# The Helmholtz Analytics Toolkit (Heat)
## and its role in the landscape of massively-parallel scientific Python

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# What is Heat and what can I do with it?

# The Helmholtz Analytics Toolkit

- Free and open-source (MIT) Python library for **memory-distributed high-performance data analysis and machine learning** on CPU/GPU-clusters
- allows **scientists and engineers without an extensive background in HPC** to tackle data-intensive problems that go beyond the capabilities of a workstation
- Developed since 2018 at

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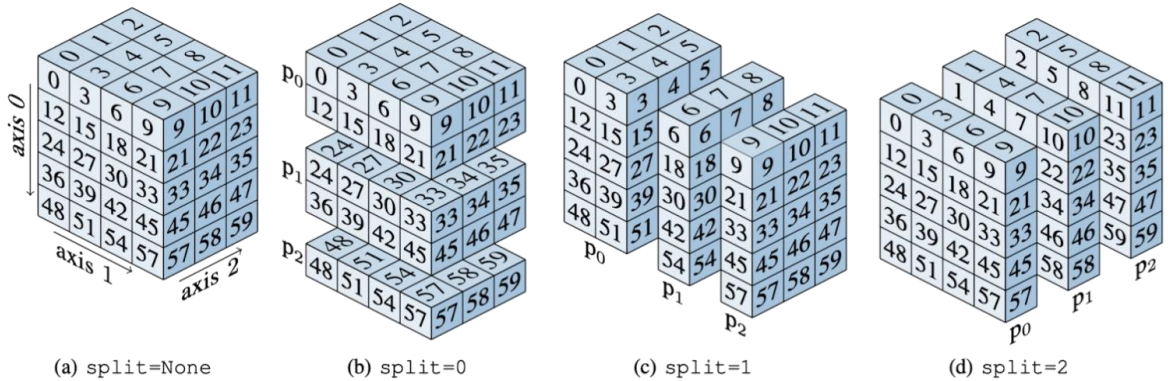
+ external *open-source contributors* on github (e.g. GSoC 2022) + *student workers*

# How it works…

**Vendor-independent GPU-support**
(Nvidia + AMD) inherited from PyTorch!

- **distributed N-dimensional array** („**`DNDarray`**“) as basic data type




(a) split=None (b) split=0 (c) split=1 (d) split=2

  - composed of „local“ **`torch`**-Tensors on each MPI-process
  - „MPI-glue” using **`mpi4py`**
  - **`numpy`**-like API

HEAT
Helmholtz Analytics Toolkit

**Clustering**
**(k-means, Spectral)**

**Deep Learning**
**(DASO, [3])**

**Regression**
**(QR, LASSO)**

**Naive Bayes**

***and more…***

PyTorch

Tensors
Linear Algebra

Automatic
Differentiation

NumPy-like
interface

GPU-support
(vendor-independent)

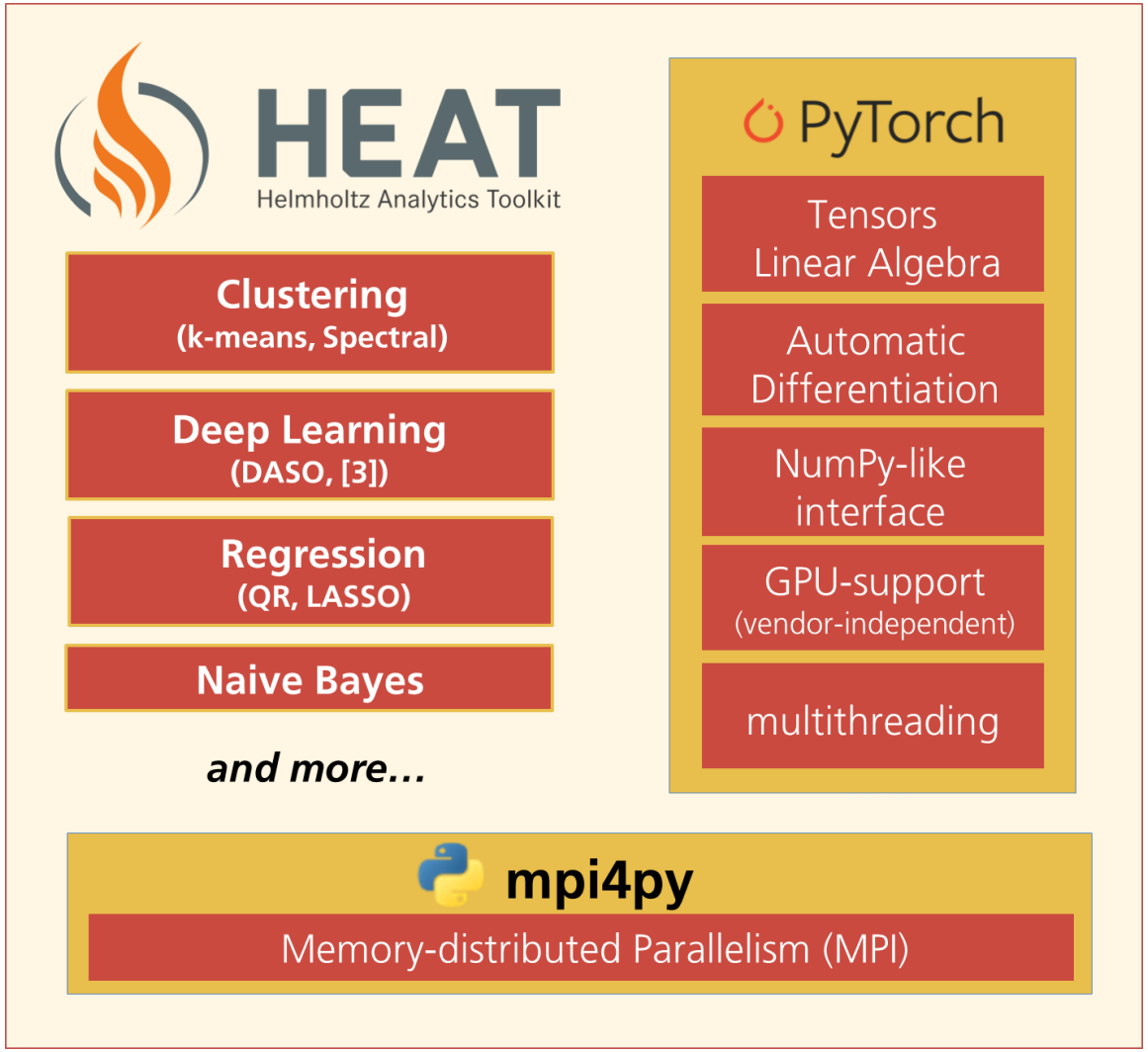
multithreading

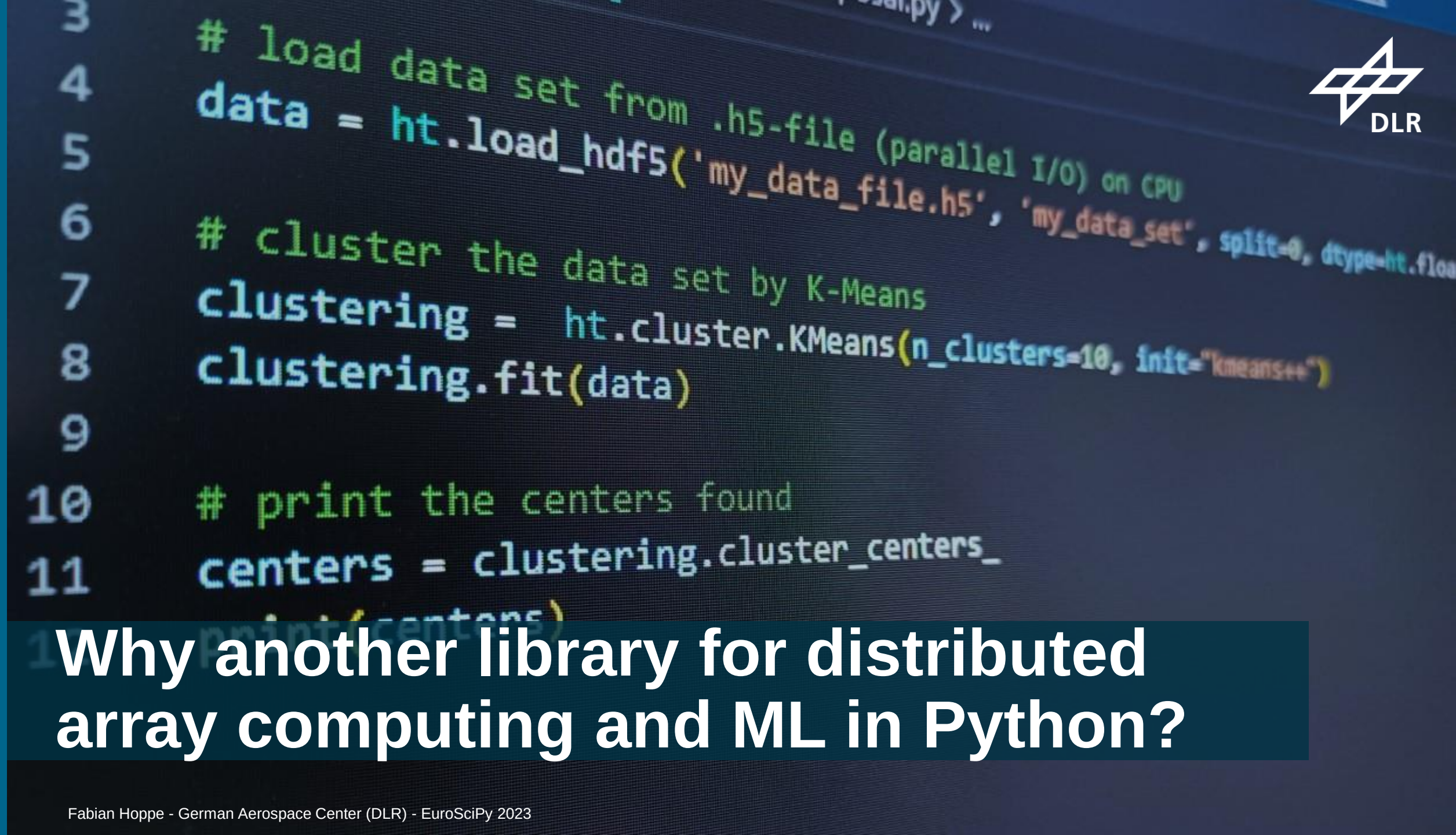
**mpi4py**

Memory-distributed Parallelism (MPI)

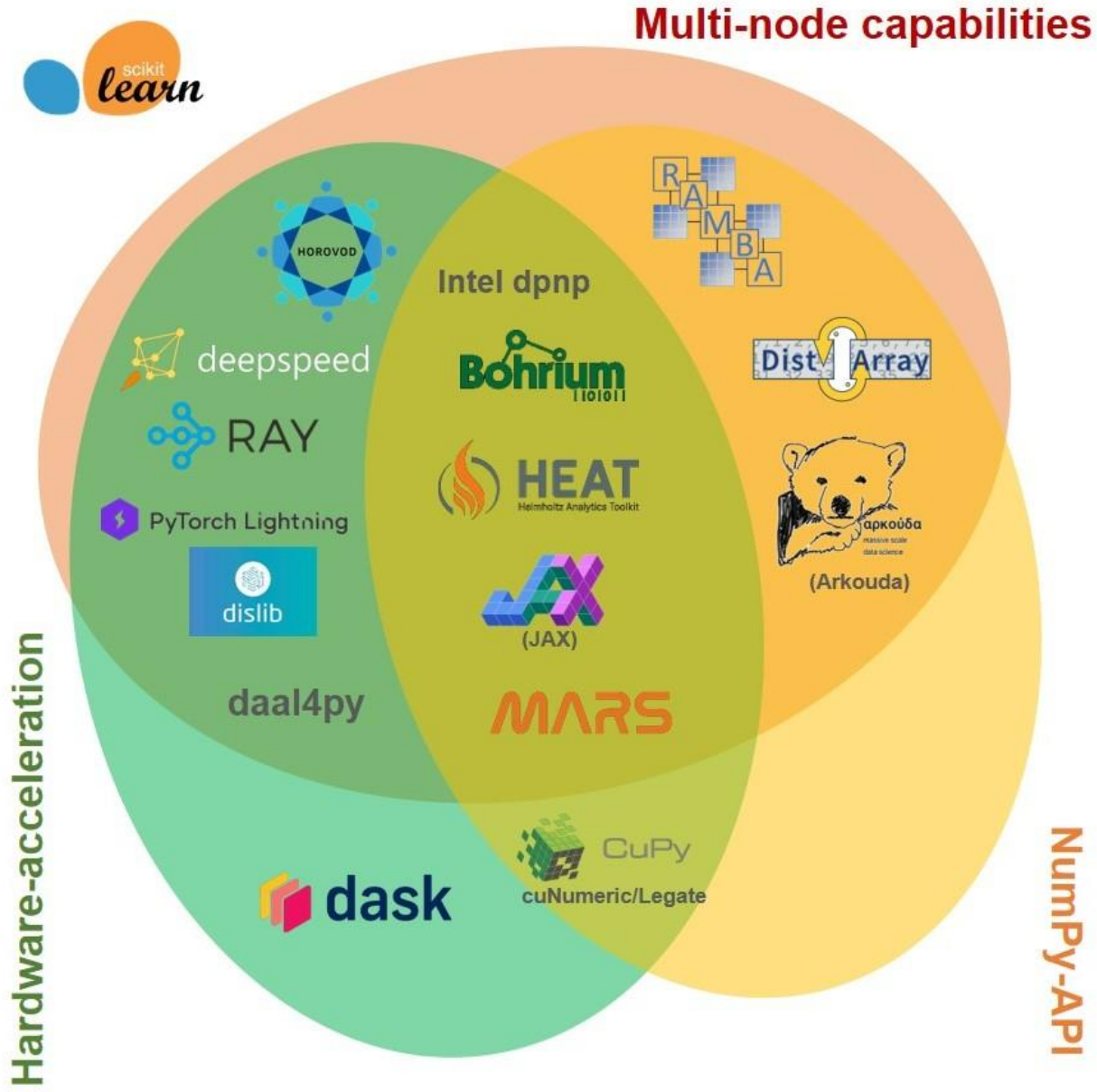
# …and what you can do with it
## (`main`-branch as of August 2023)

- **Parallel I/O** via hdf5, csv, netcdf
- **Array creation and manipulation:** get/set item, concatenate, reshape, zeros, ones, arrays with random entries, math functions…
- basic sparse array class
- **Statistics:** min, max, mean, percentile, variance, …
- **Linear algebra:** transpose, matmul, QR, Lanczos, (approximate) SVD, …
- **Machine learning:** Clustering (k-means, spectral), Regression (LASSO), Naive Bayes, …
- **Data parallel NNs** („DASO“)



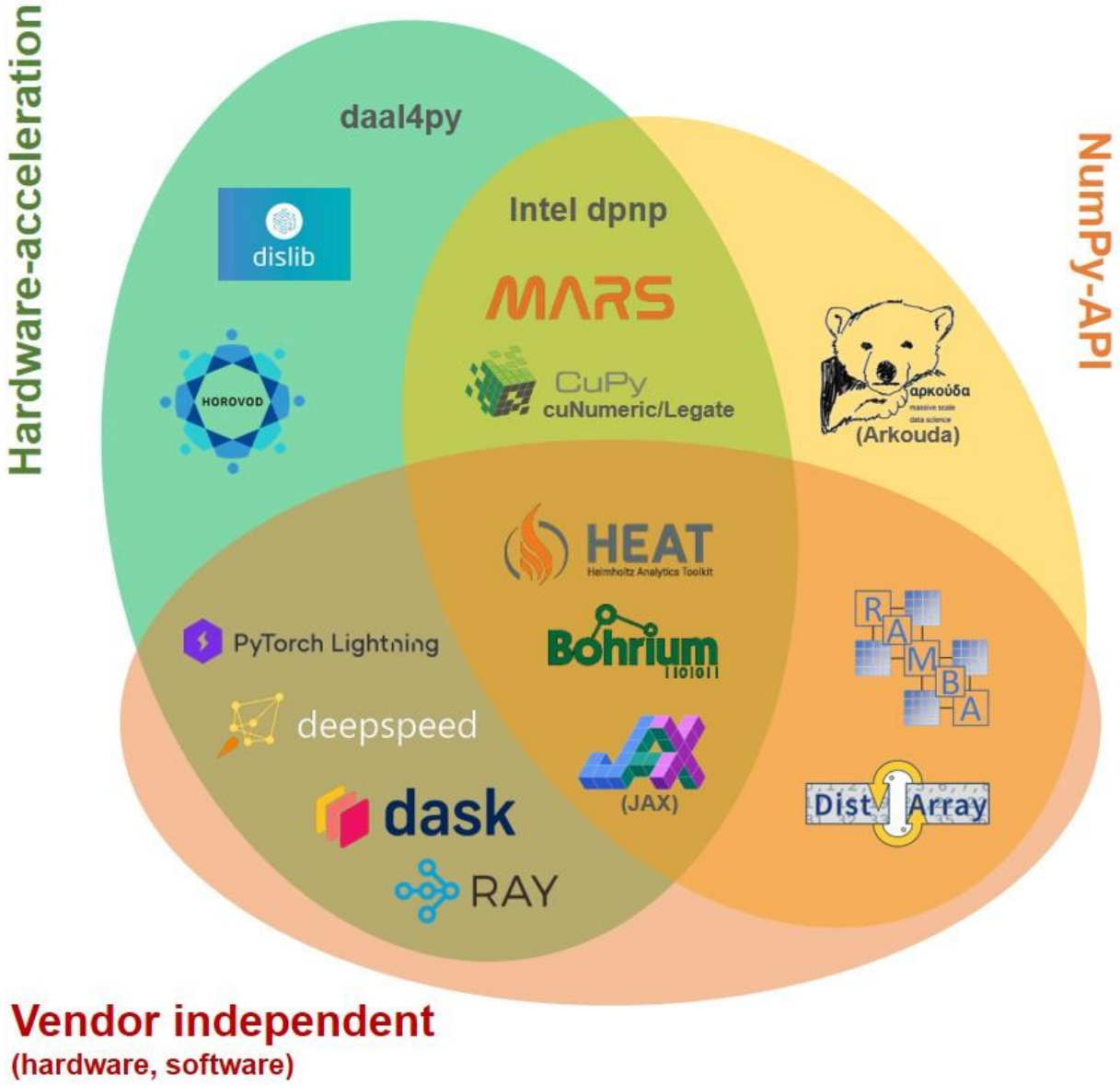



# Why another library for distributed array computing and ML in Python?




Heat…

- …allows for **memory-distributed**, i.e. **multi-node**, parallelism and is not limited to embarrassingly parallel applications
- …supports **hardware acceleration** (GPU)
- …has a **simple NumPy-/scikit-learn-like API** that allows for easy adaption of legacy code

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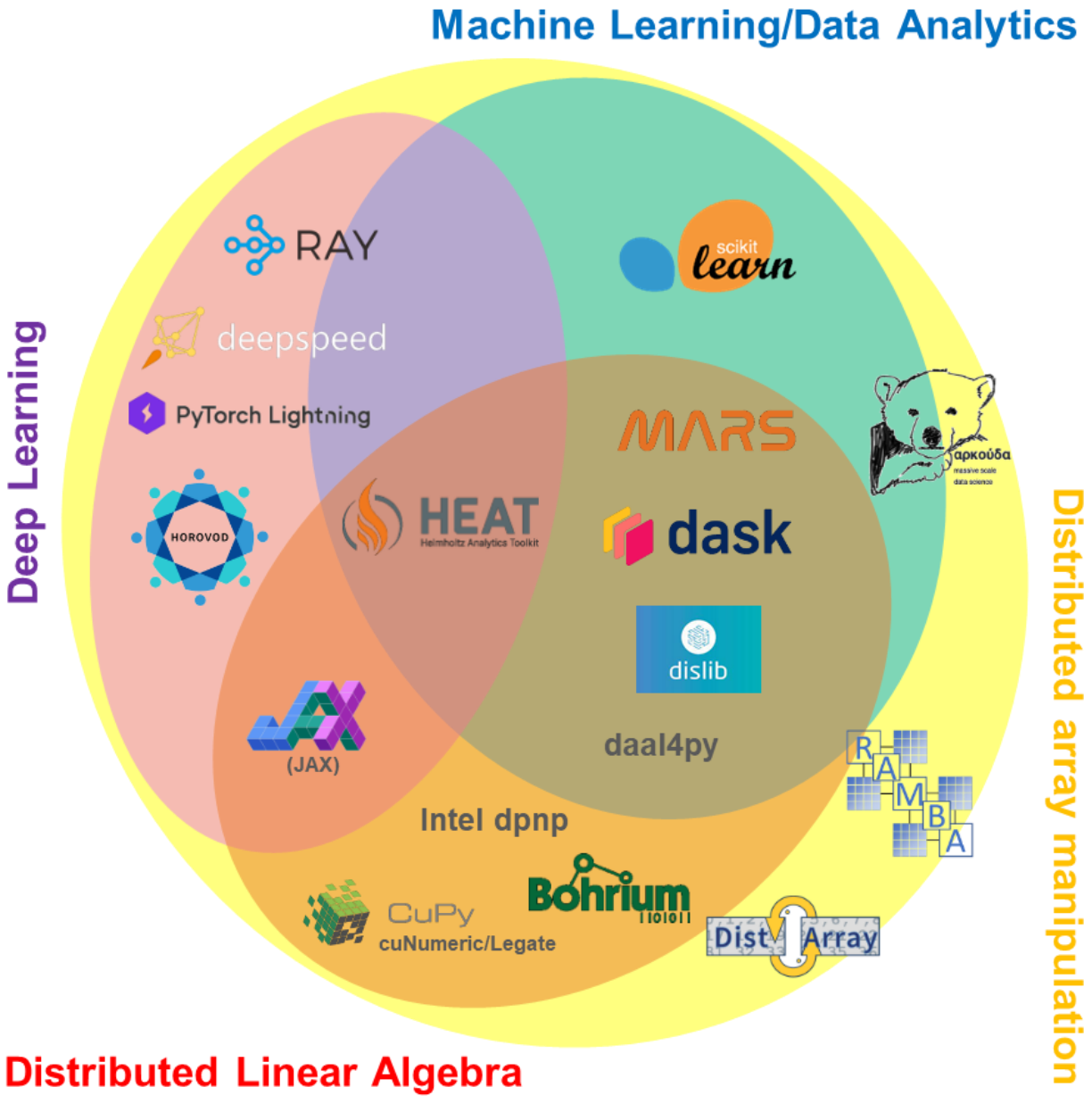
- …is **interoperable** (PyTorch)

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- …is **vendor-/platform-independent**
- …is **interoperable** (PyTorch)
- …is **general-purpose**
- …is developed **by scientists for scientists**.

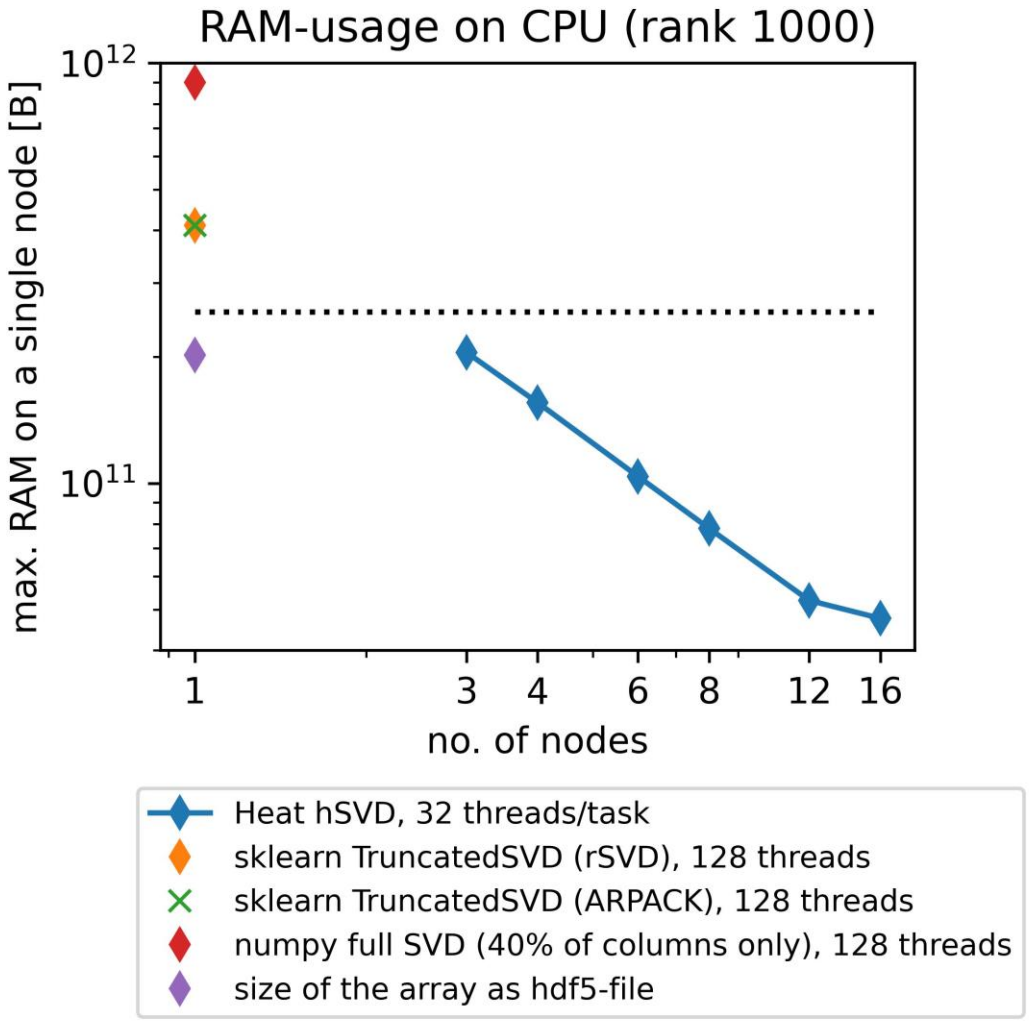

# In a bit more detail…

# Avoid memory becoming a bottleneck
## (a use-case from DLR)

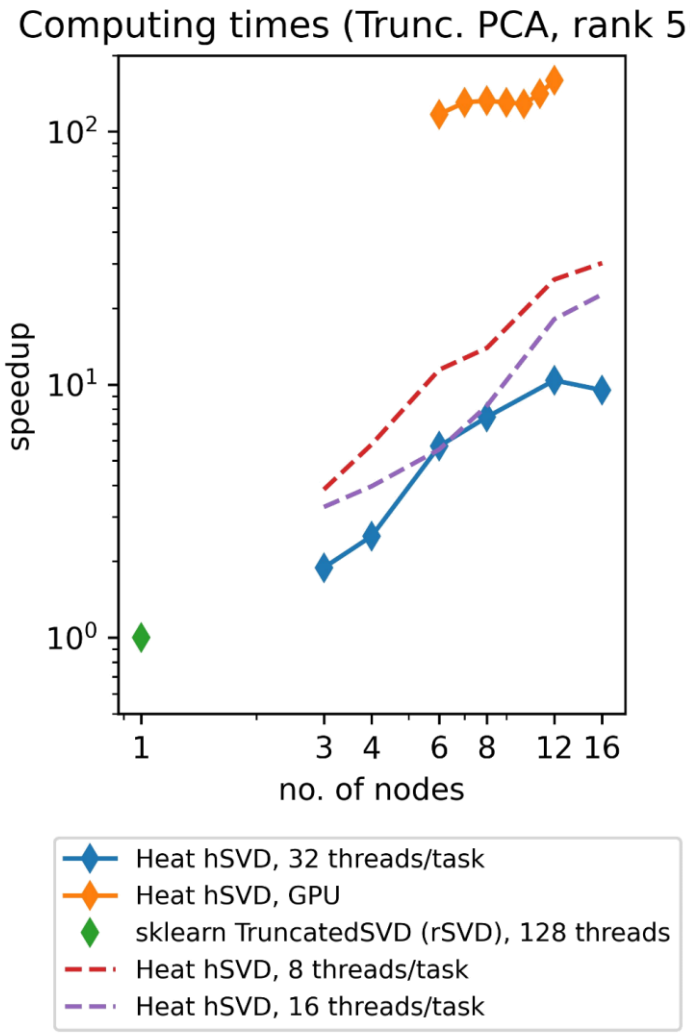
**Use-case:**
**analysis of a data set of 85487 RGB-images with 1024x192 pixels**

- 589824 x 85487 matrix **(~200GB)**
- PCA (here: ***truncated PCA with rank 1000***) and other typical tasks (e.g. clustering, matmul) are not data-parallel
- embarrassingly parallel batch-processing not possible!
- memory becomes a hard limit easily…

Experiments conducted on up to 16 ‚`medium`‘ compute nodes (Heat) and a single ‚`bigmem`‘ node (sklearn, numpy) of DLRs cluster CARO

# Exploit your existing hardware: strong scaling
## (use-case from DLR continued)



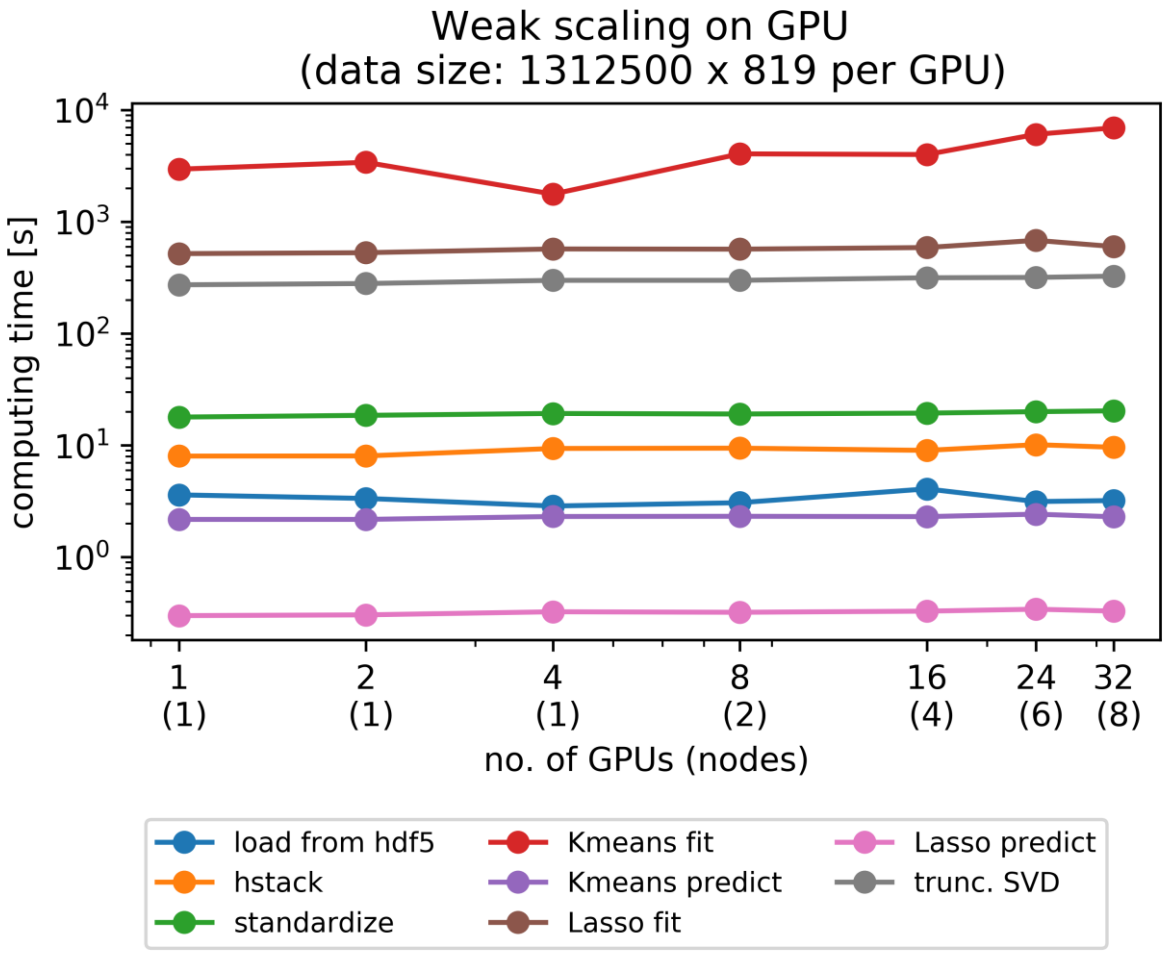

- **CPU:** hybrid parallelism (MPI+OpenMP) may achieve significant speedup compared to single node/single process
- **GPUs:** multi-GPU/multi-node setting is sometimes unavoidable due to memory limitations
- Heat so far runs on:
  - Intel and AMD CPUs
  - Nvidia GPUs
  - AMD GPUs (helmholtz.codebase runners)
  - Apple CPU+GPU (developers notebook, experimental)

Experiments conducted on:

- **sklearn:** one ‚`bigmem`‘ node of CARO
- **Heat CPU:** up to 16 ‚`medium`‘ compute nodes of CARO
- **Heat GPU:** up to 12 nodes (with 4 Nvidia A100 80GB each) of DLRs cluster Terrabyte


terrabyte

# Scale your applications: weak scaling




(Load with split=0, hstack along axis=1, Kmeans with 4 clusters, Lasso with regularization parameter 0.1 and tolerance 0.01, truncated SVD by hSVD with rel. tolerance 0.01)

**Test data set:**

*ATLAS Top Tagging Open Data Set* (42 mio. entries with 819 features each ~ 129GB (“train” part) )

[ATLAS collaboration (2022). ATLAS Top Tagging Open Data Set. CERN Open Data Portal. DOI:10.7483/OPENDATA.ATLAS.FG5F.96GA]

Experiments conducted on up to 8 GPU-nodes of DLRs cluster Terrabyte (with 4 Nvidia A100 80GB each)

# Benefits of the simple API

- Straight-forward **adaptation of legacy NumPy-/scikit-learn-workflows**:

```
import heat as ht


data = ht.load("your_hdf5_data_set.h5",
dataset="name_of_the_data", split=1, device="gpu")
clustering =  ht.cluster.KMeans(n_clusters=10,
init="kmeans++")
clustering.fit(data)
print(clustering.cluster_centers_)
```

- Simple specification of devices (similar to PyTorch) allows to **use GPUs with almost no additional effort**

# Benefits of the simple API

- Except for prescribing a split-direction, **parallelization does not enter your python-script** explicitely
  - no explicit chunking of the data required
  - easy to run on HPC-systems using SLURM:

```
# on GPU
srun --nodes=8 --ntasks-per-node=4 --gres:gpu=4 python
script.py
```

```
# on CPU (incl. multithreading)
srun --nodes=8 --ntasks-per-node=8 --cpus-per-task=20
python script.py
```

# Comparison with Dask (CPU)

## 129GB data set* on 8 CPU-nodes

| | HEAT | DASK |
|---|---|---|
| *load from hdf5* | **3 s** | 3 min |
| *stack data* | 3 s | **18 ms** |
| *standardize data* | **2 s** | 5 min |
| *K-means fit (4 clusters)…* | **40 min** | 12 h |
| *…and predict* | **1 s** | 7 min |
| *PCA (trunc. to rank 100)* | **31 s** | 10 min |
| *randn…* | 9 s | **3 ms** |
| *…and save to hdf5* | **41 s** | **48 s** |
| ***MaxRSS for all this:*** | **14 GB** | 460 GB |

Experiments conducted on up to 8 CPU-nodes of DLRs cluster Terrabyte (with 2 Intel Xeon Platinum 8380 40C 270W 2.3GHz each)

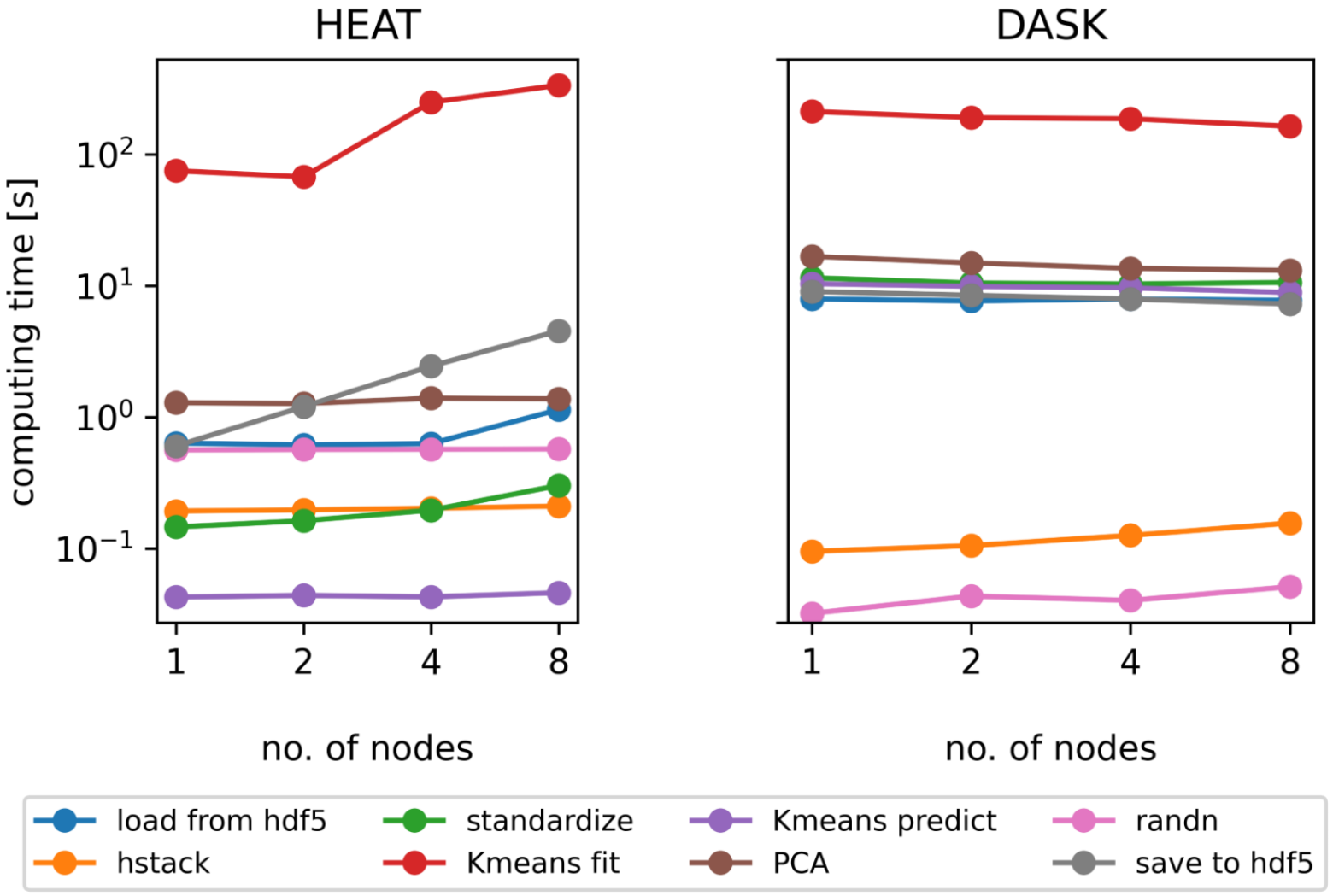
8 tasks per node, 20 threads per task


**Disclaimer:** These experiments have been run by a „Heat-Expert“, but a „Dask-Non-Expert“ – code available upon request.

***** „train“ part of *ATLAS Top Tagging Open Data Set*

# Comparison with Dask (CPU)

## Weak scaling of runtime on a small data set* (7.6GB)

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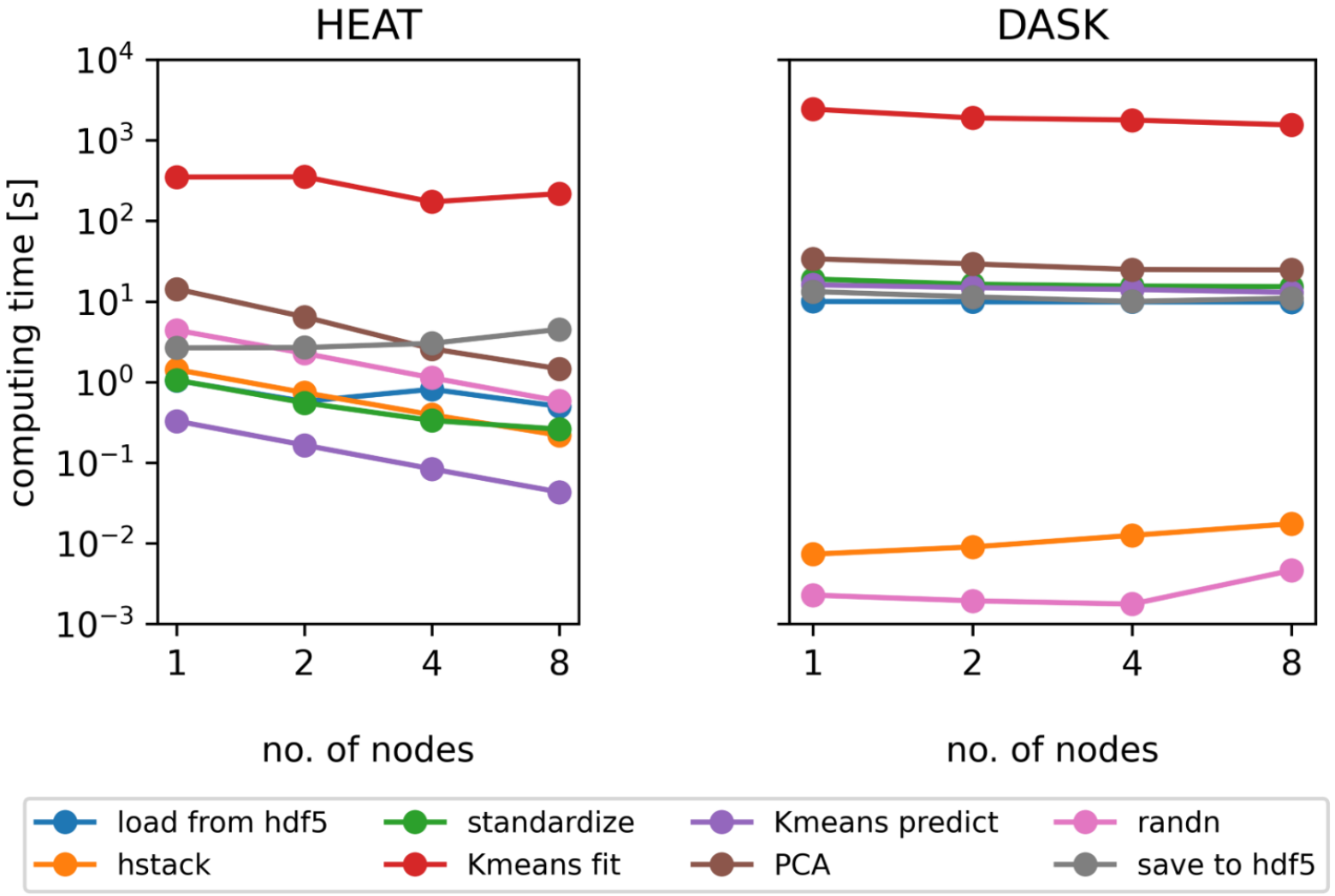
powered by terrabyte

***** „test“ part of *ATLAS Top Tagging Open Data Set*

# Comparison with Dask (CPU)

## Strong scaling of runtime on a small data set* (7.6GB)

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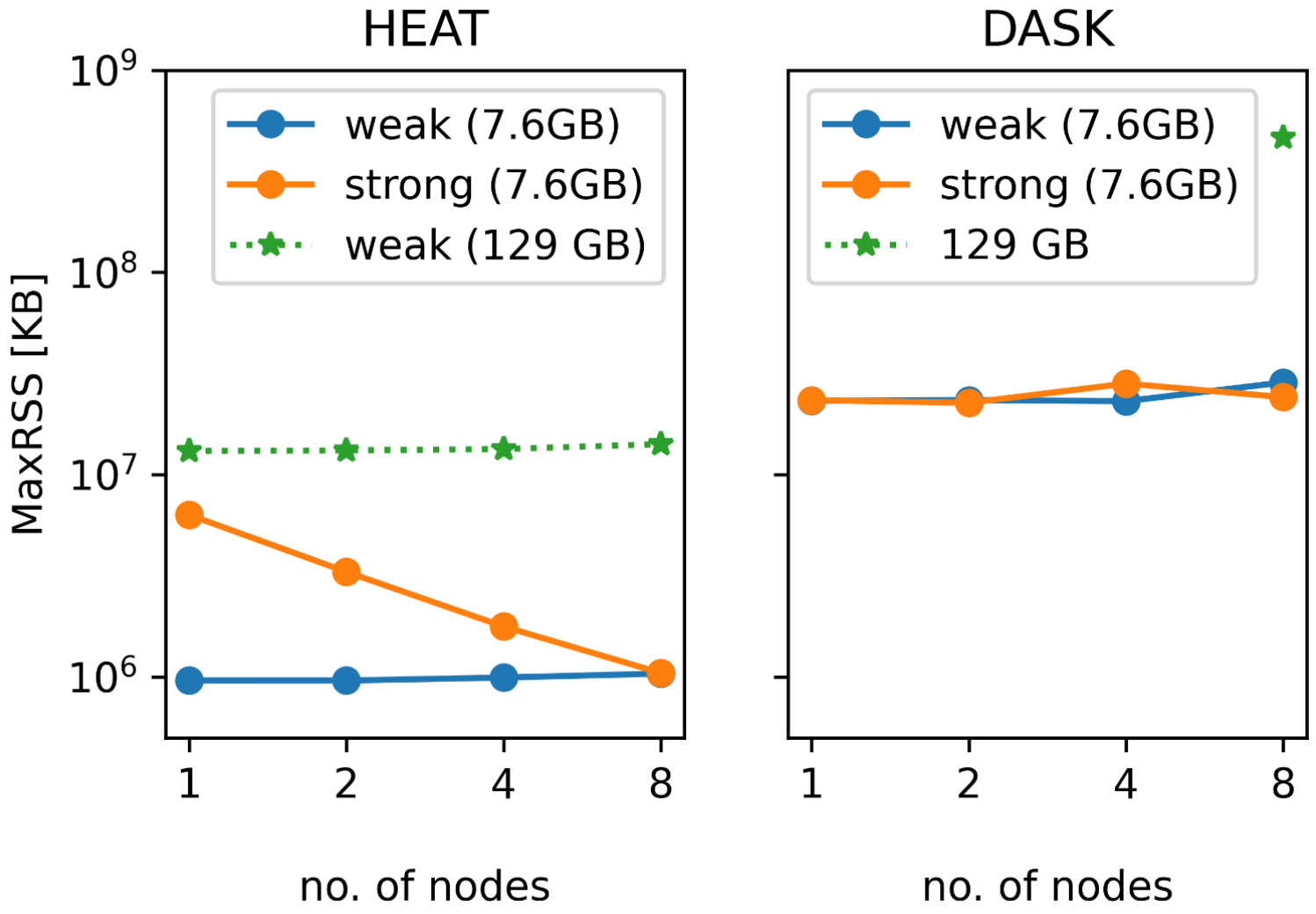
# Comparison with Dask (CPU)

## Weak and strong scaling of used RAM on a small data set* (7.6GB)

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***** „test“ part of *ATLAS Top Tagging Open Data Set*


# Future development and challenges

# Future development and challenges

- **Software engineering:** keep/increase *software quality* by, e.g., …
  - continuous benchmarking of runtime, memory consumption, and energy consumption („green HPC“)
  - keep/extend interoperability w.r.t. the evolving ecosystem
- **Extend fuctionality**, e.g.,
  - implementation of support for distributed **`xarray`**‘s has just started (➔EOC-community)
  - implementation of an SVD/PCA/DMD-module (➔ ESA)
  - preprocessing module, FFT, … ➔ ***or maybe your suggestion?***
- **Community interaction**, e.g., …
  - extend documentation by tutorials/use cases etc.
  - user-support by workshops and/or individual collaboration/help:
    ***If you want to try out/use Heat for your research, we are glad to help you; we do <u>not</u> expect you to contribute to Heat.***

# Feel free to try out, to suggest features, or to contribute!


visit us on **github**:

# Impressum

| | |
|---|---|
| Thema: | **The Helmholtz Analytics Toolkit (Heat)** and its role in the landscape of massively-parallel scientific Python |
| Datum: | 2023-08 |
| Autor: | Fabian Hoppe (+ the Heat development team) |
| Institut: | Institut für Softwaretechnologie, High-Performance Computing |
| Bildcredits: | Alle Bilder „DLR (CC BY-NC-ND 3.0)“, sofern nicht anders angegeben |