4. draft

KET Input zu ErUM Data Call

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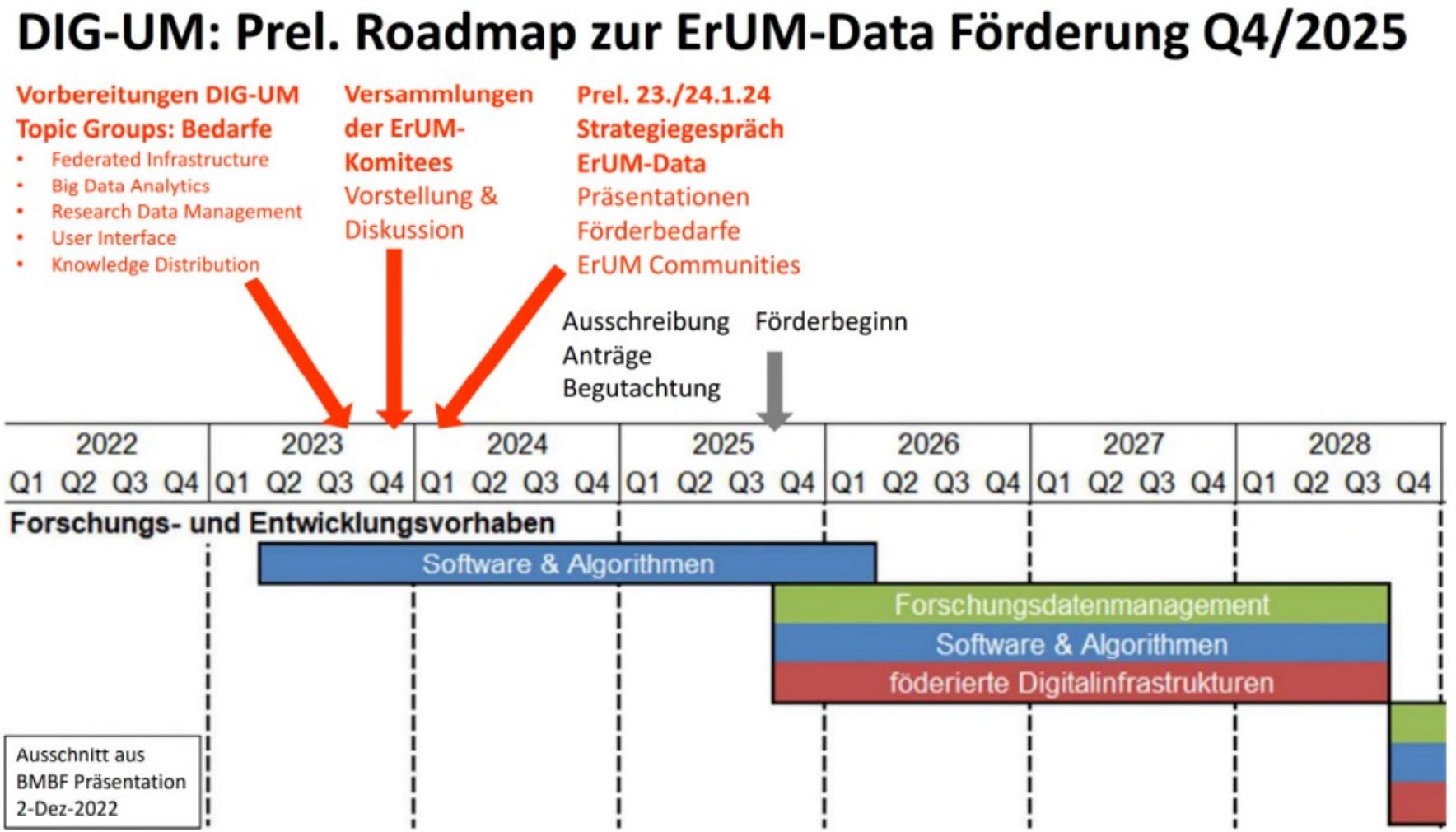
für KET
Computing
Panel

- Einführung
- ErUM Data Ausschreibung und Zeitplan
- Themen in
  - Federated infrastructures
  - Software and algorithms
  - Research data management
- Diskussion

Einführung

- BMBF plant Finanzierung von Forschungsprojekten in ErUM Data ab Q4/2025 in diesen Themengebieten:
  - Federated digital infrastructures
  - Software & algorithms
  - Research data management
- ErUM communities (KAT, KET, KfB, KFN, KFS, KFSI, KhuK, RDS) können über DIG-UM Topic Groups Input zur Gestaltung der Ausschreibung geben
- Laufende ErUM Projekte mit KET Beteiligung:
  - Fidium ("Föderierte Digitale Infrastrukturen für die Erforschung von Universum und Materie"):
    - gemeinsames Projekt von KET und KhUK, 2021-2024 (+2025)
  - KISS ("Künstliche Intelligenz zur schnellen Simulation von wissenschaftlichen Daten") und AISafety im Bereich Software & Algorithmen (2023-2026)
    - Gemeinsame Projekte KET + weitere Communities

Roadmap (M. Erdmann)



KET Themenliste – Federated Infrastructures

1) Building a federated compute infrastructure for all ErUM data communities
   - Ongoing for HEP but potentially interesting also for HEP, HuK, ATP, astronomy and photon-science
   - Possible involvement of industrial partners (e.g. dynamic clouds)
2) Building a federated data infrastructure (data lake + data caches, etc.)
   - Needed for 1) - essentially a combination of centers with storage systems and high bandwidth in a data federation.
3) Analysis facilities:
   - Platforms using resources in 1) with dynamical setup and scaling (COBalD/TARDIS). Based on industry standards Apache Spark or Dask.
   - dCache to federate storage infrastructure for efficient analysis
4) Development and validation of methods for simulating data lakes, distributed data, caches
5) Monitoring and communication infrastructure for federated compute and data resources
   - accounting, controlling, availability, CO2e footprint (Fidium/Auditor as basis)
6) SDN (Software Defined Networking)
   - penalties for unscheduled transfers (already emerging in the USA)

Sustainability as overarching topic

Software and Algorithms

- Real time algorithms
- Algorithms for heterogeneous computing
- Implementation of new computational methods in dedicated hardware
- Inverse problems
- Generative models
- Foundational models
- Algorithms for sparse data
- Resource savings by software optimization
- Experiment overarching algorithms (e.g. tracking, ACTS)
- Quantum computing algorithms
- Further development/upgrade of existing software
- Application of LLM/genAI for software development, operation, etc

Topic list for KET – Research Data Management

1) Workflow management systems
   - Services to organize complex workflows (Luigi, Snakemake, …)
   - How to apply in our environment
   - following FAIR principles
2) Open data – not only outreach but for research
   - Active discussion in LHC experiments on policy details
   - Requires long-term commitment and support
   - Cooperation among experiments and with theory groups
   - following FAIR principles
3) Data lake & caching
   - overlap with topic in ‘federated infrastructure’
     - Integration with data management systems required
4) Combining meta-data and data-management systems

Diskussionspunkte

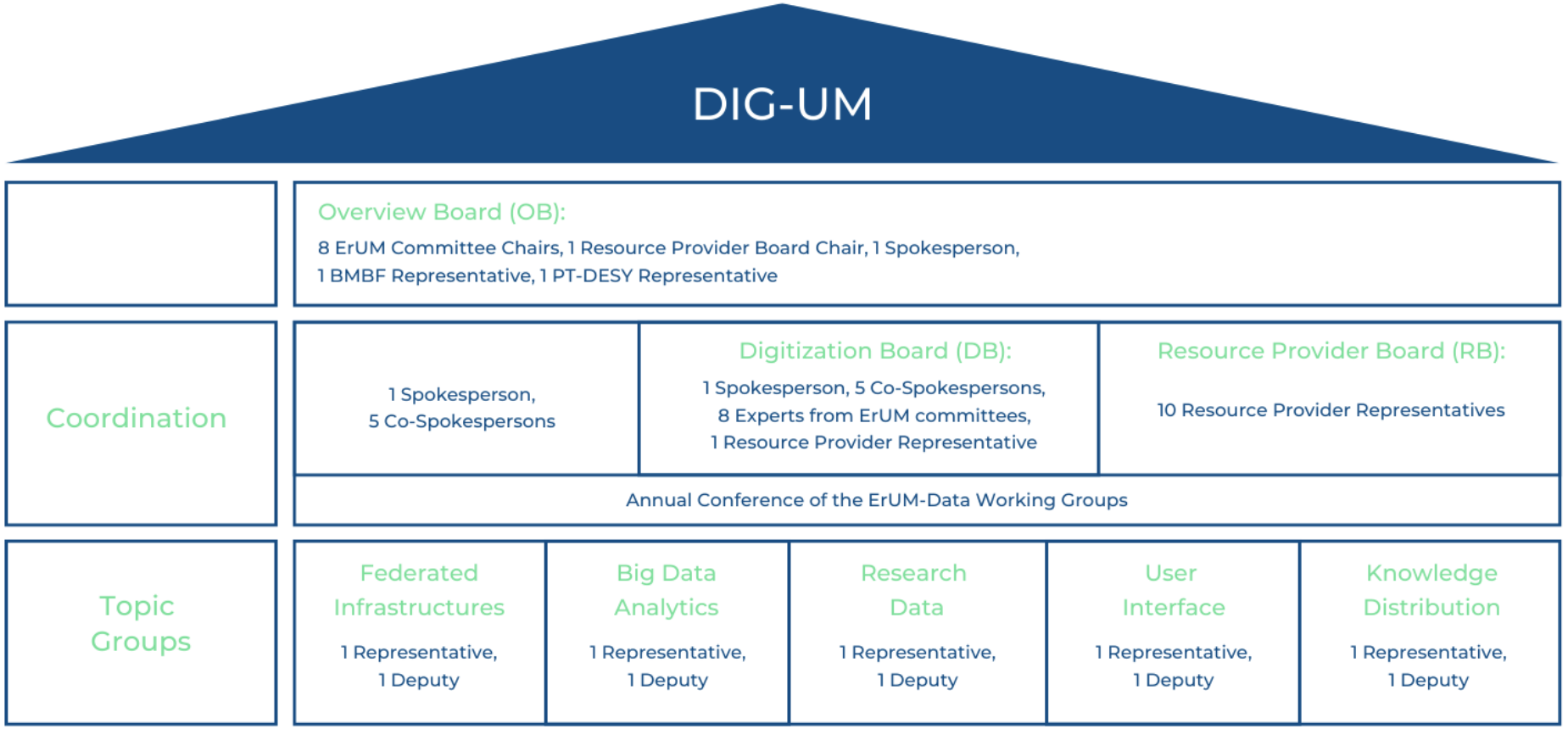
- Themenliste
- Blue-Sky Forschung vs. langfristige Nutzbarmachung von Entwicklungen
- Deutsche Beiträge zu Experimenten mit Potential von experiment-/community übergreifendem Nutzen
- Nachhaltigkeit
- Zusammenarbeit mit anderen Communities und Industrie
- Antragsverfahren:
  - Größe der Verbünde bzw ergänzende Verbünde
  - 1-oder 2-stufig
  - Kategorisierung in Themenbereiche
  - Begutachtung
- Hardware Funding

Input bis 7. Dez. 2023 an KET Computing und Software Panel bzw DIG-UM Topic groups

Backup

DIG-UM

DIG-UM = Digital Transformation in the Research of Universe and Matter: Self-organization to compile the needs and requirements of the 8 ErUM communities on digitization issues



Federated Infrastructures

Fidium

Task areas

- TA1: Tools for integrating heterogeneous computing resources:
  - COBalD/Tardis, Auditor
- TA2: Data lakes & caches
  - XCache deployment, data management integration
- TA3: Tests and deployment of services in production and analysis environments

Resulting tools and services are basis

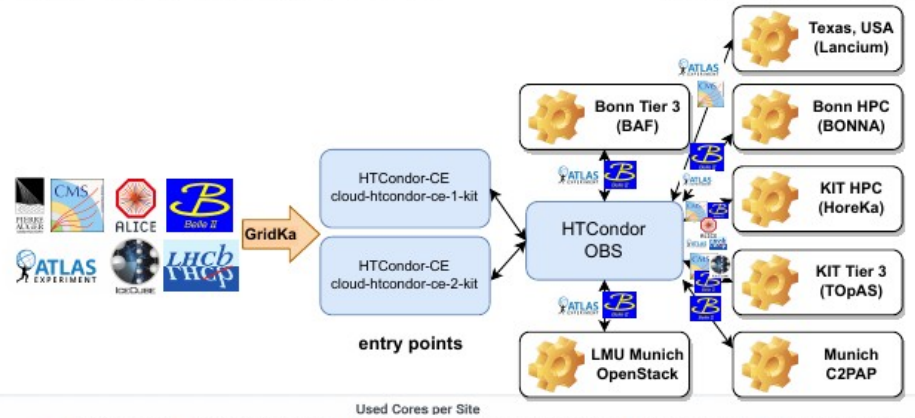
- for ongoing transition from dedicated WLCG Tier-2 centers at universities to NHR centers (Compute) and HGF (Storage)
- Compute4Punch (Compute resources for PUNCH4NFDI) project

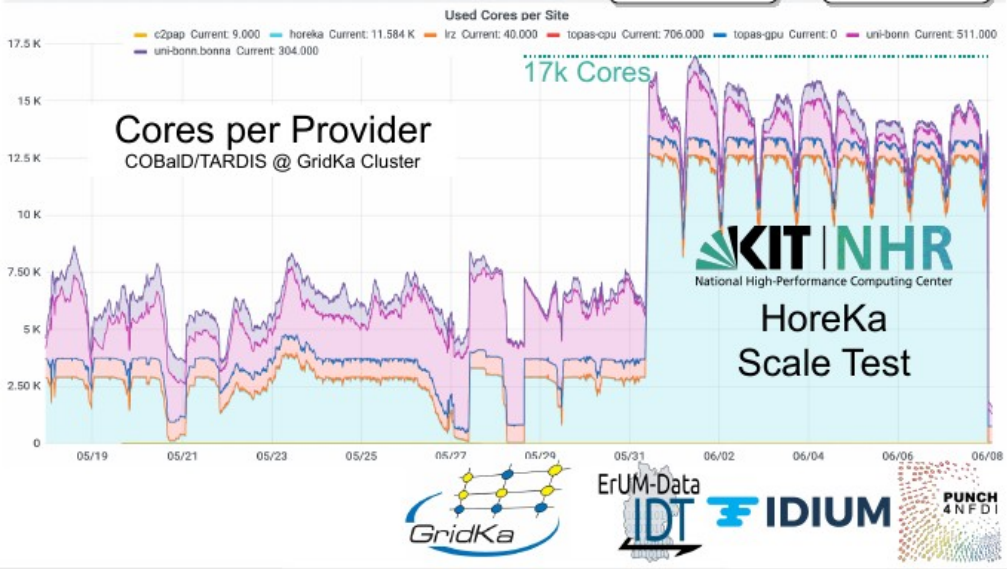
Opportunistic Compute @ FIDIUM in a Nutshell

Karlsruhe Institute of Technology

Simplify provisioning and utilization of third-party compute resources for the various communities:

- Dynamic, transparent and on-demand integration via COBalD/TARDIS (in-house development)
- Provide community-overarching unified entry points to a variety of resources (HPCs, Clouds, …)
- Demonstrated production scale operation during scale test together with HoreKa (KIT HPC cluster)
- Production deployment across HEP institutes & HPC resources coordinated by KIT/GridKa
- Central building block of the Compute4PUNCH infrastructure within PUNCH4NFDI





Fidium - continuation

- Tools & services developed in Fidium require
  - Long-term commitment and support
- NHR sites to be used for ATLAS & CMS – transition in progress
  - Potential to serve as prototype for other HEP projects and ErUM communities
- Extend functionality to keep up with developments and further requirements
  - GPU resources
  - Integration into parallel analysis workflows
  - Adjust demand to availability of renewable energy
    - E.g. include dedicated farms exclusively power by wind turbines

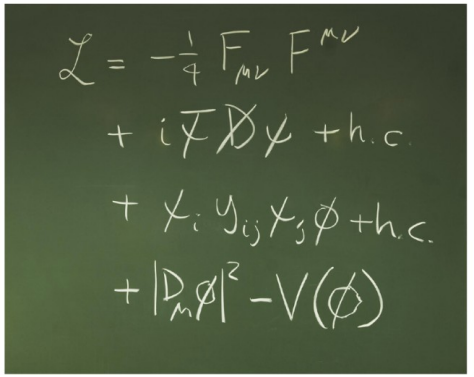
Federated storage – data lakes and caches

- Federated storage infrastructures
  - KIT and Desy-HH as ‘data-lake hubs’ for ATLAS, CMS, LHCb, Belle II
  - In combination with caching services at NHR sites and Tier-3s
  - Basic caching services tested and deployed in Fidium on small scale
  - Further activities:
    - deploy on larger scale
    - integrate into WLCG data management and workflow systems
- Similar services at GSI for Alice and Fair (KHuK)
- Desy-ZN similar role for KAT ?

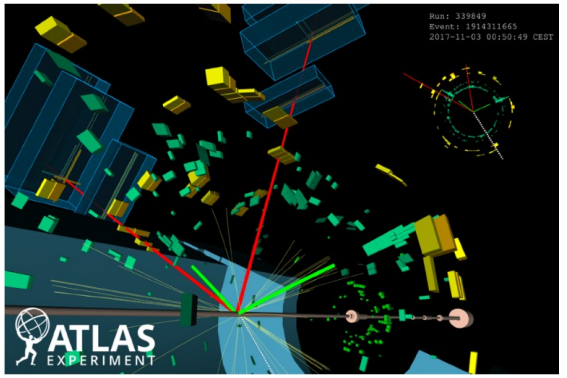
Software and Algorithms

KISS

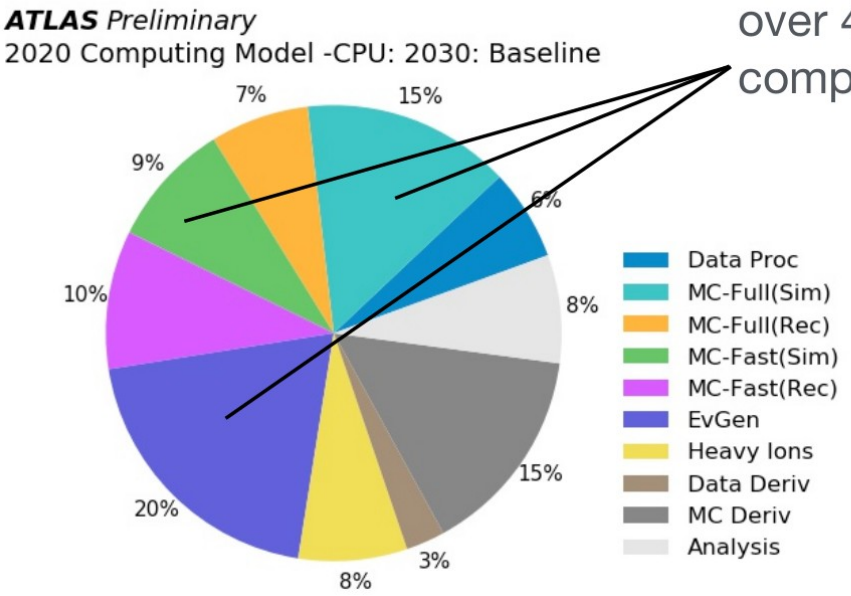
- **K**ünstliche **I**ntelligenz zur **s**chnellen **S**imulation von wissenschaftlichen Daten



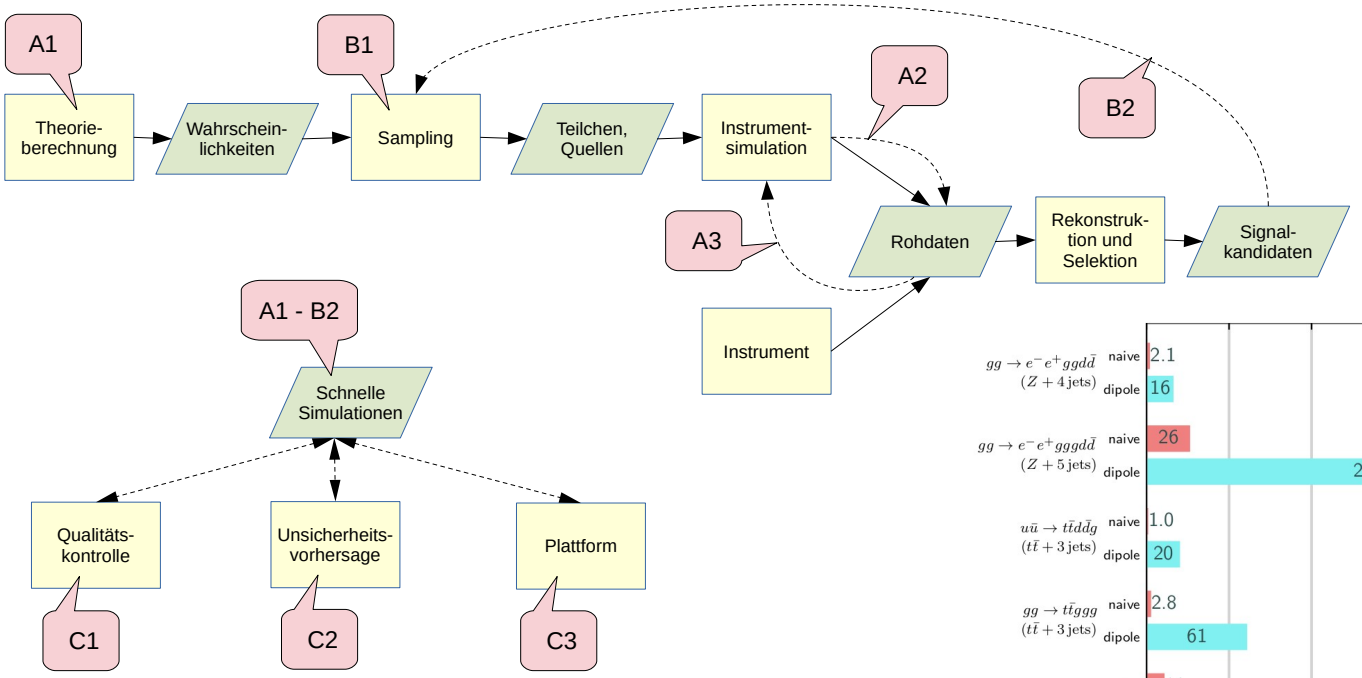
Complex chain of simulations

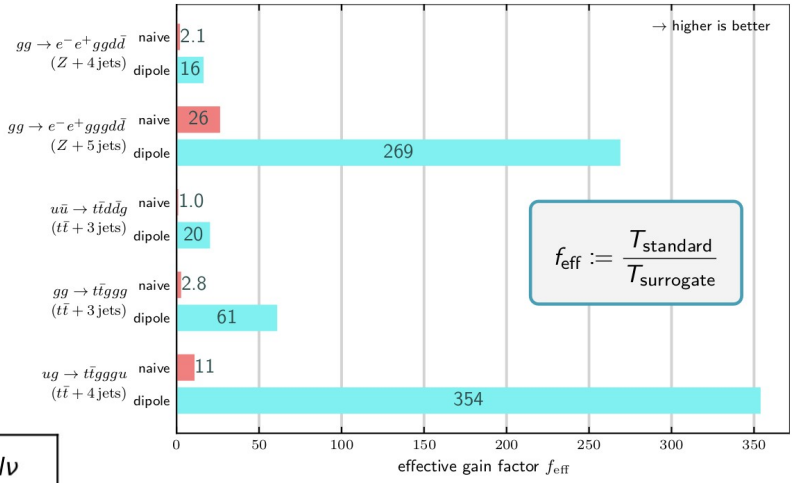


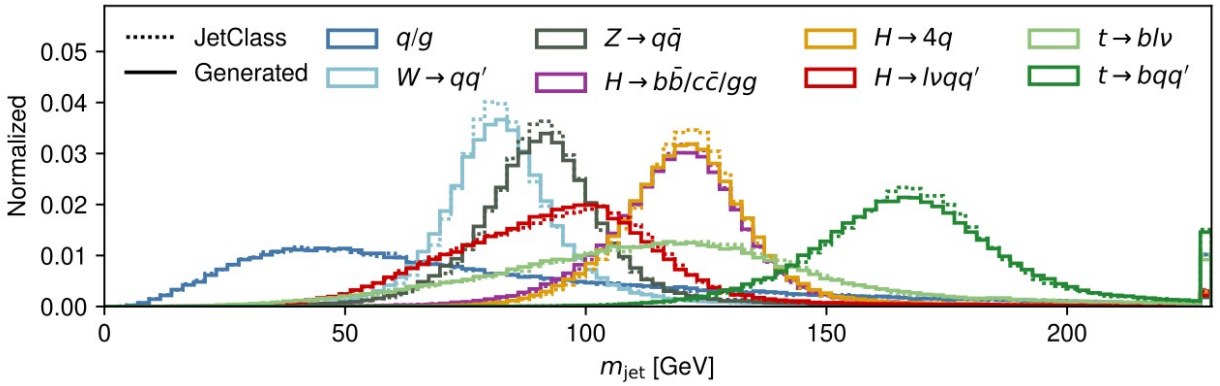
Simulation and Generation steps over 40% of ATLAS compute effort..

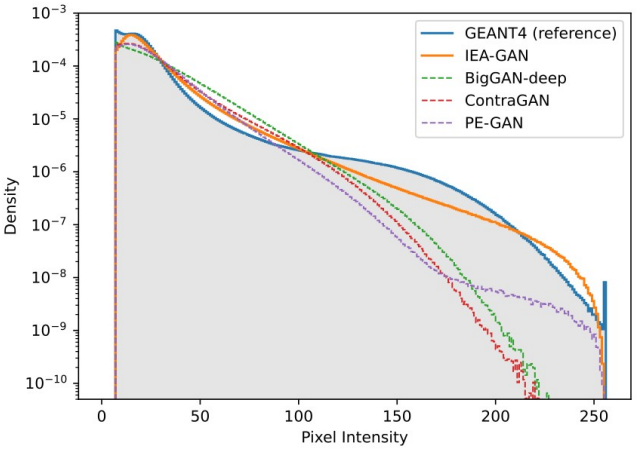


KISS


A1
Theorie-berechnung
Wahrschein-lichkeiten
B1
Sampling
Teilchen, Quellen
Instrument-simulation
A2
B2
A3
Rohdaten
Rekonstruk-tion und Selektion
Signal-kandidaten
Instrument
A1 - B2
Schnelle Simulationen
Qualitäts-kontrolle
Unsicherheits-vorhersage
Plattform
C1
C2
C3


→ higher is better
naive
dipole
2.1
16
26
269
1.0
20
2.8
61
11
354
$f_{\text{eff}} := \frac{T_{\text{standard}}}{T_{\text{surrogate}}}$
effective gain factor f_{eff}

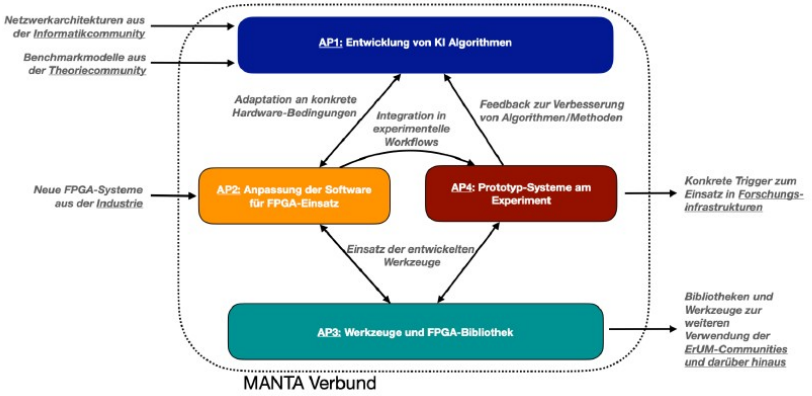

JetClass
Generated
q/g
$W \to qq'$
$Z \to q\bar{q}$
$H \to b\bar{b}/c\bar{c}/gg$
$H \to 4q$
$H \to l\nu qq'$
$t \to bl\nu$
$t \to bqq'$
Normalized
m_{jet} [GeV]

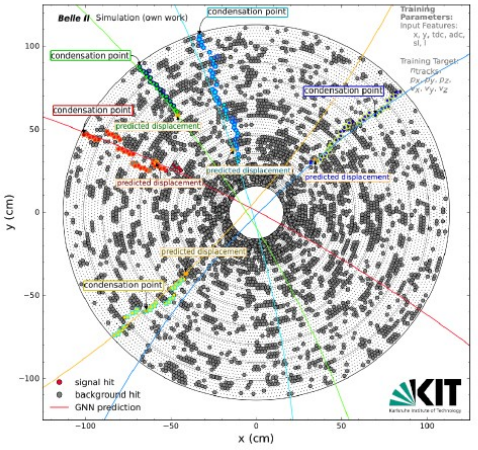

GEANT4 (reference)
IEA-GAN
BigGAN-deep
ContraGAN
PE-GAN
Density
Pixel Intensity

Real Time Algorithms

MANTA **MA**schinelles Lernen und **N**euronale Netze für Echtzeit-**T**riggersysteme mit FPG**A**s an Großgeräten der Teilchenphysik

- Real-time data processing is crucial for experiments like ATLAS, CMS, and Belle II, using FPGAs for trigger decisions with latency of <3µs
- FPGAs can now handle complex algorithms, including neural networks, for real-time decision-making in particle physics.
- MANTA aimed to develop and optimize FPGA-based ML methods for triggers, involving algorithm development, system configuration, tool creation, firmware modules, and prototype testing.
- Collaboration between experts in microelectronics, computer engineering, and particle physics is essential to efficiently implement ML algorithms on FPGAs and address common challenges.
- Next generation trigger boards with Xilinx VERSAL?





Example R&D: **GNN tracking for Belle II** with very low fake rates for displaced and low momentum tracks in high occupancy.

Referenzen

- BMBF Aktionsplan ErUM Data
- ErUM-Data: https://erumdatahub.de/
- DIG-UM: https://erumdatahub.de/en/dig-um/
- FIDIUM: https://fidium.erumdatahub.de/
- KISS: https://kiss.pages.desy.de/website
- PUNCH4NFDI: https://www.punch4nfdi.de/
- dCache: https://www.dcache.org/
- FAIR data principles: https://en.wikipedia.org/wiki/FAIR_data
- KET-computing-panel