

Monte Carlo Particle Lists : MCPL

Neutrons cradle to grave workshop, SINE2020 GA, Coimbra, Portugal, 2016-09-06

Thomas Kittelmann, ESS Detector Group
(thomas.kittelmann@esss.se)

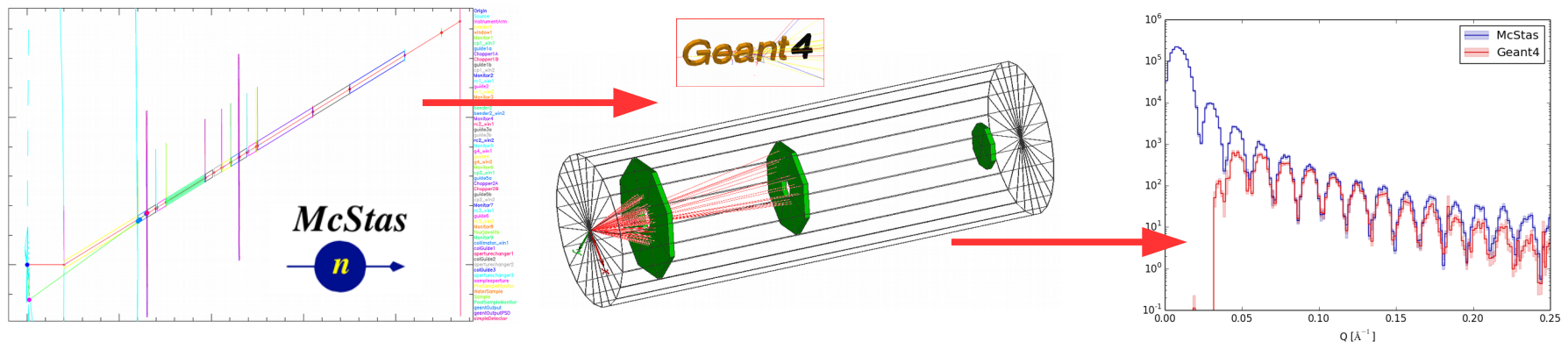
MCPL developed with contributions from:

*E. Klinkby (DTU), E. Knudsen (DTU), P. Willendrup (DTU, ESS),
K. Kanaki (ESS), X. X. Cai (ESS, DTU)*



Background / Motivation

- Many different applications in use at ESS for particle simulations.
- Desirable to be able to transfer particles between applications.
- Or reuse within a single application.
- For detector simulations in Geant4, we are interested in grabbing post-sample output of instrument simulations (usually McStas), and use those as a source.



- Or, grab background particles from MCNP or Geant4 simulations to study shielding and background issues.

Monte Carlo vs. ray tracing – where are we heading?

- MCNP**: target, moderator, reflector design
- McStas** (+guide_bot) for instrument design
- GEANT4** for shielding and backgrounds
- Vitess & NADS & Particle swarms: shielding & optics
 - design documentation for the instrument
- MCNP**: safety, dose-rates (future use of FLUKA or MARS)
- GEANT4**: detector design

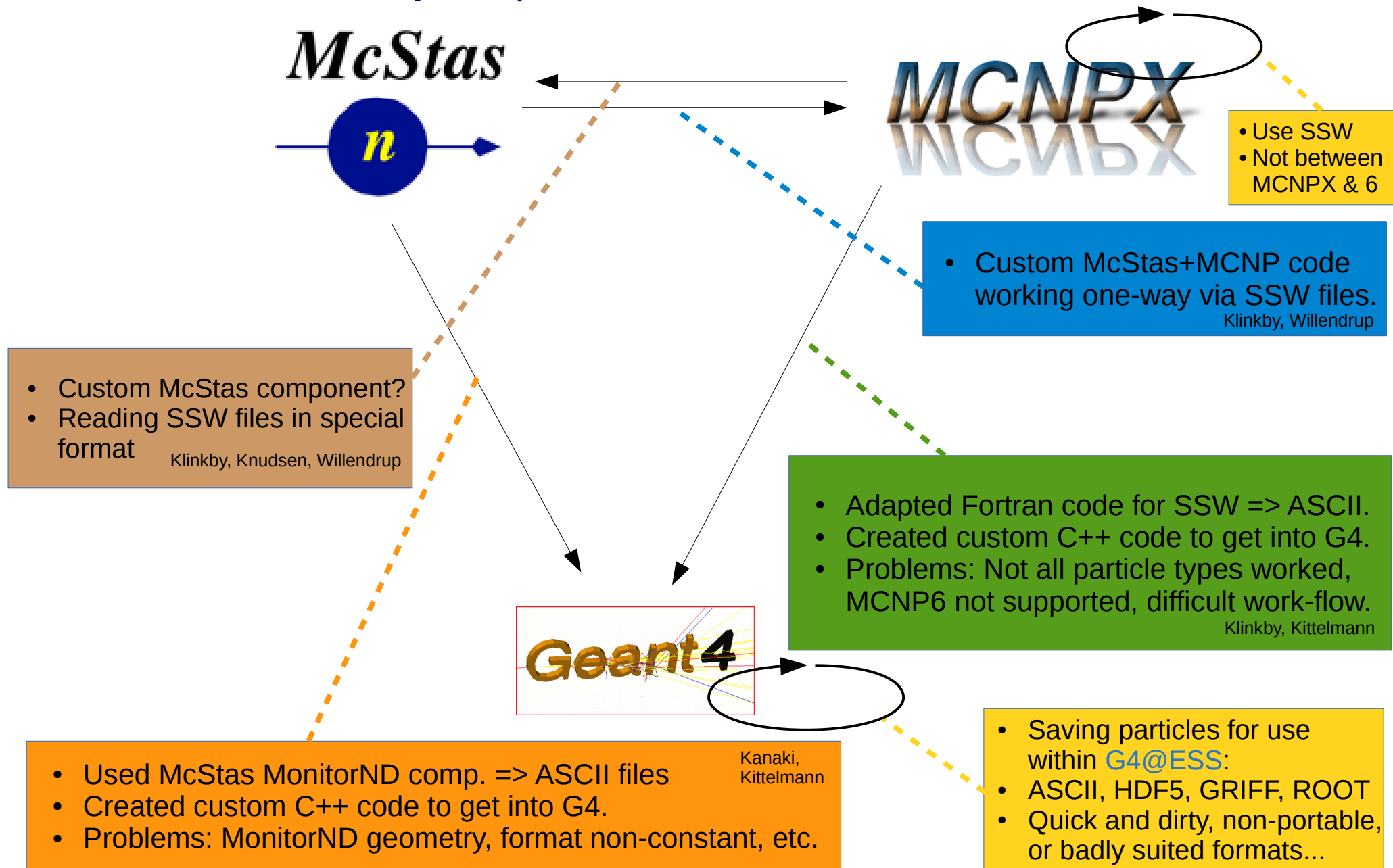
⇒ Interfacing is important.
Efforts ongoing to merge and benchmark

ESS EUROPEAN SPALLATION SOURCE

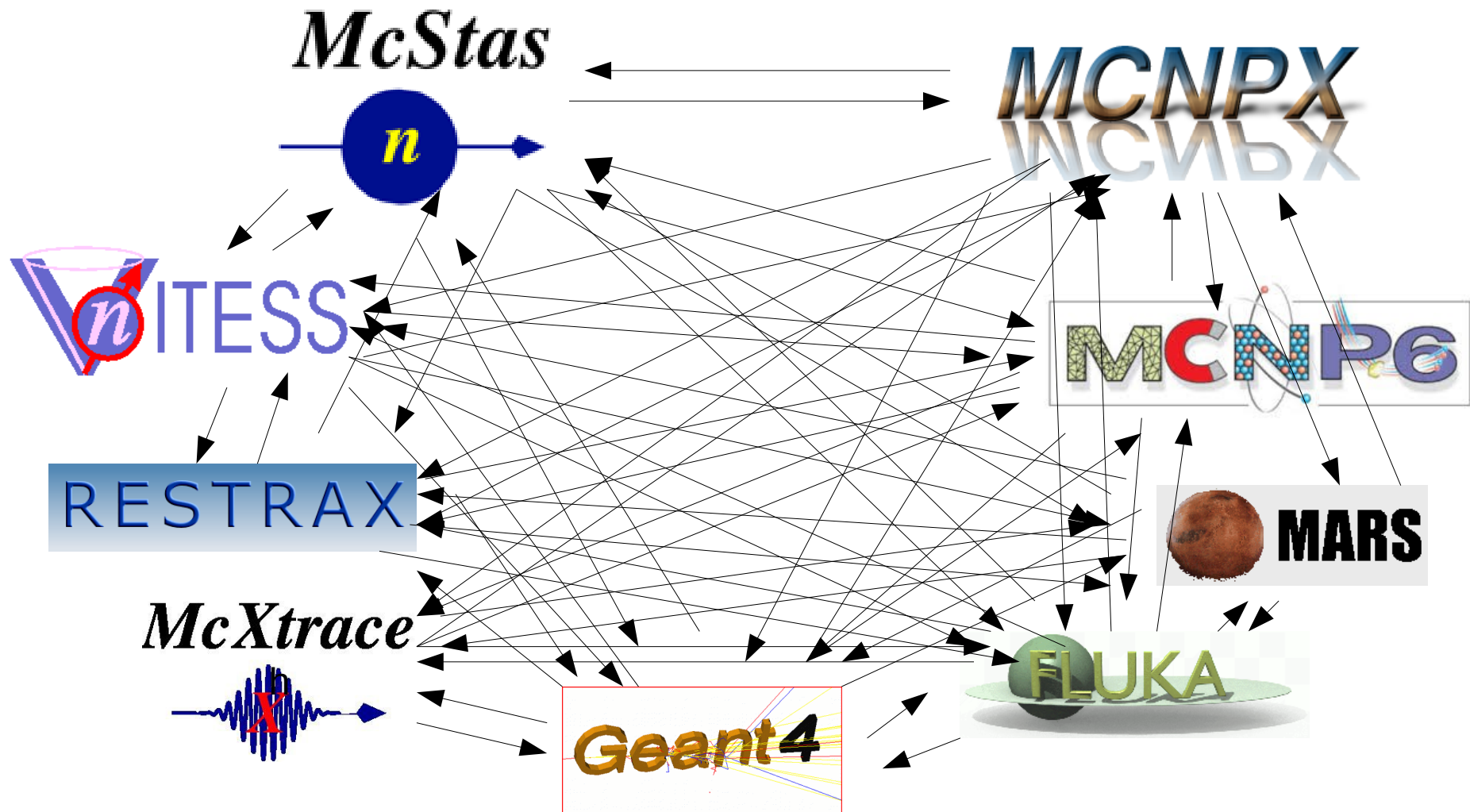
Klinkby, 2014

How to store and transfer particles? By 2015 we had a jungle of custom solutions at ESS for just 3 apps...

NB: illustration here is surely incomplete...

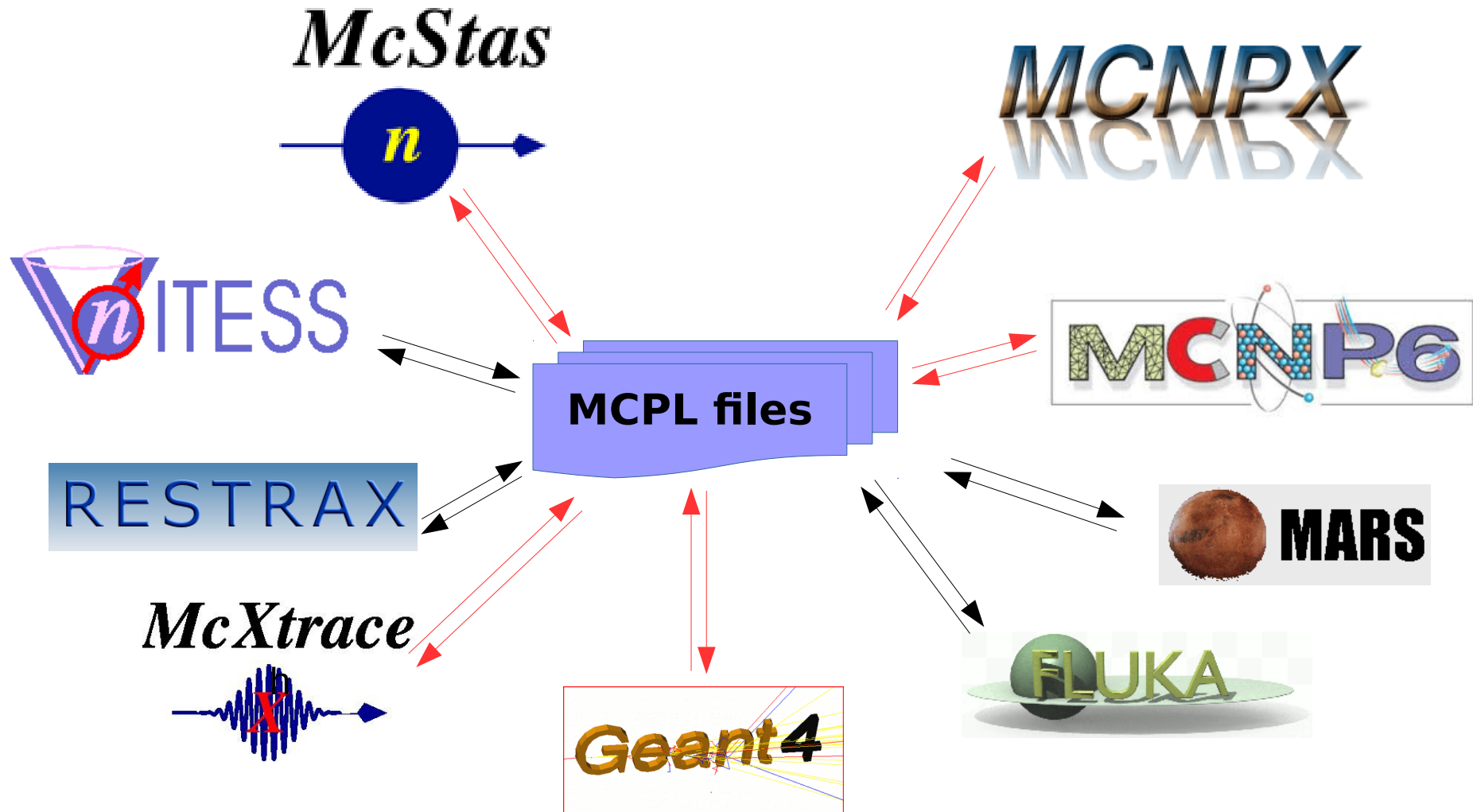


Consider more apps : The jungle gets impossibly tangled...



The solution: A common interchange format.

MCPL: Monte Carlo Particle Lists



In **red** : already available now (Sep 2016).

Disclaimer: Non-exhaustive list of applications...

What is MCPL?

MCPL : Monte Carlo Particle Lists

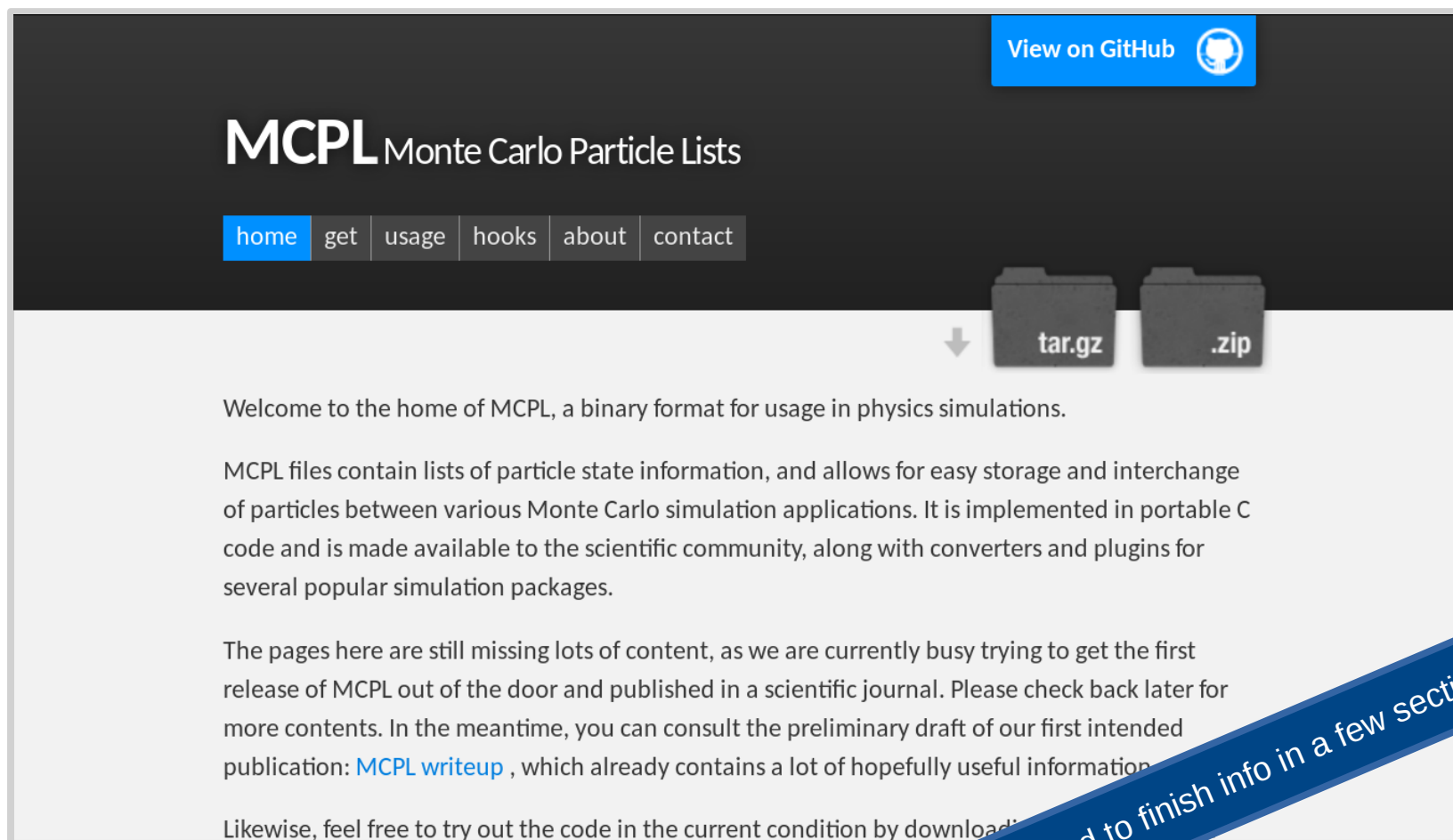


MCPL files

- It is a simple file-format. Each file contains a list of particles.
- The format is flexible: can contain a lot of information if needed, or can contain only minimal information if small file-size is important.
- It is easy to make code dealing with MCPL, so it is easy to make plugins & converters for the various Monte Carlo frameworks. End-users will simply use those converters.
- MCPL files can contain meta-data. This makes it possible to tell what data is in a file, where it came from, how it should be interpreted.
- MCPL comes with tools, such as for inspecting contents.

Official website & code @ GitHub:

<https://mctools.github.io/mcpl/>



Still need to finish info in a few sections...

Paper describing MCPL in detail about to be submitted

Monte Carlo Particle Lists : MCPL

T Kittelmann^{a,*}, E Klinkby^b, E Knudsen^c, P Willendrup^c, X X Cai^{a,b},
K Kanaki^a

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^b*DTU Nutech, Technical University of Denmark, Denmark*

^c*DTU PHYSICS, Technical University of Denmark, Denmark*

Draft version available
on MCPL website

Abstract

A binary format with lists of particle state information, for interchanging particles between various Monte Carlo simulation applications, is presented. Portable C code for file manipulation is made available to the scientific community, along with converters and plugins for several popular simulation packages.

Lots of details!
More than most end-users
will need to know or care about :-)

Browsing an MCPL file with the MCPL tool

Just run: **"mcpltool <name-of-MCPL-file>"**

Opened MCPL file myfile.mcpl.gz:

Basic info

Format : MCPL-2
No. of particles : 5037156
Header storage : 818 bytes
Data storage : 181337616 bytes

Custom meta data

Source : "Geant4"
Number of comments : 8
-> comment 0 : "Created with the Geant4 MCPLWriter in the ESS/dgcode framework"
-> comment 1 : "MPCLWriter volumes considered : ['RecordFwd']"
-> comment 2 : "MPCLWriter steps considered : <at-volume-exit>"
-> comment 3 : "MPCLWriter write filter : <unfiltered>"
-> comment 4 : "MPCLWriter user flags : <disabled>"
-> comment 5 : "MPCLWriter track kill strategy : <none>"
-> comment 6 : "ESS/dgcode geometry module : G4StdGeometries/GeoSlab"
-> comment 7 : "ESS/dgcode generator module : G4StdGenerators/SimpleGen"

Number of blobs : 2
-> 74 bytes of data with key "ESS/dgcode_geopars"
-> 231 bytes of data with key "ESS/dgcode_genpars"

Particle data format

User flags : no
Polarisation info : no
Fixed part. type : no
FP precision : single
Endianness : little
Storage : 36 bytes/particle

index	pdgcode	ekin[MeV]	x[cm]	y[cm]	z[cm]	ux	uy	uz	time[ms]	weight
0	2112	4.0061e-08	-11.518	-2.744	40	-0.60697	-0.093797	0.78917	0.22354	1
1	2112	2.5e-08	0	0	40	0	0	1	0.1829	1
2	22	7.7251	7.8603	-6.7903	40	0.072796	-0.20272	0.97653	0.33498	1
3	2112	1.8481e-08	-21.168	4.4662	40	-0.70384	0.1485	0.69466	0.24732	1
4	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
5	22	0.031	-30.093	19.067	40	0.10979	0.84395	0.52507	0.27059	1
6	22	1.592	-50	2.7616	27.847	-0.66425	0.66981	0.33186	0.27059	1
7	22	1.4402	16.313	-15.255	40	0.062836	-0.14628	0.98724	0.11248	1

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Columns of particle data (1 row = 1 particle)
In this file: No userflags or polarisation

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95	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
96	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
97	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
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99	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1

PDG codes: 2112 = neutron, 22 = gamma

More at <http://pdg.lbl.gov/2015/reviews/rpp2015-rev-monte-carlo-numbering.pdf>

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Custom meta-data

- This file is from ESS-DG Geant4
- Comments reminding us of setup used to create file
- Binary "blobs" keep more complete configuration details (here ESS-DG geo/gen parameters, could be McStas instrument file or MCNP input deck).

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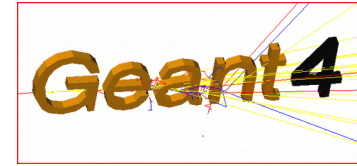
Columns of particle data (1 row = 1 particle)
In this file: No *userflags* or *polarisation*

index	pdgcode	ekin[MeV]	x[cm]	y[cm]	z[cm]	ux	uy	uz	time[ms]	weight
0	2112	4.0061e-08	-11.518	-2.744	40	-0.60697	-0.093797	0.78917	0.22354	1
1	2112	2.5e-08	0	0	40	0	0	1	0.1829	1
2	22	7.7251	7.8603	-6.7903	40	0.072796	-0.20272	0.97653	0.33498	1
3	2112	1.8481e-08	-21.168	4.4662	40	-0.70384	0.1485	0.69466	0.24732	1
4	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
5	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
6	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
7	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
8	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
9	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
10	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
11	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
12	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
13	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
14	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
15	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
16	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
17	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
18	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
19	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
20	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
21	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
22	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
23	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
24	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
25	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
26	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
27	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
28	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
29	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
30	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
31	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
32	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
33	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
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35	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
36	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
37	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
38	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
39	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
40	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
41	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
42	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
43	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
44	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
45	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
46	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
47	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
48	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
49	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
50	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
51	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
52	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
53	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
54	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
55	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
56	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
57	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
58	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
59	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
60	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
61	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
62	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
63	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
64	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
65	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
66	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
67	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
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69	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
70	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
71	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
72	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
73	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
74	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
75	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
76	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
77	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
78	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
79	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
80	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
81	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
82	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
83	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
84	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
85	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
86	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
87	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
88	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
89	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
90	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
91	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
92	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
93	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
94	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
95	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
96	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
97	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
98	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
99	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1

PDG codes: 2112 = neutron, 22 = gamma

More at <http://pdg.lbl.gov/2015/reviews/rpp2015-rev-monte-carlo-numbering.pdf>

Using MCPL with Geant4



- Provided as C++ classes extending G4 interfaces, since that is the usual M.O. for working with Geant4.
 - MCPL as input through custom G4VUserPrimaryGeneratorAction (G4MCPLGenerator).
 - MCPL as output through Custom sensitive detector (G4MCPLWriter) capturing particles entering selected volumes.
 - Many possibilities for fine-tuning behaviour.
- Users of the ESS detector group Geant4-framework don't need to deal with C++ classes, but can simply specify desired input/output behaviour with a few lines of python or at the command line.

**More info on MCPL website
& in section 3.1 of writeup!**

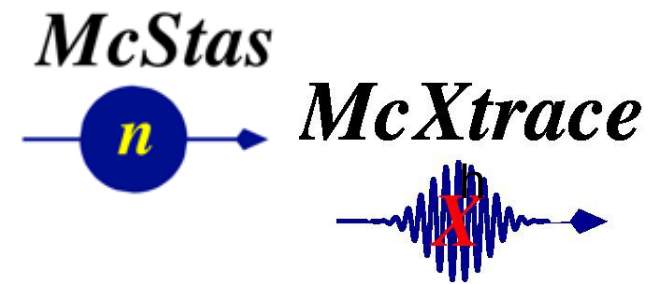
Using MCPL with MCNP



- Provided as two dependency-free command-line applications written in portable C, for converting between MCNP Surface Source Read/Write files (aka SSW files aka WSSA files) and MCPL:
 - **mcpl2ssw** and **ssw2mcpl**
- For instance run: **ssw2mcpl <my-ssw-file> output.mcpl**
- Easy to get access to one of those commands: Download a single file from the MCPL website and compile it into the executable.
- Supports MCNP5, MCNPX & MCNP6 (despite incompatible SSW formats).

**More info on MCPL website
& in section 3.2 of writeup!**

Using MCPL with McStas or McXtrace



- MCPL_output and MCPL_input components were already included upstream.
- For output, just add two lines in your instrument file at the appropriate position (for instance, right after the sample component):

```
COMPONENT mcpout = MCPL_output(filename="myfile")  
AT(0,0,0) RELATIVE PREVIOUS
```

- This captures into myfile.mcpl.gz the full state of all neutrons as they leave the previous component (with coordinates relative to that component).
- Using particles in an MCPL files as a *source* in McStas is equally simple.
- Also works when running McStas with MPI.
- Example instruments using are included with McStas:
 - [mcstas-comps/examples/Test_MCPL_output.inst](#)
 - [mcstas-comps/examples/Test_MCPL_input.inst](#)

**More info on MCPL website
& in section 3.3 of writeup!**

NOTE: The MCPL code is already part of McStas 2.3, but a few bugs were fixed late, so need to copy a fixed version of [MCPL_output.comp](#) into your rundir. From McStas 2.4 and McXtrace 1.3, everything will work out of the box.

C-code for reading MCPL file

Note: This is shown in case someone is wondering if they could implement converters for their own application. End-users should normally just activate pre-written converters & plugins for their applications

Listing 1: Simple example for looping over all particles in an existing MCPL file

```
#include "mcpl.h"

void example()
{
    mcpl_file_t f = mcpl_open_file("myfile.mcpl");

    const mcpl_particle_t* p;

    while ( ( p = mcpl_read(f) ) ) {

        /* Particle properties can here be accessed
           through the pointer "p":

           p->pdgcode
           p->position[k] (k=0,1,2)
           p->direction[k] (k=0,1,2)
           p->polarisation[k] (k=0,1,2)
           p->ekin
           p->time
           p->weight
           p->userflags
        */

    }

    mcpl_close_file(f);
}
```

C-code for creating MCPL file

Note: This is again shown in case someone is wondering if they could implement converters for their own application...

Listing 2: Simple example for creating an MCPL file with 1000 particles.

```
#include "mcpl.h"

void example()
{
    mcpl_outfile_t f = mcpl_create_outfile("myfile.mcpl");
    mcpl_hdr_set_srcname(f, "MyAppName-1.0");

    /* Tune file options or add custom comments or
       binary data into the header:

       mcpl_enable_universal_pdgcode(f, myglobalpdgcode);
       mcpl_enable_userflags(f);
       mcpl_enable_polarisation(f);
       mcpl_enable_doubleprec(f);
       mcpl_hdr_add_comment(f, "Some comment.");
       mcpl_hdr_add_data(f, "mydatakey",
                        my_datalength, my_databuf)
    */

    mcpl_particle_t* p = mcpl_get_empty_particle(f);

    int i;
    for ( i = 0; i < 1000; ++i ) {

        /* The following particle properties must
           always be set here:

           p->position[k] (k=0,1,2)
           p->direction[k] (k=0,1,2)
           p->ekin
           p->time
           p->weight

           These should also be set when required by
           file options:

           p->pdgcode
           p->userflags
           p->polarisation[k] (k=0,1,2)
        */

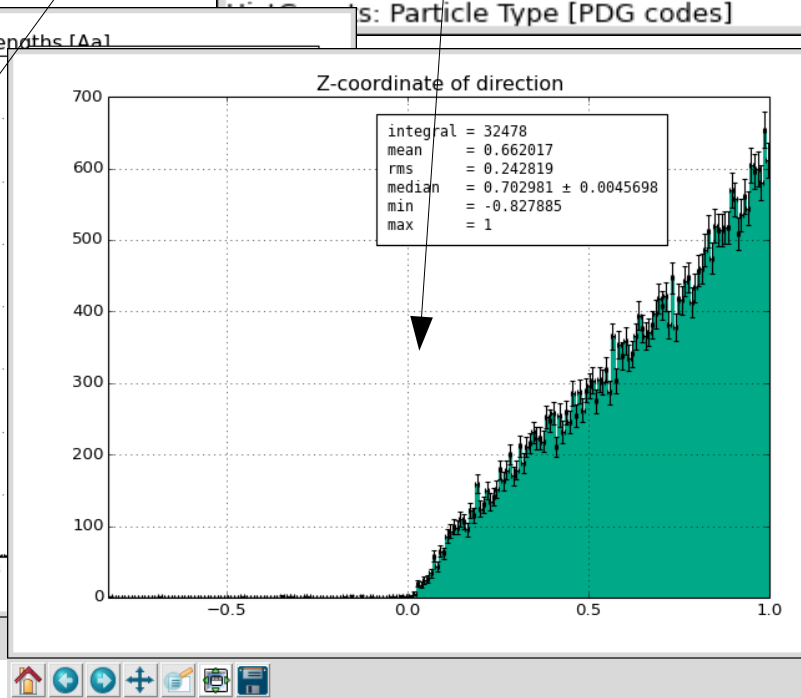
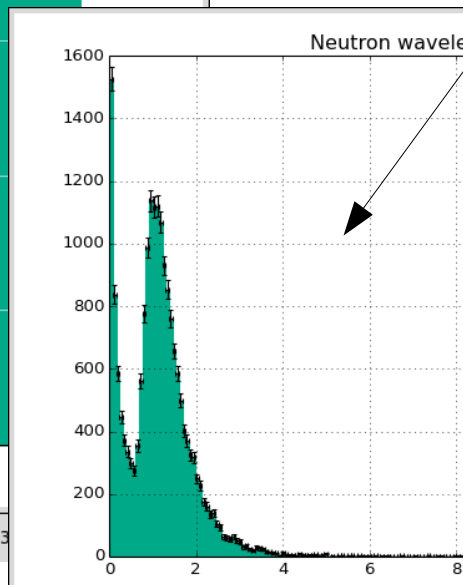
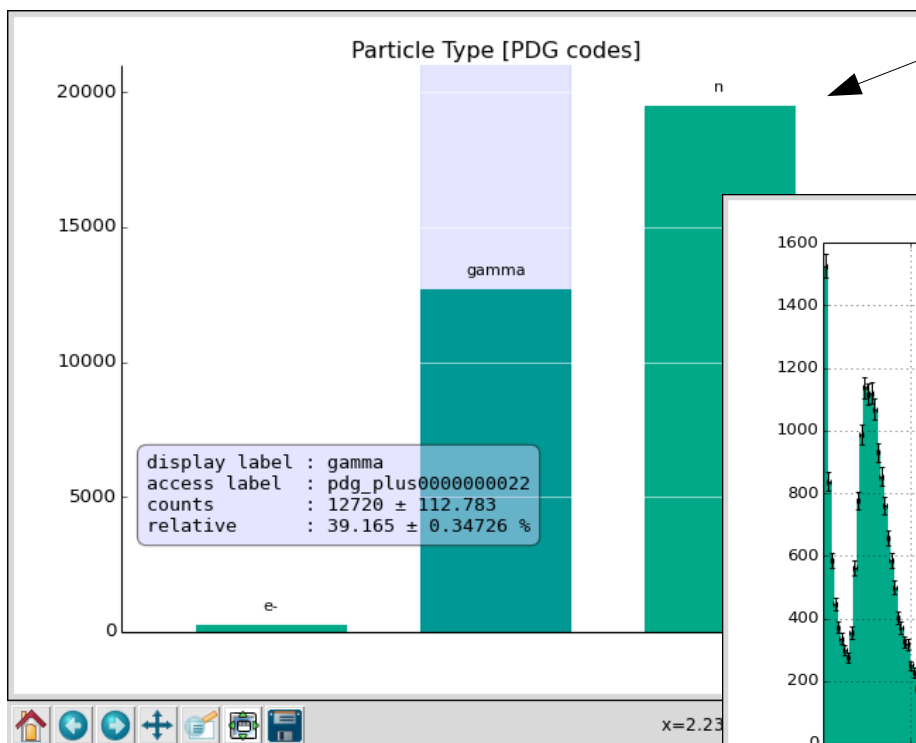
        mcpl_add_particle(f, p);
    }

    mcpl_close_outfile(f);
}
```

In the ESS detector group, we have many extra MCPL tools which we hope to make available externally as well... Example shown here is a “browser”.

`$> ess_mcplextra_browser myfile.mcpl.gz`

```
[ 0 : dirx      ]
[ 1 : diry      ]
[ 2 : dirz      ]
[ 3 : ekin       ]
[ 4 : neutron_wl ]
[ 5 : pdgcode    ]
[ 6 : posx       ]
[ 7 : posy       ]
[ 8 : posz       ]
[ 9 : time       ]
[10 : weight     ]
```



Can also produce 2D plots
of variable correlations...

And impose filters, to study
subset of particles

Summary and outlook

- Collaboration between ESS detector group (focus:Geant4), McStas developers & the ESS target group (focus:MCNP), have resulted in a new standard particle interchange format.
- It can be (and is) used for serious studies already now!
- We hope to be able to provide more MCPL tools in the future.
- Still a few loose ends to tidy up:
 - Several sections on MCPL website needs more contents.
 - Submit publication (this week!)
- We welcome any application-specific experts who might be interested in extending the list of MCPL-aware applications from the current (G4+MCNP+McStas). **Get in touch if you are interested!**



Additional material

Meta-data in MCPL header

File header information	
<i>Field</i>	<i>Description</i>
File type magic number 0x4d43504c ("MCPL")	All MCPL files start with this 4-byte word.
Version	File format version.
Endianness	Whether numbers in file are in little- or big-endian format.
Number of particles in file	64 bit integer.
Flag : Particles have polarisation info	If false, all loaded particles will have polarisation vectors (0,0,0).
Flag : Particles have "userflags" field	If false, all loaded particles will have userflags 0x00000000.
Flag : Particle info use double-precision	If true, floating points storage use double-precision.
Global pdgcode	If this 32 bit integer is non-zero, all loaded particles will have this pdgcode.
Source name	String indicating the application which created the MCPL file.
Comments	A variable number of comments (strings) added at file creation.
Binary blobs	A variable number of binary data blobs, indexed by keys (strings). This allows arbitrary custom data to be embedded.

Table 1: Information available in the header section of MCPL files.

Reference: C-code for extracting subset of particles from one MCPL file into a new one

Listing 3: Example extracting low-energy neutrons (pdgcode 2112) from an MCPL file.

```
#include "mcpl.h"

void example() {

    /* open files, transfer meta-data, add comment */

    mcpl_file_t fi = mcpl_open_file("myfile.mcpl");
    mcpl_outfile_t fo = mcpl_create_outfile("new.mcpl");
    mcpl_transfer_metadata(fi, fo);
    mcpl_hdr_add_comment(fo, "Extracted neutrons with ekin<0.1MeV");

    /* transfer selected particles */

    const mcpl_particle_t* particle;
    while ( ( particle = mcpl_read(fi) ) ) {
        if ( particle->pdgcode == 2112 && particle->ekin < 0.1 )
            mcpl_add_particle(fo, particle);
    }

    /* finish up */

    mcpl_closeandgzip_outfile(fo);
    mcpl_close_file(fi);
}
```