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MCPL
Monte Carlo Particle Lists

Developments in the MCPL project

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EUROPEAN SPALLATION SOURCE

brightness

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Overview

- Recap of the MCPL project, capabilities, tools
  - Focus mostly on more recently added features marking those added post-Coimbra or after the MCPL paper was published as NEW!
- Discuss future plans, ideas, wishes

Recap: Key MCPL features

MCPL: Monte Carlo Particle Lists

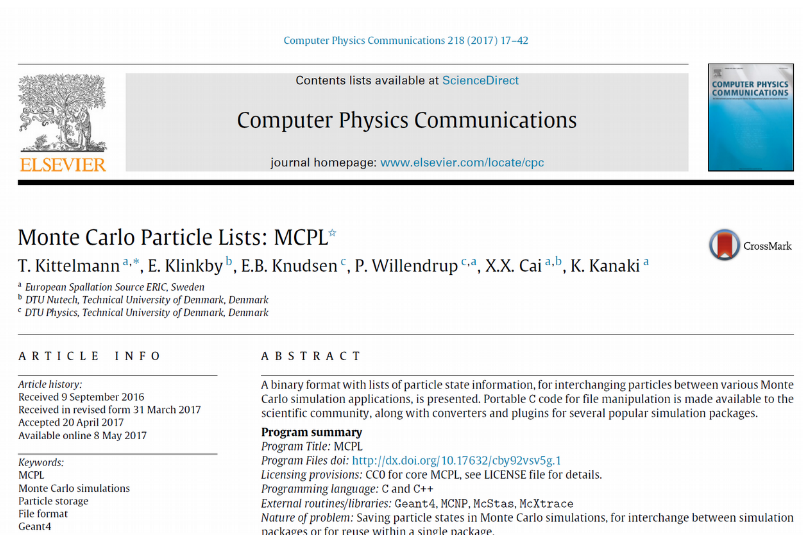
- It is a ***simple*** binary file-format. Each file contains a list of MC particles with enough info to seed simulations.
- MCPL files can contain ***meta-data***. This makes it possible to tell what data is in a file, where it came from, how it should be interpreted.
- The format is ***flexible***: can contain a lot of information if needed, or can contain only minimal information if small file-size is important. Can be gzip'ed.
- 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 comes with ***tools and APIs***, such as for inspecting or editing contents.
- ***Well-defined*** versioned format, focus on backwards compatibility.

… focus on availability:

- Extremely liberal license (CC0) encourage bundling.
- API for C/C++/Python code (all versions).
- “fat” single-file versions of all C code (even embedding zlib)
- Can “pip install” Python API+pymcpltool.

Download, follow, and report issues @GitHub

… and documentation: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Monte Carlo Particle Lists: MCPL

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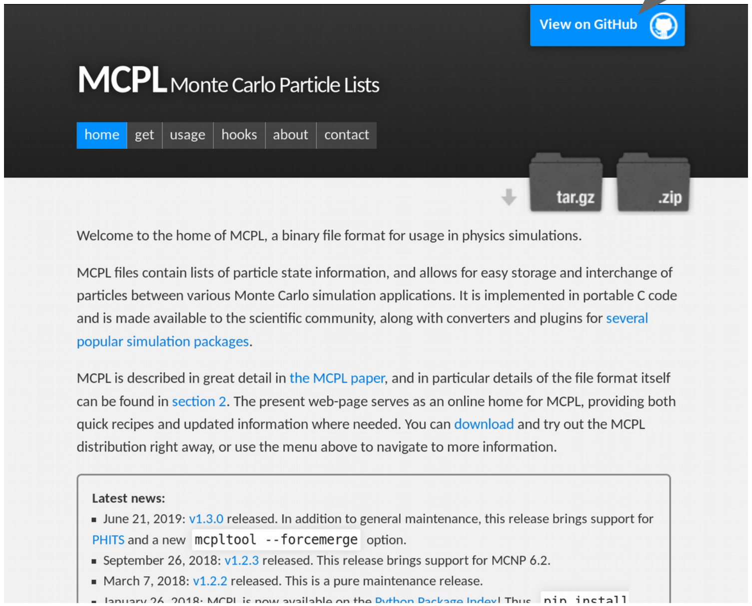
ABSTRACT

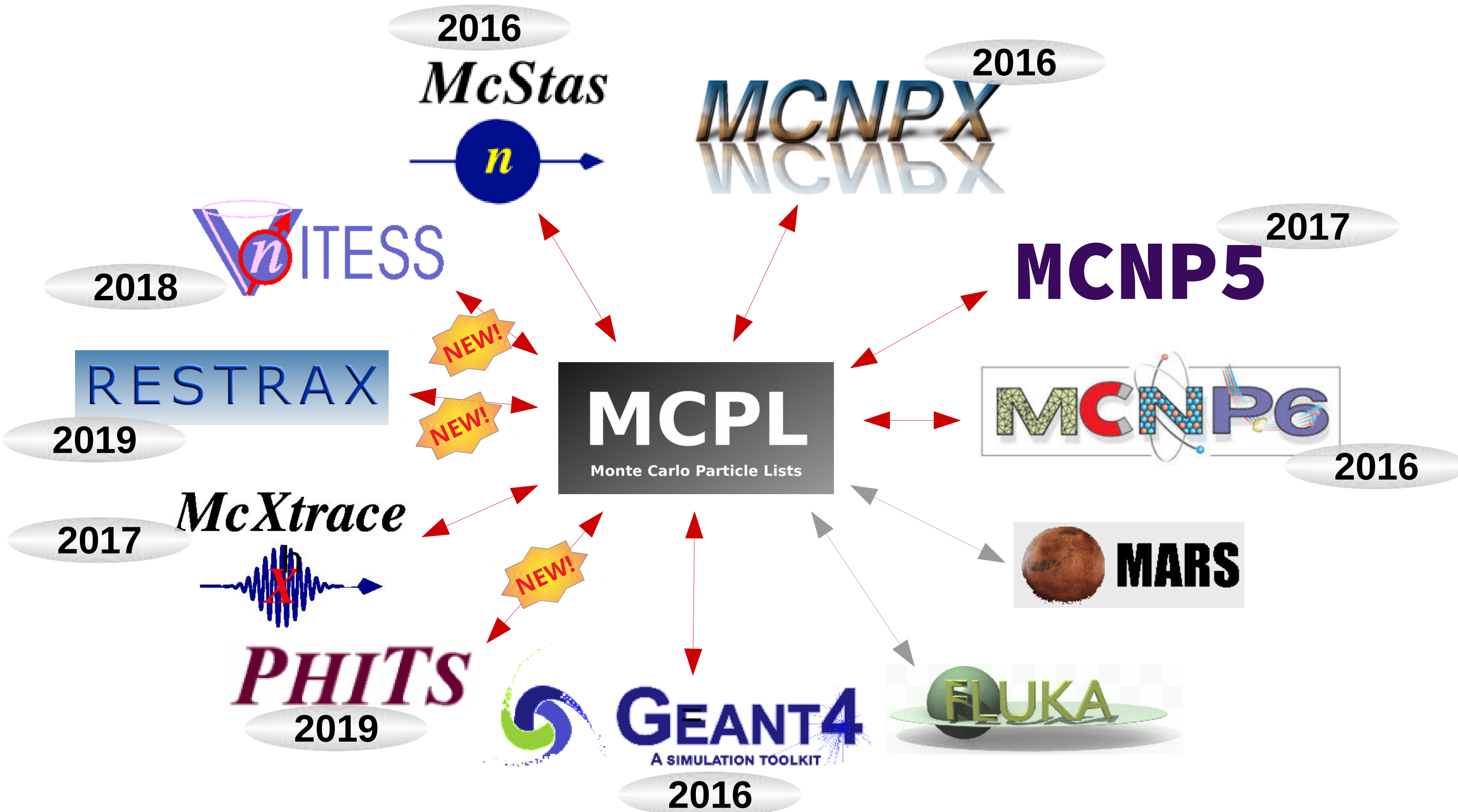
A binary format with lists of particle state information, for interchanging particles between various Monte Carlo simulation applications, is presented. Portable C code for file manipulation is made available to the scientific community, along with converters and plugins for several popular simulation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

Program summary
Program Title: MCPL
Program Files doi: http://dx.doi.org/10.17632/cby92vsv5g.1
Licensing provisions: CC0 for core MCPL, see LICENSE file for details.
Programming language: C and C++
External routines/libraries: Geant4, MCNP, McStas, McXtrace
Nature of problem: Saving particle states in Monte Carlo simulations, for interchange between simulation packages or for reuse within a single package.



- Detailed paper for release 1.1.0: (DOI 10.1016/j.cpc.2017.04.012)
- Online docs with recipes (https://mctools.github.io/mcpl/)

Codes with MCPL support



Certainly have critical mass by now! :-)

Available   Missing

What form does MCPL support take?

- Built-in support in instrument simulation codes:
  - McStas, McXtrace, VITESS, RESTRAX/SIMRES (NEW! NEW!)
  - Batteries included → great for users!

Most work done by developers of these applications!

- C++ helper classes for particle capture or event seeding available for Geant4 (in line with how most Geant4 users work)

Me

- MCNP support relies on inbuilt ability to dump particles to/seed from "SSW" files.

Me+E. Klinkby

  - We provide **ssw2mcpl** and **mcpl2ssw** tools.
  - Somewhat high maintenance burden due to plethora of MCNP flavours + closed nature of programme.
  - Complication is that particles need "surface ID". Can be provided as MCPL userflags or via global setting.
  - **mcpl2ssw** must be provided with sample SSW files from target setup.
- PHITS support: Like MCNP, but simpler. More details later. (NEW!)

Me+D. Di Julio

Data in MCPL files

All generic parameters always Available to reading code, no matter source of MCPL file.

Particle state information	
Field	Description
PDG code	32 bit integer indicating particle type.
Position	Vector, values in centimetres.
Direction	Unit vector along the particle momentum.
Kinetic energy	Value in MeV.
Time	Value in milliseconds.
Weight	Weight or intensity.
Polarisation	Vector.
User-flags	32 bit integer with custom info.

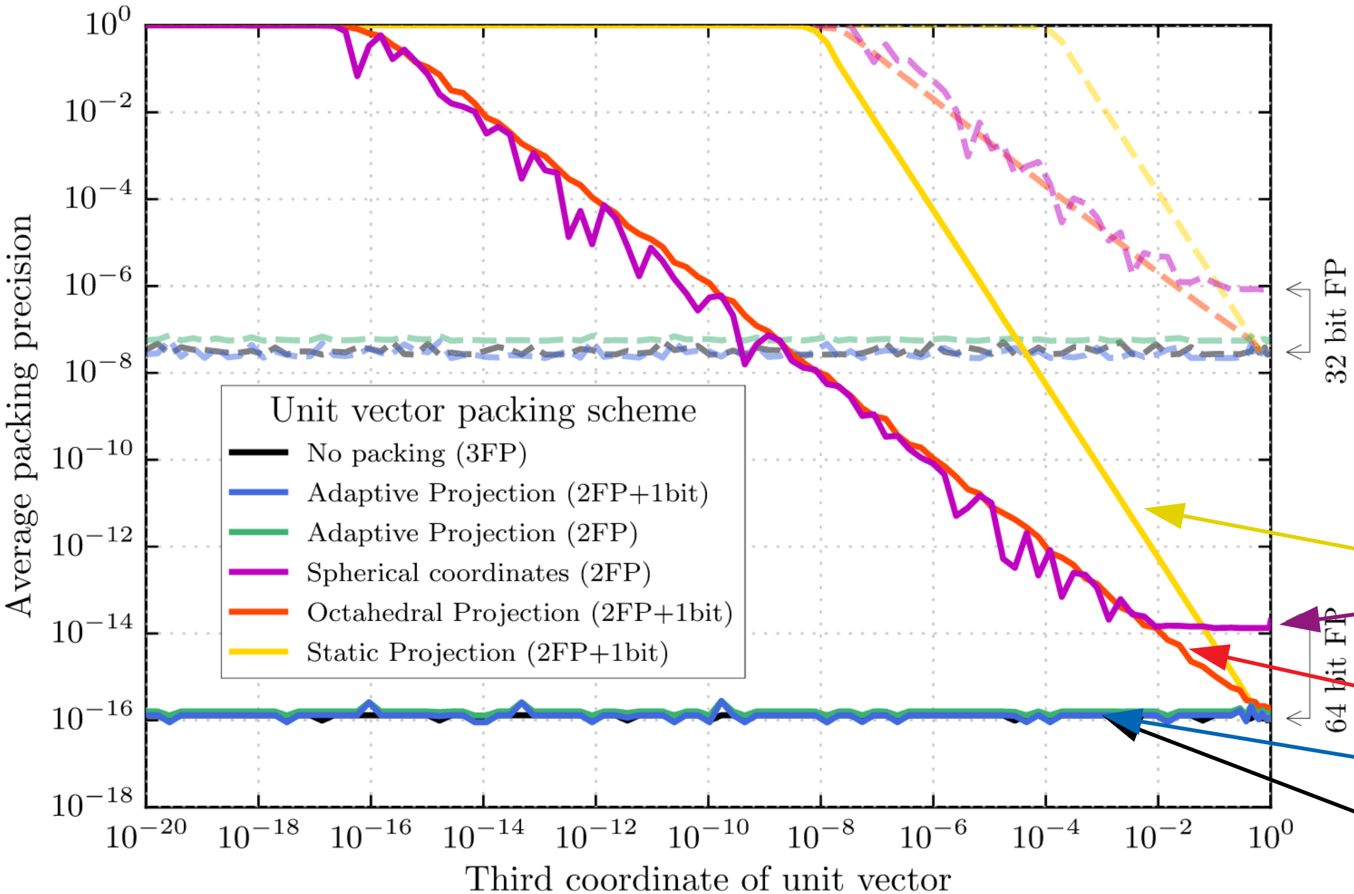
Flexibility in how this is actually stored!

Detailed layout of the data associated with each particle in an MCPL file.

Particle data layout		
Presence	Count & type	Description
OPTIONAL	$3 \times$ FP	Polarisation vector (if enabled in file).
ALWAYS	$3 \times$ FP	Position vector
ALWAYS	$3 \times$ FP	Packed direction vector and kinetic energy.
ALWAYS	$1 \times$ FP	Time.
OPTIONAL	$1 \times$ FP	Weight (if file does not have universal weight).
OPTIONAL	$1 \times$ INT32	PDG code (if file does not have universal PDG code).
OPTIONAL	$1 \times$ UINT32	User-flags (if enabled in file).

This implies from 28 to 96 bytes/particle. Already good, but most files are gzip'ed (by MCPL or user) and consume less. (NB: MCPL code can read .mcpl.gz files directly)

Novel packing of direction vectors: Optimal storage size without precision loss!



Breakdown of the Adaptive Projection Packing method, in which a unit vector, (u_x, u_y, u_z) is stored into two floating point numbers, FP1 and FP2, and one extra bit of information.

Adaptive Projection Packing				
Scenario	FP1	FP2	+1 bit	Packed signature
$\lvert u_x \rvert$ largest	$1/u_z$	u_y	sign(u_x)	$\lvert FP1 \rvert > 1, \lvert FP2 \rvert < 1$
$\lvert u_y \rvert$ largest	u_x	$1/u_z$	sign(u_y)	$\lvert FP1 \rvert < 1, \lvert FP2 \rvert > 1$
$\lvert u_z \rvert$ largest	u_x	u_y	sign(u_z)	$\lvert FP1 \rvert < 1, \lvert FP2 \rvert < 1$

Example file

Inspected with (py)mcpltool

```
Opened MCPL file recordfwd.mcpl.gz:

  Basic info
    Format             : MCPL-3
    No. of particles   : 542199
    Header storage     : 826 bytes
    Data storage       : 17350368 bytes

  Custom meta data
    Source             : "Geant4"
    Number of comments : 8
          -> comment 0 : "Created with the Geant4 MCPLWriter in the ESS/dgcod
          -> 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/GeoSl
          -> comment 7 : "ESS/dgcode generator module : G4StdGenerators/Simpl
    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
    Fixed part. weight : yes (weight 1)
    FP precision       : single
    Endianness         : little
    Storage            : 32 bytes/particle

index     pdgcode   ekin[MeV]      x[cm]      y[cm]      z[cm]         ux         uy         uz   time[ms]
    0          22      1.2238    -13.327     3.5344         40   -0.43426  -0.036564    0.90005    0.14113
    1          22     0.12059    -15.976     14.788         40   -0.63971   0.082934    0.76413    0.14113
    2          22     0.10212    -22.452    -7.1864         40   -0.58735   -0.35527    0.72718    0.14113
    3          22       7.695     12.547     36.899         40    0.19775    0.47066    0.85987    0.20354
    4        2112     2.5e-08          0          0         40          0          0          1     0.1829
    5          22    0.077251    -33.171     15.428         40   -0.81854    0.33885    0.46387  0.0047377
                                                                      666    0.38747    0.91761  0.0047367
                                                                      866  -0.075343    0.97717    0.12339
                                                                        0          0          1     0.1829
    9        2112     2.5e-08          0          0         40          0          0          1     0.1829
```

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, input deck from MCNP/PHITS, etc.

NB: compresses to 19.2bytes/particle

Columns of particle data
In this file: No *userflags* or *polarisation*

PDG codes: 2112 = neutron, 22 = gamma
More at http://pdg.lbl.gov/2015/reviews/rpp2015-rev-monte-carlo-numbering.pdf

C API

- Stable C API for reading/creating/editing MCPL
- Use to create most application-specific hooks
- Some users use it to analyse or tailor MCPL files

```
#include "mcpl.h"
void read_example()
{
  mcpl_file_t f = mcpl_open_file("myfile.mcpl");
  const mcpl_particle_t* prtcl;
  while ( ( prtcl = mcpl_read(f) ) ) {
    //<Access here: prtcl->ekin, prtcl->time, ...>
  }
  mcpl_close_file(f);
}
```

```
#include "mcpl.h"
void create_example()
{
  mcpl_outfile_t f = mcpl_create_outfile("myfile.mcpl");
  mcpl_hdr_set_srcname(f,"Custom C code");
  mcpl_hdr_add_comment(f,"Just an example.");
  mcpl_enable_doubleprec(f);
  int i;
  mcpl_particle_t * prtcl = mcpl_get_empty_particle(f);
  for ( i = 0; i < 1000; ++i ) {
    //<Set here: prtcl->ekin, prtcl->time, ...>
    mcpl_add_particle(f,prtcl);
  }
  mcpl_close_outfile(f);
}
```

C not C++ to support more apps (C is “lingua franca” of SW)

Despite being C, interface is “object oriented” and hopefully easy.

Custom filtering via C API

Filtering files with custom code in very few lines:

mcpl_transfer_metadata does all the hard work of configuring output file

```
#include "mcpl.h"
void filter_example()
{
  mcpl_file_t fi = mcpl_open_file("all.mcpl");
  mcpl_outfile_t fo = mcpl_create_outfile("lowEneutrons.mcpl");
  mcpl_transfer_metadata(fi, fo);
  mcpl_hdr_add_comment(fo,"Only neutrons, ekin<0.1MeV");
  const mcpl_particle_t* prtcl;
  while ( ( prtcl = mcpl_read(fi) ) ) {
    if ( prtcl->pdgcode == 2112 && prtcl->ekin < 0.1 )
      mcpl_transfer_last_read_particle(fi,fo);
  }
  mcpl_close_outfile(fo);
  mcpl_close_file(fi);
}
```

NEW!

mcpl_transfer_last_read_particle from MCPL v1.3.0 prevents lossy unpacking+repacking of data. If need to edit particles fields, replace with:
mcpl_add_particle(fo,prtcl);

Python API (from MCPL v1.2.0) NEW!

To enable MCPL Python module, download mcpl.py or do
python -mpip install mcpl
(this incidently also installs the pymcpltool…)

Technical details:
- Pure Python, does not use mcpl.c
- Usage of Numpy for efficiency.
- Works with both Python 2 and 3.
- Readonly access for now.

```
import mcpl
myfile = mcpl.MCPLFile("myfile.mcpl")
for p in myfile.particles:
   print( p.x, p.y, p.z, p.ekin )
```

Accessing particles is straight-forward

Can also process blocks of N particles at a time, for increased efficency.

```
for p in myfile.particle_blocks:
   print( p.x, p.y, p.z, p.ekin )
```

Numpy arrays of length N

```
print( myfile.sourcename,
       myfile.nparticles,
       myfile.opt_singleprec )
for cmt in myfile.comments:
    print( 'Comment: "%s"' % cmt )
```

Can of course access meta data as well.

Command-line tools

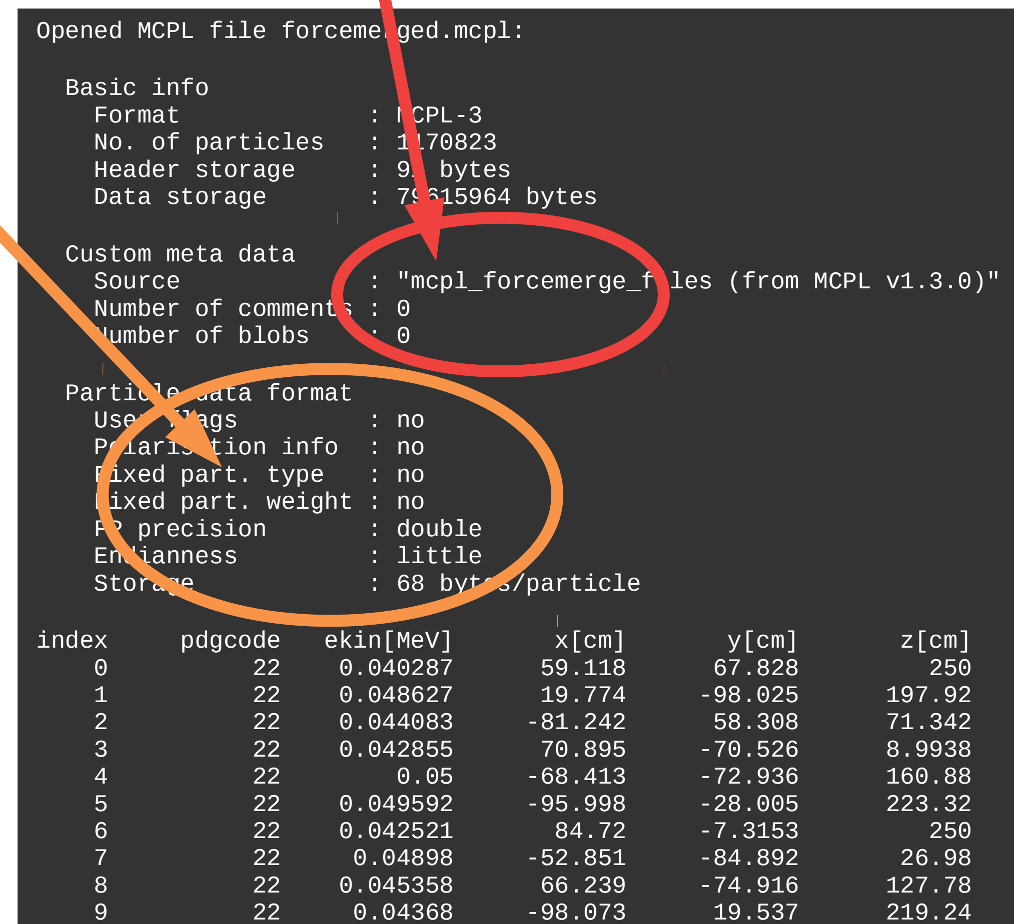
- **mcpltool** and **pymcpltool** NEW!, both can:
  - **Inspect** files, extract binary blobs to stdout
  - Convert MCPL to (inefficient) **ASCII** files for interoperability with software lacking MCPL support.
  - Show all options with **--help**
- The **mcpltool**:
  - Compiled executable with C compiler (from “fat” or proper linked code)
  - Can edit files:
    - **Merge** files
    - **Extract** subset of particles to smaller file (select by type or file idx)
    - **Repair** files leftover by crashed jobs
- The **pymcpltool** NEW!:
  - Built upon Python API (fast because of Numpy)
  - Download 1 file + run, or “pip install mcpl”
  - Can provide **statistics** (see next slide)

Merging files

- Ability to merge files is crucial for collecting output of concurrent simulations.
  - But other use-cases exists for combining files.
- Done via “**mcpltool --merge**” or “**mcpl_merge_files**“ in C API.
- As a quality concern, MCPL is conservative about not producing files with misleading meta-data.
- All meta-data must be identical and will be transferred to the newly created file.
- On several occasions this restriction has caused problems...

New “mcpltool --forcemerge” in release 1.3.0 NEW!

- Can always merge, but will ***throw away all meta-data***.
  - Should be considered as a last resort only!
- ***Particle data format options adapted*** to accommodate particles from all input files.
  - Double-prec, polarisation, fixed pdg/weight on demand.
  - Discard userflags by default [override with --keepuserflags]
- Loss-less particle data transfer whenever possible.



```
Opened MCPL file forcemerged.mcpl:

  Basic info
    Format               : MCPL-3
    No. of particles     : 1170823
    Header storage       : 9[illegible] bytes
    Data storage         : 79615964 bytes

  Custom meta data
    Source               : "mcpl_forcemerge_files (from MCPL v1.3.0)"
    Number of comments   : 0
    Number of blobs      : 0

  Particle data format
    User flags           : no
    Polarisation info    : no
    Fixed part. type     : no
    Fixed part. weight   : no
    FP precision         : double
    Endianness           : little
    Storage              : 68 bytes/particle

index     pdgcode    ekin[MeV]       x[cm]       y[cm]       z[cm]
    0          22     0.040287      59.118      67.828         250
    1          22     0.048627      19.774     -98.025      197.92
    2          22     0.044083     -81.242      58.308      71.342
    3          22     0.042855      70.895     -70.526      8.9938
    4          22         0.05     -68.413     -72.936      160.88
    5          22     0.049592     -95.998     -28.005      223.32
    6          22     0.042521       84.72     -7.3153         250
    7          22      0.04898     -52.851     -84.892       26.98
    8          22     0.045358      66.239     -74.916      127.78
    9          22      0.04368     -98.073      19.537      219.24
```

File statistics with pymcpltool

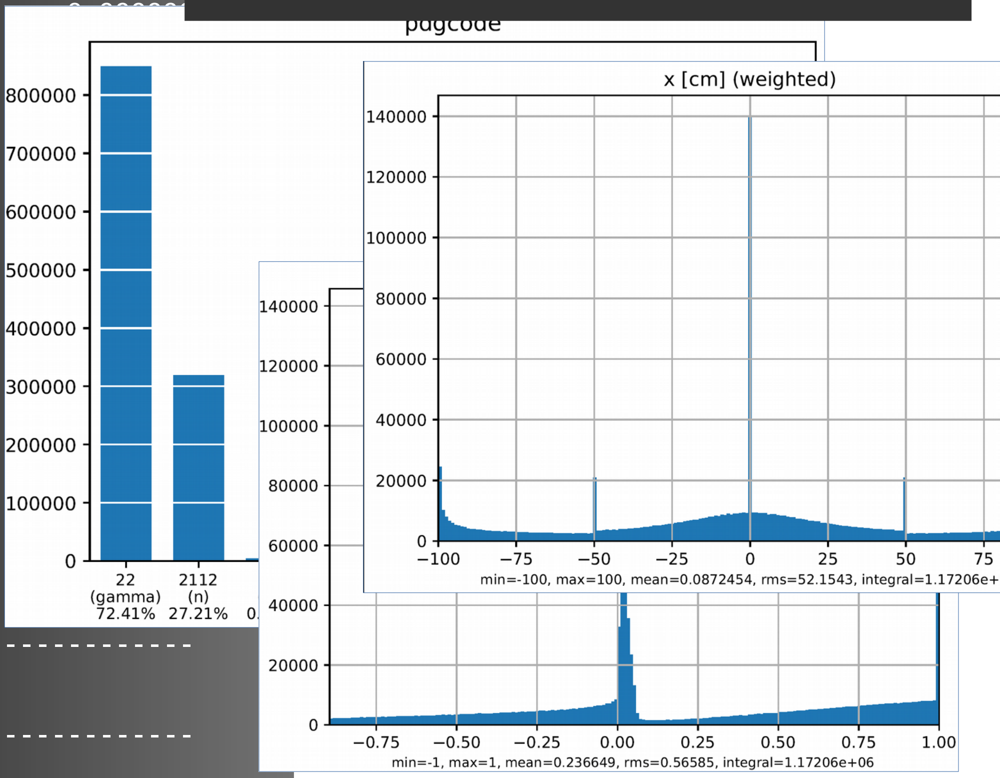
NEW!

```
pymcpltool --stats <filename>
```

```
-------------------------------------------------------------------------------
nparticles    : 1172044
sum(weights)  : 1.17206e+06
-------------------------------------------------------------------------------
              :            mean             rms             min             max
-------------------------------------------------------------------------------
ekin    [MeV] :         0.68247         14.1939      9.7657e-11         1889.44
x        [cm] :       0.0872454         52.1543            -100             100
y        [cm] :       0.0192493         52.1484            -100             100
z        [cm] :         98.2832         78.6334    -5.55112e-17             250
ux            :    -0.000322662        0.558483              -1
uy            :     6.59925e-05        0.558487       -0.999998
uz            :        0.236649         0.56585              -1
time     [ms] :           24658      4.3971e+06       1.462e-06
weight        :         1.00001      0.00483571        0.654834
polx          :     0.000415962       0.0178829               0
poly          :     0.000166385      0.00715315               0
polz          :     0.000499154       0.0214595               0
----------------------------------------------------------------------
pdgcode       :          22 (gamma)              848745 (72.41%)
                       2112 (n)                  318868 (27.21%)
                         11 (e-)                   3922 ( 0.33%)
                        -11 (e+)                    431 ( 0.04%)
                       2212 (p)                      80 ( 0.01%)
                        211 (pi+)                     5 ( 0.00%)
                        -12 (nu_e-bar)                4 ( 0.00%)
                 1000010030 (T)                       2 ( 0.00%)
                         14 (nu_mu)                   2 ( 0.00%)
                 1000020040 (alpha)                   1 ( 0.00%)
                       -211 (pi-)                     1 ( 0.00%)
                     [ values ]             [ weighted counts ]
-------------------------------------------------------------------------------
userflags     :           0 (0x00000000)  1.17206e+06 (100.00%)
                     [ values ]             [ weighted counts ]
-------------------------------------------------------------------------------
```

```
pymcpltool --stats --gui <filename>
```

```
pymcpltool --stats --pdf <filename>
```



PHITS support (new in release 1.3.0) NEW!

Added in close collaboration with Douglas Di Julio, ESS.

- Use PHITS capability to dump particles in certain tallies to so-called "dump files", and to seed runs from such files.
- Dump files can be converted to/from MCPL format via two new tools: **phits2mcpl** and **mcpl2phits**
  - Tools shipped with MCPL, but quick access by downloading "fat" versions from MCPL website.
- This all resembles how we support MCNP
  - Difference is that PHITS dump files do not have (complicated) header sections → simpler support but no self-describing meta-data available.

PHITS cfg for dump file output

NEW!

- Can be output from t-cross, t-product and t-time tallies:

```
[ t-cross ]
   part = all
   reg = 1
   r-from r-to area
    1       2   1.0
   dump = 13
   1 2 3 4 5 6 7 8 9 10 14 15 16
   file = mydump
```

Tally-specific stuff

Dump-file cfg with 13 variables
(1=type, 2=x, 8=ekin, etc.)

- Contents are flexible, but we support only the variant above, and the following with 10-variables which excludes polarisation info:

```
   dump = 10
   1 2 3 4 5 6 7 8 9 10
```

- PHITS dump files have no header, but **phits2mcpl** can detect number of variables and thus distinguish the two above variants (but don't swap/replace individual variables!)

Seed PHITS from dump files

NEW!

- Input cfg must use s-type=17 and appropriate dump file cfg:

```
[ parameters ]
   maxcas = 123456 # nparticles per batch
   maxbch = 1 # number of batches
   ...

[ source ]
   s-type =  17
   file = phits.dmp
   dump = 13
   1 2 3 4 5 6 7 8 9 10 14 15 16
```

- **mcpl2phits** outputs the 13-variable variant PHITS dump files by default, but the **--nopol** flag can be used to produce the 10-variable variant without polarisation info.

- For now recommend setting **maxbch=1** and **maxcas** to the number of particles in the file. Will revisit this over the coming months, since >1 batch might be desirable.

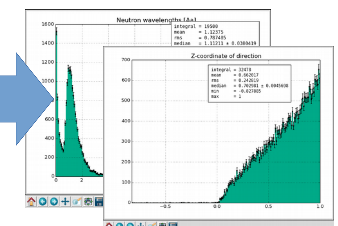
Outlook / wishful thinking

Funding missing

- Github issue 6: Mergeable statistics? E.g. “NEvtsSimulated” which would be added when files are merged. Would allow easier book-keeping.
- Github issue 44: In ESS Detector Group we have internal C++-based enhanced tools for working with MCPL files, based on our ExpressionParser and histogram classes:

```
mcplfilterfile in.mcpl.gz  out.mcpl.gz “time<2ms and is_neutron and neutron_wl>2.2Aa”
```

```
mcplbrowse in.mcpl.gz where “pdgcode!=11 and ekin<10keV”
```



GEANT4 A SIMULATION TOOLKIT

```
gen.input_file = "myfile.mcpl.gz"
gen.input_filter = "ekin>1keV && sqrt(x^2+y^2) < 10 cm"
```

  - It would be great to export these tools to the greater community, but needs significant work to disentangle and prepare.
- IMHO if the Python API would not be read-only, we could easily build and easily distribute a lot of great new tools (e.g. GUI for editing). It would also be easy for people to compose/filter their own MCPL files from cmdline or code.