

Scientific Computing in HEP

Report from FH task force

FH-retreat follow up, 14.12.2022

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The Scientific Computing Task Force



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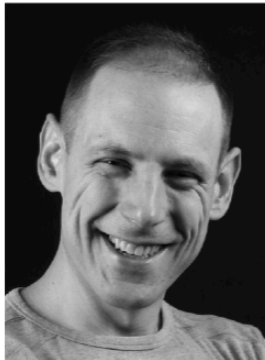
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good representation of all research groups in FH - theory, experiments and IT

The Charge

of the task force

- Review the current situation and make suggestions on how to **further develop this important area** within FH, e.g.
 - Algorithmic developments, research software developments, data management, and novel technologies such artificial intelligence, machine learning and quantum computing
- Propose strategies how to
 - Increase **DESY's visibility** in the wider HEP community
 - Strengthen DESY's **role as research hub for the German universities**
 - in preparation for **HL-LHC** and **future experiments**
 - Advance **career opportunities for young researchers**
 - Contribute to more **sustainable** computing

Points to address

as suggested in the charge

- **Review, categorise and summarise** the **activities** related to HEP scientific computing within FH
 - incl. relation to all other projects, activities, institutes (CDCS, Helmholtz, etc)
- Identify and discuss **synergies between different groups in FH** and with other scientific areas at DESY
- Propose **strategies to foster a continuous stimulating exchange** between scientists within FH and across divisions on topics of interest
- Propose **core areas of interest** where the engagement should concentrate on based on the importance for HEP, the possibilities to **exploit synergies** with other scientists at DESY and the potential for society at large
- Review the **funding landscape** and propose strategies on **how to exploit these most efficiently**, also considering potential strategic collaborations on certain topics with national or international institutes.

HEP Scientific Computing activities in FH

and relation to other projects, institutes and activities

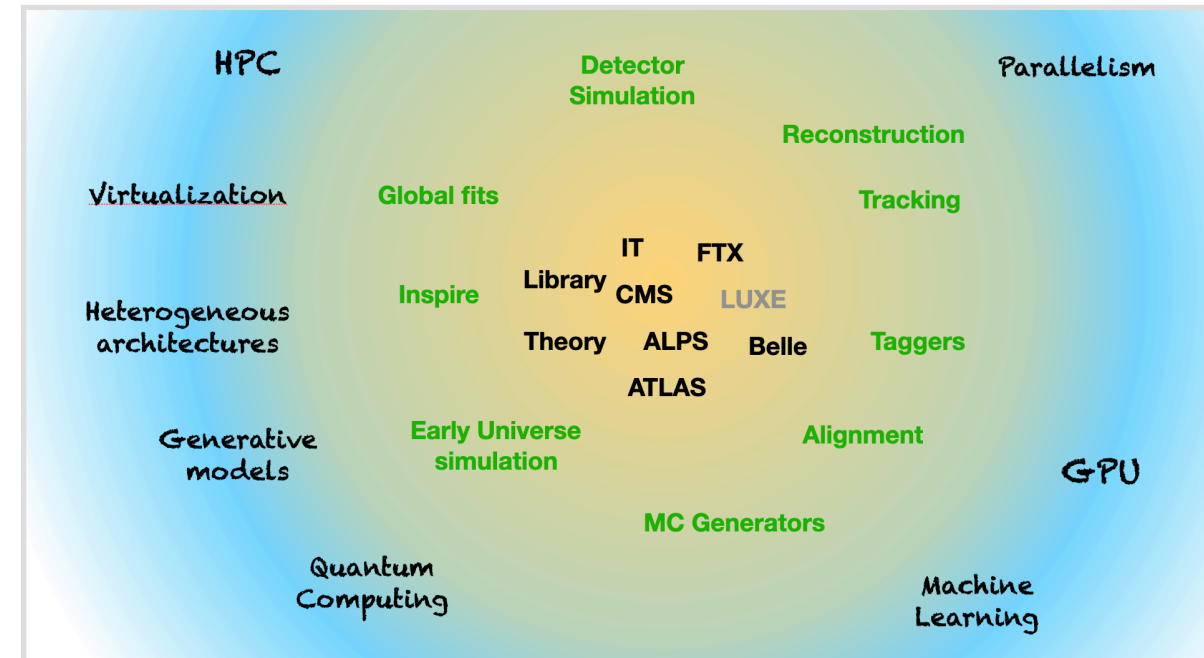
- compiled a large list of activities related to scientific computing where people from FH are involved
- useful to keep such a evolving list in the future in a suited format

3rd Party Projects -- Examples!		
AIDAInnova (Horizon 2020)	WP12: Software for Future Colliders: developments for turnkey software stack Key4hep, fast simulation, tracking and particle flow algorithms	4.2021-3.2024
ACCLAIM (Helmholtz Innovation)	Accelerating Science with Artificial Intelligence and Machine Learning	01.21-12.23
NFDI (DFG)	PUNCH4NFDI, BASE4NFDI Data Management & Infrastructure	10.2021-09.2026 (initially)
ESCAPE (EU)	Addresses challenges by future large research enterprises such as HL-LHC, SKA, FAIR and other ESFRI Roadmap projects	until 02.2023
FIDIUM (BMBF)	Federated computing infrastructures for HEP and Nuclei & Hadrons in Germany	10.2021-09.2024
HIP (Helmholtz)	Imaging, mainly Photon science	
HIFIS (Helmholtz)	IT infrastructure connecting all Helmholtz research fields & centres	
ExPaNDS (EU) –EOSC Photon and Neutron Data Service	standardised, interoperable, and integrated data sources and Data analysis services for Photon and Neutron facilities	
EOSC-Future (EU)	Implementation of the European Open Science Cloud (EOSC)	
LUXE (Innopolis)	Tracking for LUXE (incl QC methods)	
ErUM-Data/DIGUM	Computing for physics related sciences	

Institutions & Programs		
KAI Hamburg	Strategic collaboration between DESY and HAW Hamburg	Since 2021
CDCS	Astro&Particle Physics, Photon Science, Systems Biology Controls & Accelerators	Until 12.2023
CQTA	- access to quantum computer hardware - applications of use case for industry and academia - training in quantum computing- quantum sensing	
Helmholtz Topic DMA	- ST1: The MATTER Information Fabric - ST2: The Digital Scientific Method - ST3: The Digital Experiment and Machine	POF4
DASHH	Various applications, in FH often ML methods	

Infrastructures		
NAF	National Analysis Facility for German HEP. Also Belle-2 Analysis Facility (internationally)	
MAXWELL	HPC Facility serving mainly Photon Science, but also dedicated HEP applications	
Grid Center	Grid Facility for WLCG (ATLAS, CMS, LHCb Tier-2) and RAW data center for Belle-2	
Software and Middleware		
dCache	Multi purpose large scale storage middleware	
Contributions to codes (HEP-TH)	e.g. MasterCode, HEJ, WHIZARD, ChiliPDF, DEDUCTOR, Higgstools, FeynHiggs	
Contributions to codes (HEP-EXP)	e.g. Acts (A Common Tracking Software), Corvreckan (Test Beam Data Reconstruction), Key4HEP	

- the task force had several meeting with dedicated **reports by all groups** in FH
 - about their scientific computing activities
- revealing a vast range of different topics and activities that people work on
 - often driven by **personal interest** and more importantly by **the immediate needs** of the research groups
 - most certainly there is room for identifying **synergies** and possible collaboration on topics of interest
- the task force believes that this **a longer term commitment is needed** to address this - beyond the current strategy process



Transverse scientific computing platform in FH

strengthening scientific computing in the longer term

- the essential recommendation of the task force is the creation of a **transverse scientific computing platform** (aka *Virtual Scientific Computing Group*)
- ensure the long term commitment to improve the situation for this important field for the (HEP) research at DESY
 - ensure continuous and stimulating exchange
 - improve career opportunities for younger scientists
 - increase DESY's visibility in the field
- this requires the **commitment of dedicated additional resources** - in order to balance the additional overhead

Initial Ideas / Current Thoughts

- Creation of a *Virtual Scientific Computing Group* in FH
- Regular meetings to discuss and prepare 3rd party funding opportunities
- Identify and work on projects with common strategic relevance, e.g.
 - Exploiting heterogeneous resources
 - (Generative) Machine Learning
 - Quantum Computing
 - Large Scale FAIR Data Management
- Organisation of a regular FH Scientific Computing Seminar
- Organisation of HEP specific training events
- Inform about and promote *citable* software releases
- Serves as communication hub to DESY-wide Scientific Computing Group

the transverse scientific computing platform as presented - and discussed - at the FH retreat

Strategies for continuous and stimulating exchange

between the groups and beyond

- the transverse scientific computing platform - if established successfully - will naturally ensure a continuous exchange of information
- as a low-hanging fruit the task force will be in charge of organising of a **regular scientific computing seminar**:
 - current thinking, as developed together with the seminar task force:
 - **regular bi-weekly - in person/hybrid** - meetings with dedicated talks on scientific computing
 - alternating with **external invited speakers and internal speakers**
 - main goals: education and networking opportunities
- in the longer run this can be extended with additional seminars, workshop or tutorials as needed
 - need to ensure uniqueness and avoid overlap with the many existing seminar series that people can attend (virtually)

Core areas of interest

that should be addressed with dedicated funding (PhD, post doc)

- **Exploiting heterogeneous resources**
 - with increasing availability and of massively parallel hardware (GPU, FPGA, TPU) strategic interest to develop the know-how and tools to exploit this for essentially all data processing in FH and DESY
 - naturally contributes to more **sustainable** computing.
- **Large Scale FAIR Data Management**
 - efficient storage, management and access to research data following FAIR principles is a vital necessity for all research fields at DESY
 - exploiting common tools, middleware and hardware leads to a more efficient computing infrastructure
- **(Generative) Machine Learning**
 - almost all groups in FH make increasingly massive use of ML to increase computing and physics efficiencies
 - generative ML methods for fast detector simulation promise enormous speed-ups for more sustainable computing
 - here DESY has already achieved a leading role internationally with close collaboration with UHH
- **Quantum Computing**
 - not having any direct impact on ongoing research at DESY today
 - but identified as a strategic research field for DESY with great potential for future applications and methods.

Strategies for 3rd party funding

exploiting the opportunities most efficiently

- third party funding is crucial for successful research in HEP
 - and even more important with tighter budgets
 - the platform could be **very helpful in coordinating and supporting** relevant 3rd party funding proposals
 - at the same time there are also risks involved
 - often, additional and new research topics are not necessarily well aligned with the DESY/FH strategy - and require the provision of matching funds
 - the requirement for **maintenance and continuous support** after the funding ends
- the platform would be the right forum to carefully identify, discuss and coordinate funding applications matching the overall FH/DESY strategy

Summary and Outlook

- FH groups are involved in many important projects and activities in scientific computing
 - yet there is clearly the need to further strengthen this increasingly important field
- the task force suggest to establish a **transverse platform for scientific computing** that addresses this in the longer run in order to
 - **increase DESY's visibility in the wider HEP community**
 - **strengthen DESY's role as research hub for the German universities**
 - **advance career opportunities for young researchers**
 - **contribute to more sustainable computing**
 - **identify and foster synergies between the groups and divisions**
- this requires dedicated (and sufficient) funds to be available for the platform in order to start out with important projects of common strategic interest