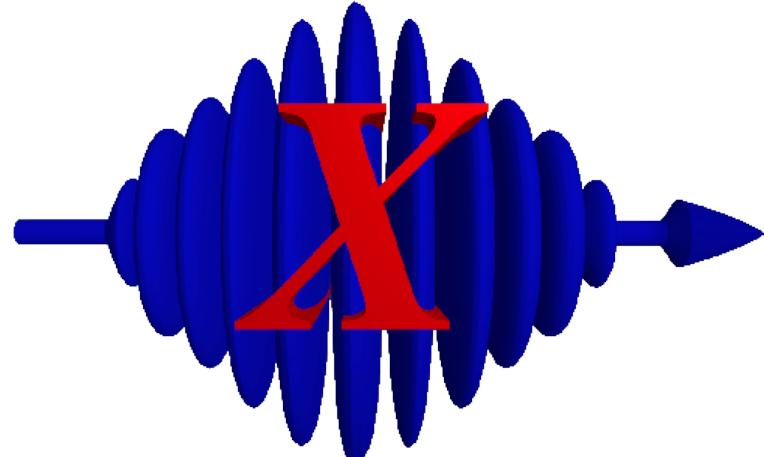


McXtrace



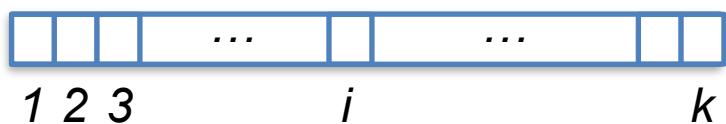
FAQ, advanced grammar, tips and tricks

Peter Willendrup (pkwi@fysik.dtu.dk)



- ❖ 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”

- Imagine a histogram, e.g. $I(\lambda)$

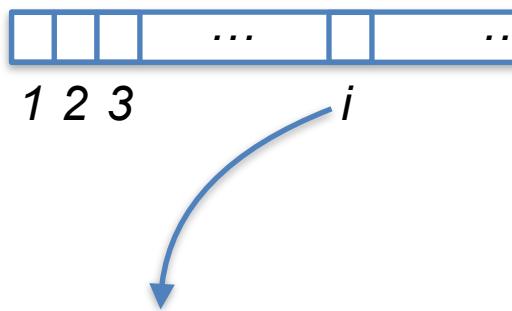


In bin i , N events each carrying a fractional intensity p_j so that

$$I = \frac{\sum p_j}{N}$$

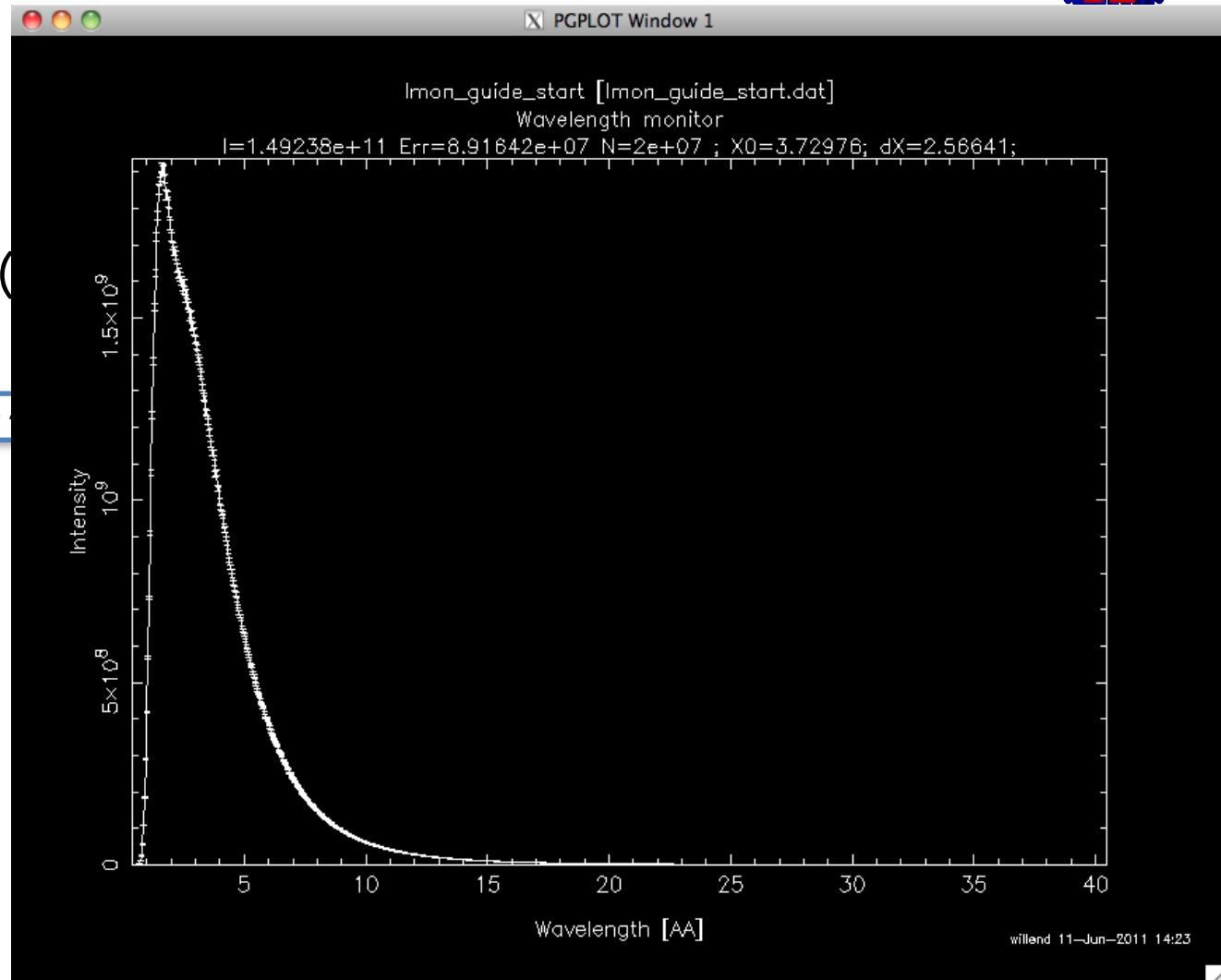
- The RMS variance over that set becomes our statistical error bar E

Imagine a histogram, e.g. $I($



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

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

$$I = \sum_{i=1}^n w_i. \quad (1)$$

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

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

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

$$C = tI, \quad (3)$$

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

$$\sigma^2(C) = t^2 \sigma^2(I). \quad (4)$$

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

$$\sigma_{\text{VE}}(C_{\text{VE}}) = \sqrt{C_{\text{VE}}}. \quad (5)$$

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

$$C_{\text{VE}} = tI + E(\Sigma). \quad (6)$$

The standard deviation for the VE becomes

$$\sigma_{\text{VE}}^2(C) = t^2 \sigma^2(I) + \Sigma^2. \quad (7)$$

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

$$\Sigma^2 = tI - t^2 \sigma^2(I). \quad (8)$$

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

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

1. On a given McXtrace histogram
2. For the non-zero bins, calculate $t_{\max} = \frac{I}{\sigma^2(I)}.$
3. The *smallest* t_{\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...

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

Lefmann, K., Willendrup, P. K., Uddy, 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:

A note about McStas errorbars

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

January 31, 2014

Contents

1	Introduction	2
2	Estimation of counting times and derivation of virtual data from simulations	2
2.1	Real vs simulated data	2
2.2	Counting time and data quality	3
2.3	Estimating the appearance of a “real” data set	3
2.4	Example	3

- ♦ 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!

- ♦ 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!

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

- 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...

- 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/1.5/examples/*
```

Examples Directory

- *Simple grep* →

They have an author name!

For instance:

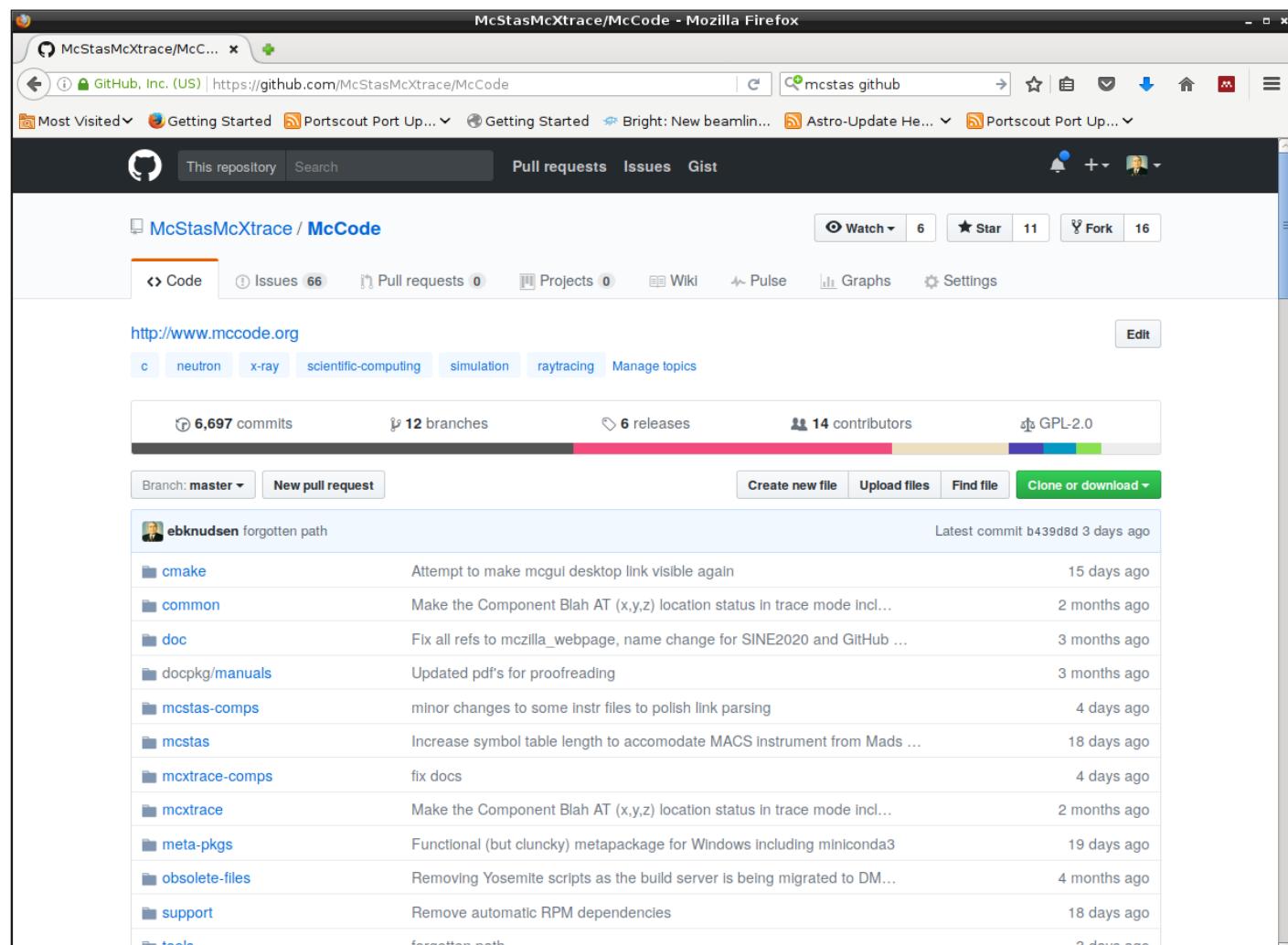
DBD_IBM_Si_analyzer → *Marcus H. Mendenhall*

Test_SX → *E. Farhi*

Pump_probe → *E. Knudsen*

GitHub.com

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



McStasMcXtrace/McCode - Mozilla Firefox

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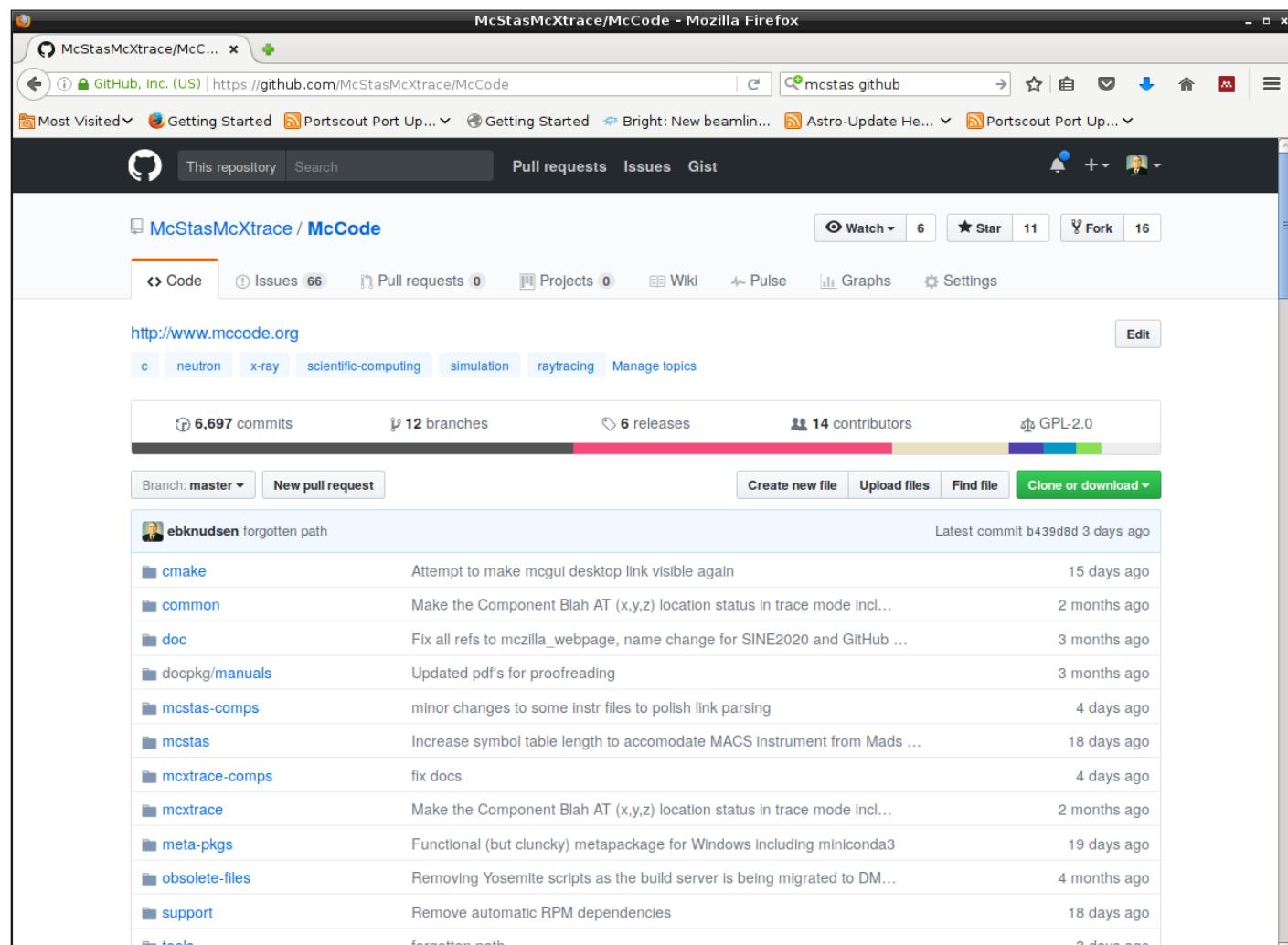
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ebknudsen	forgotten path	Latest commit b439d8d 3 days ago
cmake	Attempt to make mcgui desktop link visible again	15 days ago
common	Make the Component Blah AT (x,y,z) location status in trace mode incl...	2 months ago
doc	Fix all refs to mczilla_webpage, 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
mcxtrace	Make the Component Blah AT (x,y,z) location status in trace mode incl...	2 months ago
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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<https://github.com/McStasMcXtrace/McCode>



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docpkg/manuals	Updated pdf's for proofreading	3 months ago
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- Known issues and FAQ's
- Access to the code tree

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- 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/...)

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- 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>

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mcdisplay variants table overview

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

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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 browser
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

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✓ 610 Closed					
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① MxDisplay/MxPlot with matlab: missing 'mxdisplay' and 'mxplot' functions	C: McCode tools	P: minor bug			
#902 opened 12 minutes ago by farhi					
① McDisplay 3D rendering: not adapted to very long instruments				1	
P: minor bug					
#901 opened 14 minutes ago by farhi					
① McXtrace: Lens_parab display is very slow.	McXtrace 1.5				
annownce					
#900 opened 15 hours ago by ebknudsen					
① cif2hkl: Propagate fixes present in iFit to McCode.					
#899 opened 17 hours ago by ebknudsen					
① 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					
① McXtrace 1.5: mxdoc (py) apparently missing in suite-package(s)				1	
#897 opened 21 hours ago by willend					
① Messed-up axes with pyqtgraph plotter on Windows 10					
#896 opened 2 days ago by willend					
① 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					
① 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					
① 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

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English (USA)

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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

- Advanced language features:

*Tips and tricks for your
instrument*



```
{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] }
```



- Use the DECLARE section define user variables and functions.

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

- Use INITIALIZE for initialization of user variables and calculations.

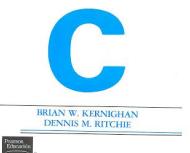
```
INITIALIZE %{
    myvar = sqrt(PI*input_var)*rand01();
%}
```

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



K & R. / GNU





Useful physics constants:

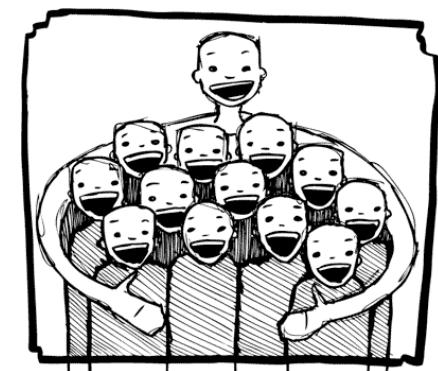
```
#define CELE      1.602176487e-19 /* [C] Elementary charge CODATA 2006*/
#define M_C        299792458   /* [m/s] speed of light CODATA 2006*/
#define E2K        0.506773091264796 /* Convert k[1/AA] to E [keV] (CELE/(HBAR*M_C)*1e-10)*1e3 */
#define K2E        1.97326972808327 /*Convert E[keV] to k[1/AA]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

- 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



- 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,AI_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





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.



- 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



BRIAN W. KERNIGHAN
DENNIS M. RITCHIE



- 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
```

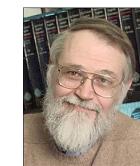
```
GROUP IN6Monoks
```

EXTEND

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



K & R. / GNU



SEGUNDA EDICION
C con base en el lenguaje C
EL
 LENGUAJE DE
PROGRAMACION

C

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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

```

- 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



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

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...)
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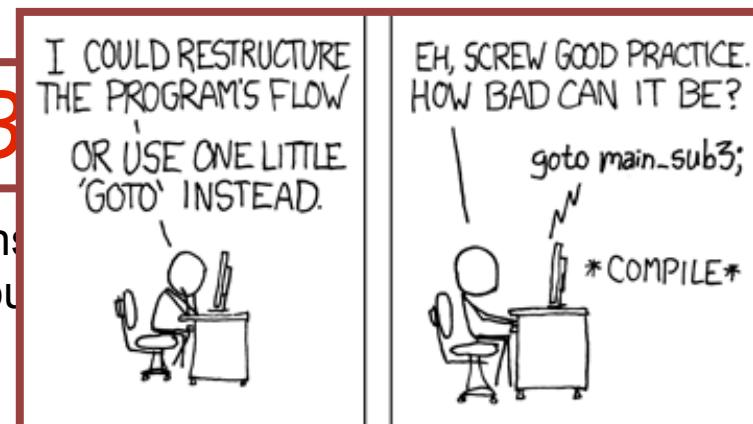


- A goto. Be careful. Can be used in two situations:

- **JUMP** to myself
- **JUMP** to an Arr

- No coordinate trans do not coincide you

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

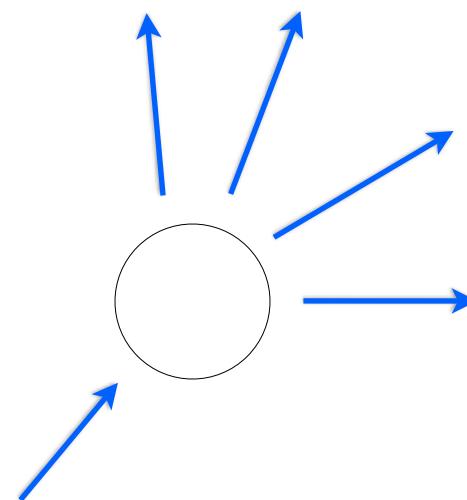


a GOTO!

at if the Arms you JUMP between)

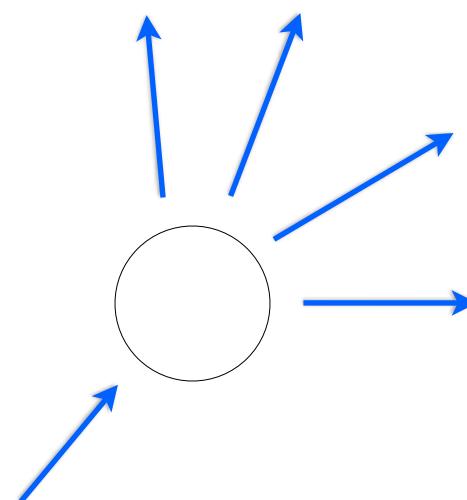


- Increase statistics beyond this point in the instrumentfile
- SPLIT n MyArm = Arm()
- AT somewhere
- will “formulate an if-statement”:
- for j=1:n
 - comp1
 - comp2
 - comp3
 - ...
- end (of instrument)
- **ONLY** meaningful in case of Monte Carlo choices after SPLIT point...



SPLIT

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

