CARME

An Open Source Framework for Multi-User, Interactive Jobs on Distributed GPU-Systems

The Carme Team
Competence Center for High Performance Computing,
Fraunhofer ITWM, Kaiserslautern, GERMANY

Fraunhofer ITWM

Machine Learning in the Wild

Why we need a tool for ML/DL on HPC Clusters

Machine Learning in the wild

Why we need a tool for ML/DL on HPC Clusters

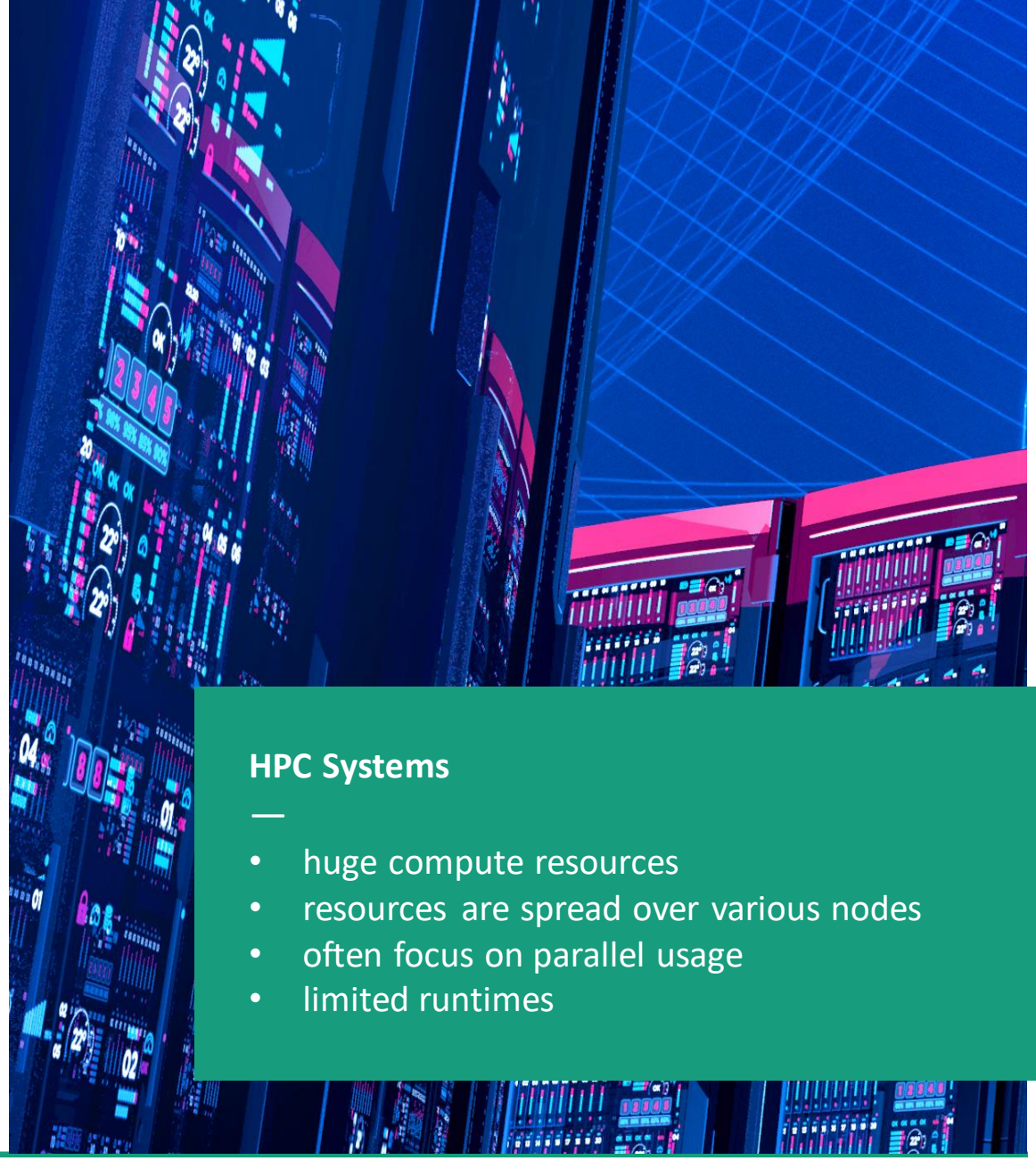
Machine Learning and Data Analytics

- showed **remarkable success** in many distinct fields
  (e.g. image processing, text translation, medical imaging, …)
- rise of **hybrid** and/or **ML/DL** supported **algorithms**
  (e.g. climate forecast, physics informed networks, …)
- **model size increases** drastically
  (needs more memory & compute power)
- generate **large investments** in new **multi-GPU hardware**

Utilize HPC Systems

The way it was for decades

- other fields use **HPC systems for decades**
  (e.g. physics, chemistry, mathematics, …)
- HPC clusters are set up to **make use of** the **hardware** that is installed
  (e.g. multi-node jobs)
- **calculate huge problems**
  (e.g. extreme memory and computationally intensive simulations)
- **commandline driven** usage
  (e.g. submit non-interactive batch jobs, jobs do not start directly)



HPC Systems

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- huge compute resources
- resources are spread over various nodes
- often focus on parallel usage
- limited runtimes

Machine Learning and HPC Systems

What we would expect

Machine Learning and HPC Systems

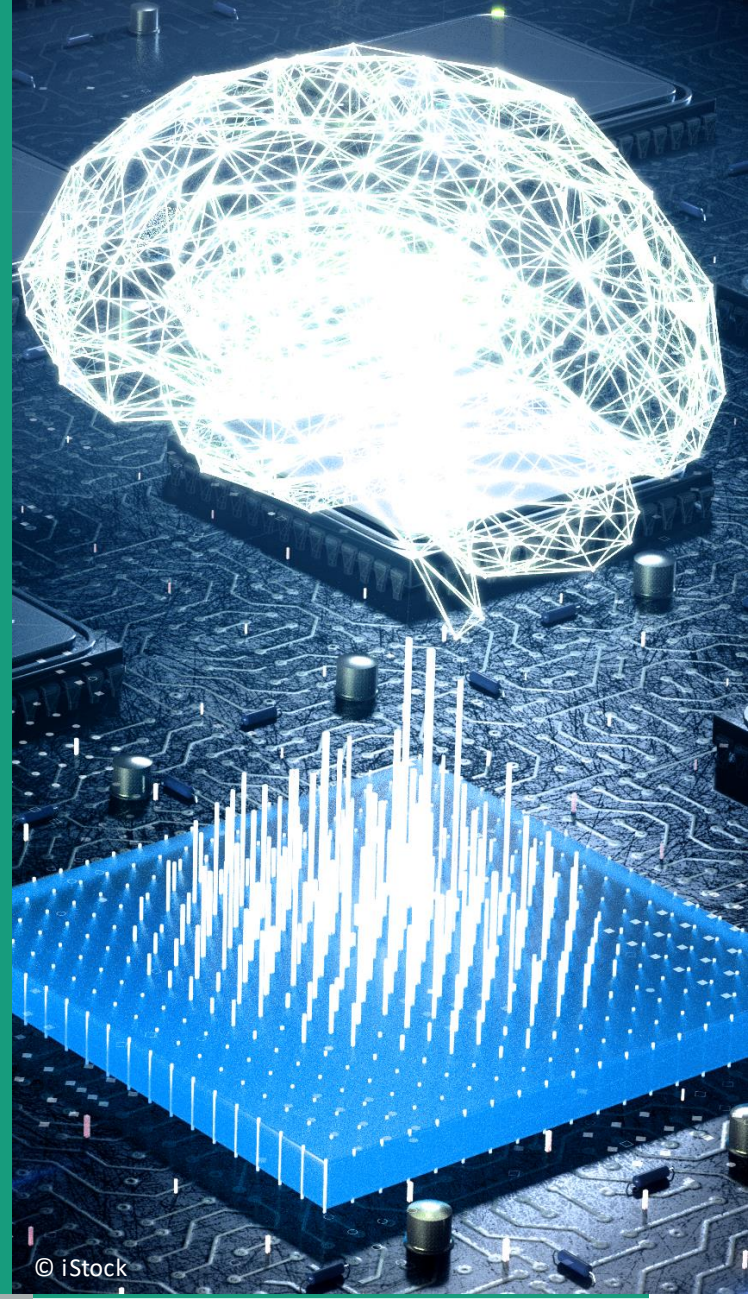
efficiently **manage** and **use** your **resources**
(how to utilize the full power of multi-GPU systems?)

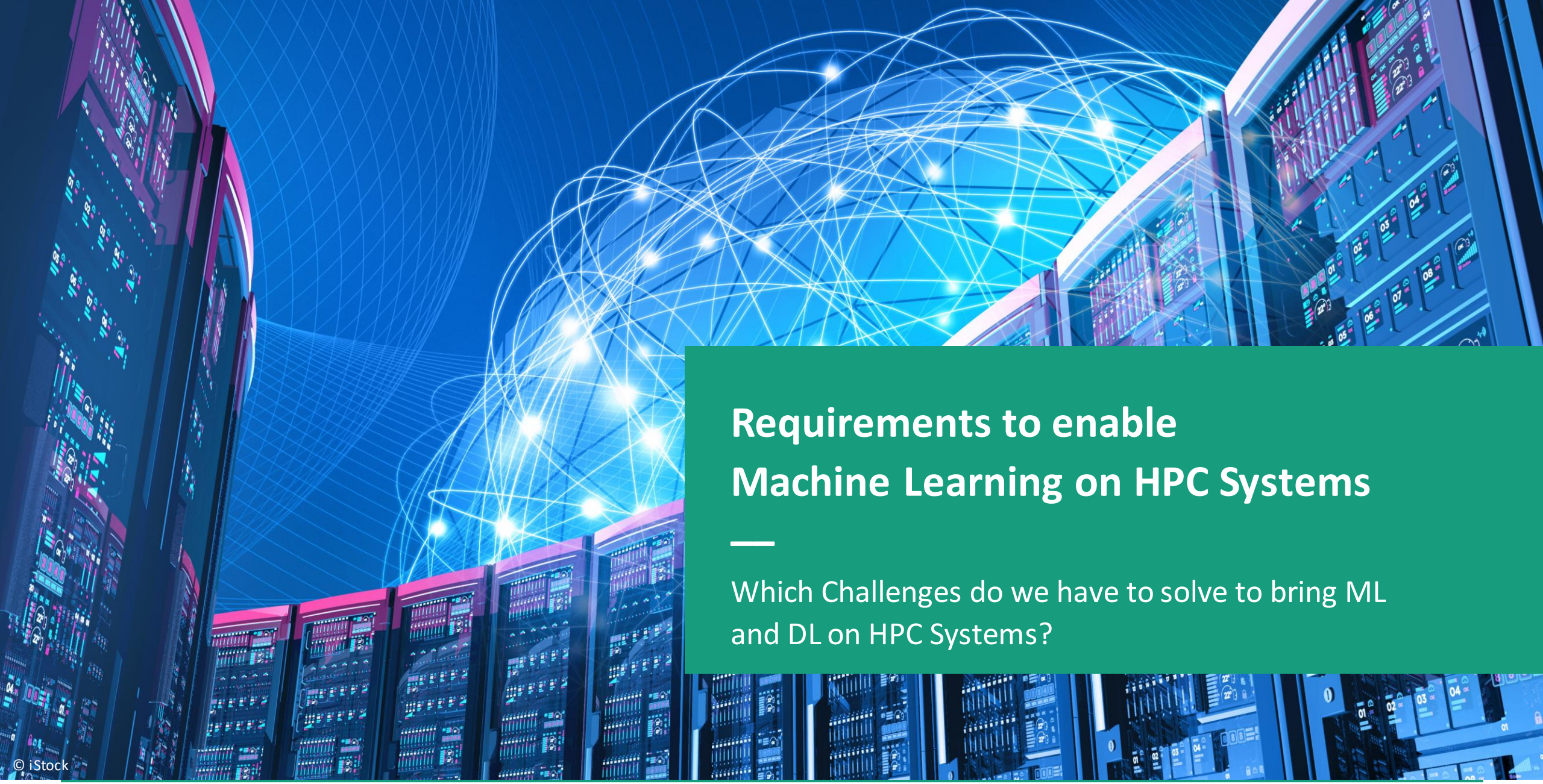
match your workflow with these resources
(how can I develop interactively?)

scale your applications to **use multiple GPUs** and/or **nodes**
(how do I easily utilize multiple GPUs in various nodes?)

manage **data I/O** and data **storage**
(how do I access my data?)

Machine Learning
and
HPC Systems
two distinct worlds?





Requirements to enable Machine Learning on HPC Systems

Which Challenges do we have to solve to bring ML and DL on HPC Systems?

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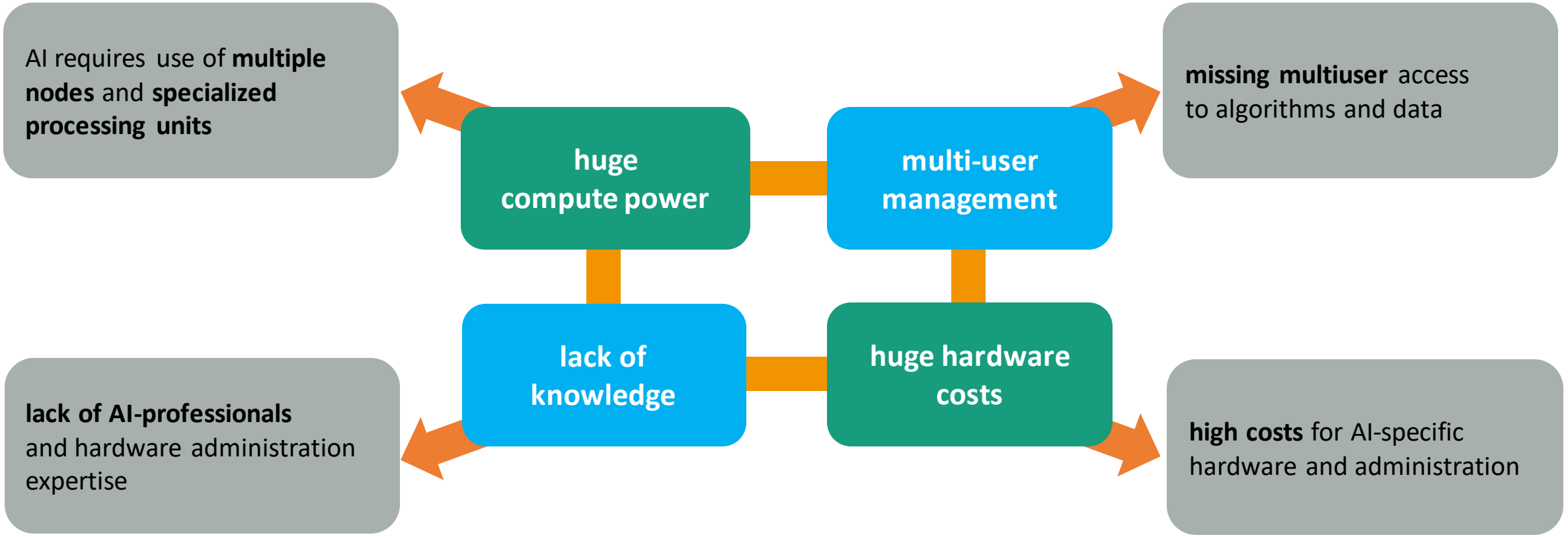
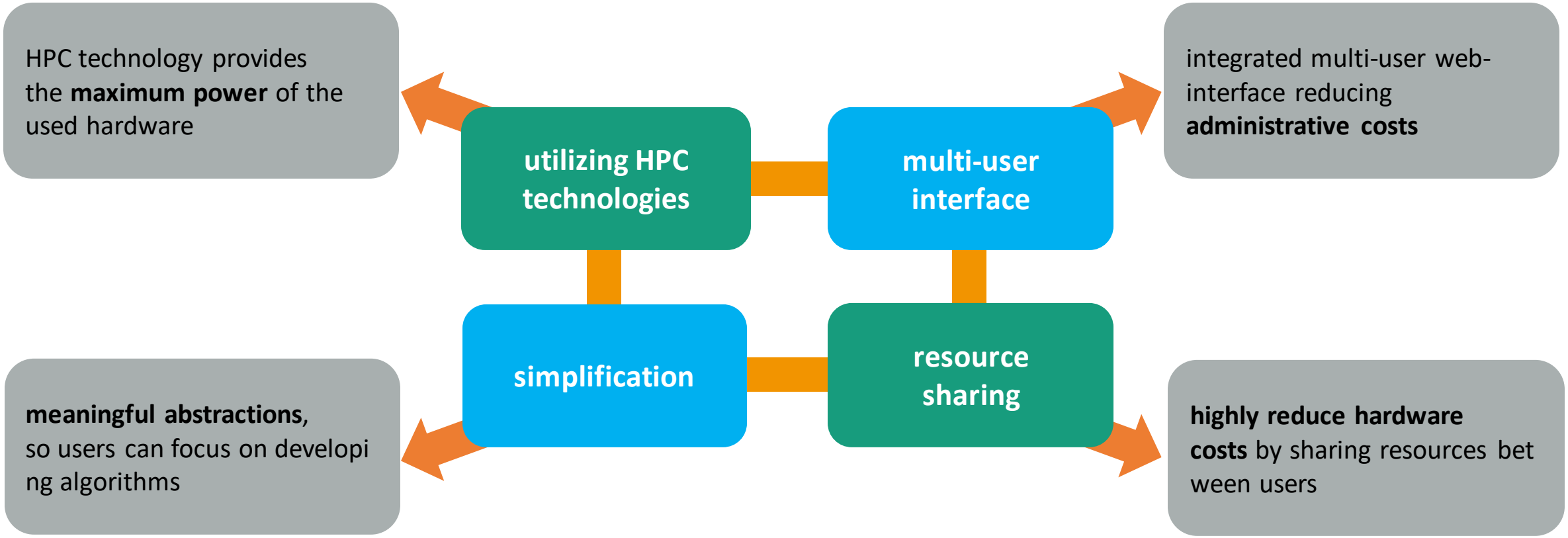
Machine Learning and HPC Systems

on an HPC system we have to take care of …



Machine Learning and HPC Systems

our proposed solutions …



Combining Open-Source ML Tools with HPC Backends

The CARME Way

Carme – an open source framework to manage resources for multiple users running interactive jobs on an HPC Clusters

combines

Data Science

- secure web frontend main GUIs
  - TheiaIDE/JupyterLab
  - TensorBoard
- anaconda environments

HPC

- user and job management
  - LDAP and SLURM
- data I/O technologies (e.g. BeeGFS)
- using containers (Singularity)
- monitoring tools (e.g. Zabbix)

Open-Source Tools

https://carmeteam.github.io/Carme/

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The Details of our Solution

What it is really about

Resource Management

How to assign resources to competing users?

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Resource Management

Proven HPC Tools

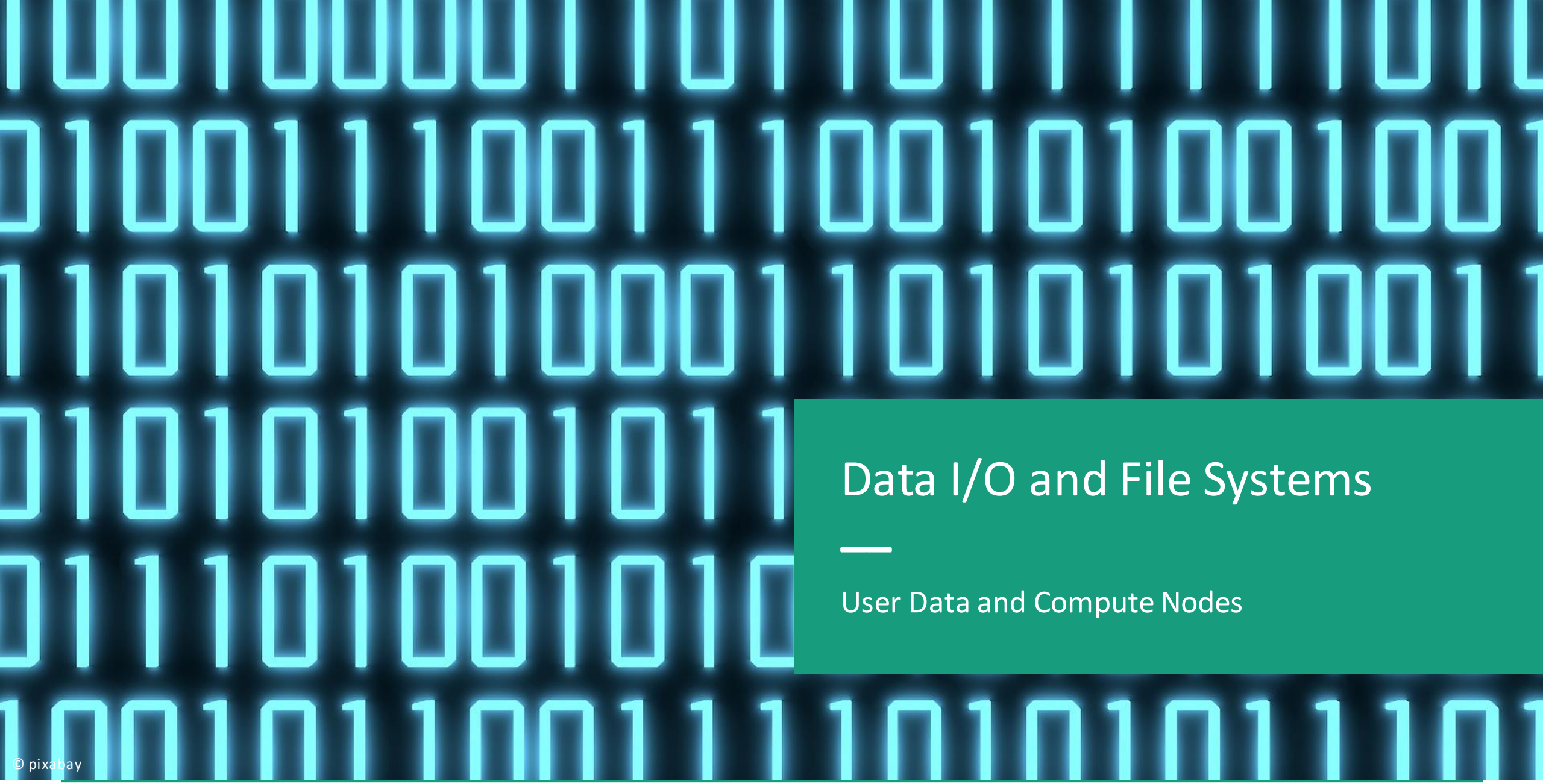
LDAP[1] (user management)

- LDAP = Lightweight Directory Access Protocol
- use **your LDAP**
- **different** user **roles**

SLURM[2] (job scheduler)

- easy **integration** in **existing installations**
- make use of **cgroups** plugins
- using **quotas**, **queues**, resource reservation
- many **useful extensions** available
  (e.g. preemtion, hiberate if idle, …)

[1] https://www.openldap.org
[2] https://slurm.schedmd.com



Data I/O and File Systems

User Data and Compute Nodes

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Data I/O and File Systems

Distributed for more Power

BeeGFS[3]

- redundant, parallel file system
- **huge** data **throughput** (via infiniband)
- temporary job FS (BeeOND) on local SSDs between node
- **open-source** (commercial support available)

[3] https://www.beegfs.io

Maintenance and Useability

Meet User Software Demands

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Maintenance and Useability

Demandings we have to care

- **using graphic cards for calculations**
  - install drivers, the corresponding libraries and TensorFlow, PyTorch, …
  - easy GPU access
- **ML/DL algorithms**
  - libraries, programs and dependencies change fast
  - different algorithms need different programs/libraries
- **programs/tools often available as deb-packages**
  - but many HPC clusters are rpm-based
- **HPC clusters have very heterogeneous users**
  - need a lot of different tools and some dependencies may collide
  - users cannot be root

Maintenance and Useability

Easy for Users and Admins

- **easy to use** (for users)
  - access via **web interface**
  - **interactive** development tools

    (e.g. TheiaIDE, JupyterLab)
  - direct **GPU access**
  - uncomplicated **multi-node/-GPU usage**

- **easy maintainable** (for administrators)
  - provide different libs for specific user groups
  - use **anaconda environments**
  - stick to **singularity containers**

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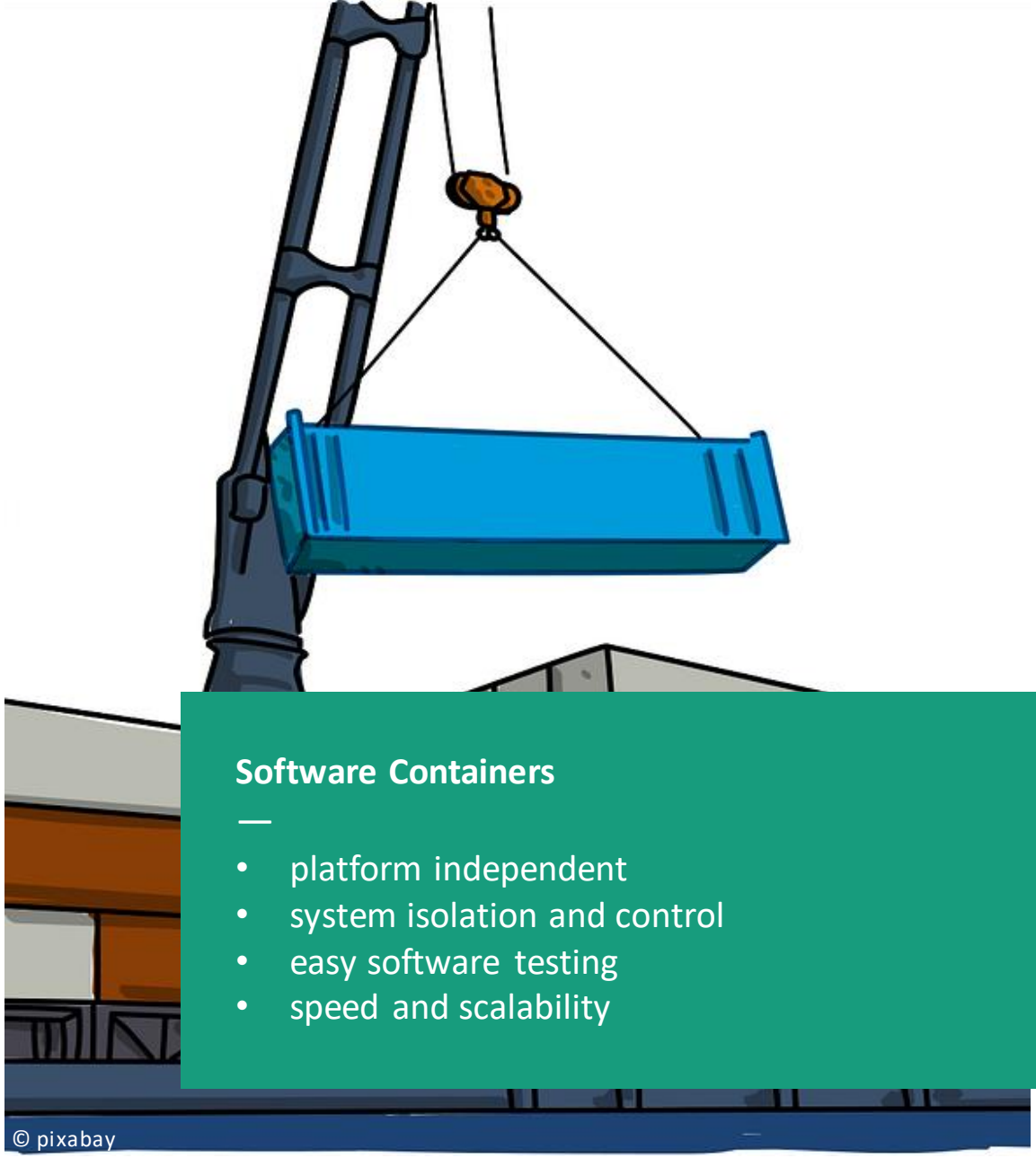
Maintenance and Useability

Portable Software Environments

singularity[4] containers

- **provide** the **OS** that ML/DL users **need**
- **on the host:** base OS and graphics drivers
  in the image: all other dependencies
- **no root-privileges** to start the container
- **only needed folders** mounted
  (e.g. /home/USERNAME, /scratch/USERNAME)
- create **images from scratch** (takes a few minutes)
  or **transform** an **existing** (clean) **docker** image



Software Containers

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- platform independent
- system isolation and control
- easy software testing
- speed and scalability

[4] https://www.sylabs.io/singularity

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Maintenance and Useability

The base Environment Carme provides

Carme Singularity "Base Image"

- set of **basig software** (e.g. vim, nano, gcc, gdb, …)
- everything **ready to use IB** (using free drivers)
- **MPI** and **GPI** are installed per default (GPISpace installation ready)
- **miniconda** and/or **mambaforge**
- **Python 3.X**
- **TheiaIDE** and **JupyterLab**
- **headless** or **web-based applications** can run inside the container

Maintenance and Useability

Userspace Package Management

anaconda[5] based environments

- **open-source** (normal and enterprice versions)
- central **miniconda/mambaforge** installation inside the image (people can use it directly)
- users have the freedom to **install** (most) of the **libs and tools** they need (precise version control)
- all **PyTorch** and **TensorFlow** versions possible
- easily **share** and **save** your environments
- supporting **cooperations**

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[5] https://www.anaconda.com

Resource Utilization

Who has access to which Resources?

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Resource Utilization

Control the Resources you have

- CARME utilizes the **scheduler resource limits** (fully respects non-carme jobs, cgroups, queues, etc.)
- **additional limits** can be defined **on top** of the scheduler limits (modify #(nodes), #(GPUs), running jobs, etc.)
- **integrates** smoothly **in** your **existing scheduler** (only a carme feature flag is needed)
- everything **inside a job** runs inside an **isolated namespace** (programs cannot escape a job)
- inside a job you can only see the GPUs associated with the job (no access to information of other GPUs on the node)

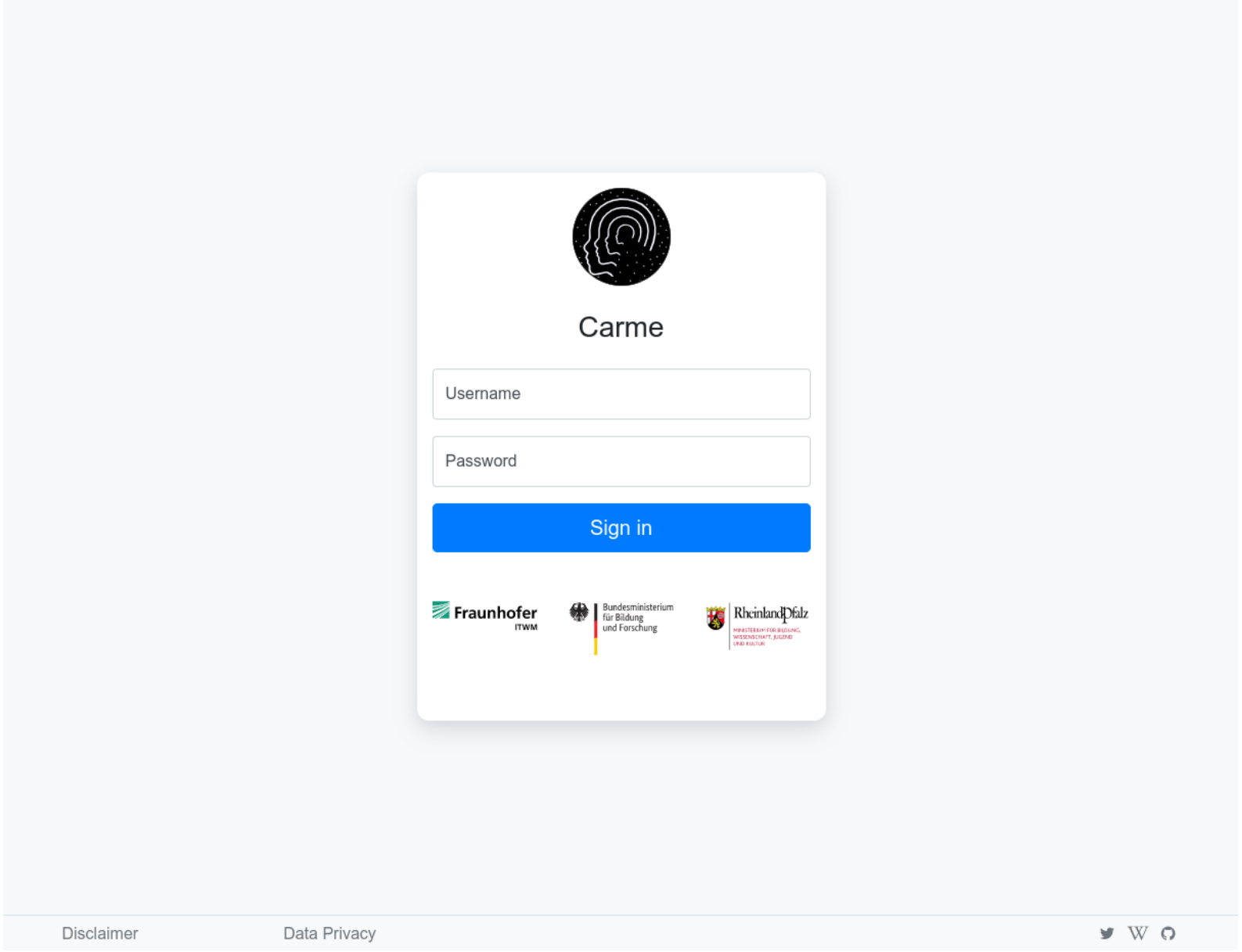
Interactive and Secure Multi-User Environments

ML/DL and Data Science Users want interactive Access

Interactive Usage

Secure and simple Access

- access via **web interface**
- **no additional software**
  (like ssh or special tool)
- runs **behind your firewall**
- **secure autehntification**
  (e.g. via LDAP) and additional
  2FA



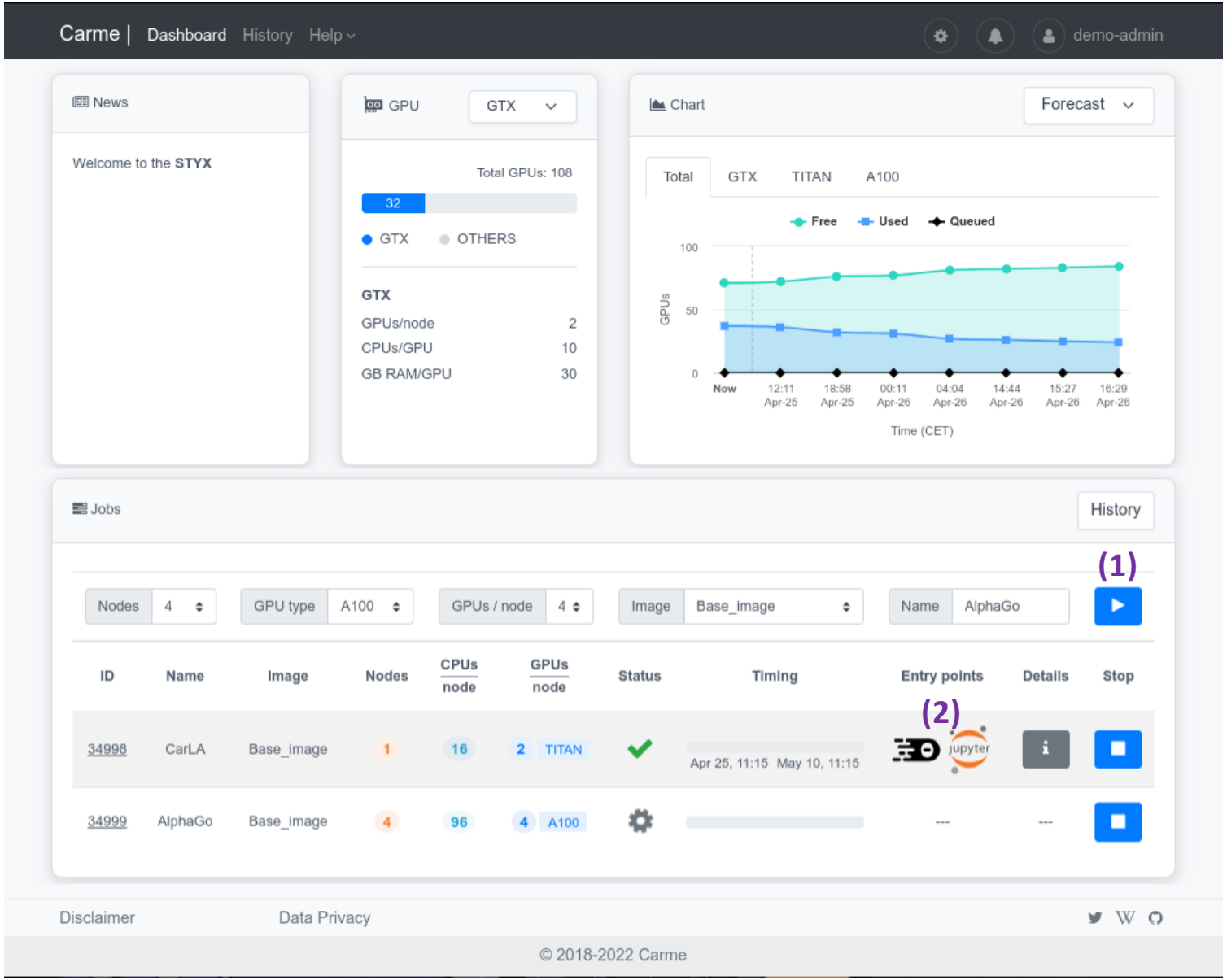
Interactive Usage

The User Control Center

two clicks to development

(1) start a job

(2) select *your* preferred **development environment**



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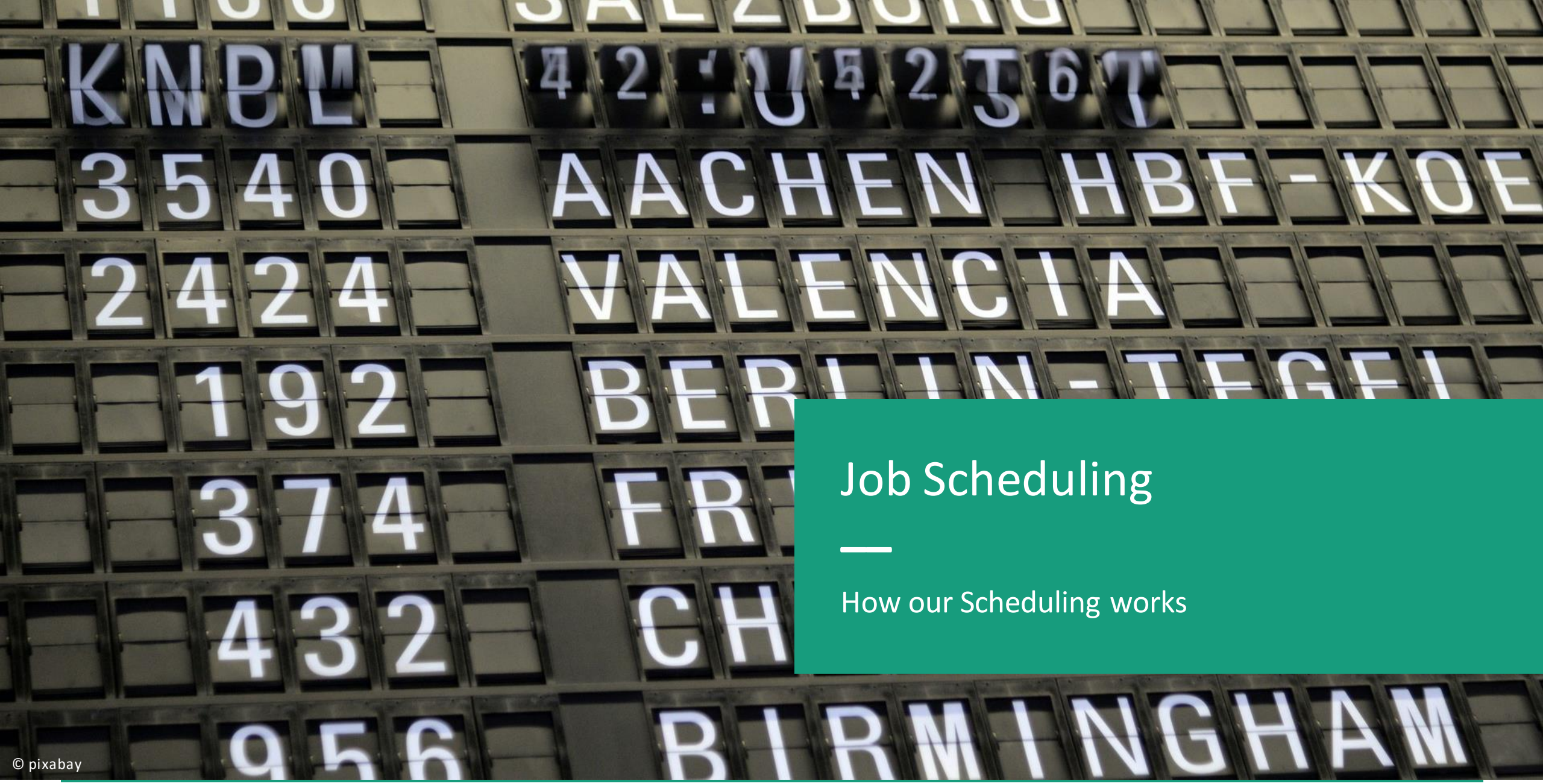

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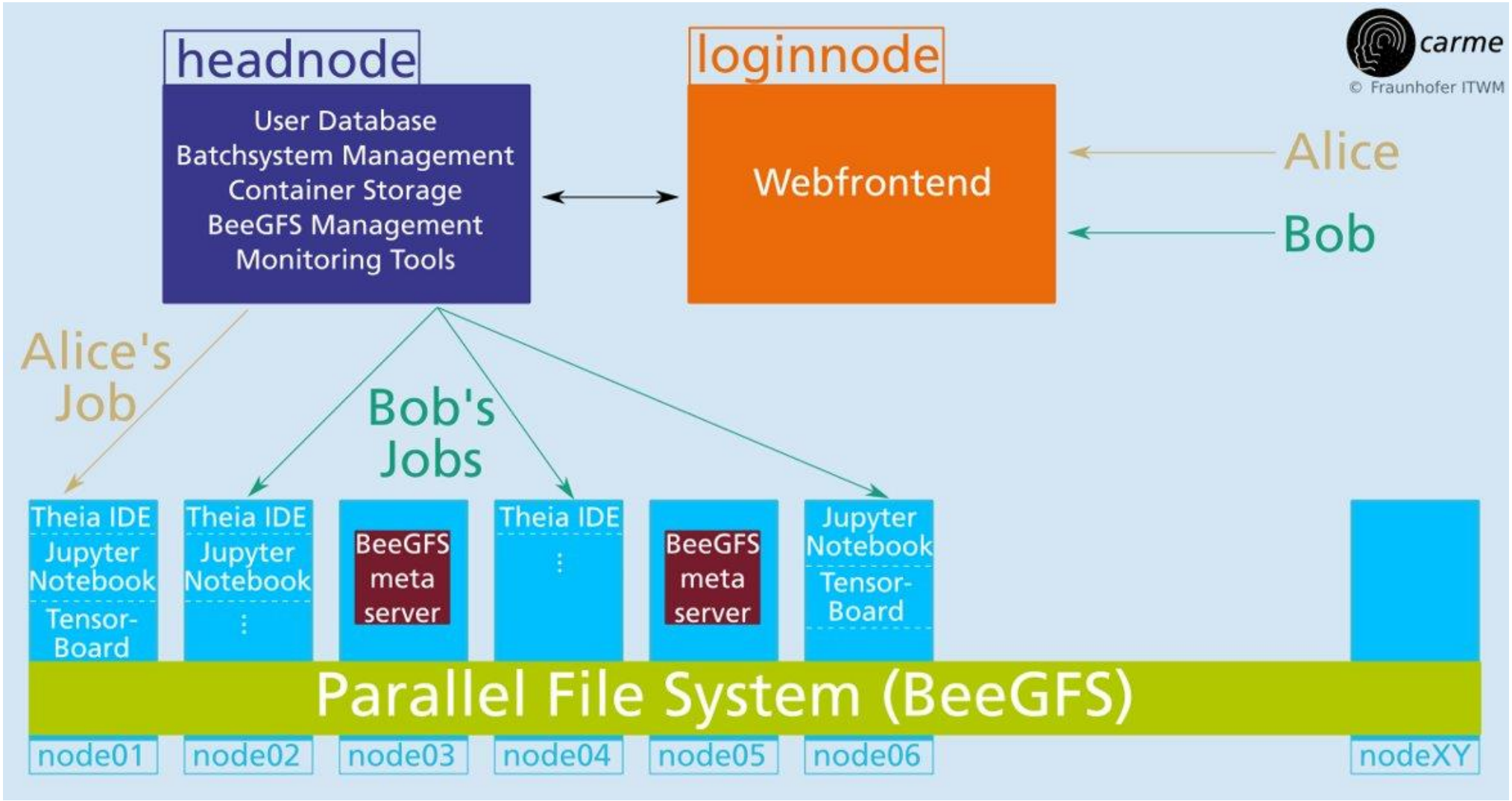
Job Scheduling

How our Scheduling works

Job Submission Scheme



Job Submission Scheme

- user login to the web interface
- user submits a job
  - request for new job is sent from the frontend to our hpc-backend
  - secure connection via rpyc and special keys
- our hpc-backend
  - gets the job information from the frontend and our data base
  - finally submits the job to the scheduler as original user
- job start script is handed over to the scheduler
  - scheduler checks handed over information (resource limits, user accounts, availability, …)
  - respective CARME prolog scripts run (only if the job belongs to us)
- job starts on the requested node(s)
- user is informed in the frontend that the job has sucessfully started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Security Concept

Our Security Idea

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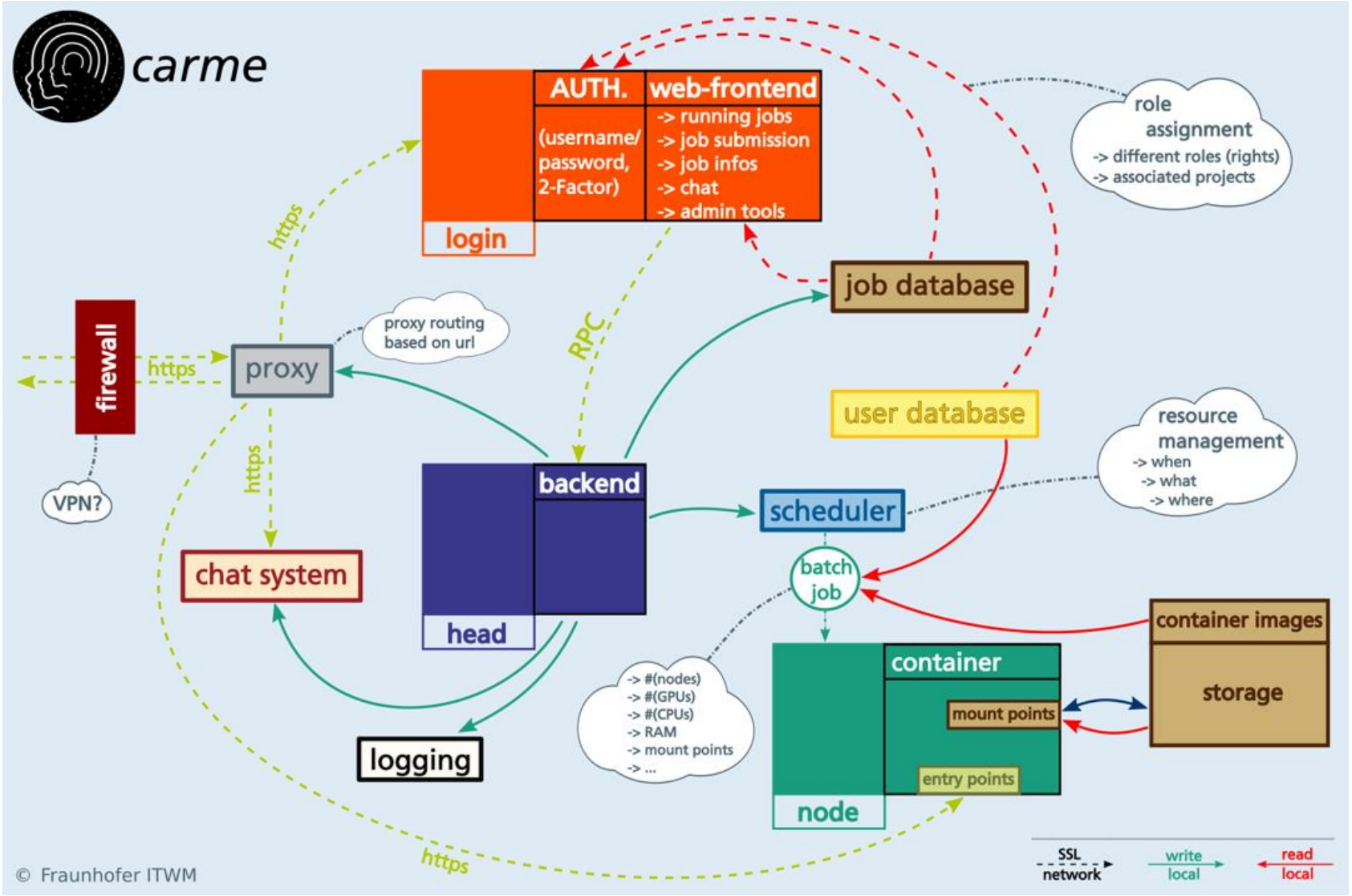
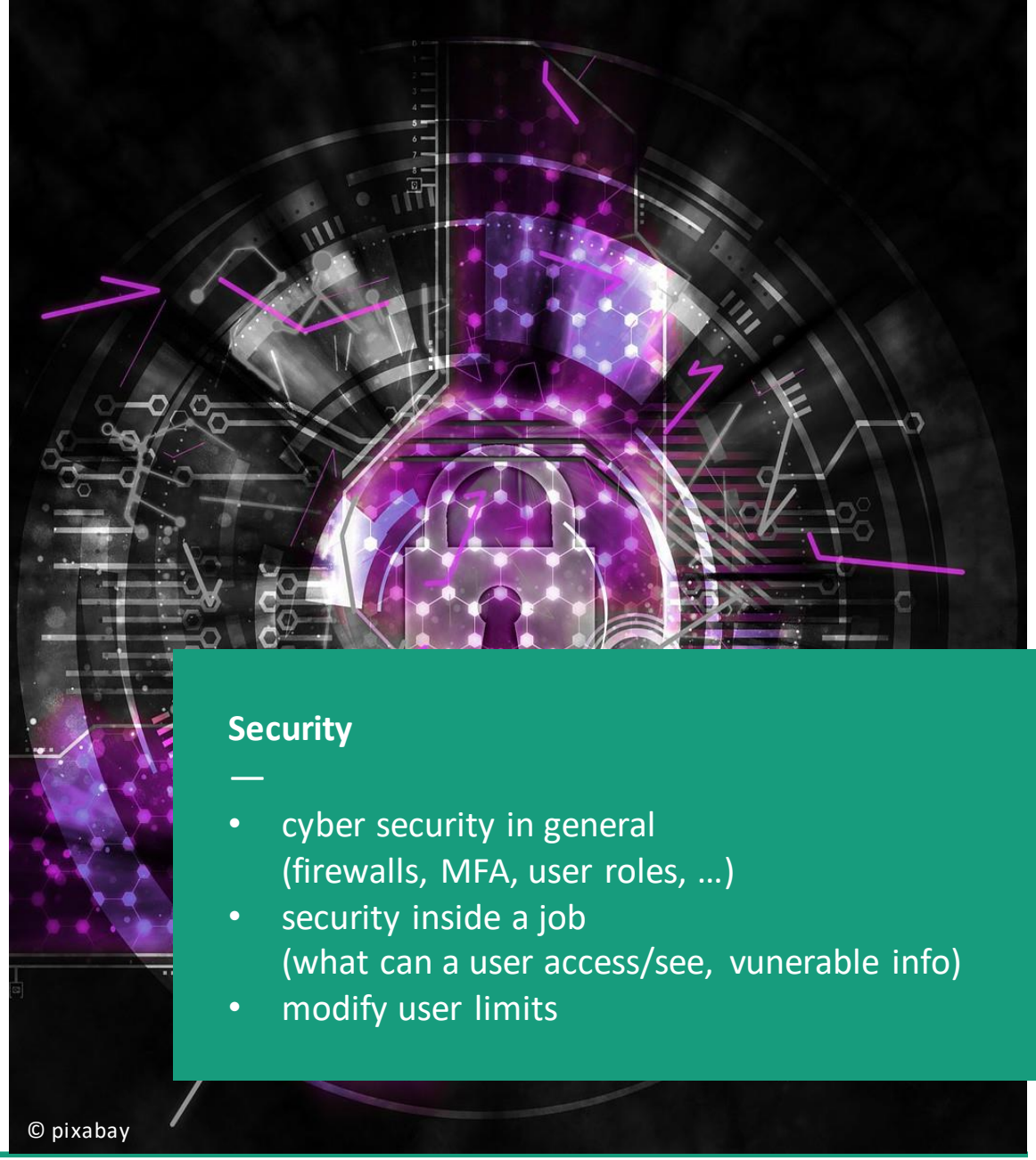
Security Concept



Security Concept

- everything can run **behind your firewall**
- we utilize our **own proxy** and **frontend**
  (both are separated singularity containers)
- **secure connection** between frontend and backend
- access **requires authentification** and **2FA**
- define what is **mounted inside** a **job**
- fully **integrate** the **limitations** of your **scheduler**
- **addinitional limitations** in CARME
  (e.g. resource limits, running jobs and singularity images)
- everything **inside** a **job** runs in its **own namespace**
  (no chance to use other resources)



Security

—

- cyber security in general
  (firewalls, MFA, user roles, …)
- security inside a job
  (what can a user access/see, vunerable info)
- modify user limits

Our Key Features

In a Nutshell

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Our Key Features

In a Nutshell

- **seamless integration** into existing HPC setups
- user-friendly **web-interface** providing **flexible** and os-**independent** access from anywhere in the world
- **interactive jobs** to develop directly **on the cluster** with your favorite **deep learning tools**
- fully **separated jobs** with **custom resources**
- **intuitive abstraction** of complex cluster topologies
- **distributed multi-node/multi-gpu jobs** with direct access to GPI, GPI-Space, MPI, Tarantella and **Horovod**
- user maintained and **containerized environments** using singularity and **anaconda**

Our Key Features

In more Detail

- **seamless integration with available HPC tools**
  - job scheduling via SLURM
  - native LDAP support for user authentication
  - integrate existing distributed file systems like BeeGFS
- **access via web-interface**
  - OS independent (only web browser needed)
  - full user information (running jobs, cluster usage, news, messages)
  - start / stop jobs within the web-interface
- **interactive jobs**
  - flexible access to GPUs
  - access via web driven GUIs like Theia-IDE and/or JupyterLab
- **distributed multi-node and/or multi-gpu jobs**
  - easy and intuitive job scheduling
  - directly use GPI, GPI-Space, MPI, Tarantella and Horovod within the jobs
- **full control about accounting and resource management**
  - job scheduling according to user specific roles
  - compute resources are user exclusive
- **user maintained, containerized environments**
  - singularity containers (runs as normal user, GPU, Ethernet and Infiband support)
  - anaconda environments (easy updates, project/user specific environments)
  - Built-in matching between GPU driver and ML/DL tools

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In Summary

What you get

In Summary

What you get

The User Side

- **interactive development** access to HPC systems
  (keep your workflow with Jupyter Notebooks or full IDE)
- **easy** way to **submit** and **get jobs** on big clusters
  (simpified submission mask, no need to write batch scripts)
- guarantee that **only you** have **access** to **your resources**
  (no need to worry about other users)
- utilize **containers** and **conda environments** to get software
  (keep track with quickly chaning and diverse tool requirements)
- **access** your **HPC cluster** via a **web browser**
  (no need to install special or additional software)

In Summary

What you get

The Administrator Side

- **easily integrate** CARME in your scheduler set up
  (a feature flag and our prolog/epilog scripts is all you need)
- **control** which **folders** user have access to
  (you can decide per image which folders are mounted or not)
- **provide** the **basic software** that ML/DL users need to do there work
  (keep the host installation small and clean)
- manage our **data base via** a simple **web interface**
- **simplify** the **support** for AI and Data Science users
- get **logs** and **error outputs** for CARME scripts and services

In Summary

What you get

The Institution Side

- CARME was and will be **developed in Germany**
  (following Fraunhofer standards and respecting data privacy)
- **license** that allows **commercial use**
- giving users a tool to **easily utilize GPU resources**
  (be sure that your investments in hardware pay off)
- **increase** the **productivitiy** of both your AI developers and researchers and your system administrators

Bringing AI Development / Education and HPC Systems together

The CARME Way

Carme – an open source framework to manage resources for multiple users running interactive jobs on an HPC Clusters

CARME

AI and Data Science Tools

THEIA

jupyter

HPC Tools

slurm workload manager

OpenLDAP

singularity

BeeGFS

ZABBIX

Open-Source Tools

enables

AI development

- develop code
- schedule & track experiments
- debug model performance

AI education

- hands-on sessions
- slides & homework
- easy Q&A

https://carmeteam.github.io/Carme/

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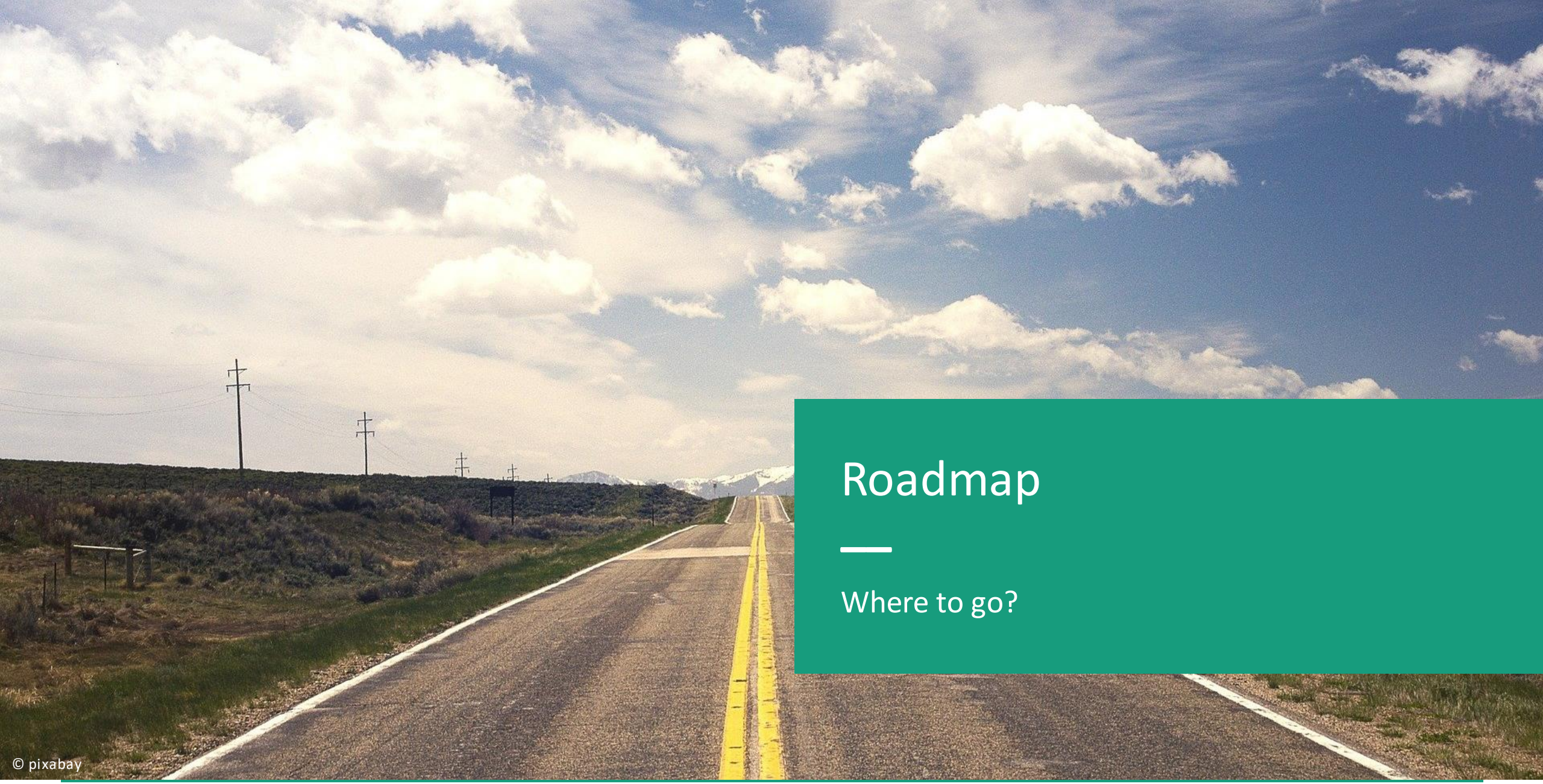
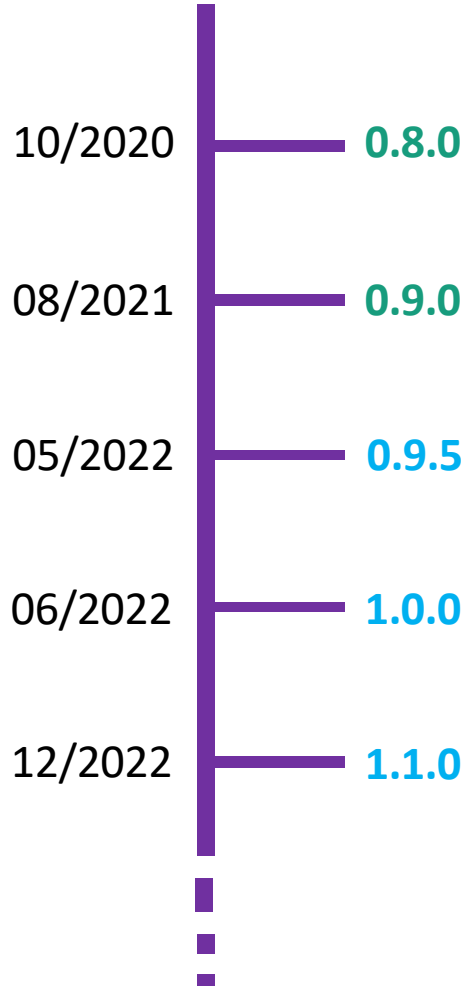


Roadmap

Where to go?

Roadmap
Where to go?

- available on **GitHub** (https://carmeteam.github.io/Carme/)
- **installation on demand** (including support)
- **release cycle:** 6–9 months
- **latest release:** r0.9.5 (05/2022)
- **next release:** r1.0.0 (06/2022)



Contact

Dr. Dominik Straßel
Competence Center High Performance Computing
Fraunhofer ITWM
Fraunhofer–Platz 1
D–67663 Kaiserslautern, GERMANY
Tel. +49 631 31600 4896
dominik.strassel@itwm.fraunhofer.de