HPC working seminar for physicists

Scientific Computing Department at HIM

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bi-weekly meeting – 28.9.2021

Today’s Topics

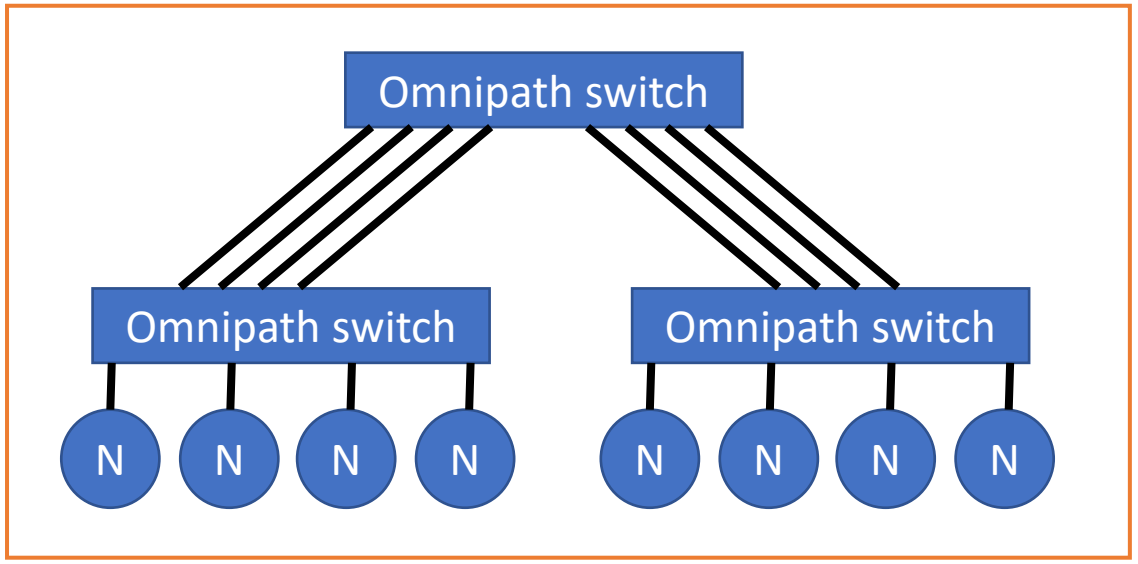
1. presentation of users / work groups
2. differentiation Mogon2 and Himster2
3. how to run Jupyter on Himster2
4. Your questions / discussion / requests to the maintainers

- compact in time (15mins + user questions/discussion).
- bring people together tackling the same problems

News

- Minutes: https://www.hi-mainz.de/research/computing/hpc-working-seminar/
- GPFS-fileserver will be retired at some point.
  - /project
  - compute node: 16.9.: read-only, 5.10.: gone
  - Login nodes: 16.9.: read-only
- Next scheduled maintanance 5.10.

Mogon 2 ⇔ Himster 2



HPC-Gate
(PrivacyIdea)

head nodes 1..3

Mogon 2:
80% of compute nodes & interconnect

GPU
nodes

home directory

Himster 2:
320 compute nodes & Fat tree interconnect

LUSTRE

Further shared:
- maintenance
- user software
- slow control

shared

Non shared hardware

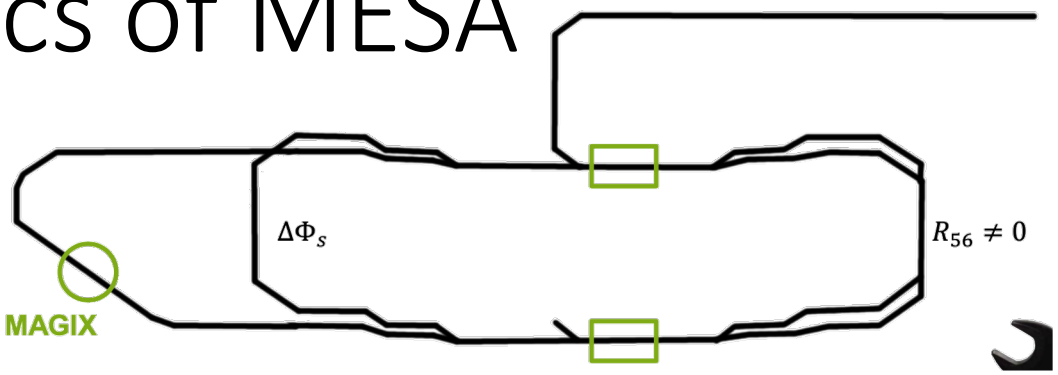
AG Denig BES III

- Working On: Detector Simulation & Data Analysis
- Christoph Florian Redmer, Riccardo Aliberti, Yasemin Schelhaas, Thomas Lenz, Max Lellmann, Yuping Guo, Tong Liu, Yaqian Wang, + MSc + BSc
- Software:
  - BOSS (BESIII internal software framework including Gaudi, Geant4, ROOT, ...)
  - "Slurm Job Submitter": small Python framework to coordinate BOSS jobs at Himster
  - Standalone event generators (with non-GNU compilers)

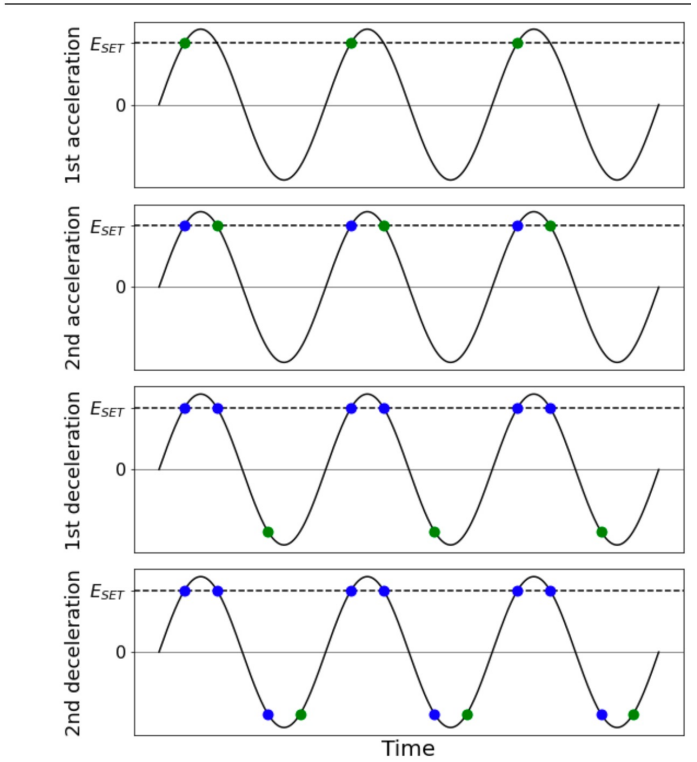
Longitudinal Beam Dynamics of MESA

- Sebastian Taubert

- OPAL: Object - Oriented Parallel Accelerator Library
- Large 3D ensemble tracking, under consideration of
  - wake fields,
  - space charge,
  - focusing and accelerating fields
  - Not a matrix code: Integration over time steps

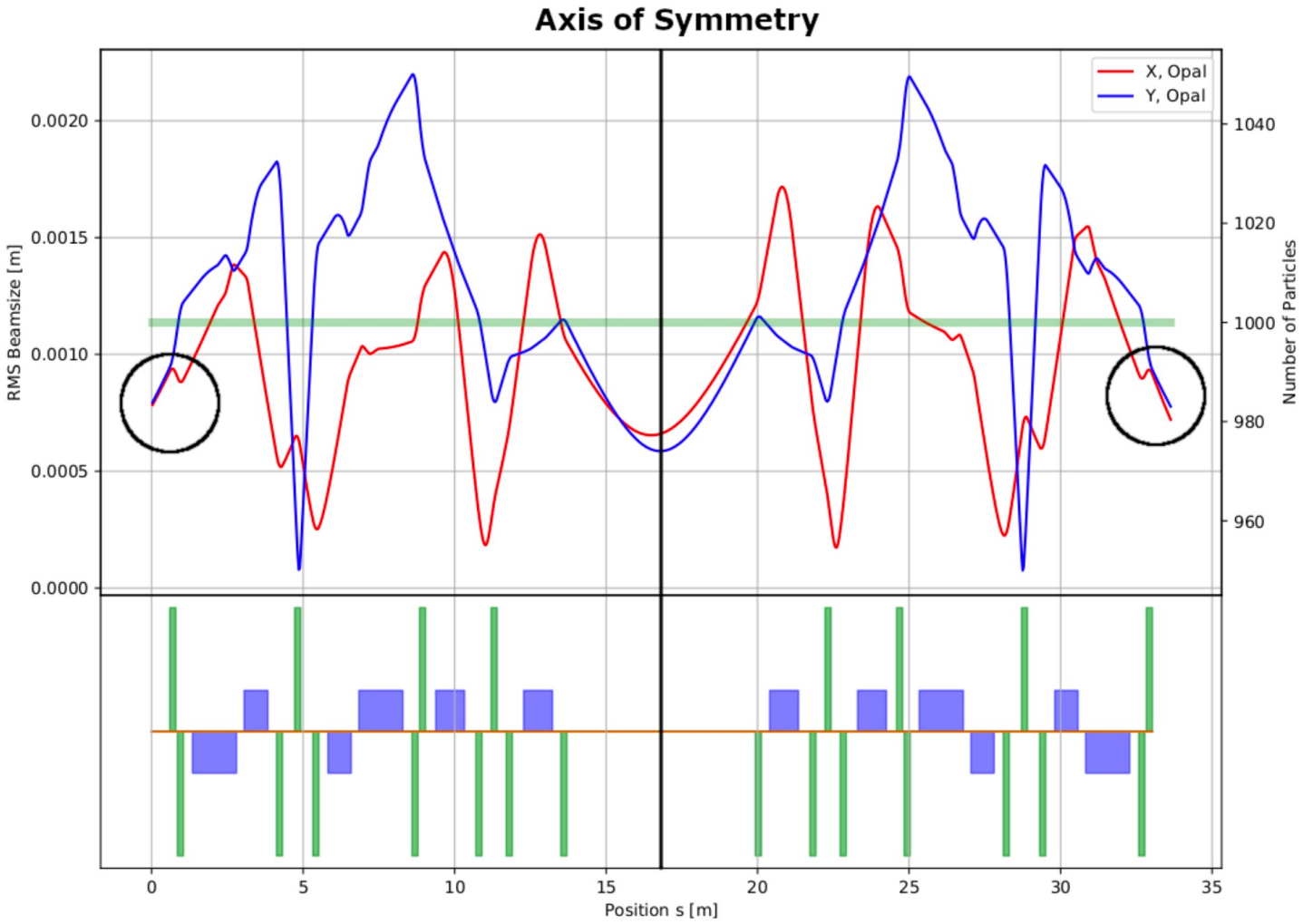


2x4 Pass ERL Mode



Simulation of Third Transferarc

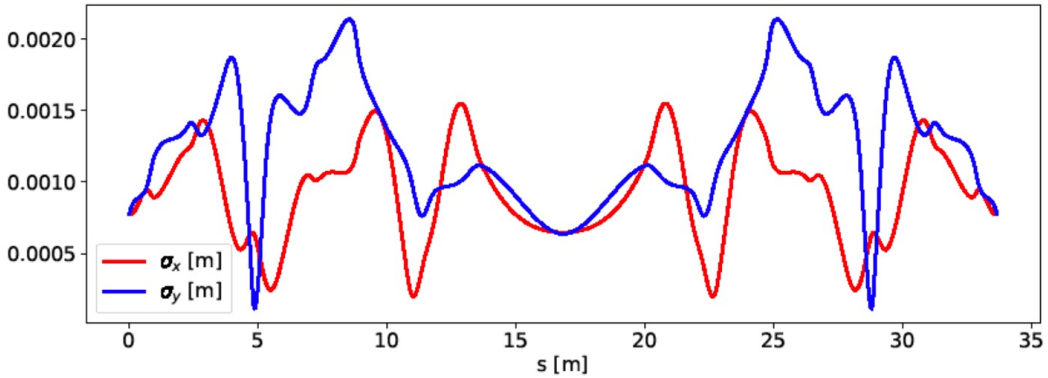
80 MeV

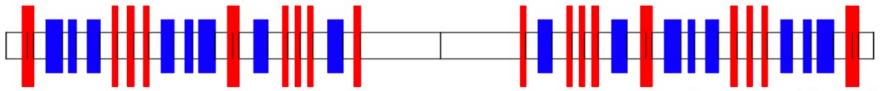


Left: Translated lattice to OPAL

Bottom: Simulation in elegant

Where do the differences come from?



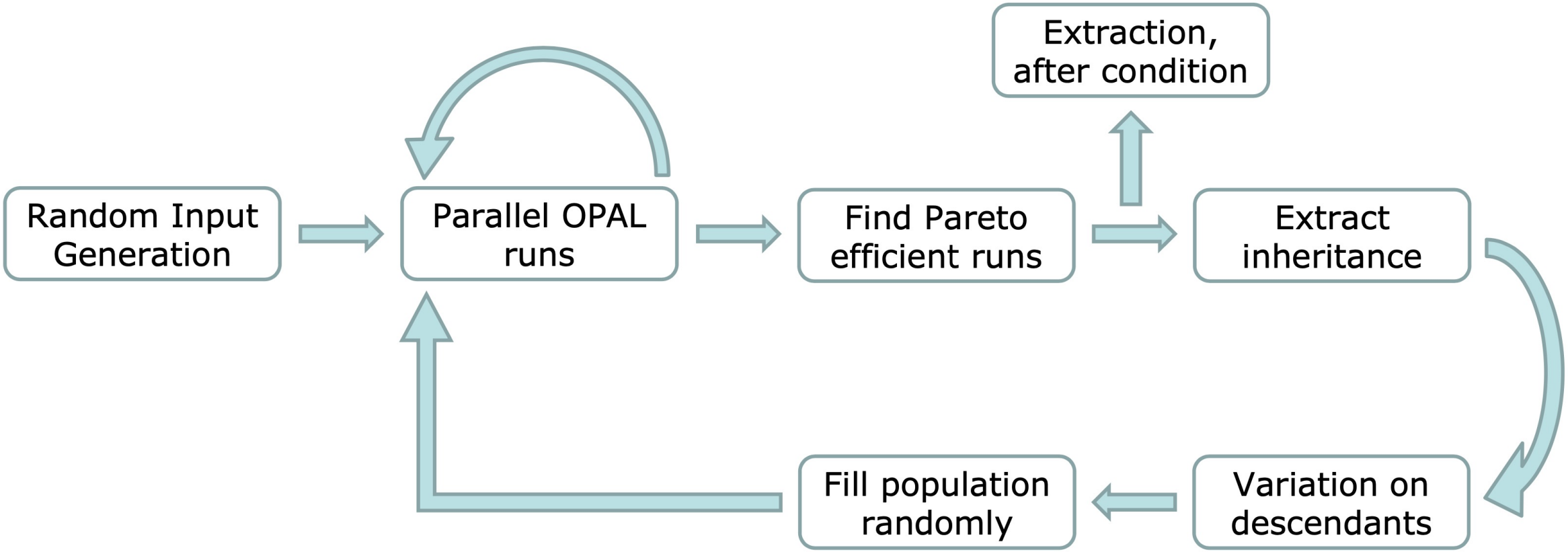


Courtesy of C. Stoll

Optimization via Python

JOHANNES GUTENBERG UNIVERSITÄT MAINZ

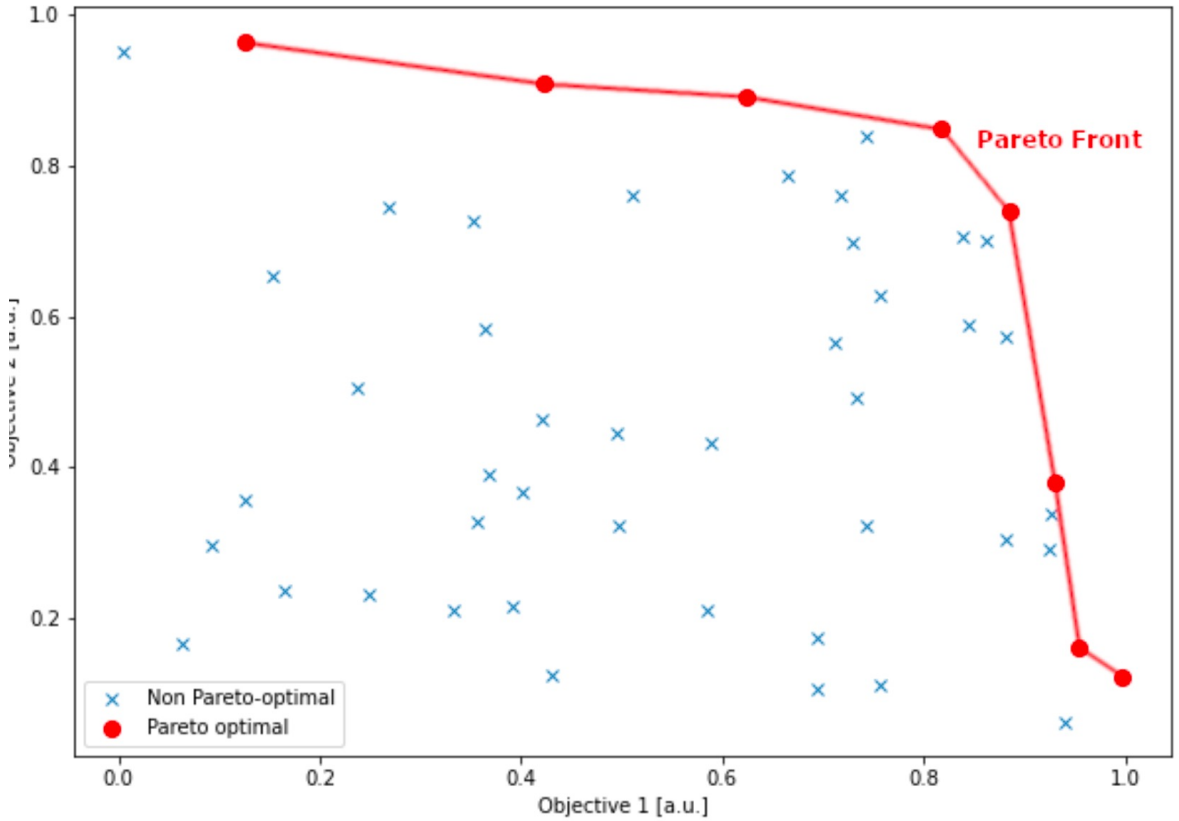
TECHNISCHE UNIVERSITÄT DARMSTADT



Python based, highly parallel program using **multiprocessing**, **OApackage**, **pandas**.

Pareto Efficiency and Pareto Front

(Or Potato Efficiency)



Example from
https://oapackage.readthedocs.io/en/latest/examples/example_pareto.html

Origin in Economics:

Allocation of limited resources to individuals

Pareto Efficiency or Optimum:

No improvement on one aspect (parameter) without taking from another

Pareto Front or Pareto Set:

- Set of Pareto efficient parameterizations
- Useful for engineering or beam optics to make focused tradeoffs

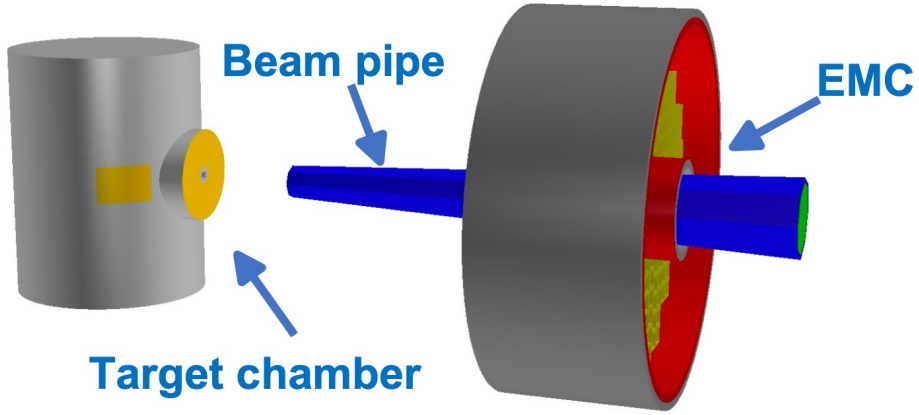
HELMHOLTZ
Helmholtz-Institut Mainz

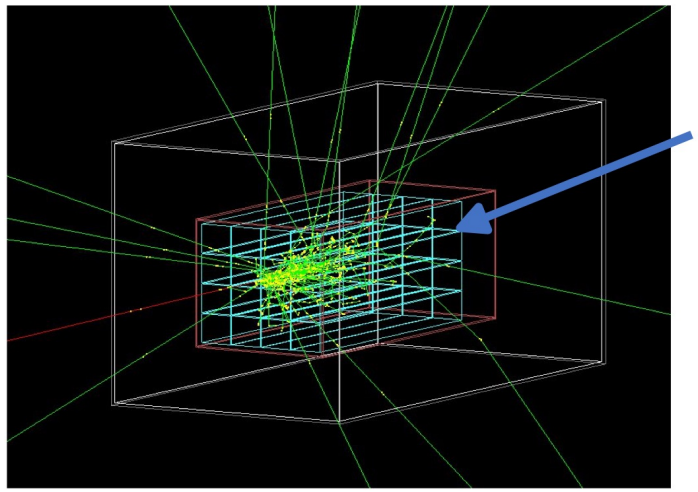
EMP (Electromagnetic Processes) on Himster

EMP - Simulation

Goal: simulation of detector signals analogue to the experiment

- Implementation of main geometry: dead material and detector components
- Generate particles (event generator)
- Particle tracking with physics processes
- Calculation of the deposited energy in the detector (in each crystal of the detector)
- Deduction of the detector signal from the deposited energy
- Storing of the signals in root files
- Analysis scripts to interpret the signals





Currently done on Himster

EMP - Simulation

Environment?

Requirements:

- Fairsoft May18
  - Root
  - Geant4
- C++
- Python
  - Pytorch
- Later: maybe Fluka

Gitlab repository:

- https://gitlab.rlp.net/emp/primasoft.git

Who is involved?

Postdocs:

- Luigi Capozza
- Dong Liu

PhD Student:

- Sahra Wolff

Master Students:

- Alexander Greiner
- Julian Moik

Jupyter on head node with plain python

Setup:

1. ssh himster2
2. [pbotte@login23 ~]$ python3 -m venv testjupyter
3. [pbotte@login23 ~]$ source testjupyter/bin/activate
4. [pbotte@login23 ~]$ pip3 install jupyter
5. Change config:
    1. [pbotte@login23 ~]$ jupyter notebook --generate-config
    2. change in ~/.jupyter/jupyter_notebook_config.py:
        1. c.NotebookApp.allow_remote_access = True
        2. c.NotebookApp.ip = '*'
        3. c.NotebookApp.open_browser = False
        4. double check that these lines are not commented out!

Jupyter on headnode with plain python

usage:

1. ssh himster2
2. [pbotte@login23 ~]$ source testjupyter/bin/activate
3. (testjupyter) [pbotte@login23 ~]$ jupyter notebook
4. Open locally: http://localhost:12345
   - Enter the code presented in terminal

- Caution:
  - others might already use port 8888.
  - If port already in use, change config file and the port forward in SSH.

Jupyter on compute node with plain python

Usage (setup like before):

1. Ssh himster2
2. [pbotte@login23 ~]$ salloc -p himster2_exp -N 2 --time=01:00:00 -A m2_him_exp
3. [pbotte@login23 ~]$ ssh x0784 #log into the computer node
4. [pbotte@x0784 ~]$ source testjupyter/bin/activate
5. (testjupyter) [pbotte@x0784 ~]$ jupyter notebook

6. ssh -L 12346:x0784.mogon:8888 himster2
7. Open locally: http://localhost:12346
   - Enter the code presented in terminal

Hot Topics we are working on

- Singularity containers for anaylsis (BES, Panda)

- Lustre mount GSI <-> HIM via T-Bit Link
  - Test IP-connection with 10GBit/s
  - Lustre mount on special head nodes
  - next: user mapping

- visualisation of usage statistics via Elastic Search
  - together with ZDV

Next

- Move selected howtos to Mogon Wiki

- Next meeting on 12.10.
  - presentation of our users (part 2)
  - singulalrity usage for EMP
  - hand in your topics!

Present your work group

work group title	
working on:	detector simulation / data analysis / …
picture	
all involved:	• names • project headline • technique (group internal analysis framework / python scripts / fancy algorithms / …)

- Please return until end of next week