

HPC working seminar for physicists

Scientific Computing Department at HIM

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bi-weekly meeting – 9.11.2021



Today's Topics

1. news
2. presentation Miguel (Lattice Group)
3. archive service from ZDV on Himster 2

Questions to the users:

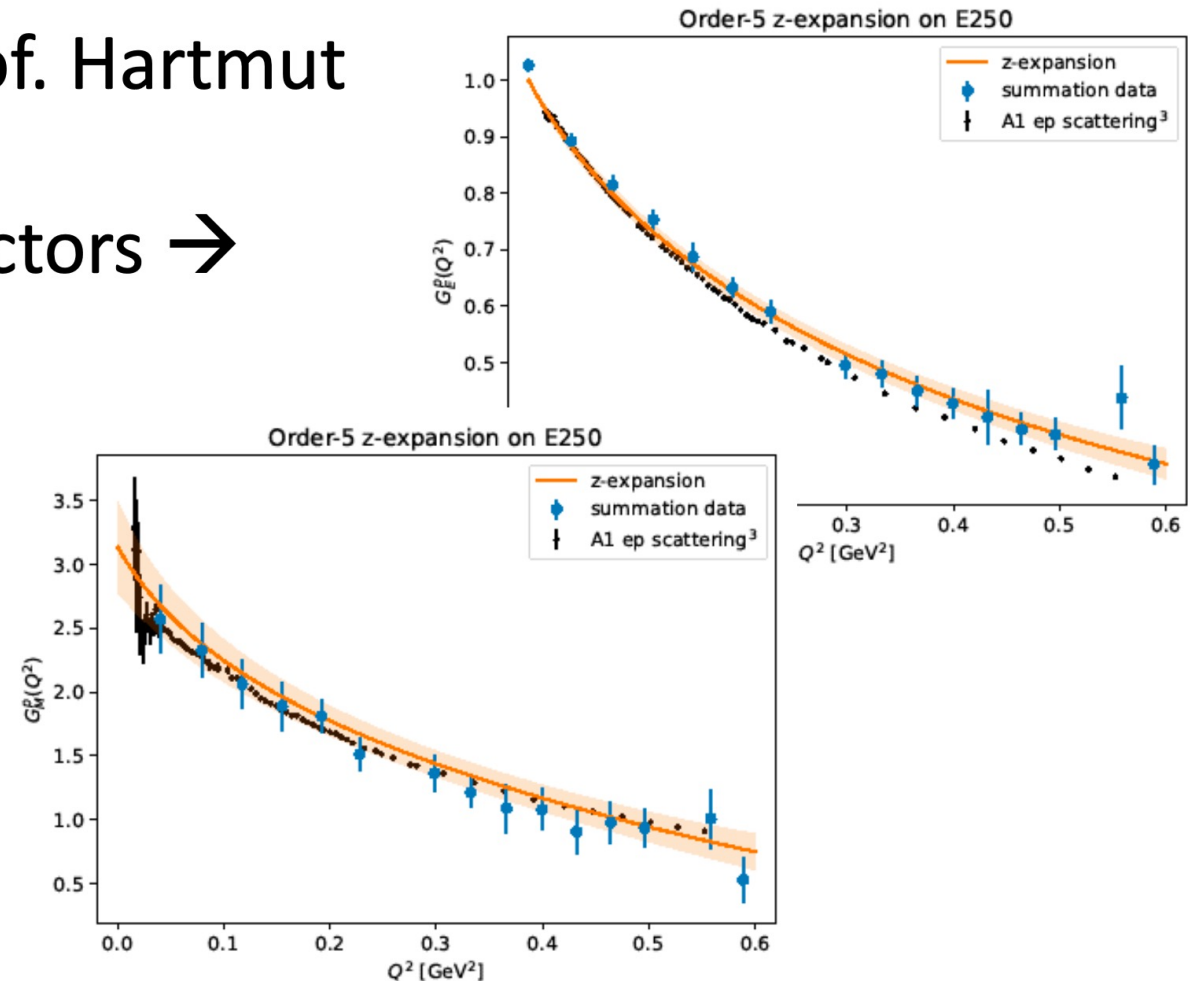
1. problematic file transfer between data centers
 2. questionnaire: best time slot for this meeting?
 3. your questions / discussion / requests to the maintainers
- compact in time (15mins + user questions/discussion).
 - bring people together tackling the same problems

News

- Minutes:
<https://www.hi-mainz.de/research/computing/hpc-working-seminar/>
- Fix: Singularity on Himster 2 with batch jobs:
https://mogonwiki.zdv.uni-mainz.de/dokuwiki/start:software:containers:singularity#using_singularity_on_mogon

Nucleon form factors from lattice QCD

- Miguel Salg (PhD student with Prof. Hartmut Wittig)
- Isoscalar electromagnetic form factors → proton, neutron
- Focus on data analysis
- Tools
 - Python
 - HDF5 file format
 - SciPy, NumPy, h5py, MPI4py, ...
 - Mainly self-written analysis scripts / notebooks



Nucleon form factors from lattice

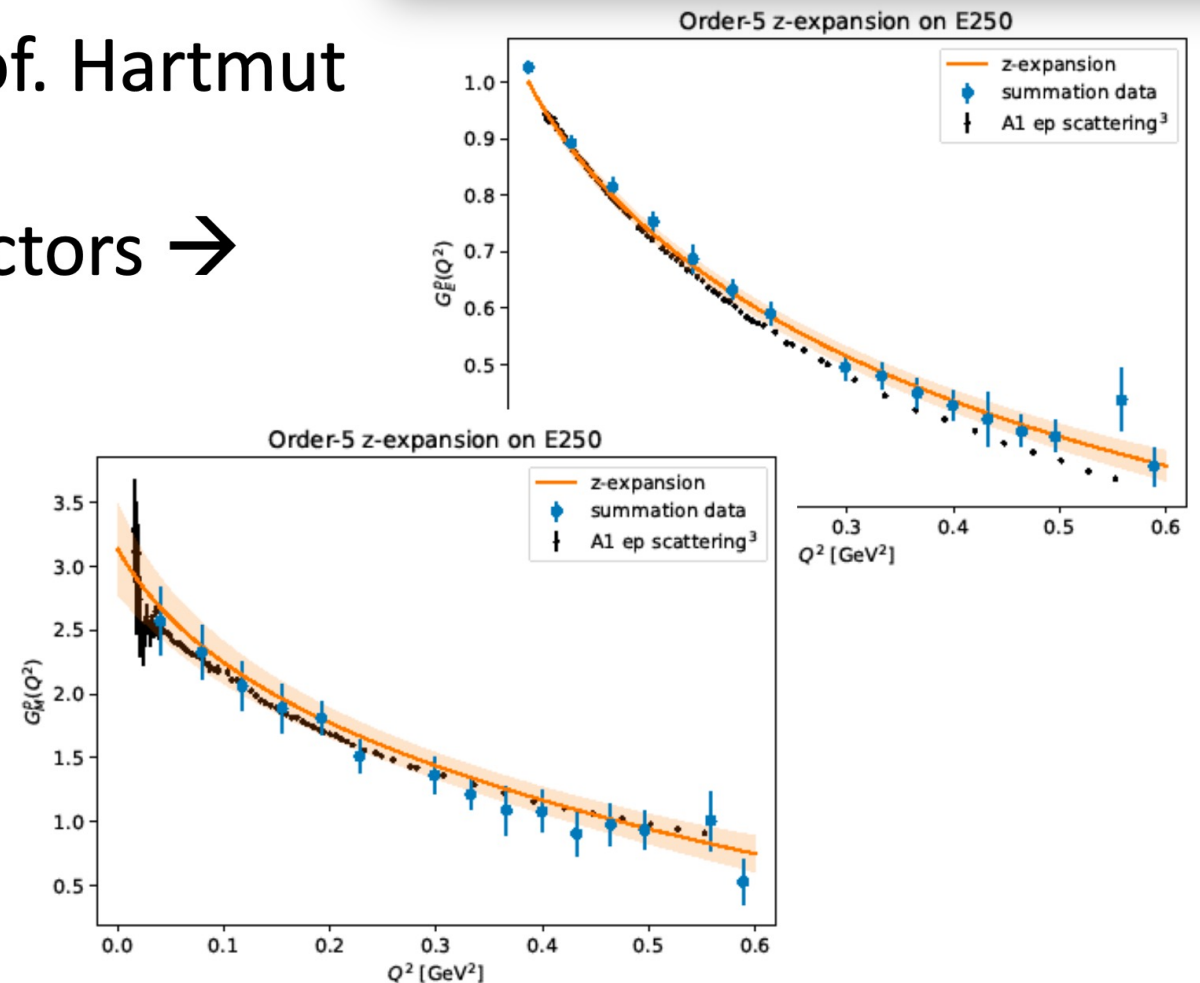
3 step process:

1st simulation/generation of gauge field

2nd perform measurement on fields

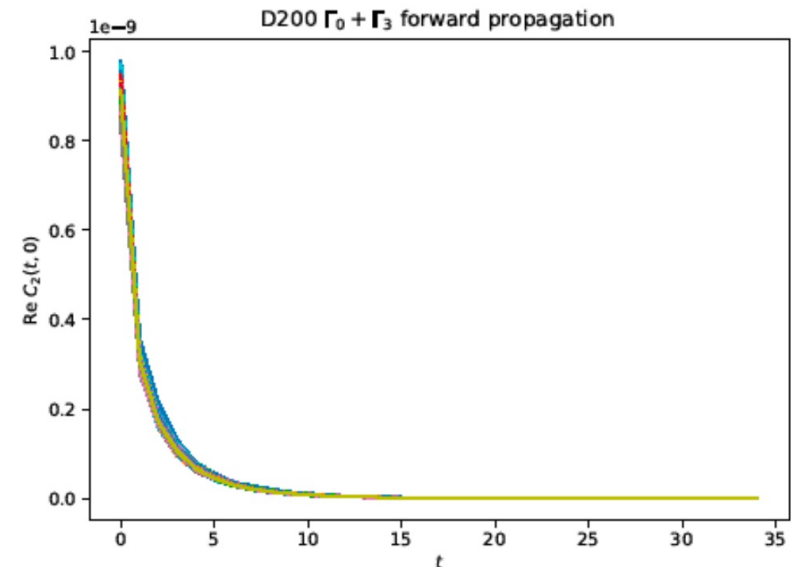
3rd post process measurement

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Nucleon form factors from lattice QCD

- Measurement of observables with the group-internal software package 'observer'
- Mixed C / C++, MPI
- Based on openQCD and QDP++
- Currently I'm running on Clover
- Typical problems:
 - Solving linear systems / matrix inversions
 - Tensor contractions
 - Fourier transforms
 - Least-squares fits (in the analysis)



Archiving Service on Himster 2/Mogon 2 (1/2)

DMP (data management plans) necessary for founding program?

- [Experts: https://researchdata.uni-mainz.de](https://researchdata.uni-mainz.de)

IRODS

- Archiving service connected to Himster 2
- No space limit (if >1TB inform support first)
- <250TB/user -> free
- combine files until they are larger than 10GB
- Idea:
 - write once, read from time to time
 - share your raw data together with paper (measurement or analysis VMs)

Archiving Service on Himster 2/Mogon 2 (2/2)

Who is interested?

IRODS, more links

- <https://researchdata.uni-mainz.de/technical-support/>
- https://mogonwiki.zdv.uni-mainz.de/dokuwiki/start:fs_dm:archiving:irods
- <https://docs.irods.org/4.2.6/icommands/user/>
- Webinterface: <https://irods-web.zdv.uni-mainz.de/irods-cloud-backend/#/home/My%20Home>

Your requests

- Problematic file transfer between data centers (Jülich, GSI, Mainz)
 - in the pipeline (GridFTP, UFTP or SCP?)
 - Who else encounters these problems? BES3 / LatticeQCD?
- Better time slot for this seminar?
 - doodle poll via email
- What else needs improvement?

Hot Topics we are working on

- Singularity containers for analysis (BES, Panda): CVMFS client
- Lustre mount GSI <-> HIM via T-Bit Link
 - Test IP-connection with 10Gbit/s
 - Lustre mount on special head nodes
 - Mapping for both directions
 - user and group mapping
 - Next: speed tests
- visualisation of usage statistics via Elastic Search
 - together with ZDV

Next

- Next meeting on 23.11.
 - Last user group presentations (EMP, SHE, MAM?)
- 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:	<ul style="list-style-type: none">• names• project headline• technique (group internal analysis framework / python scripts / fancy algorithms / ...)