HELMHOLTZ AI | ARTIFICIAL INTELLIGENCE COOPERATION UNIT

Helmholtz AI

Systematic Aware Training Meeting

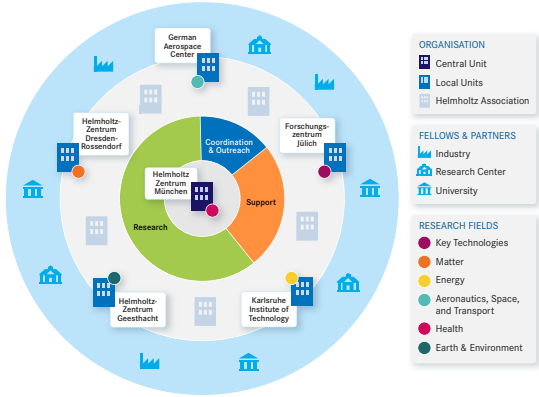
Markus Götz

Karlsruhe Institute of Technology / 2022-09-16

Helmholtz AI

Helmholtz AI
Concept

- **Helmholtz incubator** (INF) platform
- Launched **mid 2019**
- **12M € per year** (overall)
- **One central unit (30 FTEs)**
- **Five local units**
  - AI YIG (**3 FTEs**)
  - Consultant group (**5 FTEs**)

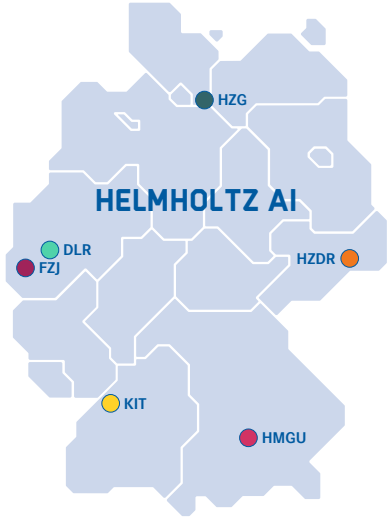


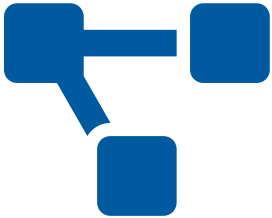
Helmholtz AI
Goals

1. **Interdisciplinary** platform for innovative **research** in **AI**

2. Compiles, develops and fosters **applied AI** methods nationwide across all **Helmholtz centers**

3. Aims to reach **international leadership** in **applied AI**





Projects

Vouchers

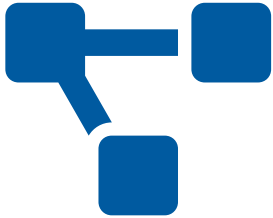
Helmholtz AI
Projects

Research on novel AI methods and applications

- **High risk, high gain AI research**
- At least **two Helmholtz centers**, external partners possible

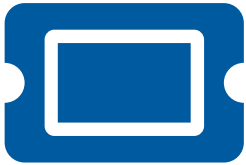
- Duration: **1-3 years** (usually: 2)
- Bi-annual, 50:50 matched funding
  - Up to 200.000 € from the INF
  - Same amount in own contribution

- Slack: helmholtzaicommunity.slack.com

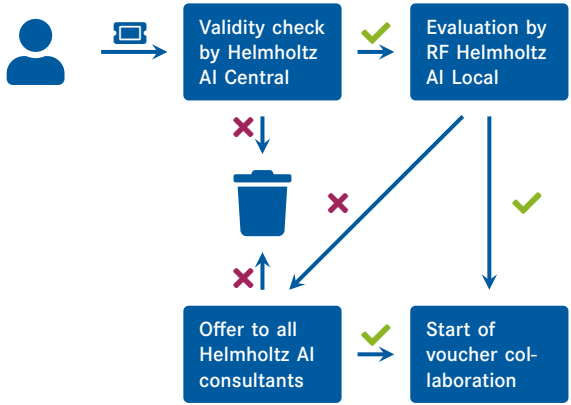


Support for Applied AI Research

- **Collaborative work** between **applied researchers** and **consultants** group
  - Method consulting
  - Implementation of AI pipelines
  - Joint publications
  - ...
- Duration: **2–26 weeks**, repeatable
- Free-of-charge for Helmholtz members
- Low-cost funding for travel, conferences, ...



- **Centralized web-based system**
  - **Log-in** via **Helmholtz** center **e-mail** address
  - **Fill out form** with voucher title, duration, abstract, ...
- Voucher system
- Formal **assignment process**



HAICORE

HAICORE
Concept

- **Compute resources** for Helmholtz AI
- **Free of charge for Helmholtz**

- Register here
- Technical details
  - **Jupyter** Notebook (browser-computing)
  - **GPU**-accelerated **HPC** systems

- Two installation sites
  - **FZJ: JUWELS** booster
  - **KIT: HoreKa** system
  - Each 72× A100-40GB GPUs, total 144

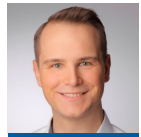
Local Unit Energy@KIT

Helmholtz AI Local Unit Energy@KIT

The Teams

YIG AI in Energy

Benjamin Schäfer



Oliver Neumann

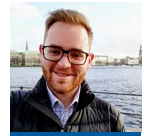
Benedikt Heidrich

AI Consultants

Markus Götz

Marie Weiel

James Kahn



Daniel Coquelin

Katharina Flügel

Helmholtz AI Consultants

Team Profile

- Typical **application domains**
  - **Renewable** energy
  - Future **energy systems** and smart grids
  - **Remote sensing** in UAV imaging
- Areas of expertise
  - Computer **vision**
  - **Time series** analysis
  - Graph processing
  - Massively **parallel** AI
- Hosting organization for **HAICORE@KIT**
- Visit us virtually:
  https://github.com/Helmholtz-AI-Energy/

Solar cell test park KIT Campus North

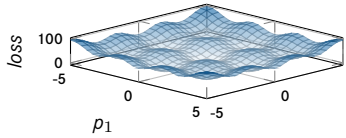
HoreKa supercomputer with HAICORE@KIT partition

Helmholtz AI Consultants

Example Vouchers

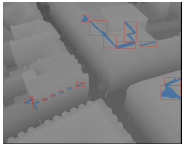
Mini Grid Operations

Propulate – Massively Parallel Genetic Optimization



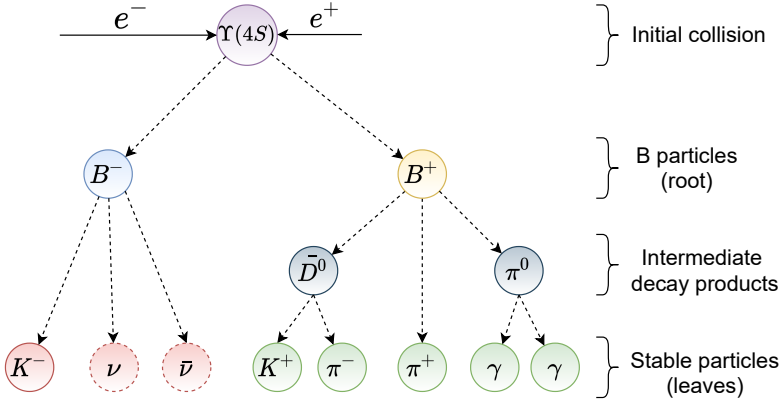
HyDe – Hyperspectral Image Denoising Toolbox

Thermal Bridge Detection



Voucher: BaumBauen

Clean Detection Environment at Belle II



Goal: identify structure of decay process up to *B* particles

Voucher: BaumBauen

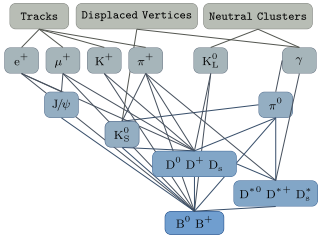
The Belle II Full Event Interpretation (FEI)

Exclusive Tagging Algorithm

- $\mathcal{O}(10.000)$ explicit decay chains
- Hierarchical approach with six distinct stages
- Multivariate classification (BDTs)

Efficiency: $\frac{\textbf{correctly reconstructed B decays}}{\text{all B decays}}$

Efficiency	$B^{\pm}$ (%)	B^{0} (%)
Hadronic	0.76	0.46
Semileptonic	1.80	2.04



Limitations

- Hard coded decay channels **restrict branching fraction** to $\sim 15\%$
- Hierarchical structure leads to **error propagation**

The Full Event Interpretation – An exclusive tagging algorithm for the Belle II experiment, Keck et al. (2018), arxiv:1807.08680

Voucher: BaumBauen

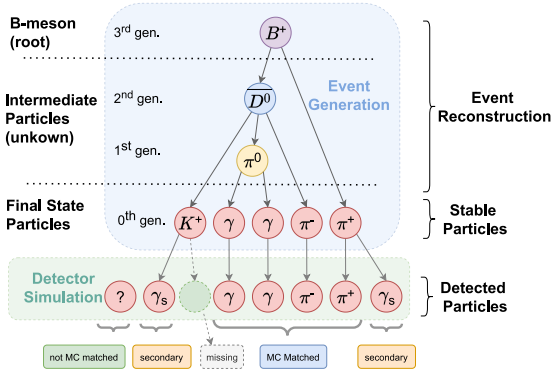
Replacing the FEI

Have: Final state particles (FSPs)

Want: Entire decay structure

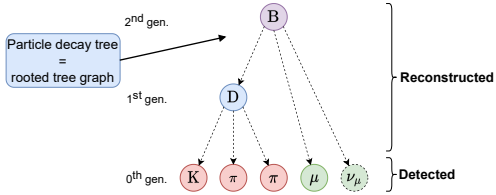
Challenges:
- Variable #FSPs
- Unknown #generations
- Unknown #ancestors
- Undetected FSPs
- Missing ground truth

Solution: Encode tree as FSP relations



Voucher: BaumBauen

Graph-based Full Event Interpretation (graFEI)



Voucher: BaumBauen

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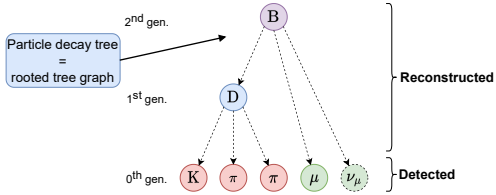

Adjacency Matrix

	B	D	K	π	π	μ
B	0	1	0	0	0	1
D	1	0	1	1	1	0
K	0	1	0	0	0	0
π	0	1	0	0	0	0
π	0	1	0	0	0	0
μ	1	0	0	0	0	0

Voucher: BaumBauen

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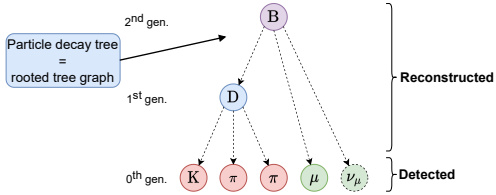

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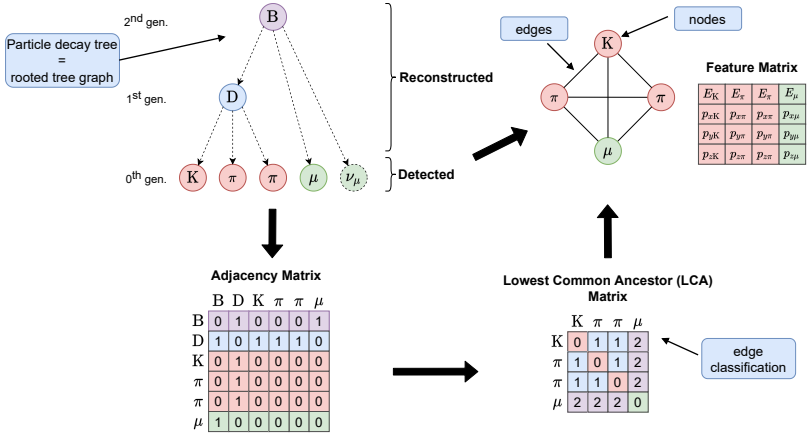
π	0	1	0	0	0	0
μ	1	0	0	0	0	0

Lowest Common Ancestor (LCA) Matrix

	K	π	π	μ
K	0	1	1	2
π	1	0	1	2
π	1	1	0	2
μ	2	2	2	0

Voucher: BaumBauen

Graph-based Full Event Interpretation (graFEI)



Voucher: BaumBauen

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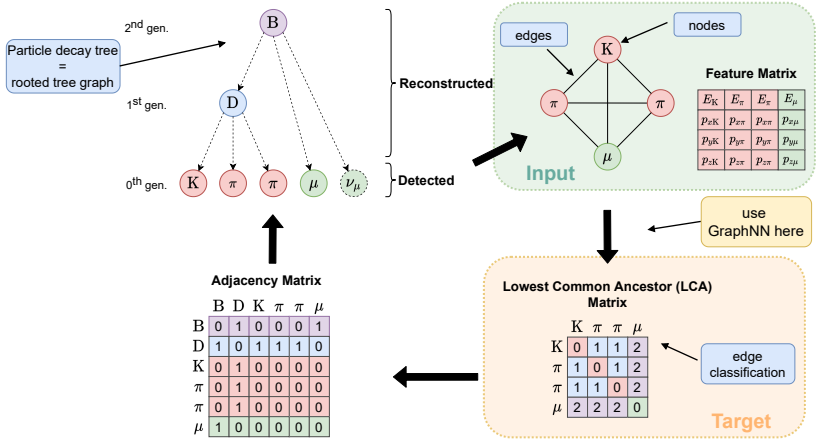
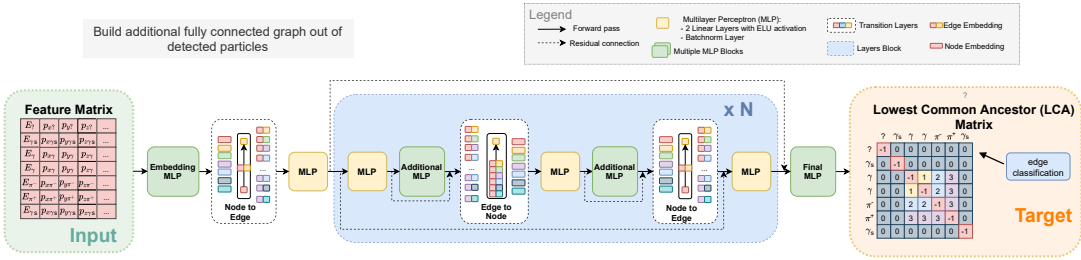


Voucher: BaumBauen

Model: Neural Relational Inference Encoder



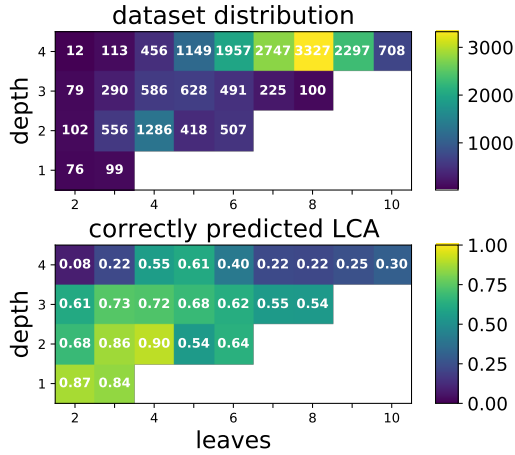
- **Iterative** node $v \leftrightarrow$ edge e **update** and hierarchical agglomeration
- Implementation in `PyTorch` and `Optuna`
- Experiments using the NVidia A100s in HAICORE

Neural Relation Inference or Interacting Systems, Kipf et al. (2018), arXiv:1802.04687v2

Voucher: BaumBauen

Mixed Belle II dataset

- Belle II Monte Carlo simulations
  - Six decay channels
  - Considered missing particles
- Correctly predicted LCAs
  - NRI: 43.2%
  - Transformer: 31.8%
- High accuracy (correctly predicted LCA entries) of 85.6% for NRI



James Kahn et al 2022 Mach. Learn.: Sci. Technol. 3 035012, doi: 10.1088/2632-2153/ac8de0