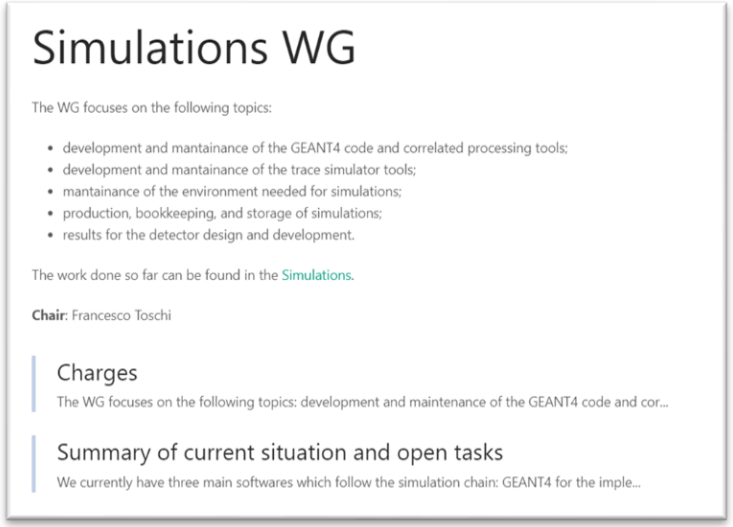
Report from Simulations WG

Francesco Toschi for the Simulations WG

DELight Collaboration Meeting, Heidelberg – 13.09.2024

Simulations WG

- Development and maintenance of
  - GEANT4 framework;
  - post-simulation processing tools;
  - trace simulator.
- “Logistics” of simulations: production, bookkeeping and storage.
- Informing design and development of the detector.


Simulations WG

The WG focuses on the following topics:

- development and mantainance of the GEANT4 code and correlated processing tools;
- development and mantainance of the trace simulator tools;
- mantainance of the environment needed for simulations;
- production, bookkeeping, and storage of simulations;
- results for the detector design and development.

The work done so far can be found in the Simulations.

Chair: Francesco Toschi

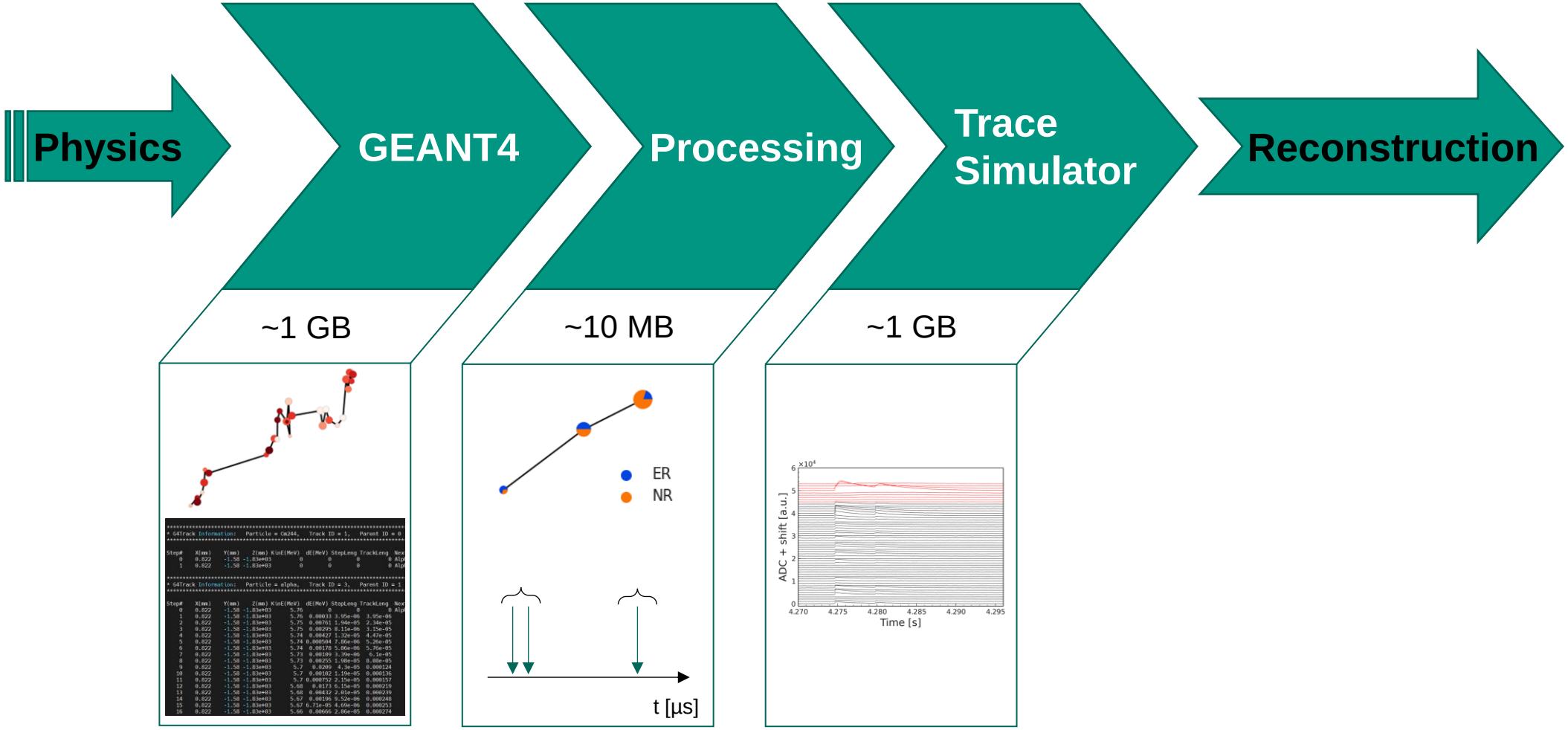
Charges

The WG focuses on the following topics: development and maintenance of the GEANT4 code and cor...

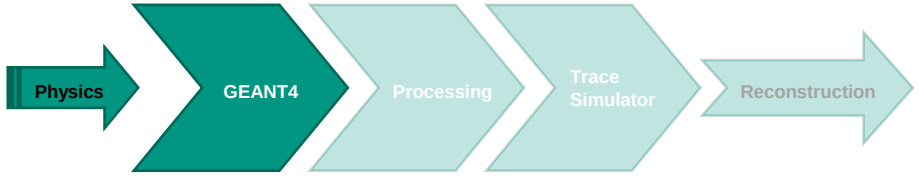
Summary of current situation and open tasks

We currently have three main softwares which follow the simulation chain: GEANT4 for the imple...

Simulation framework

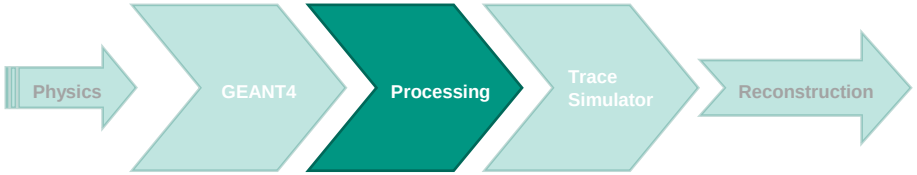


Simulation framework



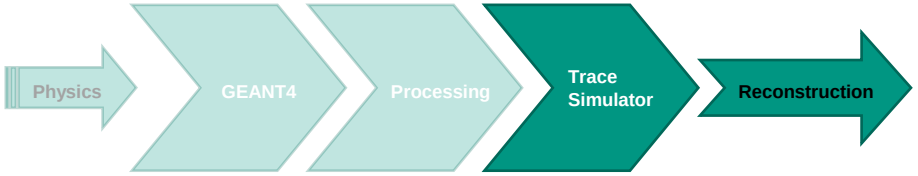
- GEANT4 v11.0.3 on ROOT v6.26.06 using multithreading:
  - currently locally stored in my kalinka‘s home directory,
  - Benedikt is working on container/singularity solution.
- Available on GitHub as private repo:
  - currently no versioning,
  - foreseen to move it to DELight GitLab (maybe starting point for version 0).
- Inclusion of external packages:
  - G4CMP logic used for implementation of quasiparticle propagation,
  - EcoMug for cosmic background,
  - SaG4n for (α,n) simulations.

Simulation framework



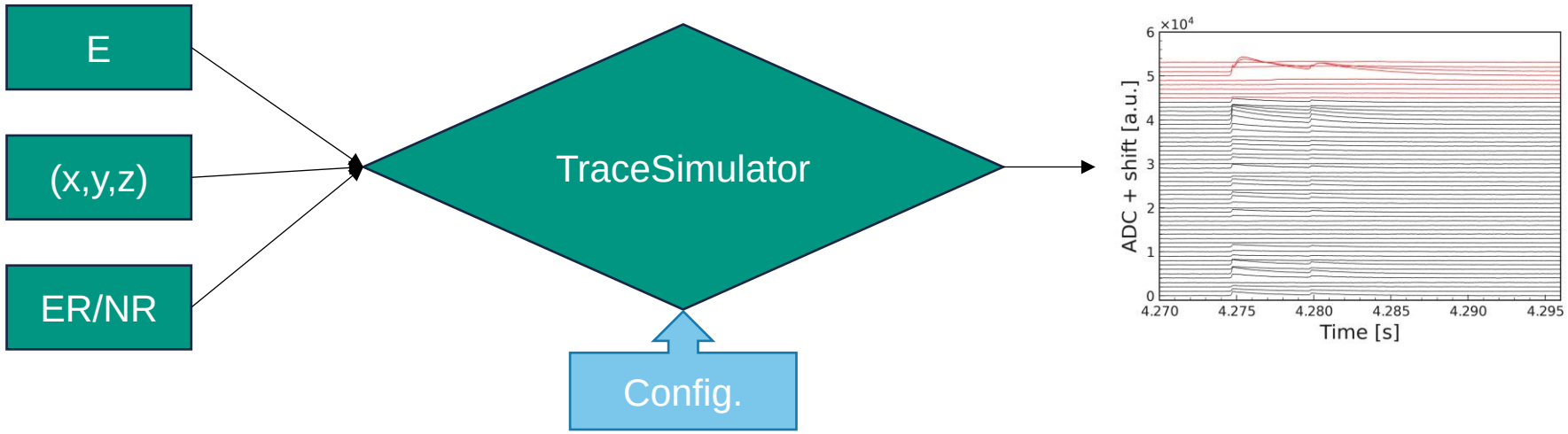
- Currently done with C++ code *procDEL.cc.*
- Developed from a „quick fix“ for
  - multiscattering ($\Delta t > 50$ µs as threshold),
  - ER vs. NR.
- Handling of quanta propagation (quasiparticles, photons and triplets).
- Still at a primitive stage.

Simulation framework

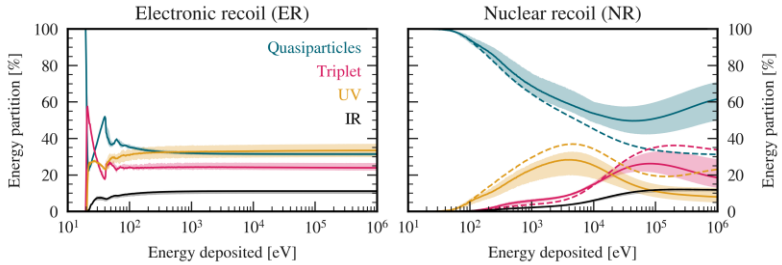


- Python-based solution: not compilable so far (e.g., numba, Cython, …).
- Detector effects from GEANT4 dedicated simulations:
  - light collection efficiency (LCE) maps for each MMC,
  - phonon collection efficiency (PCE) maps for each MMC,
  - phonon arrival time (~template) for each MMC.
- Signal partitioning from MC model (paper to be circulated).
- Noise can be sampled from a given PSD.
- Output compatible with helix.

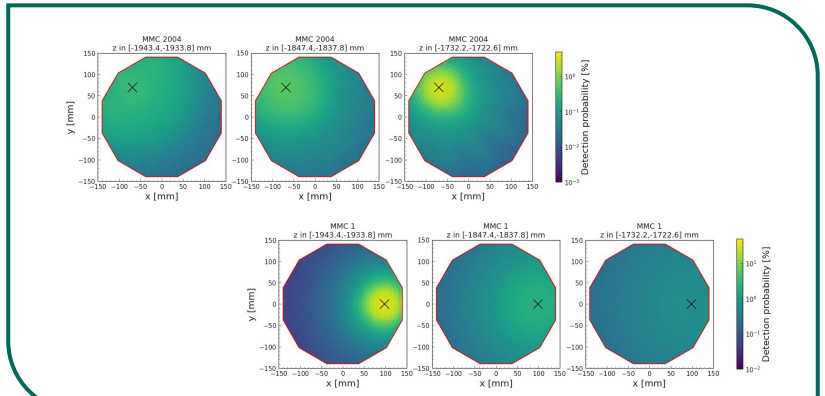
TraceSimulator: the newcomer



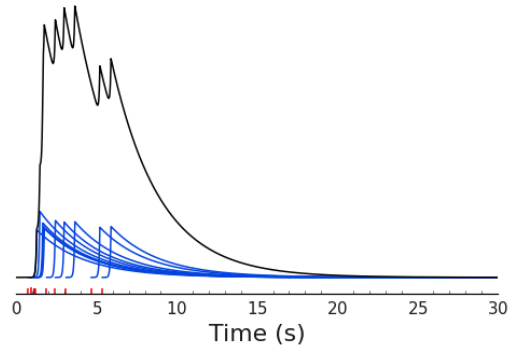
Energy partition



Detector effects



Summing individual contributions



Open tasks

- Large room for improvement and many open tasks
- Overview of open tasks on wiki (with priority and required competences)

GEANT4

Task	Description	Priority	Type	Comments
GEANT4 container	Development and mantainance of container with proper GEANT4 and ROOT version, now the environment is on Francesco's home in kalinka	Medium	Computing	Benedikt has experience with containers/singularities and will look into it
Versioning	Versioning GEANT4, possibly together with moving it to GitLab from the current GitHub	High	Development	
Documentation	Although a README exists, the code is poorly documented and the README might be outdated	Medium	Development	
Storage input	Simulation of quasiparticle requires several text files (for human readability) for a total of 50 MB, now stored locally in Francesco's homepage	Medium	Computing	
Storage output	Simulations will produce O(>10 TB) output, for the moment we have 200 TB in kalinka storage (shared with DM group, but mostly unused)	Low	Computing	
Maintenance	Currently only Francesco and Eleanor work on the code, we need to involve more people for the development and maintenance of the code	Low	Development	
Metadata	Currently no metadata are saved when producing simulations (MC version, input files used, options set, etc.)	Low	Development	
Geometry	A geometry should be discussed and eventually fixed for the sensitivity paper	High	Development	
SF-multiplicity	Implement neutron multiplicity in spontaneous fission simulations	Low	Development	
Quasiparticle in LHe	In case we see quasiparticle within LHe, we need to re-think how quasiparticles are currently propagated. Priority depends on observations	Low/High	Development	
Mass estimation	Current mass estimation of MultiUnion is very unprecise, we should implement a custom estimation for better performance	Low	Development	
UG implementation	Implementation of the VdA cavern for cosmic simulations	Medium	Development	

Processing

Task	Description	Priority	Type	Comments
Performance	Speed-up using better tools or exploiting multithread	Low	Development	
Validation	So far only minor validation, need to do a systematic check to highlight potential problems	High	Development	
Multiple scatter vs. events	Currently multiple scatters are all energy deposits separated by at least 50 µs, but this includes decay taking days or years. They should be divided into different events	Medium	Development	
Clustering	Together with validation, the clustering of the events should be assessed in order to have a more realistic final energy partition	High	Development	
Quanta	Check, validate and improve the postprocessing for quanta propagation, currently developed with a specific use case in mind	High	Development	

TraceSimulator

Task	Description	Priority	Type	Comments
Container	Development and mantainance of container with proper version and needed libraries	Medium	Computing	
Performance	Currently the module takes a long time to load and a lot of memory (>30 GB)	High	Development	
Signal model	Analytical or ML-based solution for the signal model, currently main issue of the performance of the trace simulator	Medium/High	Development	BSc thesis with Markus/Benedikt starting in September
Storage output	Simulations will produce O(>10 TB) output, for the moment we have 200 TB in kalinka storage (shared with DM group, but mostly unused)	Medium	Computing	
Triplet and IR	Add triplet and IR contribution to the traces	Medium	Development	

Simulations/analyses

Task	Description	Left to do	Link to note	Comments
Geometry	Implementation of detector geometry with proper dimension and materials	Agree on first geometry and size of cell		First geometry is there, but cell contains 2 kg of LHe, against the 1 kg we usually quote
MMC material	Study of impact of MMC material (sapphire for better QE gain, silicon for IR detection)	Entire study		Collaboration with Calorimeter WG
Aspect ratio	Study of the best shape and aspect ratio of the helium cell	Implementation of aspect ratio in real cell, distance of vacuum MMCs from surface	First study	First study by Francesco
Radiogenic ER background	Study of the radiogenic ER background and estimation of final expected spectrum (connected to shield studies)	Entire study		
Radiogenic NR background	Study of the radiogenic NR background coming from (α,n) and spontaneous fission processes	Update with final geometry	First study and systematics	Systematics and first study by Francesco
Cosmic background	Study of the background from cosmic radiation	Study for underground detector	Summary	Study by Eleanor
Cosmogenic background	Study and estimation of the cosmogenically activated background	Entire study		
Internal shield	Study of shield for ER and NR inside the fridge	Finalize geometry and impact study		First implementation by Kathrin Gerbig, further studies by Eleanor
Outer shield	Study of shield mainly for NR and cosmic	Update with final geometry and underground performance	Summary	Study by Eleanor

Open tasks

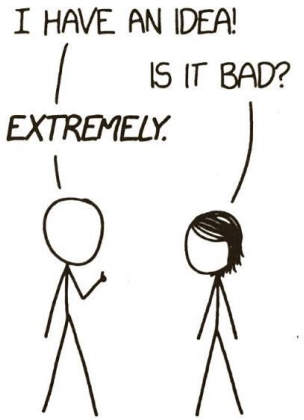
- Geometry consensus (towards sensitivity paper):
  - current geometry cells is 2 kg (25 cm x 25 cm),
  - cryostat material, is SS/Ti feasible? Proposal?
  - additional input for extra materials (cables, sensors, etc.).
- Processing studies and validation:
  - micro/macro-clustering in time and space,
  - multi- vs. single-scattering events.
- Performance of TraceSimulator is poor:
  - large memory consumption (>30 GB),
  - slow at loading and calculating.

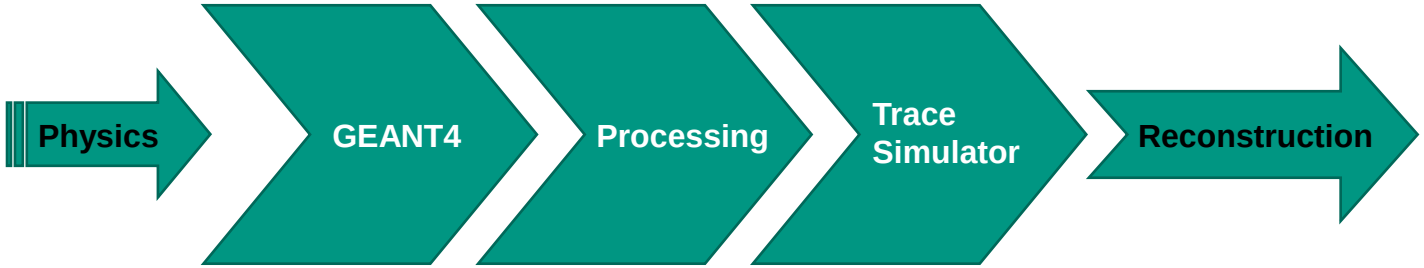
Open tasks = thesis topics!

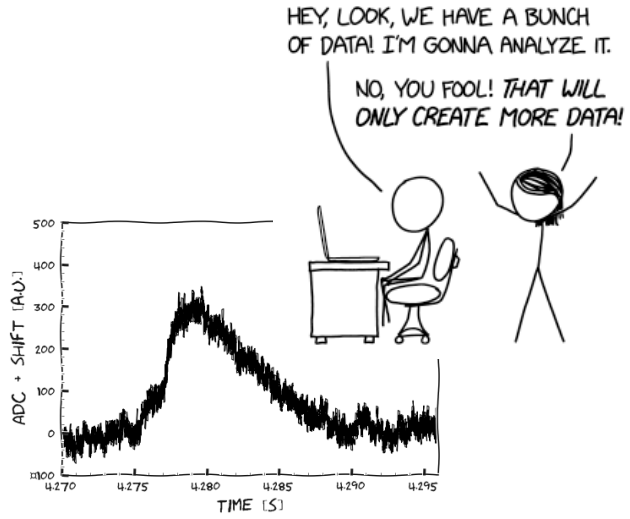
- Ayman Ratey (BSc, Markus) will work on signal partition for TraceSimulator
- Jens Reininghaus (MSc, Marc) interested in background mitigation
- Kathrin Gerbig (HiWi, Belina) will work on GEANT4 development
- Many topics for BSc and MSc theses:
  - processing validation (microphysics),
  - MMC wafer material,
  - cosmogenic activation,
  - …

Conclusion

- We have a working framework which allows for the simulations of realistic traces from scratch.
- Large room for development and improvement, with potentially nice projects.







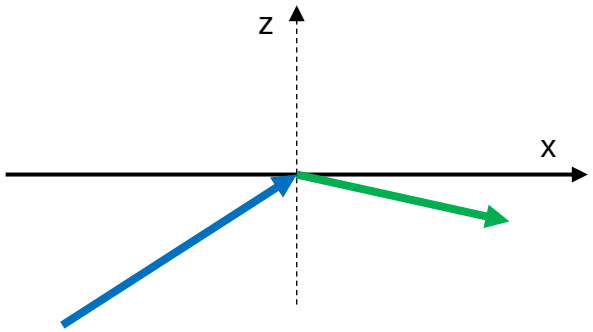
Backup slides

GEANT4 output

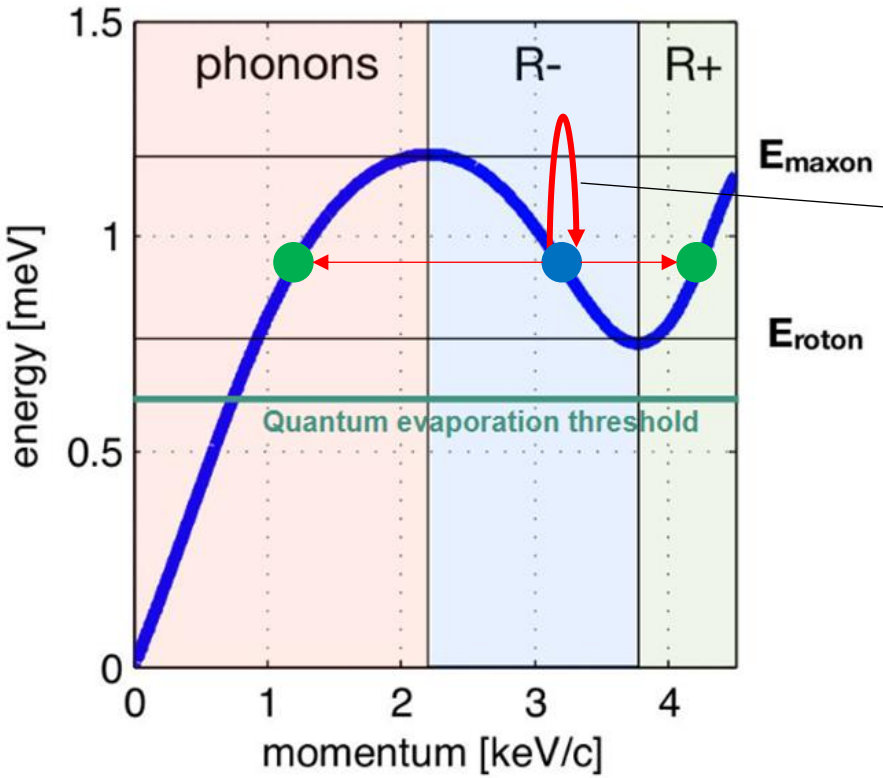
Name	Type	Description	Units
event_ID	int	Event ID	-
MMC_index	Integer	MMC hit index	-
n_neutron	int	Number of neutrons emitted	-
type_pri	string	Primary particle type	-
x_pri	double	X-coordinate of primary particle	mm
y_pri	double	Y-coordinate of primary particle	mm
z_pri	double	Z-coordinate of primary particle	mm
t_pri	double	Time of primary particle	ns
E_pri	double	Energy of primary particle	keV
E_depTot_He	double	Total energy deposited in He sensitive volume	keV
E_depTot_MMC	double	Total energy deposited in MMC sensitive volume	keV
px_pri	double	X-component of primary particle momentum	keV
py_pri	double	Y-component of primary particle momentum	keV
pz_pri	double	Z-component of primary particle momentum	keV

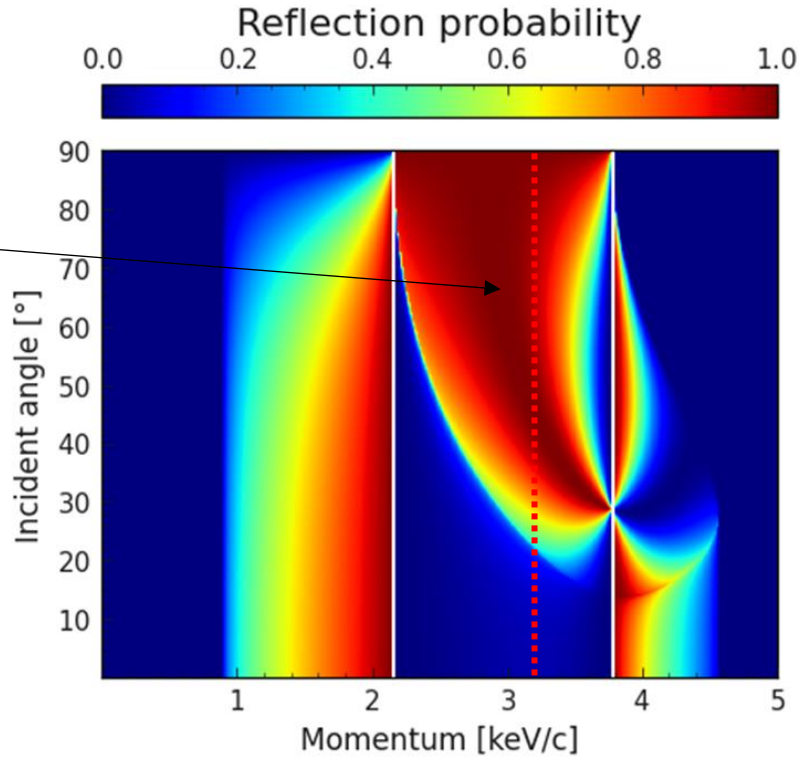
Name	Type	Description	Units
track_ID	array<int>	Track ID of particles	-
parent_ID	array<int>	Parent track IDs	-
SensVolume	array<int>	Sensitive volume IDs	-
x	array<double>	X-coordinates of particles	mm
y	array<double>	Y-coordinates of particles	mm
z	array<double>	Z-coordinates of particles	mm
t	array<double>	Times of particles	ns
E_dep	array<double>	Energies deposited by particles	keV
E_in	array<double>	Initial energies of particles	keV
L_step	array<double>	Step lengths of particles	mm
theta_in	array<double>	Incoming angles	deg
theta_out	array<double>	Outgoing angles	deg
type	array<string>	Particle types	-
creaProc	array<string>	Creation processes of particles	-
creaVol	array<string>	Creation volumes of particles	-
depProc	array<string>	Deposition processes of particles	-
parent_type	array<string>	Parent particle types	-

Quasiparticle reflection



$$\begin{cases} E^i = E^f \\ \vec{p}_{\parallel}^{\,i} = \vec{p}_{\parallel}^{\,f} \end{cases}$$

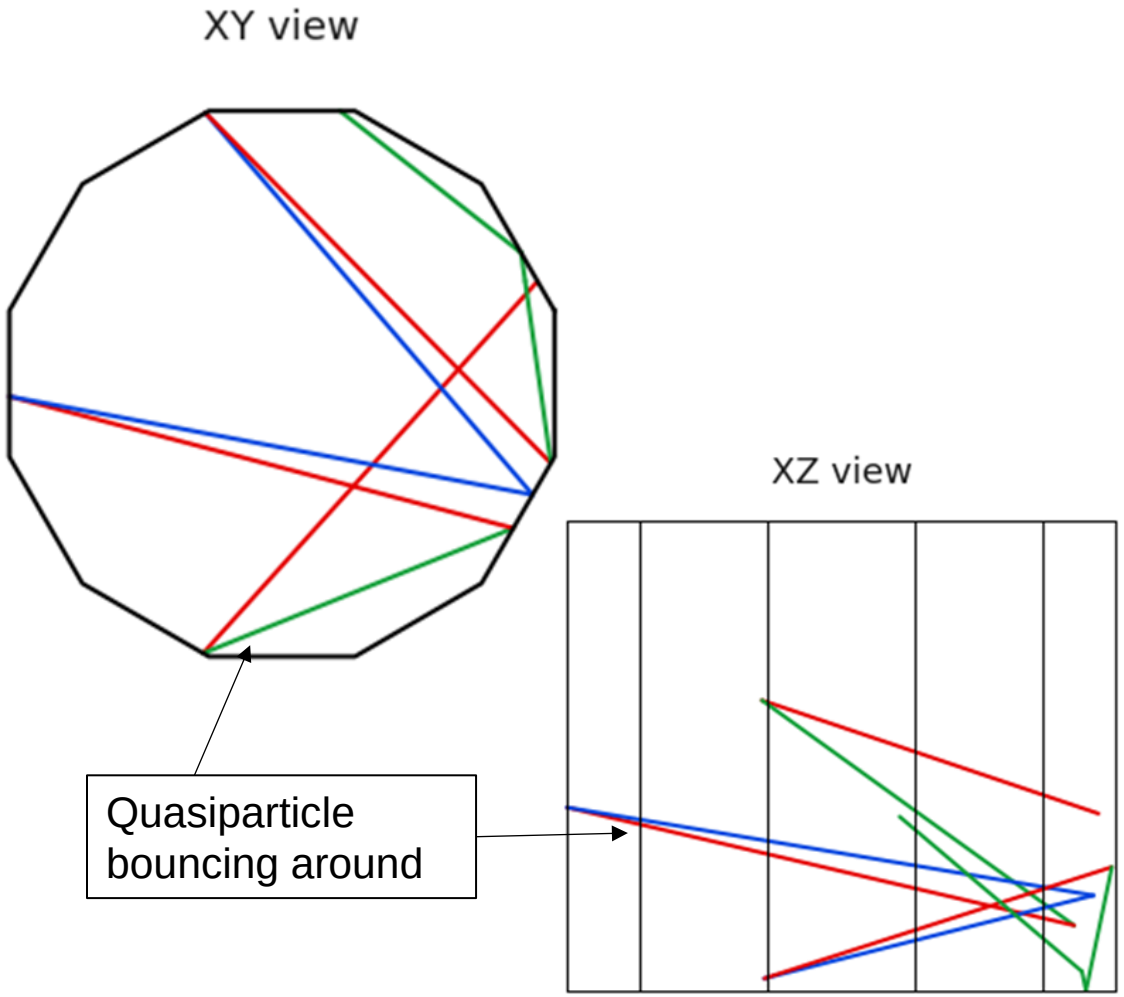


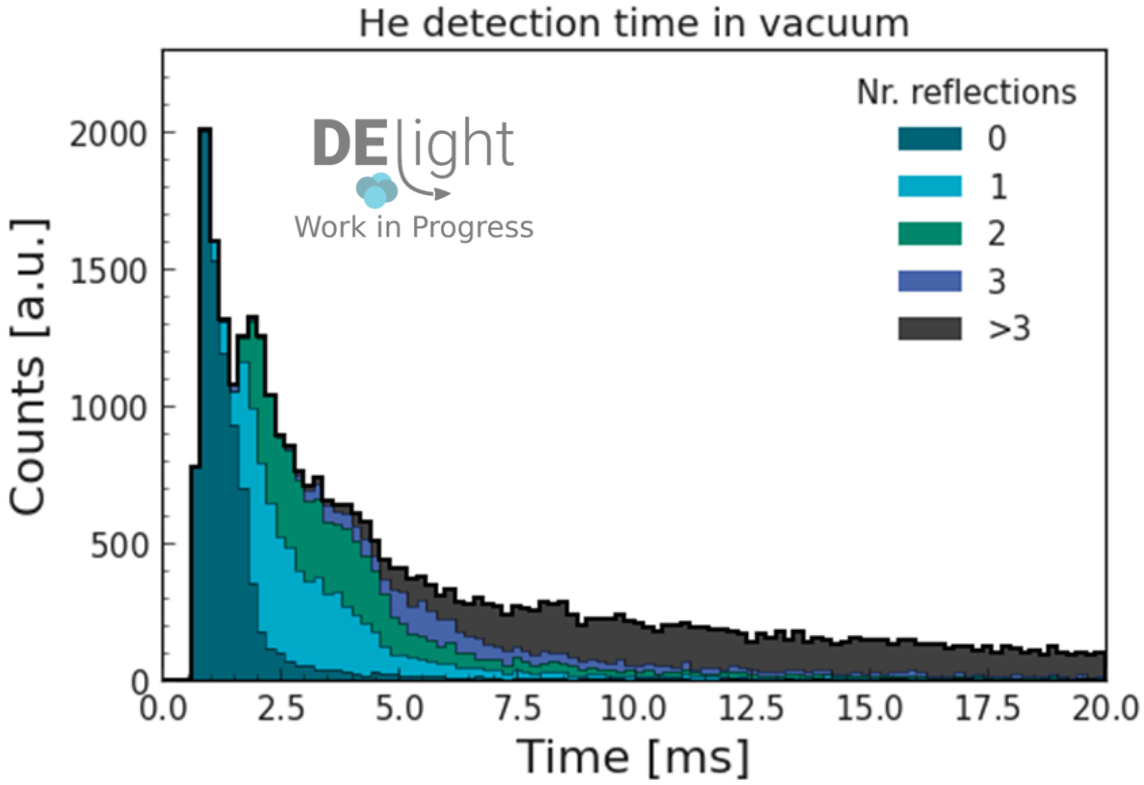


Reflection on copper

Phys. Rev. B 77, 174510

Quasiparticle reflection

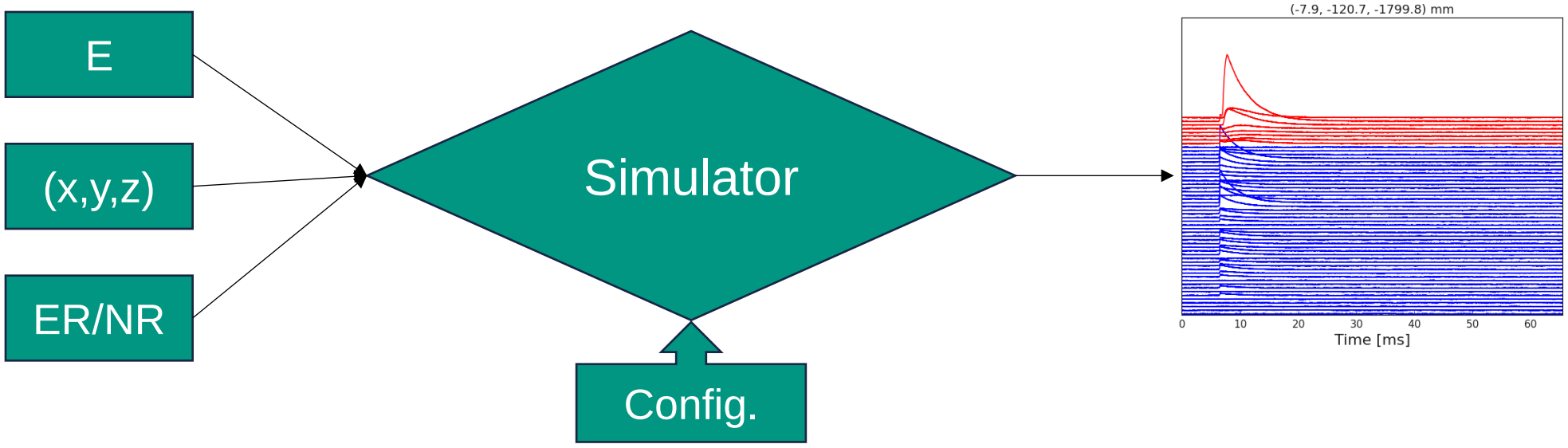




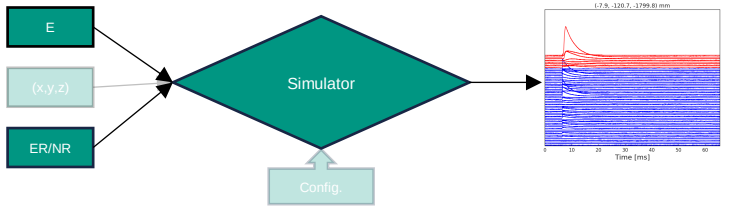
Evidences of smaller reflection probability:
tail suppression

Trace simulator

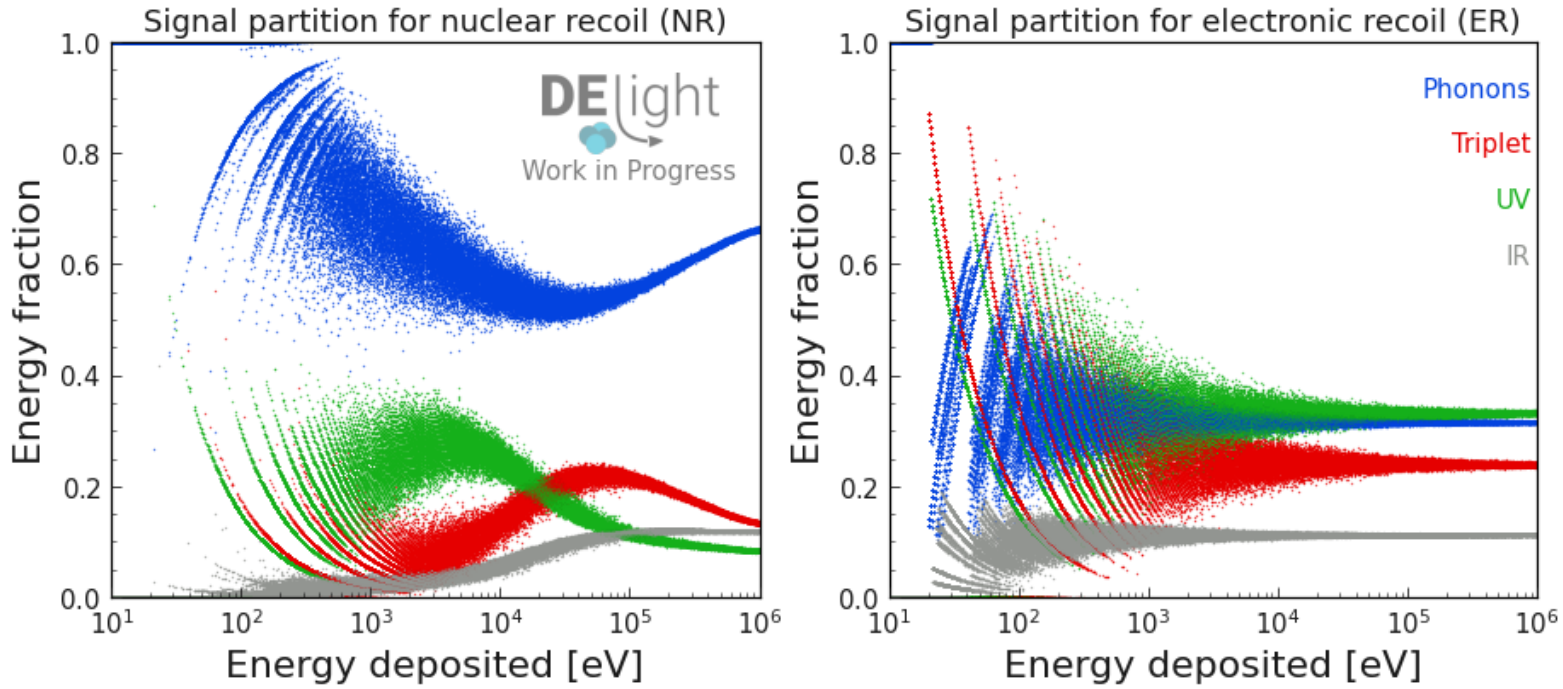
- A trace simulator should return the expected MMC output given three pieces of information:
  - Energy of the event **E**
  - Position of the event **(x,y,z)**
  - Type of the interaction (**ER** or **NR**)



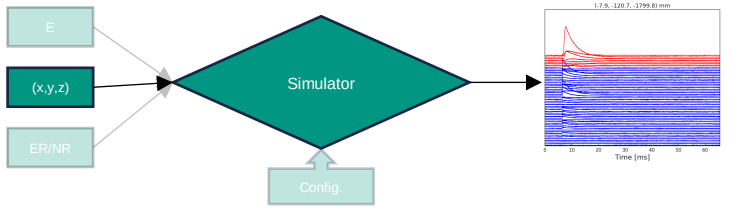
Energy information



- The energy information (together with the interaction type) is used to understand how many quanta are physically produced

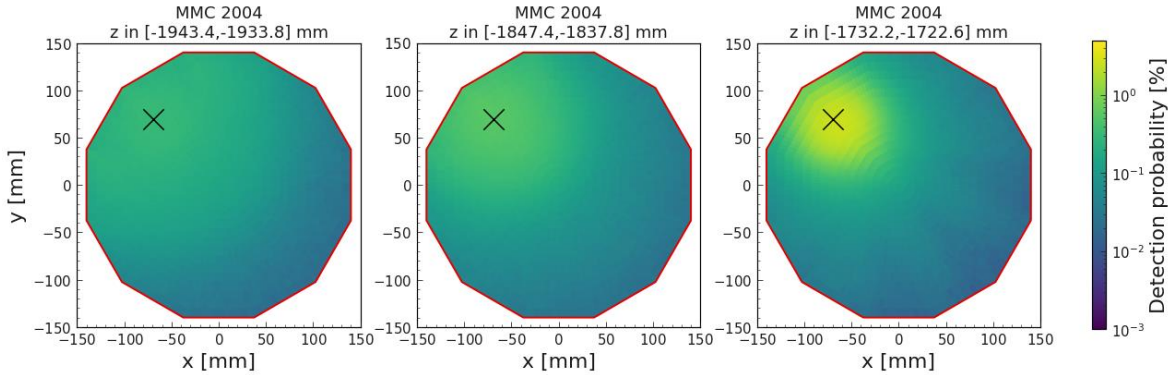


Position information



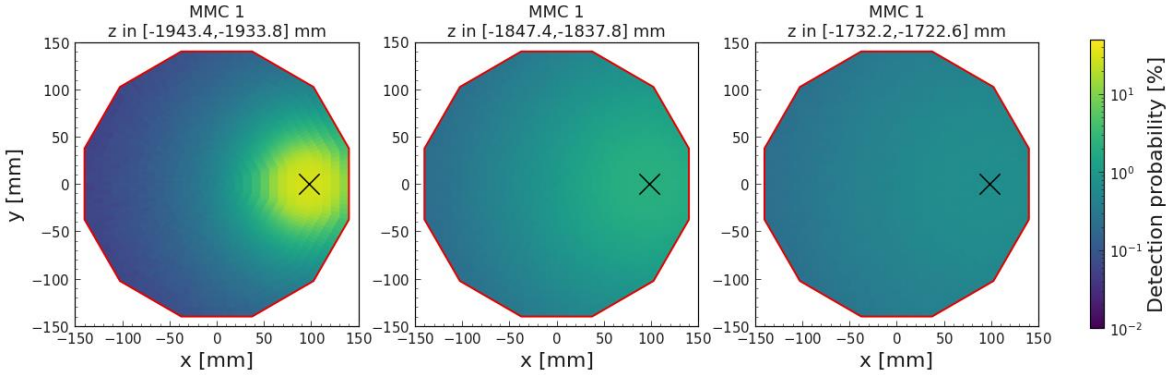
- The position information is used to estimate:
  - Light collection efficiency (LCE) and UV photons arrival time for each MMC;
  - Phonon collection efficiency (PCE) and phonon signal template for each MMC.
- The signal template is saved as array of dimension 100 with the times from the 0^{th} to the 100^{th} percentiles, used then to sample the arrival time.

PCE map



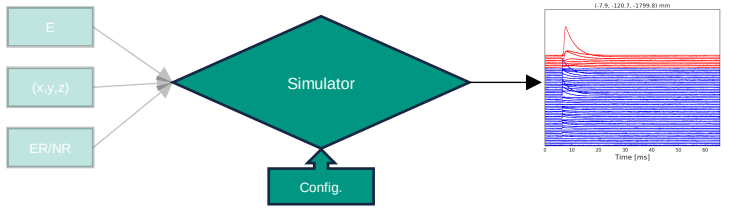
MMC in vacuum

LCE map



MMC on the bottom

Configuration

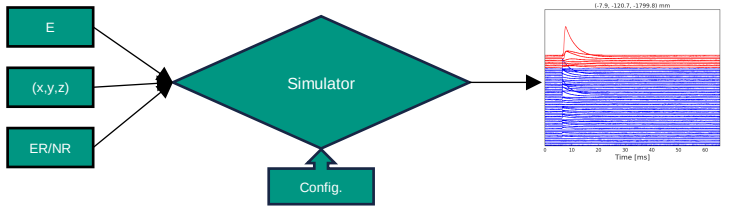


- The configuration is a dictionary taking information for the simulation of traces, such as:
  - path to the stored maps;
  - noise shape and intensity;
  - sampling information.

```
config = {'LCE': '/kalinka/storage/darkmatter/DELight/share/output/optical_simulations/optSim_LCE.npz',
          'optArrivalTime': '/kalinka/storage/darkmatter/DELight/share/output/optical_simulations/optSim_arrivalTime.npz',
          'PCE': '/kalinka/storage/darkmatter/DELight/share/output/quasiparticle/qp_map/phonSim_PCE.npz',
          'phonArrivalTime': '/kalinka/storage/darkmatter/DELight/share/output/quasiparticle/qp_map/phonSim_phonTemplate.npz',
          'sampling_frequency': 2.5e5,
          'trace_samples': 16384,
          'noise_type': 'pink'}

ws = WaveformSimulation(config)
```

Trace simulator



- Samples the observed quanta following a Binomial distribution (e.g., Bin(LCE(x,y,z), N_{UV}))
- Sums shifted template scaled w.r.t. the deposited energy in each time bin
- Repeat for each MMC