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TA3 Deliverables

Total requests/contributions

Institution	Request	Contribution
TU Dortmund	0.5	0.25
LMU	2.5	1.25
TU Munich	0.5	0.25
HZDR	0.5	1.5
Bielefeld	1.0	0.5
Regensburg	1.0	0.5
Jülich	2.25	1.0
Mainz	0.5	0.5
Uni Hamburg	2.0	1.75
MPIK Heidelberg	0.5	0.5
Total	11.25	7.75

WP1: Statistical Methods

1. Extending the BAT.jl project to large data sets, highly parallel computing and applications in HEP, astro and cosmology
 - a. Extending to large data sets including a particle-physics example (TU Dortmund: 0.50 FTE/y + 0.25 FTE/y matching)

- b. Development of MCMC techniques (parallelization, hierarchical models, discrete parameters, ... -> BAT.jl) (TU Munich / ODSL: 0.5 FTE, matching 0.25)
2. Statistical methods for astro/cosmology analyses, including, e.g., cross-correlation analyses, power spectrum analyses, MCMC samplers, python tools, cosmo toolkits-- capturing and integrating initially and extending over time, methods for combination of different datasets may benefit from particular statistical methods that account for covariances (LMU Munich: 0.5 FTE/y + 0.25 FTE/yr matching, MPIK Heidelberg: 0.25 FTE/yr + 0.25FTE/yr matching)

⇒ ?? Development of further statistical methods (GU Frankfurt)

Connected use cases:

Primary:

5.1.2 HEP/HuK: Fit of peak in very large data set

7.2 Global analysis across our consortium

In general use cases within 5 will all draw upon these methods

Secondary:

5.5.12 Clustering measurements for astrophysics and cosmology

5.5.13 Line Identification in ALMA data

Institution	Request	Contribution
TU Dortmund	0.5	0.25
LMU	0.5	0.25
TU Munich	0.5	0.25
MPIK Heidelberg	0.25	0.25

WP2: Numerical Methods and Simulations

1. Software development and support for lattice QCD data analysis on multi-GPU systems, heterogeneous compute clusters and upcoming processor generations (Bielefeld, Jülich, Regensburg)
2. Optimisation of simulation and data analysis algorithms for lattice QCD, Astrophysics and Plasma-Simulations. The focus shall be data-/compute-heavy algorithms and on algorithmic/technical aspects of scientific reproducibility (resiliency, uncertainties). (Bielefeld, HZDR: 0.5 FTE matching, Jülich, Regensburg, LRZ, Uni Hamburg 1.0 matching)

Request 1&2: Bielefeld 0.5FTE, Jülich 1.5FTE, Regensburg 1.0FTE

Comparison simulation and observation/measurement (GU Frankfurt and others)

Institution	Request	Contribution
Bielefeld	0.5	0.25
Regensburg	1.0	0.5
Jülich	1.5	0.5
HZDR	0	0.5
Uni Hamburg	0.5	1.0

WP3: Machine Learning Methods

1. Methods for automated machine learning (automated model selection and hyperparameter optimisation) and transfer learning on scientific datasets (UHH, GU Frankfurt, Uni Mainz AG Schott, Uni Siegen - participant)
2. ML on very large datasets / exascale platform (UHH, Jülich 1.0 FTE)
3. ML for image & event reconstruction (TU Munich / ODSL: 0.5 FTE requested, matching 0.25,
4. Surrogate modeling of large-scale simulations (HZDR: 0.25 FTE matching)

Institution	Request	Contribution
TU Munich	-	-
Jülich	0.5	0.25
Uni. Mainz	0.5	0.5 (Brickwedde - Landesstelle)
Uni Hamburg	1.5	0.75

WP4: Methods for Analyses Across Datasets

1. Framework for conversion of data for combined analyses on heterogeneous systems
Interfaces to optimised libraries for analysis software, workflows, and for conversion tools in Lattice QCD, Astrophysics, Plasma Physics; Provision of platform-portable libraries for single source CPU/GPU/FPGA development
(Bielefeld 0.5 FTE, HZDR: 0.5 FTE requested, 0.5 FTE matching, Jülich 0.25 FTE, LRZ)
2. Tools for low level (e.g. pixel/raw data with high volume) analyses across different datasets that will work efficiently in the limit of massive datasets. Tools to define code-to-data workflows that can be tested on small scale and then executed on distributed datasets in a heterogeneous computing environment (LMU, 1.5 FTE/yr + 0.75 FT/yr matching), provision of platform independent libraries for implementing these low level tools (HZDR: 0.25 matching)
3. Standard interface for the publication of likelihoods, including a catalog for the definition of common (nuisance) parameters (LMU, 0.5 FTE, MPIK 0.25 FTE)

Institution	Request	Contribution
LMU	2.0	1.00
Bielefeld	0.5	0.25
Jülich	0.25	
HZDR	0.5	0.75
MPIK Heidelberg	0.25	0.25

WP5*: Software Packaging and Distribution (together with TA6)?

- Software management (packaging, quality management, testing) tools for improving reproducibility of simulations and data analysis workflows (Astrophysics, LQCD) (LRZ - who likes to collaborate - we are “just” participant? - Bielefeld, Regensburg, Jülich? Interest also in GU Frankfurt)
- Provision of multi-platform CI/CD-Platform (NVIDIA GPUs, AMD GPUs, Intel CPUs, AMD CPUs, XILINX FPGAs, Windows/Linux, various compilers) (HZDR. 0.25 FTE matching)

Institution	Request	Contribution
HZDR	-	0.25

Deliver	Description	Institute	Request	Contribution
WP3.1.1	Bayesian Toolkit	TU Dortmund, TU München	0.5 + 0.5	0.25 + 0.25
WP3.1.2	Astro/APP tools	LMU-M, MPIK Heidelberg	0.5 + 0.25	0.25 + 0.25
WP3.2.1	Analysis tool for heterogeneous compute systems	Bielefeld, Jülich, Regensburg	0.25 + 0.5 + 1.0	0.25 + 0.5 + 0.25
WP3.2.2	Optimization of sim for HEP, HUK, Lattice QCD, Astro, Plasma	Bielefeld, Jülich, Regensburg, HZDR, LRZ, Hamburg	0.25 + 1.0 + 0.0 + 0.0 + 0.0 + 0.5	0.0 + 0.0 + 0.25 + 0.5 + ? + 1.0
WP3.3.1	Automated ML	Hamburg, Mainz	1.0 + 0.5?	
WP3.3.2	ML on Exascale datasets	Hamburg, Jülich	0.5 + 0.5	
WP3.4.1	Data conversion tools	Bielefeld, HZDR, Jülich, LRZ	0.5+0.5+0.25+0	0.25+0.5+0.0+?
WP3.4.2	Tools for creation of joint analysis workflows	LMU-M, LMU-K, HZDR	1.0+0.5+0.0	0.5+0.25+0.25
WP3.4.3	Standard interface for publication of likelihoods	LMU-K, MPIK Heidelberg	0.5+0.25	0.25+0.25