

Monte Carlo Particle Lists: MCPL

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Monte Carlo Particle Lists : MCPL

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

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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.

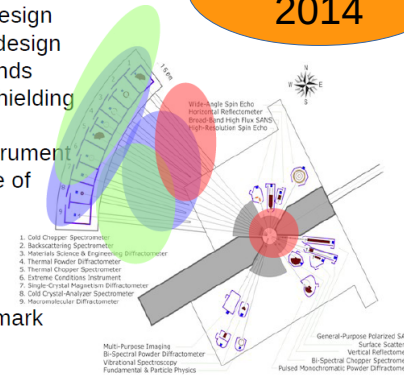
Monte Carlo vs. ray tracing – where are we heading?



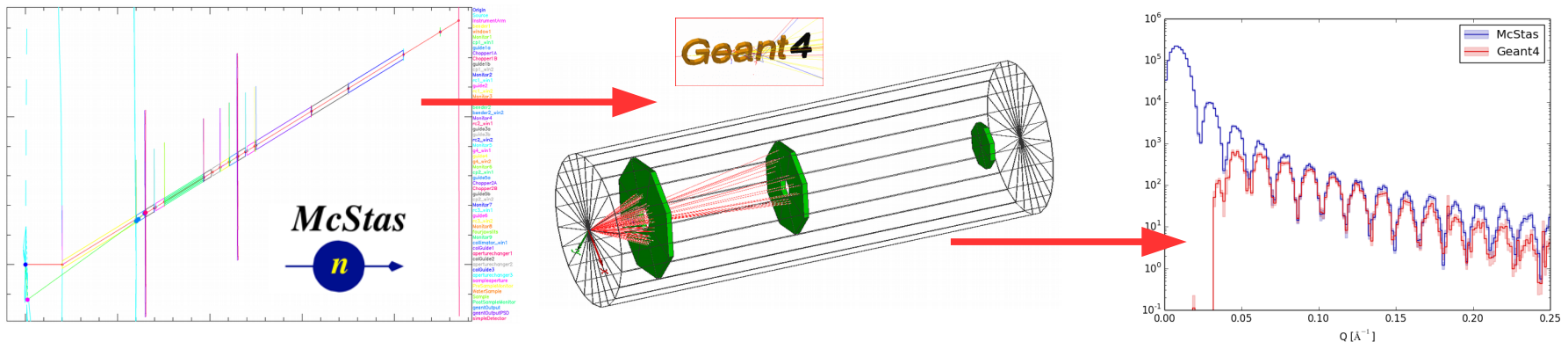
Klinkby,
2014

- **MCNP**: target, moderator, reflector design
- **McStas** (+*guide_bot*) for instrument design
- **GEANT4** for shielding and backgrounds
- Vites & 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



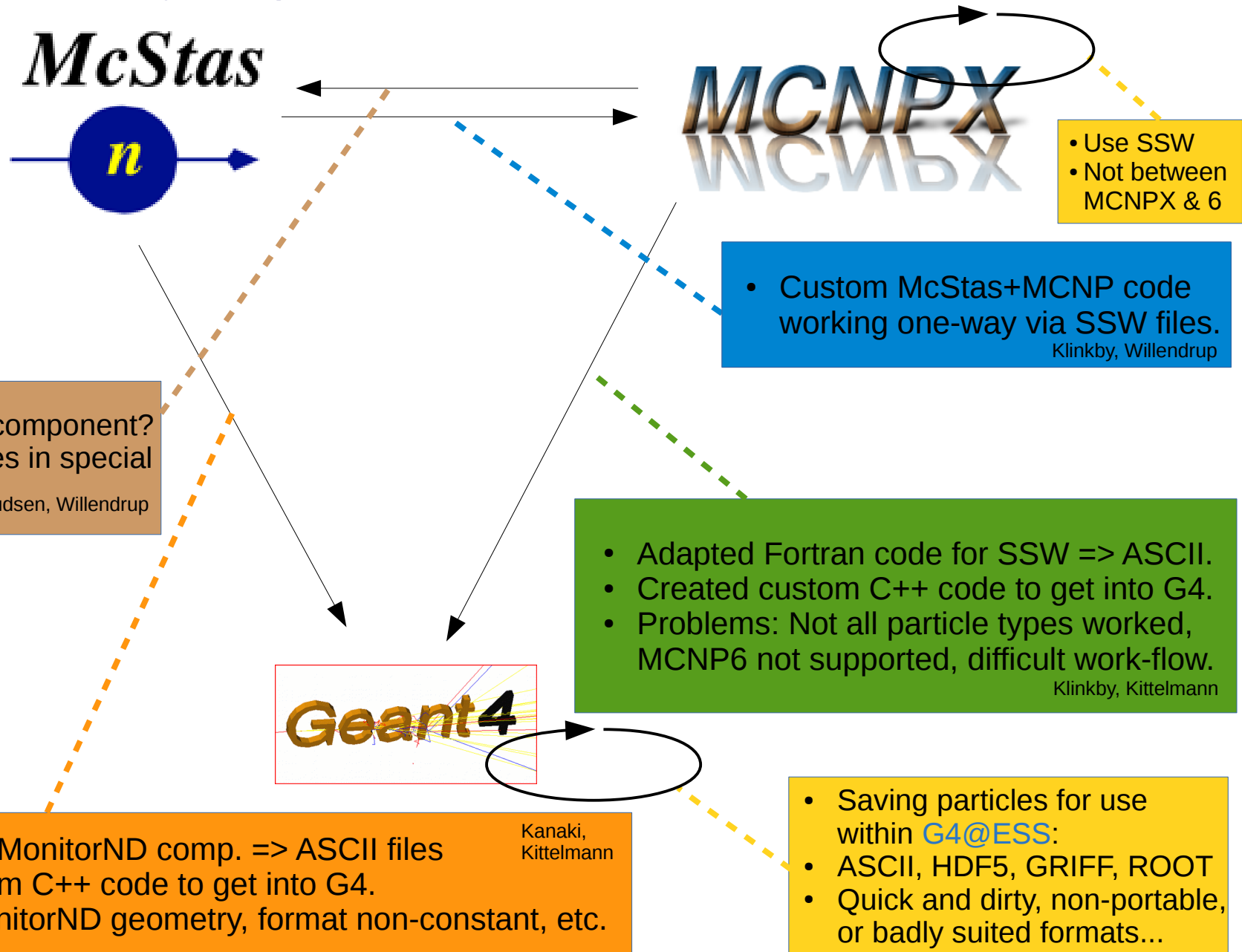
15



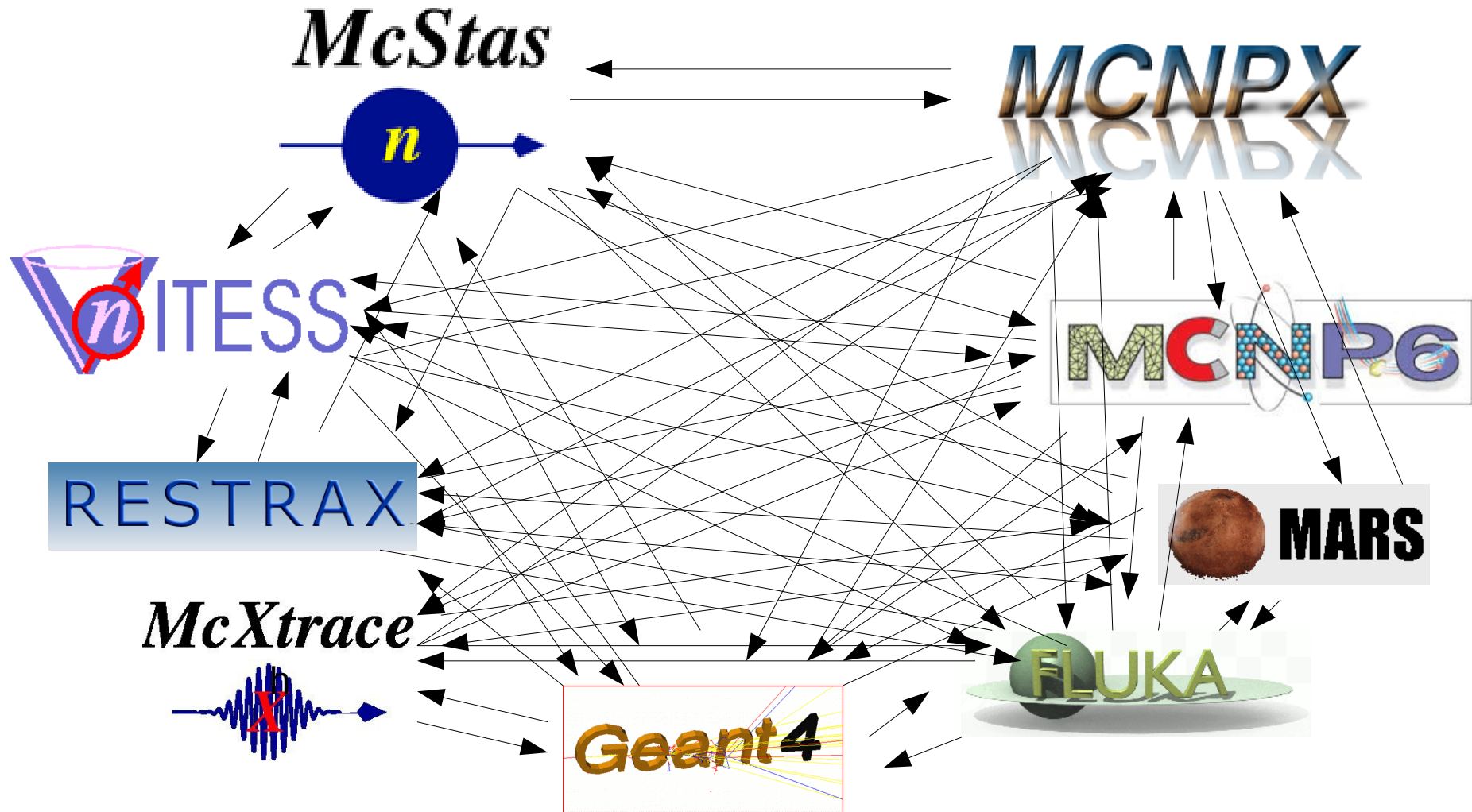
- Or, grab background particles from MCNP or Geant4 simulations to study shielding and background issues.

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...

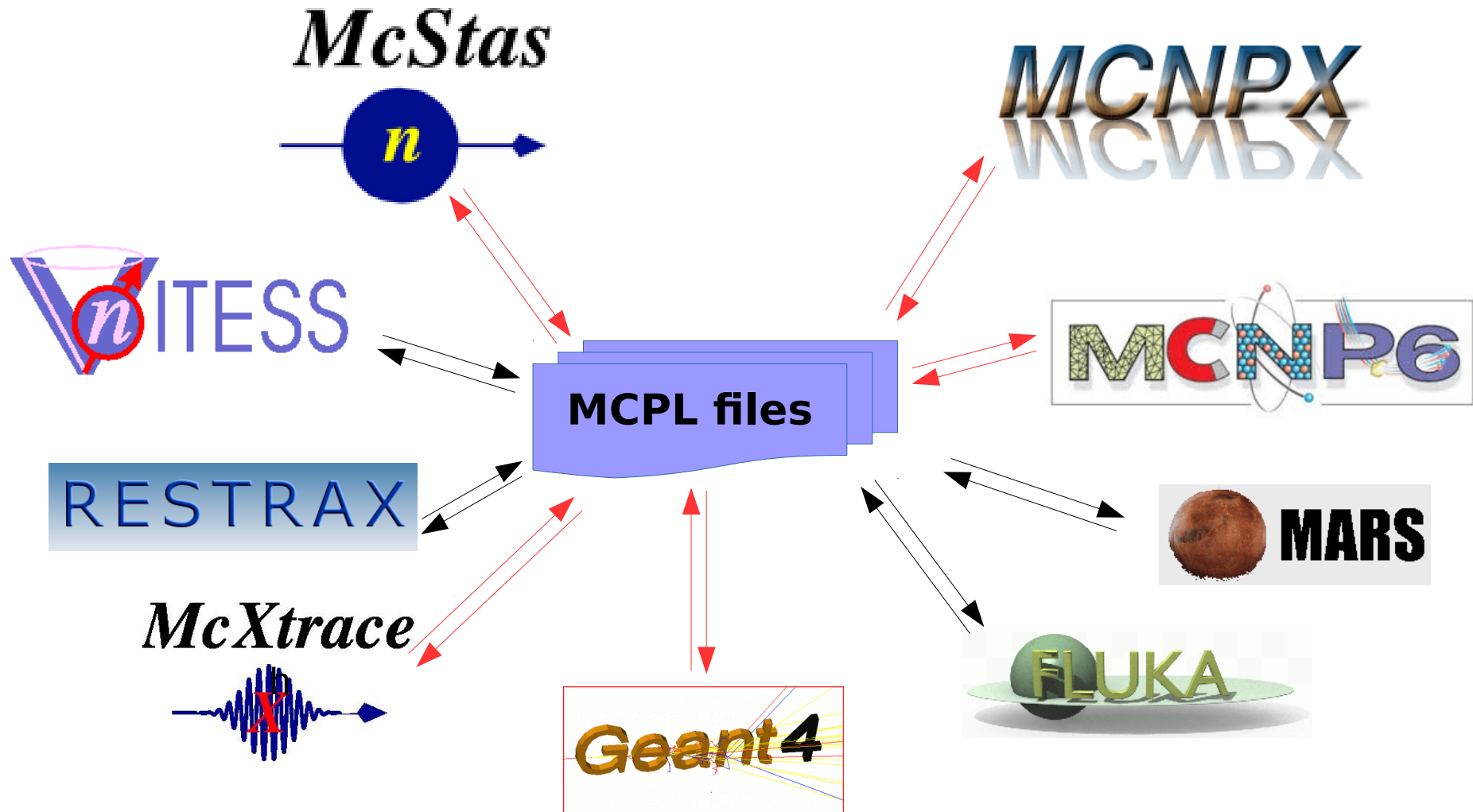


Consider more apps : The jungle gets impossibly tangled...



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

A graphic consisting of three overlapping, light blue rectangular boxes with rounded corners, arranged in a slightly offset, descending staircase pattern. The text "MCPL files" is written in bold black font across the top of the boxes.

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/>

View on GitHub 

MCPL Monte Carlo Particle Lists

[home](#) [get](#) [usage](#) [hooks](#) [about](#) [contact](#)

↓ [tar.gz](#) [.zip](#)

Welcome to the home of MCPL, a binary format for usage in physics simulations.

MCPL files contain lists of particle state information, and allows for easy storage and interchange of particles between various Monte Carlo simulation applications. It is implemented in portable C code and is made available to the scientific community, along with converters and plugins for several popular simulation packages.

The pages here are still missing lots of content, as we are currently busy trying to get the first release of MCPL out of the door and published in a scientific journal. Please check back later for more contents. In the meantime, you can consult the preliminary draft of our first intended publication: [MCPL writeup](#) , which already contains a lot of hopefully useful information.

Likewise, feel free to try out the code in the current condition by downloading the code.

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

Paper describing MCPL in detail about to be submitted

Monte Carlo Particle Lists : MCPL

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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

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

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	0.031	-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

Browsing an MCPL file with the MCPL tool

Just run: "mcp1tool <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

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
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5	22	0.511	28.693	10.867	40	0.18870	0.84395	0.52507	0.27059	1
6	22	0.511	28.693	10.867	40	0.18870	0.66981	0.33186	0.27059	1
7	22	0.511	28.693	10.867	40	0.18870	0.14628	0.98724	0.11248	1

PDG codes: 2112 = neutron, 22 = gamma

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

Browsing an MCPL file with the MCPL tool

Just run: "mcppltool <name-of-MCPL-file>"

Opened MCPL file myfile.mcppl.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 f
-> 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/SimpleGe
Number of blobs : 2
-> 74 bytes of data with key "ESS/dgcode_geopars"
-> 231 bytes of data with key "ESS/dgcode_genpars"

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).

Particle data format

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

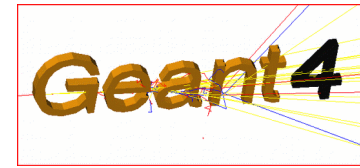
Columns of particle data (1 row = 1 particle)
In this file: No userflags or polarisation

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
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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
34	22	0.511	27.191	7.7111	40	0.12641	-0.034978	0.99136	0.13778	1
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

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!**

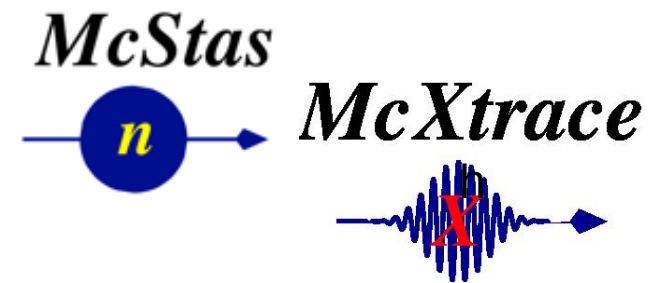
Using MCPL with MCNP



- 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.mcp1**
- 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 mcp1out = 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)
        */

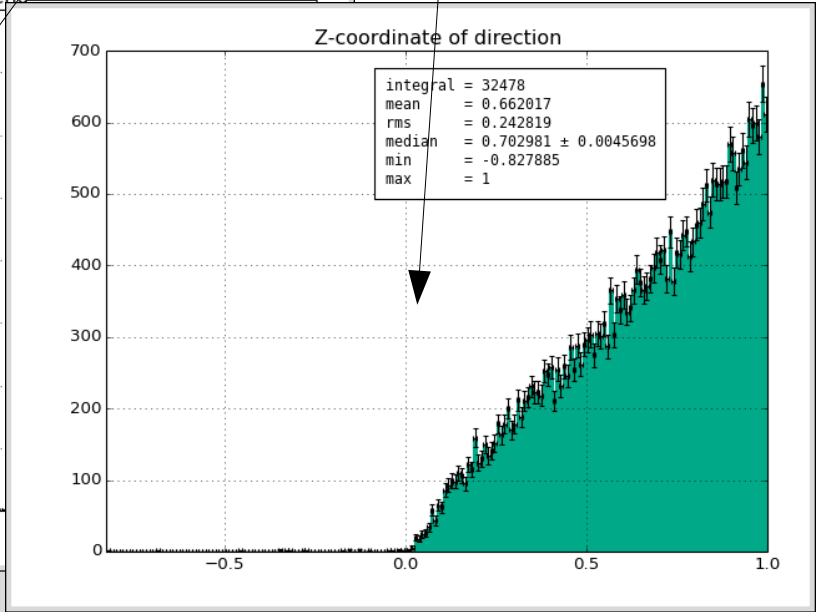
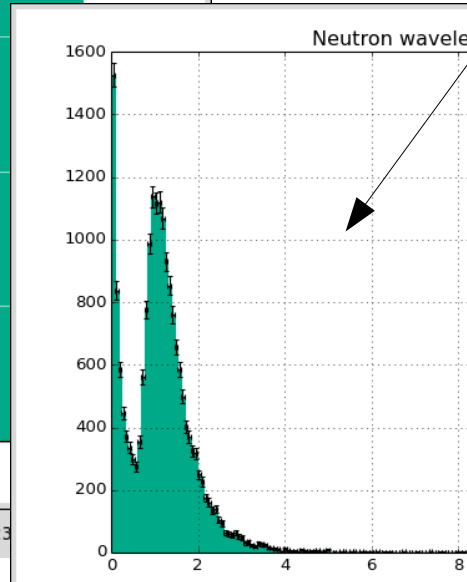
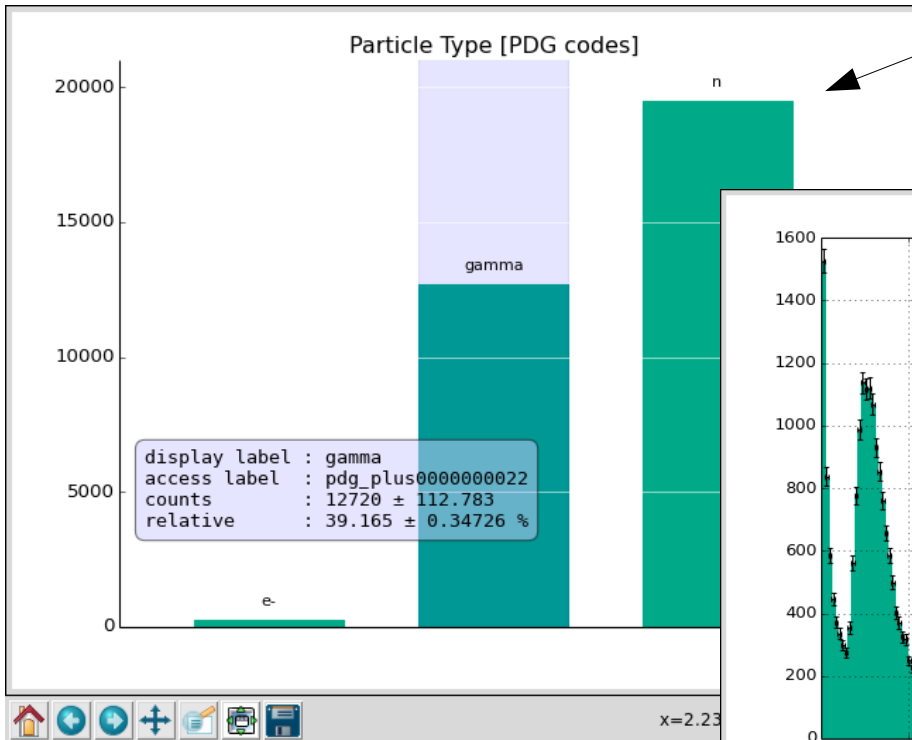
        mcpl_add_particle(f,p);
    }

    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);
}
```