HPC working seminar for physicists

Scientific Computing Department at HIM

Dr. Dalibor Djukanovic

Dr. Peter-Bernd Otte

bi-weekly meeting – 12.10.2021

Today’s Topics

1. news
2. presentation of 2 work groups
3. Your questions / discussion / requests to the maintainers

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

Jupyter on headnode with plain python

usage:

1. ssh -L 12345:localhost:8888 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

Working seminar, please do not hesitate to ask! missed a parameter last time.

Moved to Mogon Wiki:

https://mogonwiki.zdv.uni-mainz.de/dokuwiki/start:software:topical:physics:jupyter

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

News

- Minutes: https://www.hi-mainz.de/research/computing/hpc-working-seminar/

7.10.:

- updated Privacyidea
- reinstalled login nodes, all 3 available
- removed gpfs-project (/project) folder from the compute nodes (NOT /lustre/project)
- improved security

Nuclear Theory Group

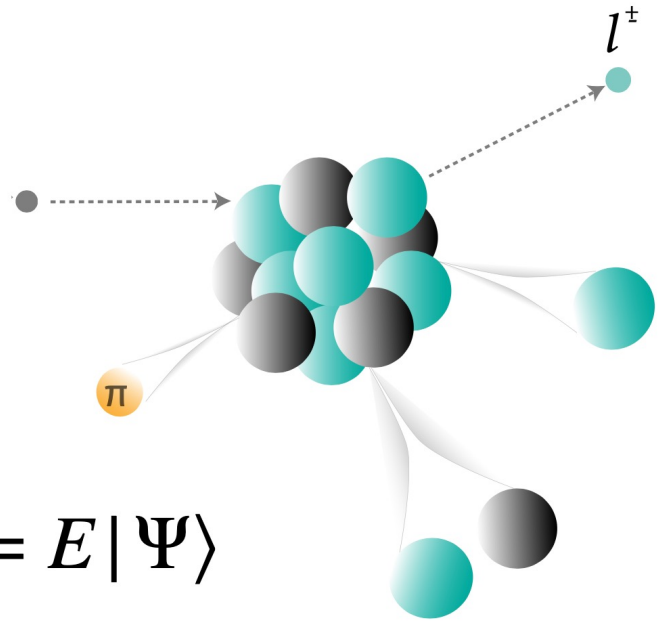
Sonia Bacca

Postdocs: Bijaya Acharya, Joanna Sobczyk

PhD students: Simone Li Muli, Francesca Bonaiti

Precision calculations of few-body and many-body systems

- ✓ Electroweak structure of nuclei
- ✓ Motivation: neutrino physics, astrophysical interest, precision calculations for BSM searches, ...



$$\hat{\mathscr{H}} \, |\Psi\rangle = E \, |\Psi\rangle$$

Nuclear Theory Group

Tools

- Hyperspherical-harmonics
  - light systems (up to 6 nucleons)
- Coupled-cluster framework
  - Medium-mass systems

✦ solving systems of coupled equations

✦ matrix operations (diagonalization) for large spaces

- Fortran90
- Algebraic operations: OpenBLAS, LAPACK, EISPACK
- HDF5 file format
- (post-processing done in Python)

JOHANNES GUTENBERG UNIVERSITÄT MAINZ JG|U

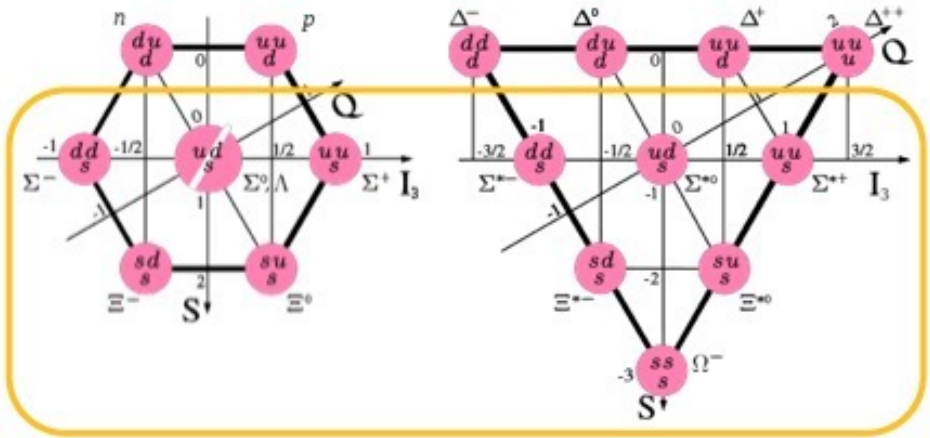
panda

HELMHOLTZ
Helmholtz-Institut Mainz

Himster2 usage by SPECF-Hyp

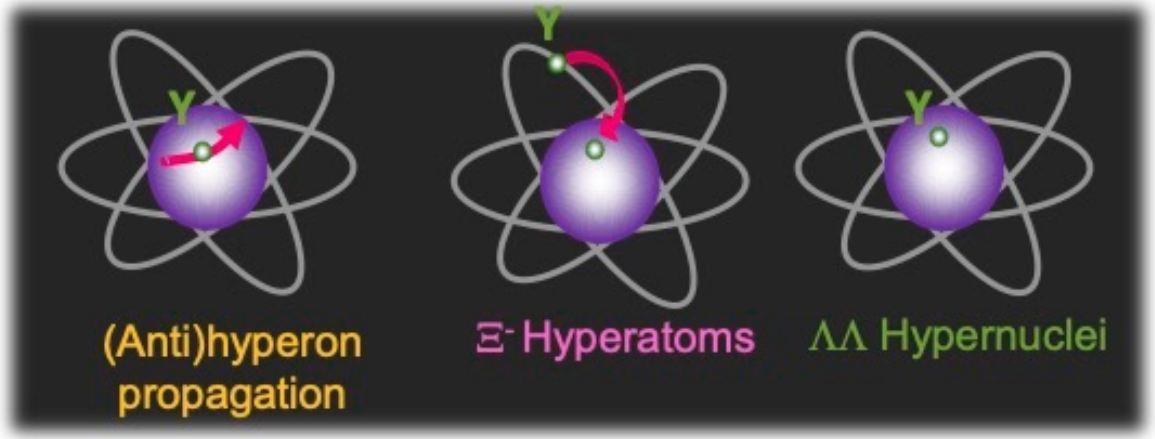
Marcell Steinen

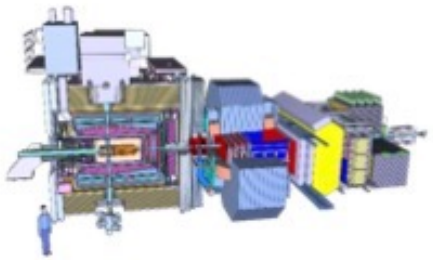
Hyperon



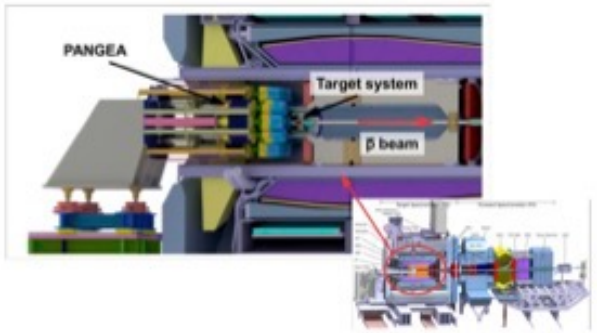
- Baryon with s quark (Y)
- Weak decay -> τ ~ 100 ps
- Short lifetime prevents scattering experiments!
- Interaction of YN, YY, $\bar{Y}$N barely/not known
  - Important parameters for the understanding of neutron stars!

Strangeness nuclear physics at $\bar{P}$ANDA



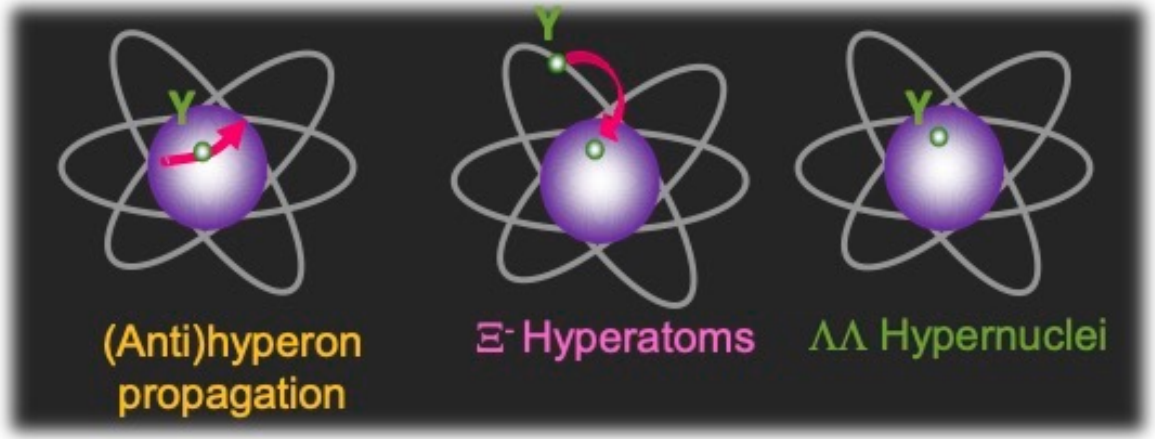


Phase 1 setup



Dedicated setup

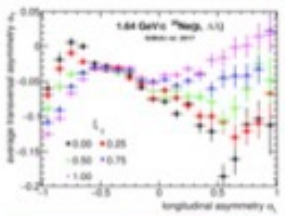
GiBUU

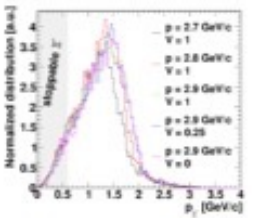


$\bar{P}$ANDA: H gas target

Ne gas target

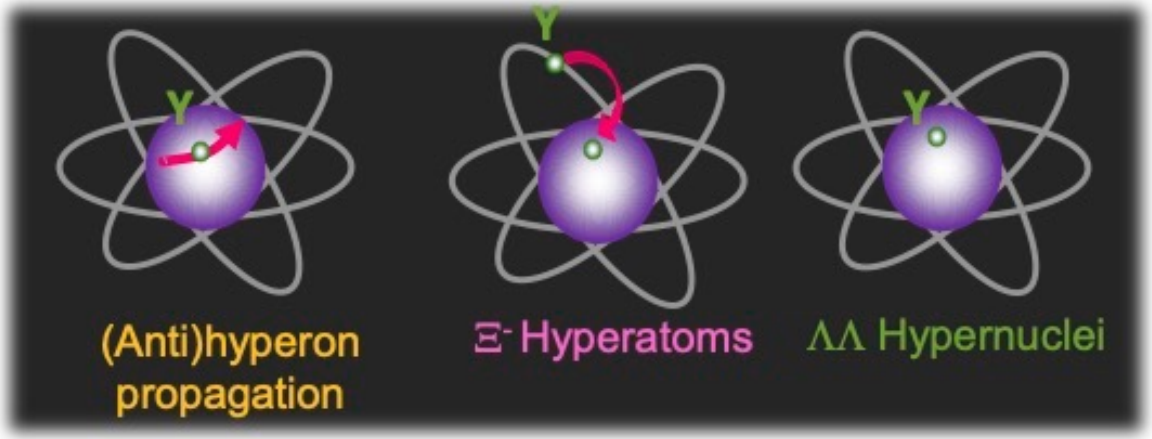
Solid C target





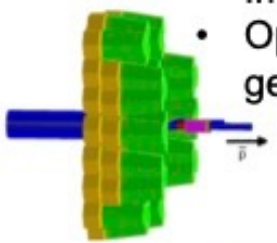
Himster2: event generation of primary interactions
in **GiBUU** transport code to study nuclear effects

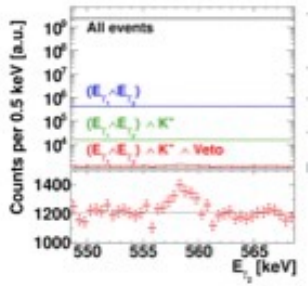
PandaRoot



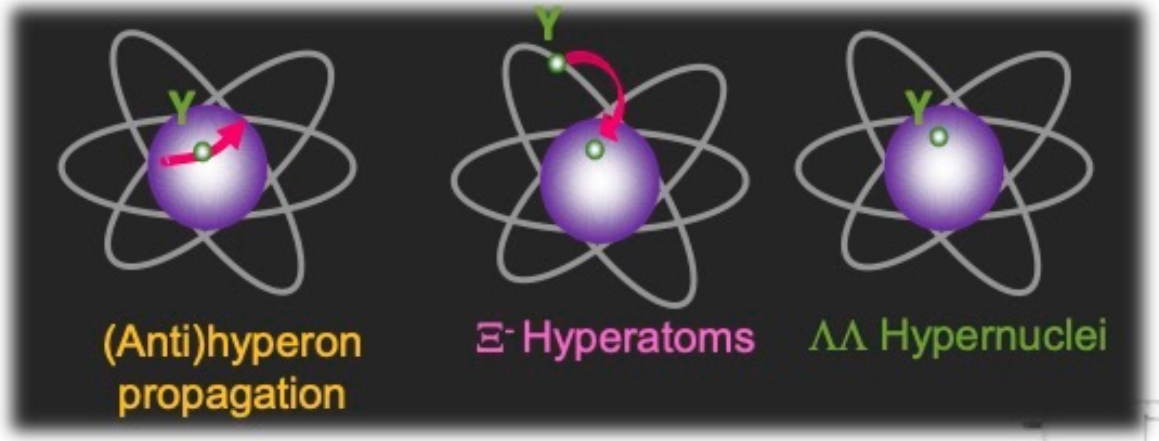
PandaRoot used on Himster2 for detector simulation (Geant3/Geant4)

- Feasibility studies
- Optimization of tracking
- Implementation and optimization of dedicated setup
- Optimization of gamma energy reconstruction in germanium detectors in background environment



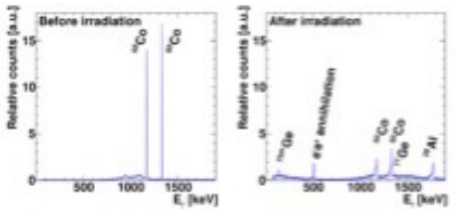


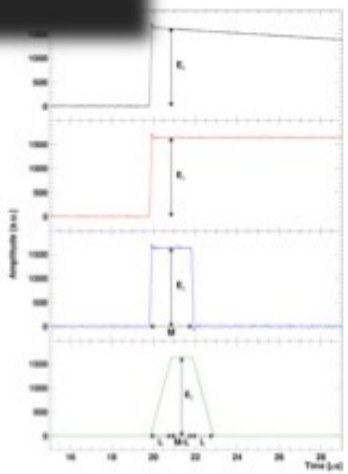
Strangeness nuclear physics at $\bar{P}$ANDA



Go4:

- Offline analysis of test beam data of germanium detectors using digital readout





Tools

- GiBUU (Gi)
  - Fortran
- PandaRoot (Pr)
  - C++
- GO4 (G4)
  - C++

Bash used for automatization

Users

- Sebastian Bleser (Gi, Pr)
- Michael Bölting (Pr, G4)
- Martin Christiansen (Gi)
- Falk Schupp (Gi, Pr)
- Marcell Steinen (Pr, G4)

Hot Topics we are working on

- Singularity containers for analysis (BES, Panda)

- Lustre mount GSI <-> HIM via T-Bit Link
  - Test IP-connection with 10GBit/s
  - Lustre mount on special head nodes
  - Mapping for both directions
  - next: Fix GSI side, then user mapping

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

Your requests

- Problematic file transfer between data centers (Jülich, GSI, Mainz)
- What else needs improvement?

Next

- Next meeting on 26.10.
  - presentation of our users (part 3)
  - PandaRoot with cvmfs (localy and with docker)

- Planning ahead:
  - detailed presentation of algorithms

- 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 / …)