CORSIKA Workshop 2022 - Cherenkov Simulation

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Thesis - Optimization of HPC code for Gamma Ray experiments

https://gitlab.iap.kit.edu/AirShowerPhysics/corsika/-/tree/275-Cherenkov-module
Last merge with the master branch : 6b6d8af2583bc6a5a062c56e227cbe86b42034c7

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07/13/22

Context

CTA (Cherenkov Telescope Array)

- Next generation ground-based observatory for gamma-ray astronomy at very-high energies
  - 2 sites in the two hemispheres and counts more than 50 of telescopes of three different sizes
- Simulation represents 80% of CPU time
  - Consumes almost 100 million HS06 CPU hours/year
  - Uses CORSIKA 7 with the Cherenkov module
  - Runs on the EGI grid

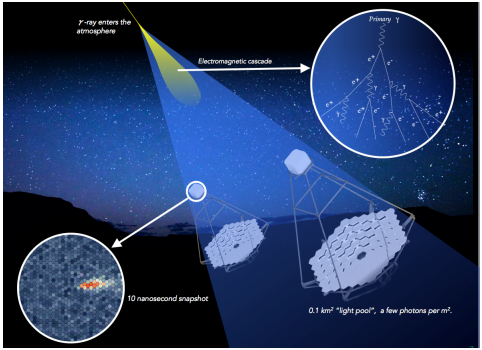
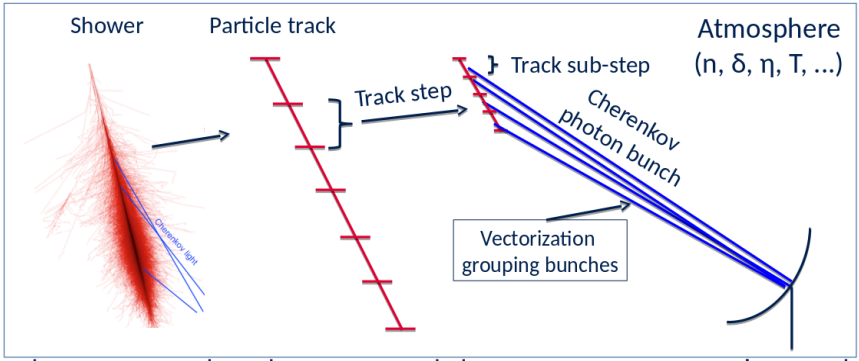


Figure 1: Representation of electromagnetic cascade with production and reception on telescopes of Cherenkov photons

Cherenkov Simulation in CORSIKA 8



Cherenkov module - Classes

Cherenkov	Generate and propagate Cherenkov photons
Vector-libm	C library of vectorized elementary functions
Interpolation	Linear and cubic spline interpolations
StackBunches	Store and load photon bunches for different classes (Cherenkov, TelescopeGrid, etc)
AtmosphereTabulated	Create a CORSIKA 7 tabulated atmosphere and calculates some values
LongitudinalProfileCherenkov	Calculate the longitudinal profile for photons
TelescopeGrid	Create and manage telescopes
Telescope	Generic telescope which manages bunches recorded (multiple geometries)
Bunch	Store a bunch information (coordinates, number of photons, etc)
CherenkovParquet	Store data on hard disk
TelescopeParquet	
LongitudinalCherenkovParquet	

Cherenkov module - Initialization

```
1   // Init the tabulated atmosphere
2   corsika::cherenkov::AtmosphereTabulated atmosphere{
3         myExperiment.atmosphereTabulatedNumber_,
4         injectionHeight,
5         constants::EarthRadius::Mean,
6         observationHeight,
7         thetaRad,
8         phiRad};
9
10  // Init the telescope grid
11  corsika::cherenkov::TelescopeGrid<TelescopeParquet> telescopeGrid{
12        myExperiment.telConfig_, atmosphere, stackbunches};
13
14  // Init the stack bunches
15  corsika::cherenkov::StackBunches stackbunches;
16
17  // Init the Cherenkov simulation
18  corsika::cherenkov::Cherenkov<NoOutputCherenkov>
19          pCherenkov{atmosphere, stackbunches};
20
21  // Init the longitudinal profile for the Cherenkov simulation
22  corsika::cherenkov::LongitudinalProfileCherenkov
23      <LongitudinalCherenkovParquet
24          <longitudinalOption>,longitudinalOption>
25          longitudinalCherenkov(atmosphere, stackbunches);
```

Strategy

- Profiling -> Optimization -> Validation of results
- Profiler : *Perf Linux* (with *stat* and *record* modules)
- Performance counters and ratios : cycles, instructions, cache-misses, etc
- Hardware :

CPU	GCC	OS
AMD Ryzen 9 3950X 4.4Ghz (fixed) CPU caches: 1MB/8MB/64MB	9.4	Ubuntu 20.04

- Compilation flags for the Release Version : -O3 -mavx2 (-std=c99 for CORSIKA 7)

CORSIKA - Tested versions

- One tested version for CORSIKA 7
- Two tested versions for CORSIKA 8 with custom examples and based on the last 275-Cherenkov-module branch
  - Last merge with the master branch : 6b6d8af2583bc6a5a062c56e227cbe86b42034c7

Version	Sub-Version	Mathematical Library
CORSIKA 7	77100	Vector-Libm
CORSIKA 8	275-Cherenkov-module-tests	Libm
CORSIKA 8	275-Cherenkov-module-tests-opt1	Vector-Libm

The experiment

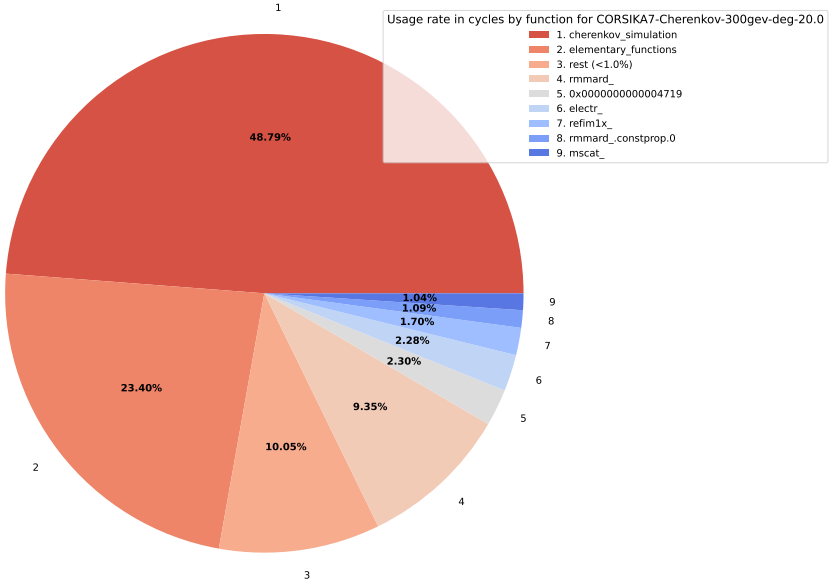
Incident particle	electron (PROPOSAL 7.3.1) or gamma (physics results)
Nb showers	500
Initial energy	3 GeV to 330TeV (physical results) and 300 GeV (performance results)
Angles	0.01-20° (zenith) et 180° (azimuth)
Cut energy	20 MeV
Magnetic field	0.01mT
C8 Atmosphere	Analytic model for the shower and the tabulated model for the Cherenkov photons
C7 Atmosphere	Tabulated model
Atmosphere height	112.8 km
Number of telescopes	None or 99
Seed	fixed

CORSIKAs - Cherenkov Simulation - The experiment

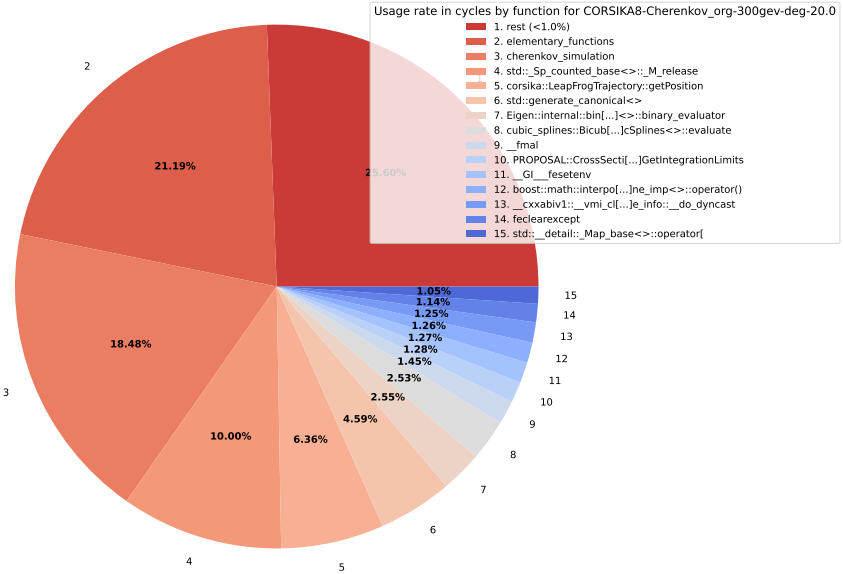
- We compare CORSIKA 7 and CORSIKA 8 for the Cherenkov simulation
- A comparison without telescope grid

Incident particle	electron
Nb showers	500
Angles	20° (zenith) et 180° (azimuth)
Initial energy	300 GeV
Number of telescopes	None

CORSIKA 7 - Cherenkov Simulation - Profiling



CORSIKA 8 - Cherenkov Simulation - Profiling



CORSIKAs - Cherenkov Simulation - Profiling - Usage

Category	CORSIKA7	CORSIKA8
Cherenkov Simulation	48.79%	18.48%
Elementary functions	23.40%	21.19%
Rest	27.81%	**60.33%**

- The use of Cherenkov functions is less important in CORSIKA 8
- News functions appeared :
  - `std::_Sp_counted_base` : 10%
  - `LeapFrogTrajectory::getPosition` : 6.36%
  - `std::generate_canonical` : 4.59%
  - ...

CORSIKAs - Cherenkov Simulation - Profiling

Example : std::_Sp_counted_base

- A classical problem for smart pointers and more particulary: the shared pointer
- Basically, there are two smart pointers in C++ :
  - `unique_ptr` : almost the same raw pointer in C (practically free cost)
  - `shr_ptr` : thread safe but generate a time overhead (complexe structure with multiple allocations, reference counting)
- Solutions :
  - Use `make_shared` to allocate a `shr_ptr`
  - Pass the `shared_ptr<T> const` by reference
  - Replace some `shr_ptr` by `unique_ptr` ?

CORSIKAs - Cherenkov Simulation - Profiling - Resume

General and calculations events

counter	CORSIKA7	CORSIKA8	C8/C7
task-clock	215s	615s	x2.86
IPC	2.08	1.79	-0.29
cycles	9.47e+11	2.71e+12	x2.86
instructions	1.97e+12	4.86e+12	x2.47
fp_ret_sse_avx_ops.all	8.64e+11	1.05e+12	x1.21
fp_ret_sse_avx_ops.div_flops	3.99e+10	4.48e+10	x1.12
μOPC	0.91	0.39	-0.52
branch-misses	3.93e+09	7.25e+09	x1.84
branches	2.62e+11	6.56e+11	x2.50
branch-misses-ratio	2%	1%	-1%

- An increase of a 2.86 factor in time
- A stable ratio in branches
- Less time is spent on calculations

CORSIKAs - Cherenkov Simulation - Profiling - Resume

Memory aspect events

counter	CORSIKA7	CORSIKA8	C8/C7
task-clock	215s	615s	**x2.86**
IPC	2.08	1.79	-0.29
cycles	9.47e+11	2.71e+12	**x2.86**
cache-misses	9.21e+08	1.04e+10	**x11.3**
cache-references	2.99e+10	1.17e+11	x3.91
cache-misses-ratio	3%	9%	**+6%**
stalled-cycles-frontend	9.22e+09	3.17e+10	x3.43
stalled-cycles-backend	3.84e+11	1.45e+12	x3.78

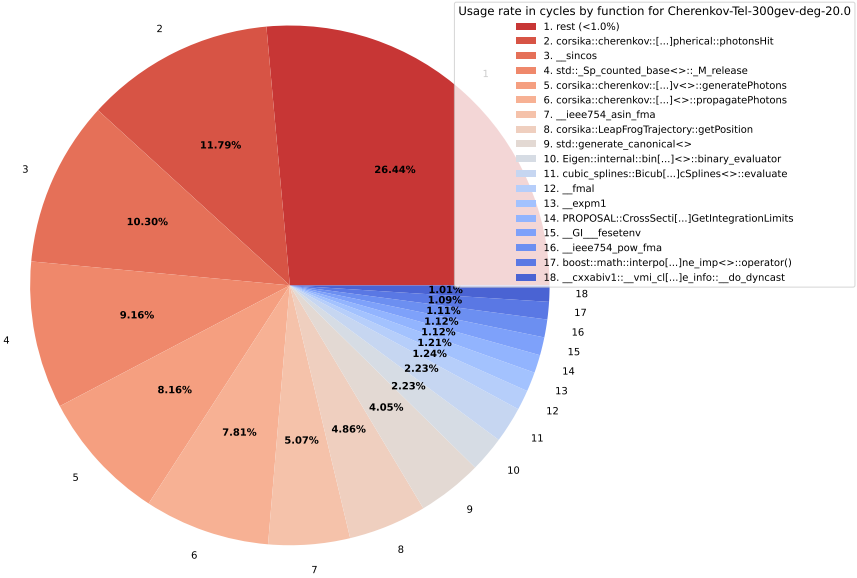
- An increase of a factor of 11.3 in cache misses
- A bottleneck in the backend -> The CPU has to wait ressources in memory
- Need to investigate

CORSIKA 8 - Cherenkov Simulation - Telescope experiment

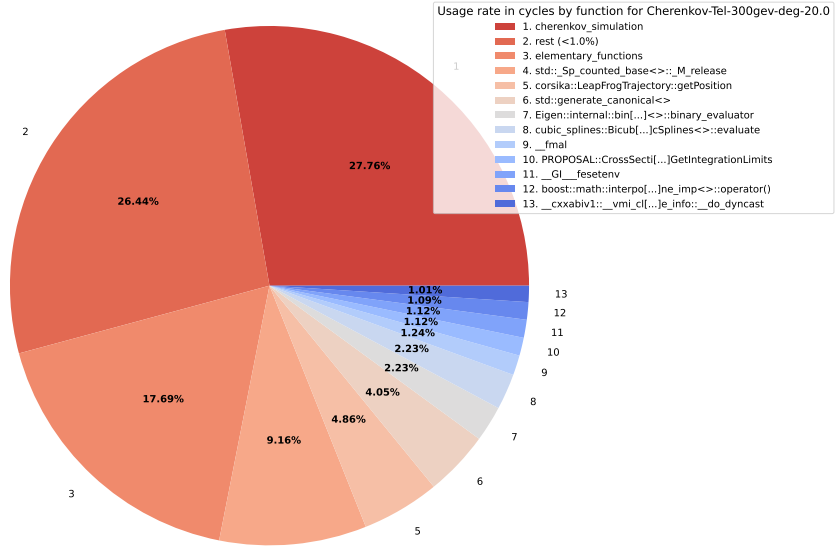
- A telescope grid -> telescopes -> bunches of photons
- We detect if a bunch hit a telescope and save data about the bunch

Incident particle	electron
Nb showers	500
Angles	20.° (zenith) et 180° (azimuth)
Initial energy	300 GeV
Number of telescopes	99

CORSIKA 8 - Cherenkov Simulation - Telescope Grid



CORSIKA 8 - Cherenkov Simulation - Telescope Grid - By Categorie



CORSIKA 8 - Cherenkov Simulation - With and without the telescope grid

counter	No_Tel	Tel	Tel/No_Tel
IPC	1.79	1.81	+0.02%
cache-misses-ratio	0.09	0.04	-5.%
branch-misses-ratio	0.01	0.01	<1.%
cycles	2.71e+12	3.12e+12	+15.%
instructions	4.86e+12	5.65e+12	+16.%
task-clock	615s	710s	+15.%
cache-misses	1.04e+10	9.57e+09	-8.%
cache-references	1.17e+11	2.13e+11	+85.%
fp_ret_sse_avx_ops.all	1.05e+12	1.05e+12	<1.%
fp_ret_sse_avx_ops.div_flops	4.48e+10	4.49e+10	<1.%
stalled-cycles-frontend	3.17e+10	3.21e+10	+1.%
stalled-cycles-backend	1.45e+12	1.67e+12	+15.%
branches	6.56e+11	7.76e+11	+18.%
branch-misses	7.25e+09	7.52e+09	+4.%

CORSIKA 8 - Cherenkov Simulation - Telescope Grid

- Only a 15% increase in time
- Some cache references but a cache misses level controled
- The feature works but :
  - Keep less photons than CORSIKA 7
  - Need to investigate to fix this bug

CORSIKA 8 - Cherenkov Simulation - Optimization work

- Goal : have a binary more efficient (use all the arithmetic units on the CPU) and preserve same physical results.
- Like in our last works[1][2], we tried to vectorize the Cherenkov simulation for CORSIKA 8
- A writing and a C library for the elementary functions : Vector-libm[3]
  - Interface in C++ with unit tests
  - Used some functions to compare with the Libm library
- Work in progress

[1] "A C++ Cherenkov photons simulation in CORSIKA 8"

[2] "Optimizing Cherenkov Photons Generation and Propagation in CORSIKA for CTA Monte–Carlo Simulations"

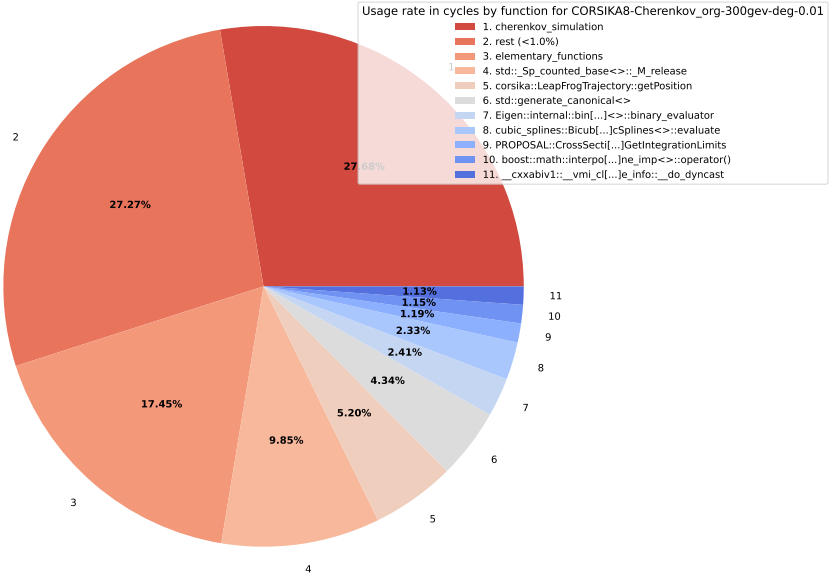
[3] https://gitlab.com/cquirin/vector-libm/-/tree/master

CORSIKA 8 - Cherenkov Simulation - Vector-libm experiment

Incident particle	electron
Nb showers	500
Angles	0.01° (zenith) et 180° (azimuth)
Initial energy	300 GeV
Number of telescopes	99

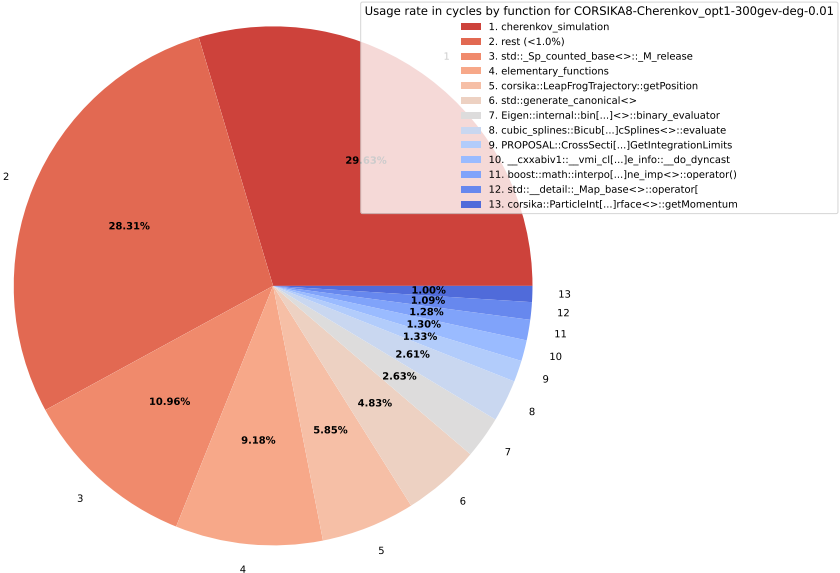
CORSIKA 8 - Cherenkov Simulation - Vector-libm

With the Libm and telescopes



CORSIKA 8 - Cherenkov Simulation - Vector-libm

With the Vector-libm and telescopes



CORSIKA 8 - Cherenkov Simulation - With and without the Vector-libm

counter	Libm	Vector-Libm	Libm/Vector-Libm
IPC	1.82	1.74	1.05
μOPC	0.36	0.47	+0.11
cycles	2.92e+12	2.61e+12	-10.62%
instructions	5.32e+12	4.54e+12	-14.66%
task-clock	664s	594s	-10.54%
cache-misses	9.55e+09	9e+09	-5.76%
cache-references	1.97e+11	1.85e+11	-6.09%
fp_ret_sse_avx_ops.all	1.04e+12	1.22e+12	+17.31%
fp_ret_sse_avx_ops.div_flops	4.5e+10	4.99e+10	+10.88%
stalled-cycles-frontend	3.73e+10	2.72e+10	-27.08%
stalled-cycles-backend	1.52e+12	1.46e+12	-3.95%
branches	7.36e+11	6.18e+11	-16.03%
branch-misses	7.54e+09	3.18e+09	-57.82%

Physics results - Protocol

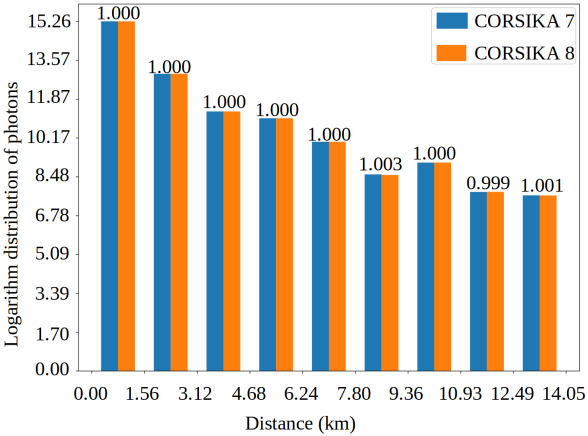
- For the different performance tests, we produced almost : 12 billions of photons with a difference less than 5% between C7 and C8
- We started a comparison between C7 and C8 for the photon positions in these conditions but we need more investigations
- For the rest of the presentation : we'll do a comparison for physics results with ten showers of C7 we read with the Cherenkov Simulation in C8
  - Produced almost $4{,}9.10^6$ on the ground

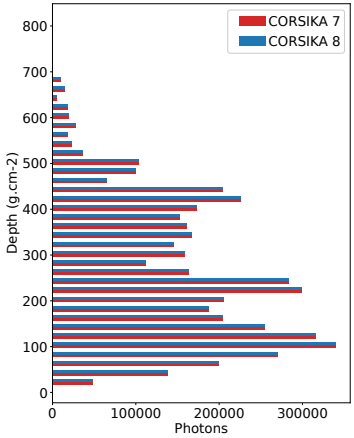
Physics results - the experiment

Incident particle	gamma
Nb showers	10
Initial energy	3 GeV to 330 TeV (power law in energy)
Angles	20° (zenith) et 180° (azimuth)
Cut energy	20 MeV
Magnetic field	21mT
CORSIKA shower	Created in C7
Atmosphere height	112.8 km
Seed	fixed

Physics results comparison for the Cherenkov Module C8/C7

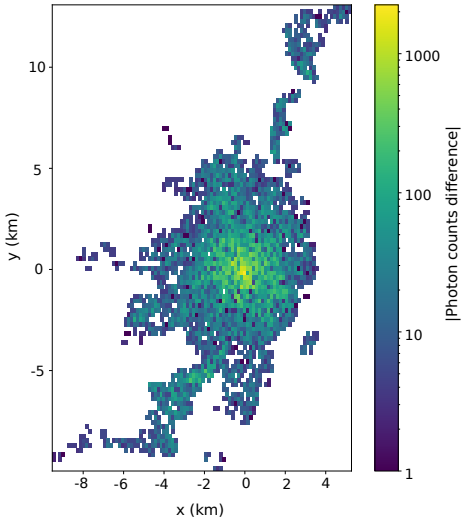
(Left) Lateral distribution of photon density with respect to the shower axis (Right) Longitudinal distribution





Physics results comparison for the Cherenkov Module C8/C7

2D map of the photon counts difference on the ground



	Pearson	Kolmogorov
NbPhotons	1.000	1.000
PosZ	1.000	1.000
DistXY	0.996	0.994
DirX	0.982	0.963
DirY	0.986	0.939
Time	0.991	0.972

Conclusion

Some numbers for the Cherenkov Simulation

counter	C7	C8	C8-opt1
IPC	2.08	1.82	1.74
μOPC	0.90	0.36	0.47
cycles	9.62e+11	2.92e+12	2.61e+12
instructions	2e+12	5.32e+12	4.54e+12
task-clock	219s	664s	594s
cache-misses	8.66e+08	9.55e+09	9e+09
stalled-cycles-backend	3.89e+11	1.52e+12	1.46e+12
branch-misses	4.03e+09	7.54e+09	3.18e+09

- We are "only" 2.71 times slower for the moment
- A small optimization improved the performance with a decrease of 10%
- Results are close for a same shower

Next Steps

- Verify physics results for a complete simulation in CORSIKA 8
- Optimize the Cherenkov Module
  - Test different appropriate mathematical libraries for CORSIKA 8
  - Remove some useless variables and reduce the memory footprint
  - Evaluate the single precision to improve vectorization efficiency
- Fix the Cherenkov Telescope Grid to have a real comparison between CORSIKA 7 and CORSIKA 8
- Interface the CORSIKA 8 atmosphere for the Cherenkov module and resolve this atmosphere tabulated dependence

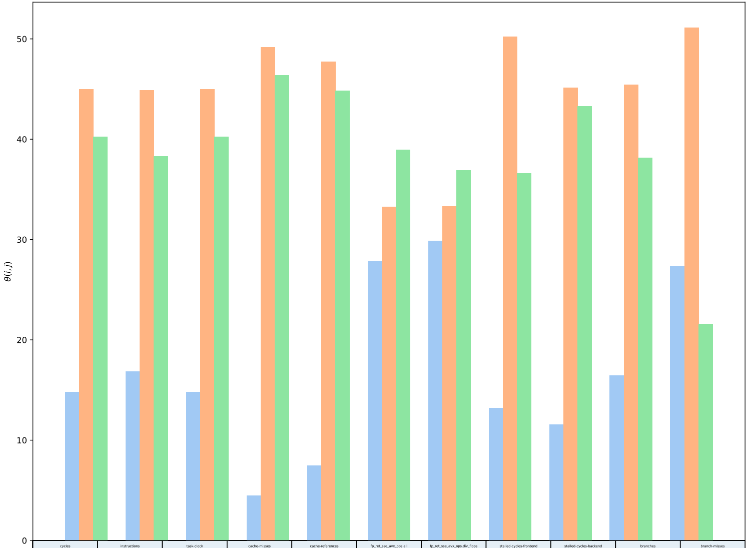
Thank you for your attention

Backups

Conclusion - details

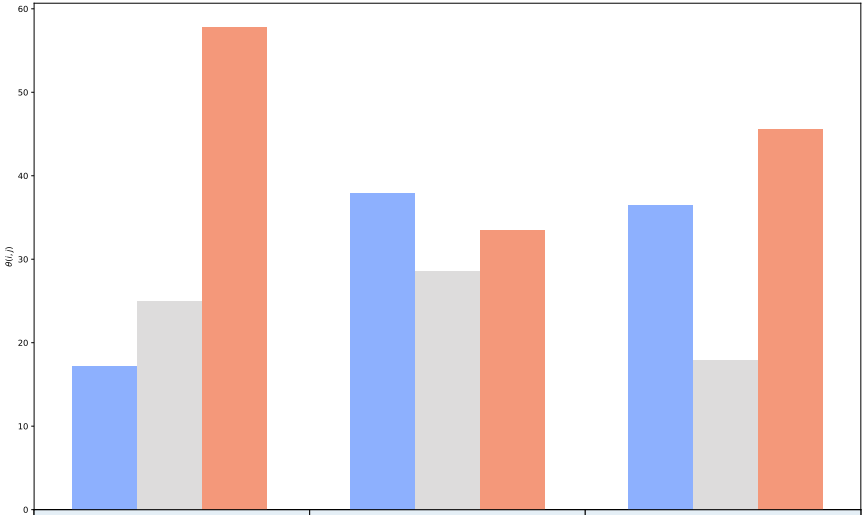
counter	C7	C8	C8-opt1
IPC	2.08	1.82	1.74
μOPC	0.90	0.36	0.47
cache-misses-ratio	0.03	0.05	0.05
branch-misses-ratio	0.02	0.01	0.01
cycles	9.62e+11	2.92e+12	2.61e+12
instructions	2e+12	5.32e+12	4.54e+12
task-clock	219s	664s	594s
cache-misses	8.66e+08	9.55e+09	9e+09
cache-references	3.08e+10	1.97e+11	1.85e+11
fp_ret_sse_avx_ops.all	8.73e+11	1.04e+12	1.22e+12
fp_ret_sse_avx_ops.div_flops	4.04e+10	4.5e+10	4.99e+10
stalled-cycles-frontend	9.79e+09	3.73e+10	2.72e+10
stalled-cycles-backend	3.89e+11	1.52e+12	1.46e+12
branches	2.66e+11	7.36e+11	6.18e+11
branch-misses	4.03e+09	7.54e+09	3.18e+09

CORSIKA 7 - Cherenkov Simulation - Stat total



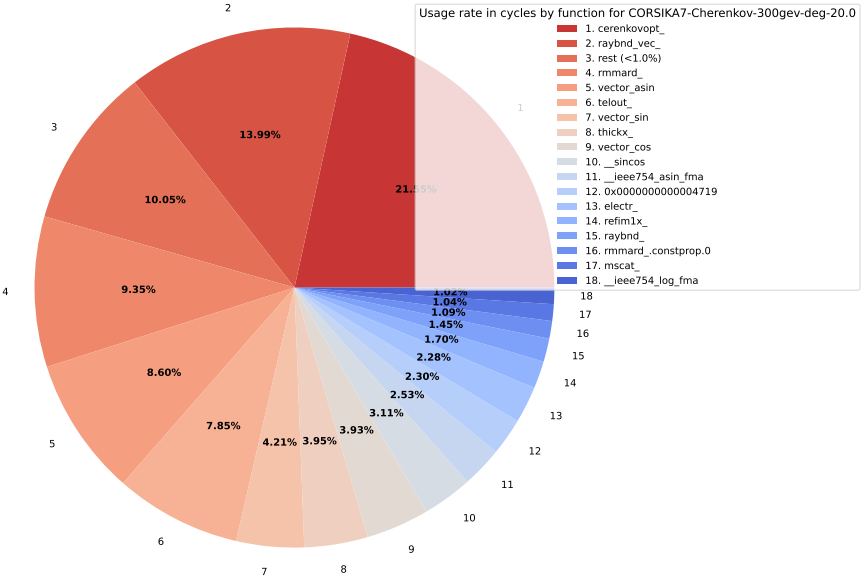
	cycles	instructions	task-clock	cache-misses	cache-references	fp_ret_sse_avx_ops.all	fp_ret_sse_avx_ops.div_flops	stalled-cycles-frontend	stalled-cycles-backend	branches	branch-misses
CORSIKA7-Cherenkov-300gev-deg-0.01	9.6222e+11 (+0.00%)	1.9986e+12 (+0.00%)	2.1872e+05 (+0.00%)	8.6613e+08 (+0.00%)	3.0828e+10 (+0.00%)	8.7259e+11 (+0.00%)	4.0380e+10 (+0.00%)	9.7905e+09 (+0.00%)	3.8859e+11 (+0.00%)	2.6617e+11 (+0.00%)	4.0338e+09 (+0.00%)
CORSIKA8-Cherenkov_org-300gev-deg-0.01	2.9218e+12 (+203.65%)	5.3172e+12 (+166.04%)	6.6412e+05 (+203.64%)	9.5473e+09 (+1002.29%)	1.9674e+11 (+538.18%)	1.0428e+12 (+19.51%)	4.5018e+10 (+11.49%)	3.7287e+10 (+280.85%)	1.5177e+12 (+290.57%)	7.3611e+11 (+176.56%)	7.5413e+09 (+86.95%)
CORSIKA8-Cherenkov_opt1-300gev-deg-0.01	2.6145e+12 (+171.72%)	4.5372e+12 (+127.02%)	5.9428e+05 (+171.71%)	8.9991e+09 (+939.01%)	1.8481e+11 (+499.49%)	1.2213e+12 (+39.96%)	4.9873e+10 (+23.51%)	2.7193e+10 (+177.75%)	1.4555e+12 (+274.55%)	6.1764e+11 (+132.05%)	3.1815e+09 (-21.13%)

CORSIKA 7 - Cherenkov Simulation - Record total

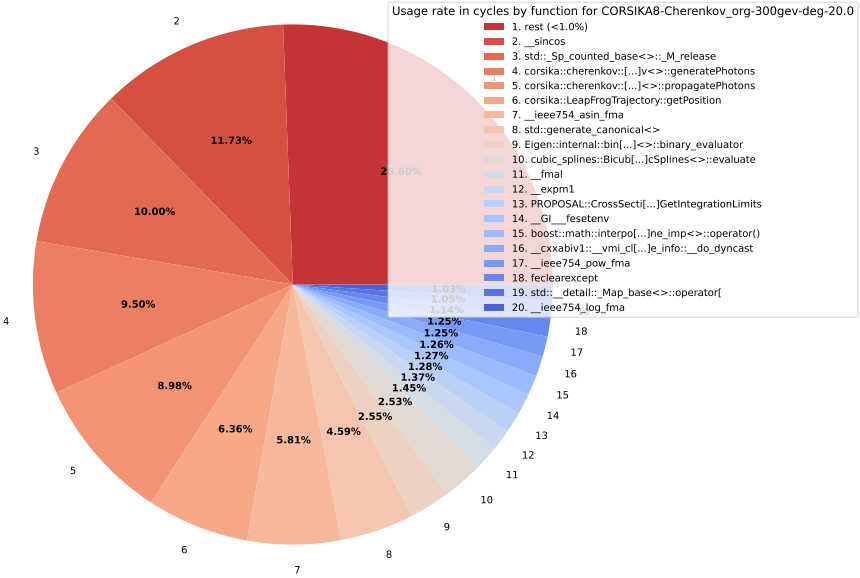


	CORSIKA7-Cherenkov-300gev-deg-0.01 - fp_rel_sse_avx_sps.all	CORSIKA8-Cherenkov_org-300gev-deg-0.01 - fp_rel_sse_avx_sps.all	CORSIKA8-Cherenkov_opt1-300gev-deg-0.01 - fp_rel_sse_avx_sps.all
rest	1.5054e+11 (+0.00%)	3.9577e+11 (+163.24%)	4.4606e+11 (+196.89%)
elementary_functions	2.1812e+11 (+0.00%)	2.9789e+11 (+36.57%)	2.1099e+11 (+0.40%)
cherenkov_simulation	5.0408e+11 (+0.00%)	3.4901e+11 (-30.76%)	5.5618e+11 (+10.33%)

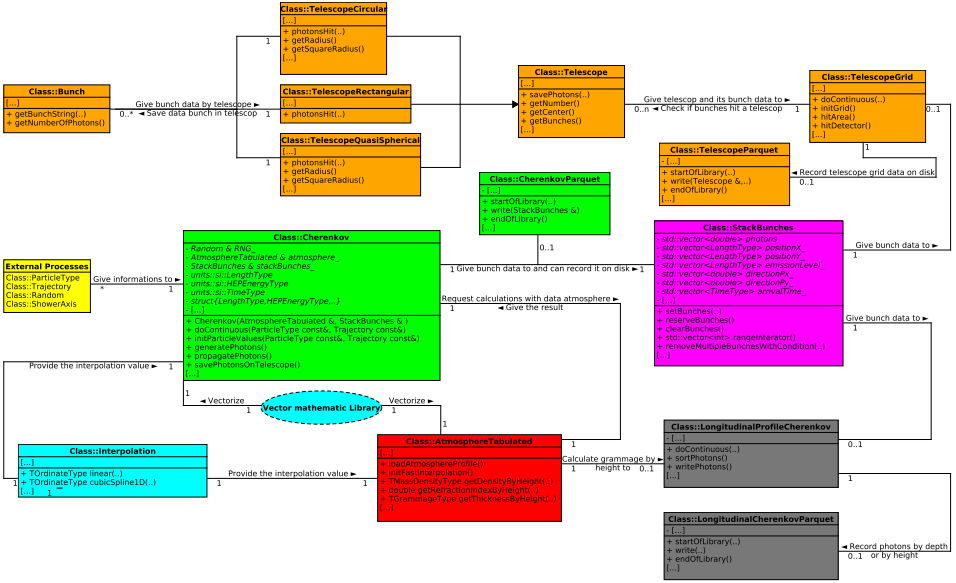
CORSIKA 7 - Cherenkov Simulation - Profiling



CORSIKA 8 - Cherenkov Simulation - Profiling



UML diagram for the Cherenkov Simulation



Performance comparison for Cherenkov Module C8/C7 (2021)

I7 CPU - with *vlibm* - 10 showers - Energy spectrum E^{-2} from 3 GeV to 330 TeV

Version	Instructions	Cycles	Wall clock time
C8 / C7	1.02	1.57	1.39

Version	Scalars[1] (Mi)	Vectors (Mi)	Vectorization Ratio
C7	108	53	66.4%
C8	219	29	34.8%

- Number of instructions is almost the same
- Vectorization rate decreased
- An increase of number of cycles

[1] Scalars : scalars double precision floating-point instructions, Vectors : vectorized double precision floating-point instructions

Performance comparison for Cherenkov Module C8/C7 (2021)

I7 CPU - with *vlibm* - 10 showers - Energy spectrum E^{-2} from 3 GeV to 330 TeV

Version	BM/B[(1)]	CM/CR	LLCM/LLC
C7	3.0%	6.0%	9.8%
C8	3.3%	32.7%	41.8%

- Similarly BM/B = same algorithms
- Cache misses and L3 load misses increase
- We need more investigations

[1] BM: branch misses, B: branch, CM: cache misses, CR: cache reference, LLCM: last level cache misses, LLC: last level cache load