Task Force on Scientific Computing in HEP

Findings and current discussion for next steps

FH Fellow Meeting, 21 April 2023

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HELMHOLTZ RESEARCH FOR GRAND CHALLENGES

DESY.

The Scientific Computing Task Force

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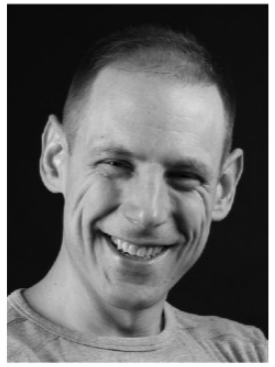

Jürgen Reuter (TH)

Stefan Schaefer (NIC)

Frank Schluenzen (IT)

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David South (ATLAS)

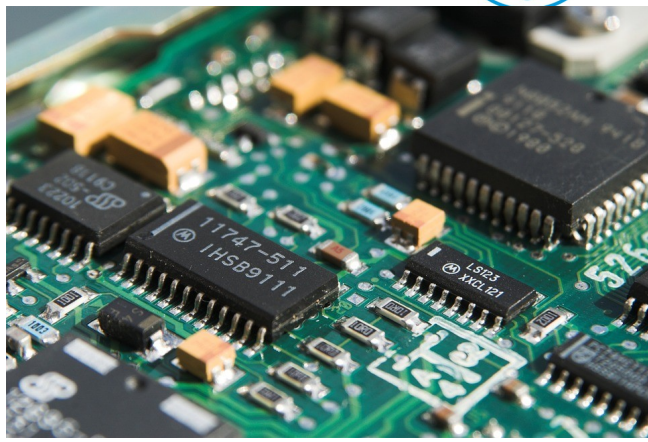
good representation of all research groups in FH - theory, experiments and IT

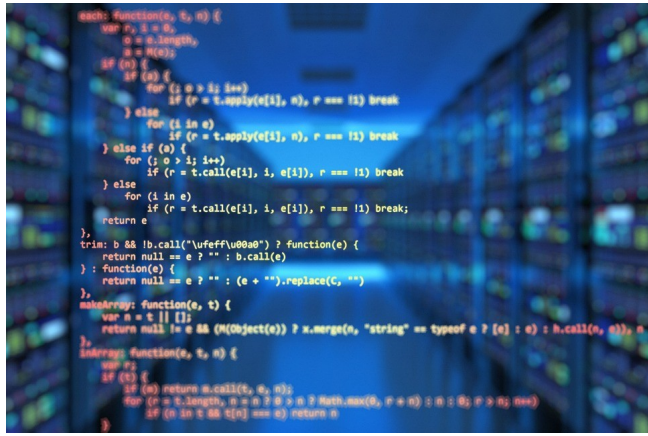
Scientific Computing

Enabling fundamental research

- Particle physics research employs custom instruments and methods
- Computing and software are everywhere – Examples:
  - Detector front end electronics
    - Highly specialised firmware & control software
  - Reconstruction & calibration codes
  - Physics in computer programs
    - MC generators
    - Detector simulation
  - Processing frameworks and data management for distributed computing
  - Statistical and AI & ML tools for data analysis

- Better computing and clever software enhance the scientific harvest and help lowering the required energy footprint





The Charge

of the task force

- Scientific Computing has been one of about dozen tasks forces that were appointed ~1y ago
- 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

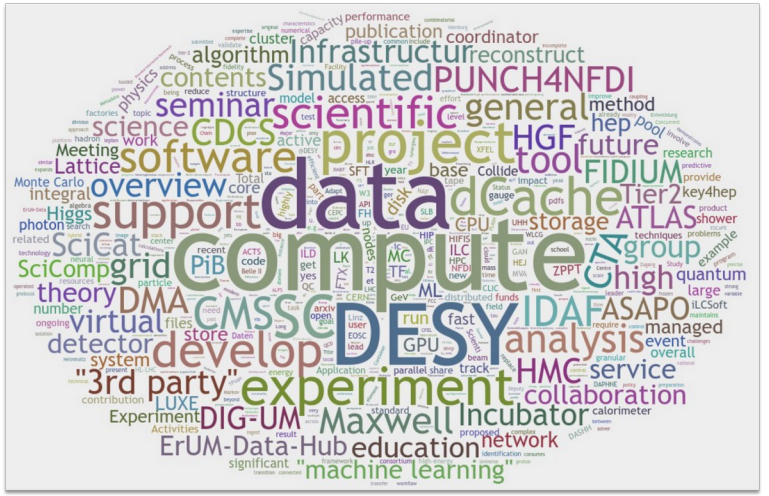
Propose strategies how to

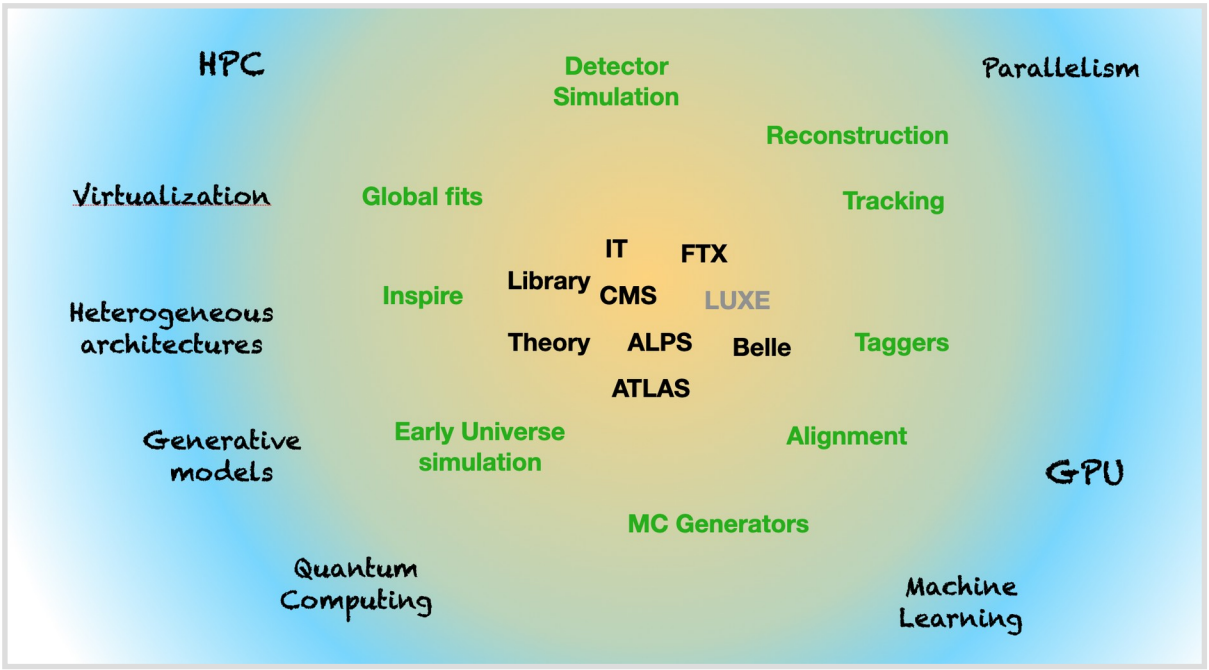
- Increase **DESY's visibility** in the wider HEP community
- Strengthen DESY's **role as research hub for the German universities**
  - in preparation for **HL-LHC** and **future experiments**
- Advance **career opportunities for young researchers**
- Contribute to more **sustainable** computing

Identification of Synergies

between the FH groups and others at DESY

- 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 across groups

- the essential recommendation of the task force is the creation of a **transverse scientific computing platform**
- 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
- the TF strongly suggests **commitment of dedicated additional resources**

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 FH groups and beyond

- the transverse scientific computing platform - once 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**:
  - together with the seminar task force the following is about to be implemented:
    - **regular bi-weekly - in person/hybrid** - meetings with dedicated talks on scientific computing
    - primarily internal speakers and occasionally external invited speakers
    - main goals: **education and networking** opportunities
- in the longer run this can be extended with additional seminars, **workshops or tutorials** as needed
  - need to ensure uniqueness and avoid overlap with the many existing seminar series that people can attend (virtually)

Identified core areas of interest

Possible topics to be strengthened in DMA in POF-V

- **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.

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

- a **transverse platform for scientific computing** is planned and the mandate is being worked out. It will likely address efforts to

  - **identify and foster synergies between the groups and divisions**
  - **strengthen DESY's role as research hub for the German universities**
  - **increase DESY's visibility in the wider HEP community**
  - **advance career opportunities for young researchers**
  - **contribute to more sustainable computing**

Some Questions to the Audience

Assignment of Home Work

- What can we do, in the field of scientific computing, to exchange information more effectively and to prevent reinventing the wheel? How can we better use synergies and foster intellectually stimulating discussions to provide the basis for innovation/developing novel ideas?

- How do we provide the best training in software & computing so that we can work efficiently and concentrate on the physics?