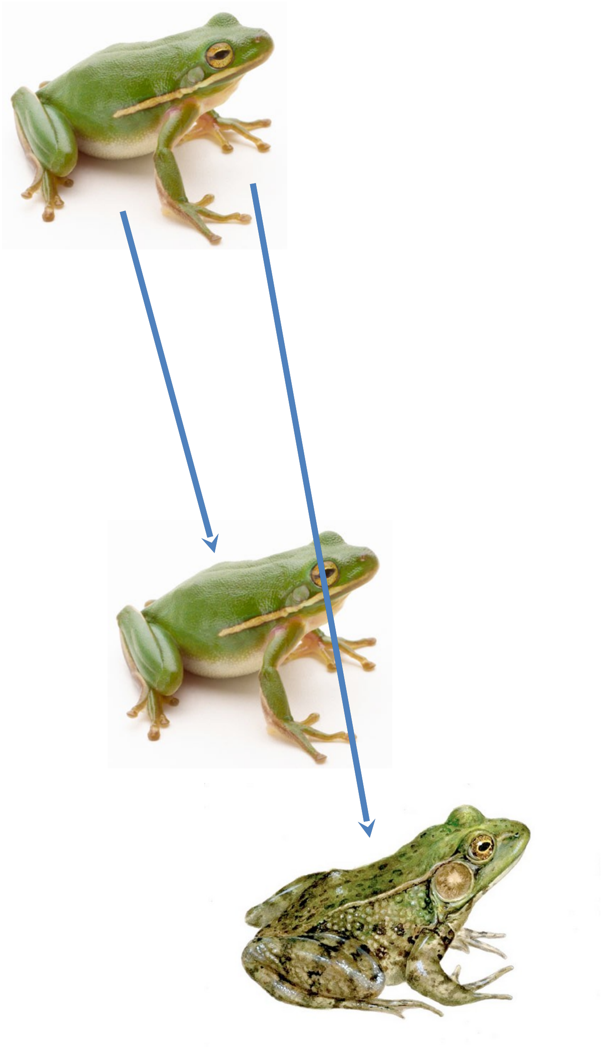
COPY- inside instruments

- In instruments: (see e.g. 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,Al_Thickness+gGap) RELATIVE PREVIOUS
- ROTATED (0,Rh_H25_1,0) RELATIVE PREVIOUS

- COMPONENT **MYcopy** = **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



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 particle is “tried” in sequential order until the it becomes SCATTERED.

WHEN

- Syntax:

COMPONENT Mine = Yours(blah, blah)

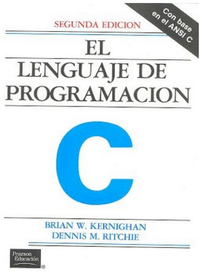
WHEN (c-expression) AT (....)

- 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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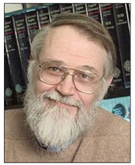
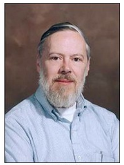
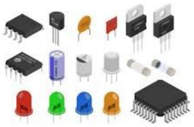
EL LENGUAJE DE PROGRAMACION
C
BRIAN W. KERNIGHAN
DENNIS M. RITCHIE
Pearson Educación


Brian Kernighan


Dennis Ritchie

EXTEND

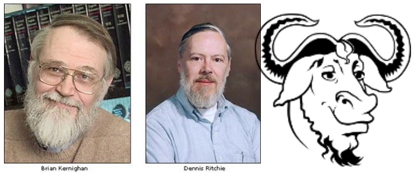


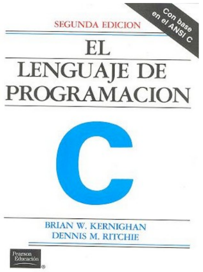
- Enrich component behaviour using EXTEND:

```
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
EXTEND
%{
  if (SCATTERED) { myvar = 2 ;}
%}
```

K & R. / GNU





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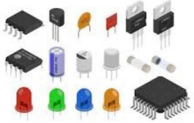
Combined example: Decompose multiple scattering from Single_crystal



```
DECLARE %{
    double multiple_scatt;
%}
…
COMPONENT Crystal = Single_crystal(… order=0 …)
AT (0,0,0) RELATIVE somewhere
EXTEND %{
    multiple_scatt=SCATTERED;
%}
…
COMPONENT PSD_single=PSD_monitor(…)
WHEN (multiple_scatt==1) AT (0,0,0) RELATIVE somewhere_else

COMPONENT PSD_multiple=PSD_monitor(…)
WHEN (multiple_scatt > 1) AT (0,0,0) RELATIVE somewhere_else
```

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 photons...)

- Syntaxes:
- COMPONENT a=b(...)
- **WHEN** (expr) AT (...) **JUMP** somewhere

- COMPONENT a=b(...)
- **WHEN** (expr) AT (...) **JUMP** myself

JUMP

- A goto. Be careful. Can be used in two situations:
- **JUMP** to myself
- **JUMP** to an Arm

BEWARE - This IS a GOTO!

- 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

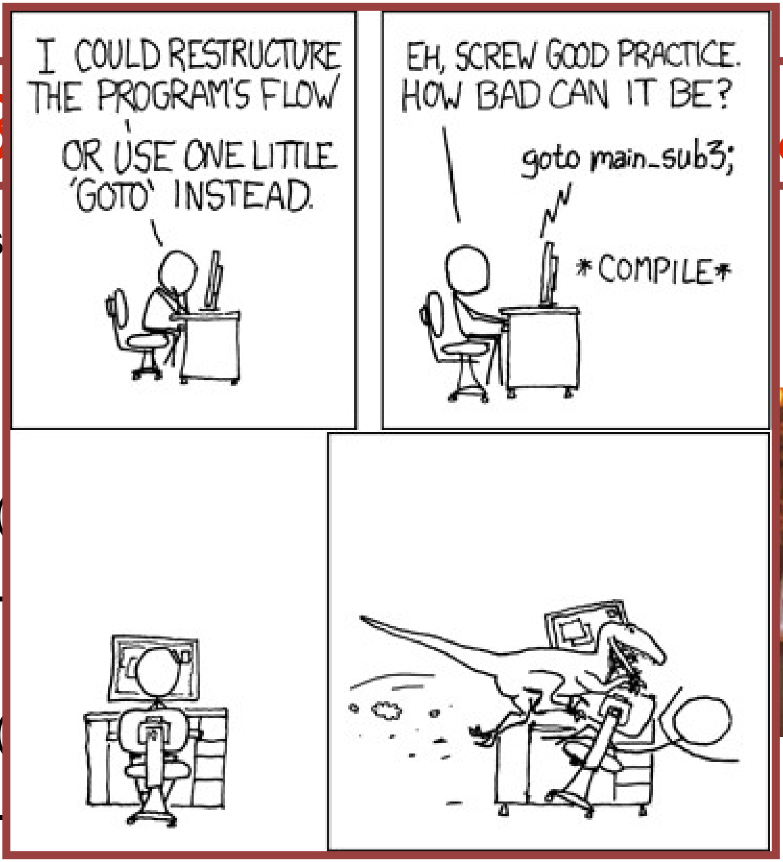
- COMPONENT a=b(...)
- **WHEN** (expr) AT (...) **JUMP** myself

JUMP

- A goto. Be careful. Can be used in two situations:
- **JUMP** to myself
- **JUMP** to an Arm

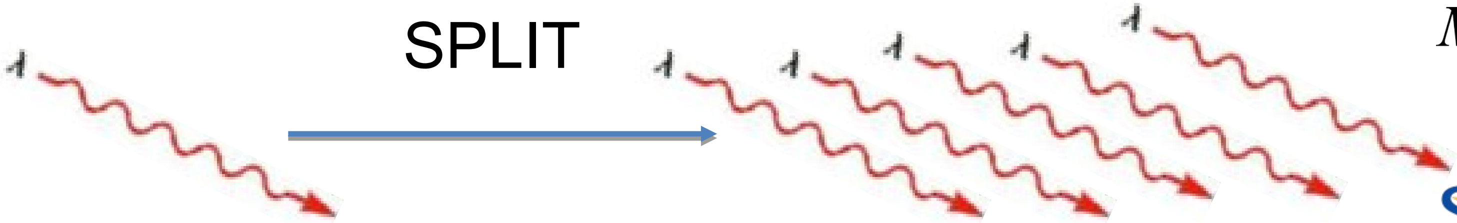
B a GOTO!

- No coordinate trans if the Arms you JUMP between do not coincide you wil


I COULD RESTRUCTURE THE PROGRAM'S FLOW
OR USE ONE LITTLE 'GOTO' INSTEAD.
EH, SCREW GOOD PRACTICE. HOW BAD CAN IT BE?
goto main_sub3;
COMPILE

- Syntaxes:
- COMPONENT a=b(
- **WHEN** (expr) AT (...
- COMPONENT a=b(
- **WHEN** (expr) AT (...

SPLIT

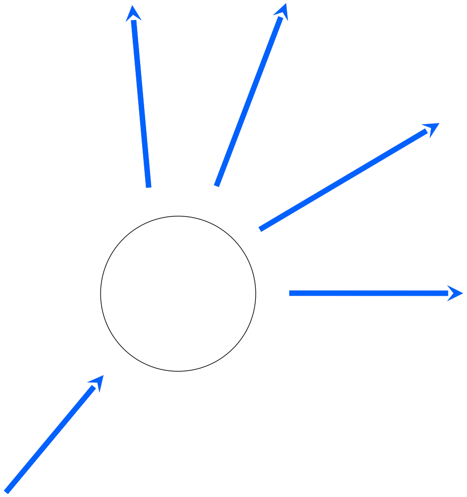


- Increase statistics beyond this point in the instrumentfile

- SPLIT n MyArm = Arm()
- AT somewhere

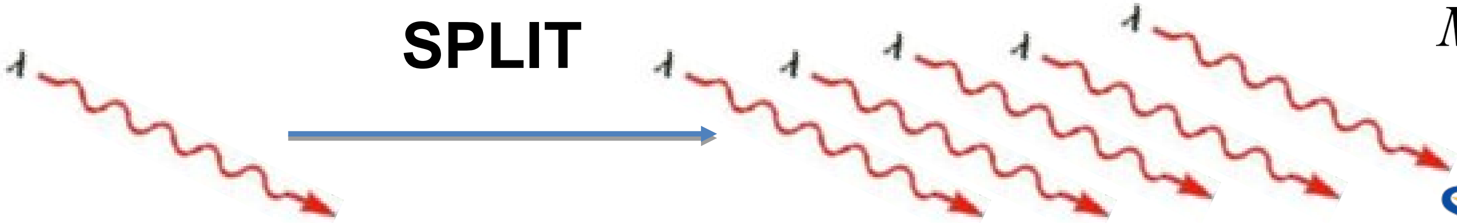
- will “formulate an if-statement”:

- for j=1:n
-    comp1
-    comp2
-    comp3
-    ...
- end (of instrument)



- **ONLY** meaningful in case of Monte Carlo choices after SPLIT point...

SPLIT



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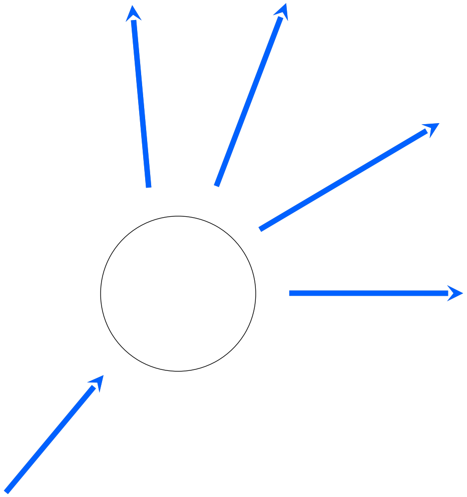

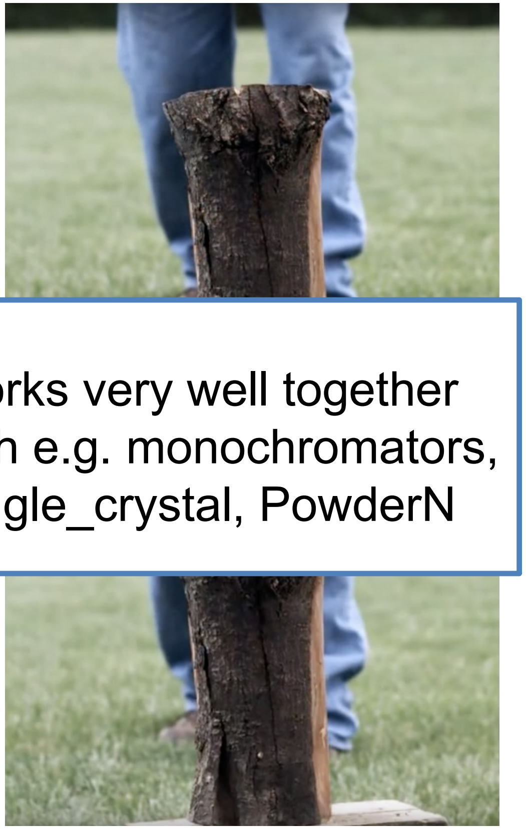

Works very well together with e.g. monochromators, Single_crystal, PowderN