



DRESDEN LEIPZIG

CENTER FOR SCALABLE DATA ANALYTICS AND  
ARTIFICIAL INTELLIGENCE

# Big Data Processing on HPC

Siavash Giashvand, Apurv D. Kulkarni, Christoph Lehmann, Elias Werner

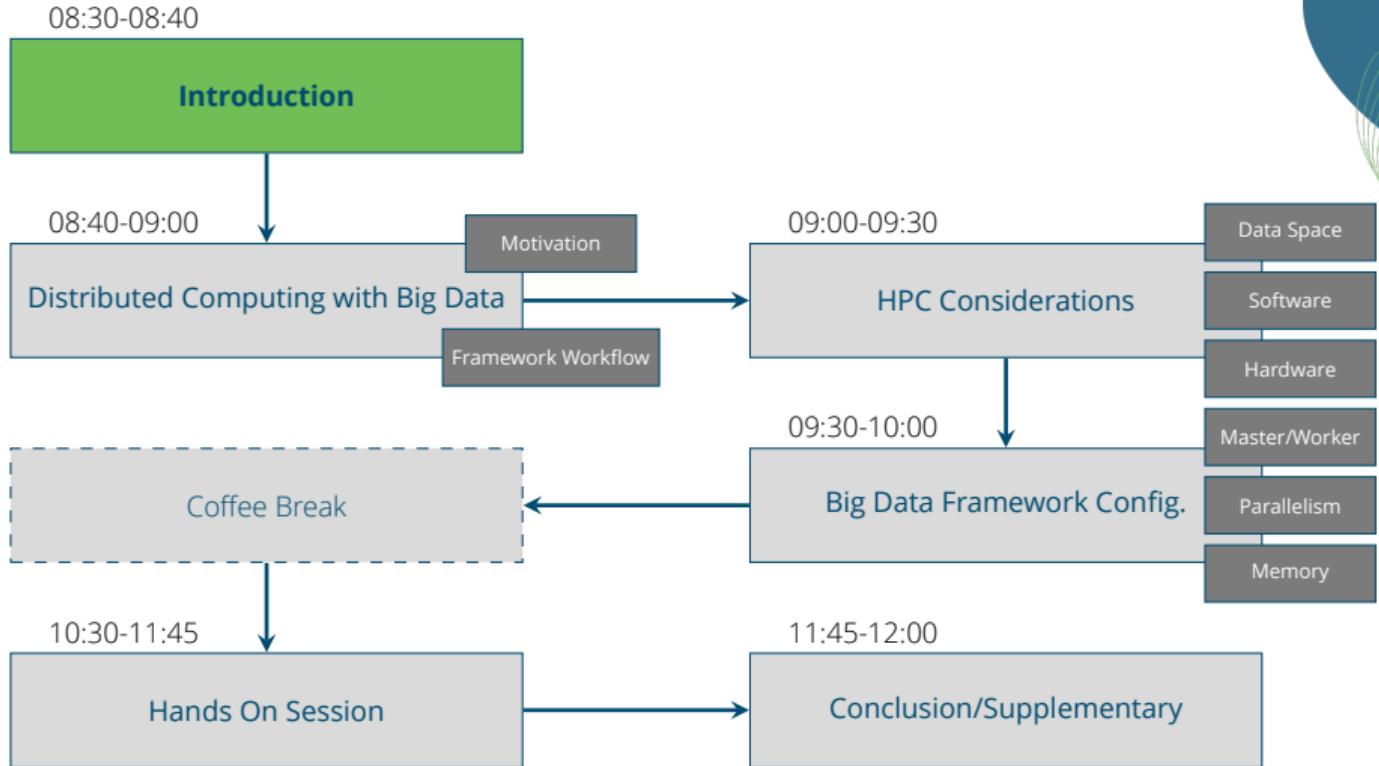
May 2025

GEFÖRDERT VOM



Bundesministerium  
für Bildung  
und Forschung

SACHSEN Diese Maßnahme wird gefördert durch die Bundesregierung aufgrund eines Beschlusses des Deutschen Bundestages.  
 Diese Maßnahme wird mitfinanziert durch Steuermittel auf der Grundlage des von den Abgeordneten des Sächsischen Landtags beschlossenen Haushaltes.



# Intention of the Training

- Making things understandable from a user's point of view
- Show interplay between Big Data frameworks and HPC environment
- Interactive sessions with toy examples

## Note

- We do **not** want to show everything that is possible. We do **not** want to show the best optimized big data processing pipeline.
- We want to provide an overview of using a big data processing engine on an HPC machine.

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## 💡 Hint

<https://compendium.../application/overview/> ↗

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ZIH HPC System

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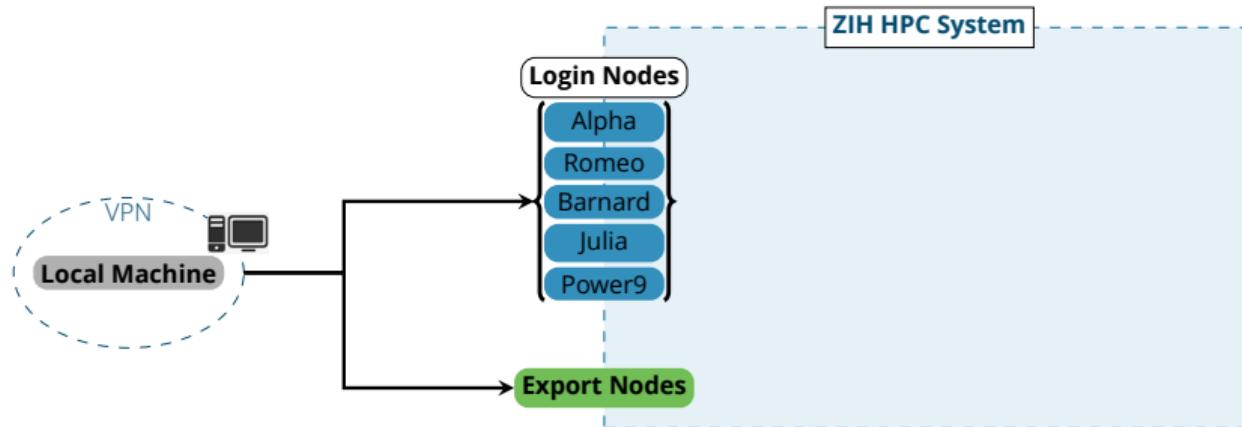
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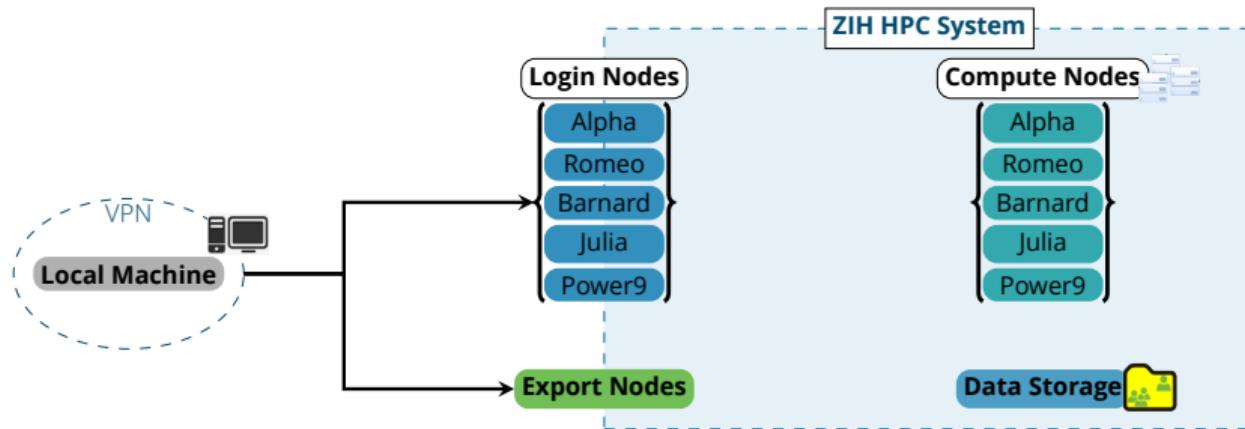
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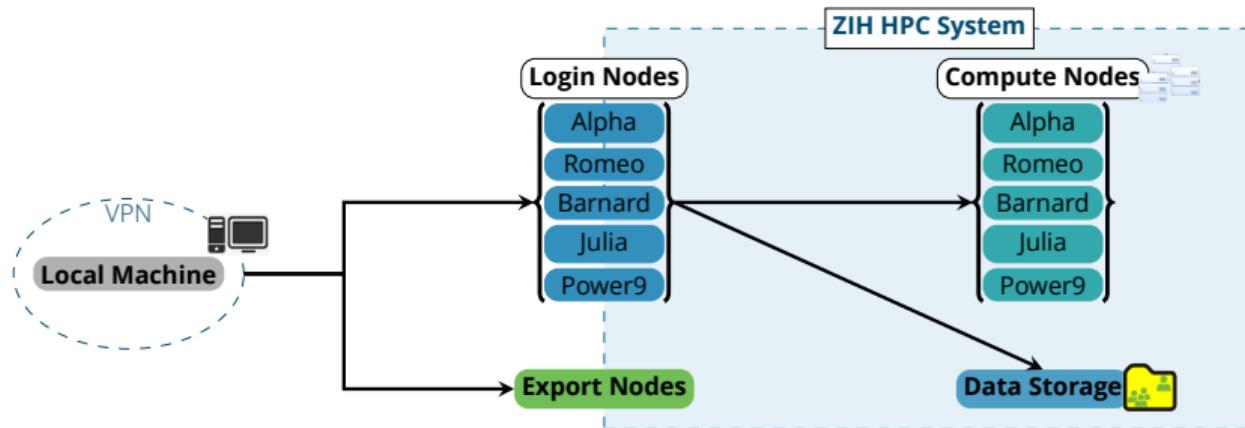
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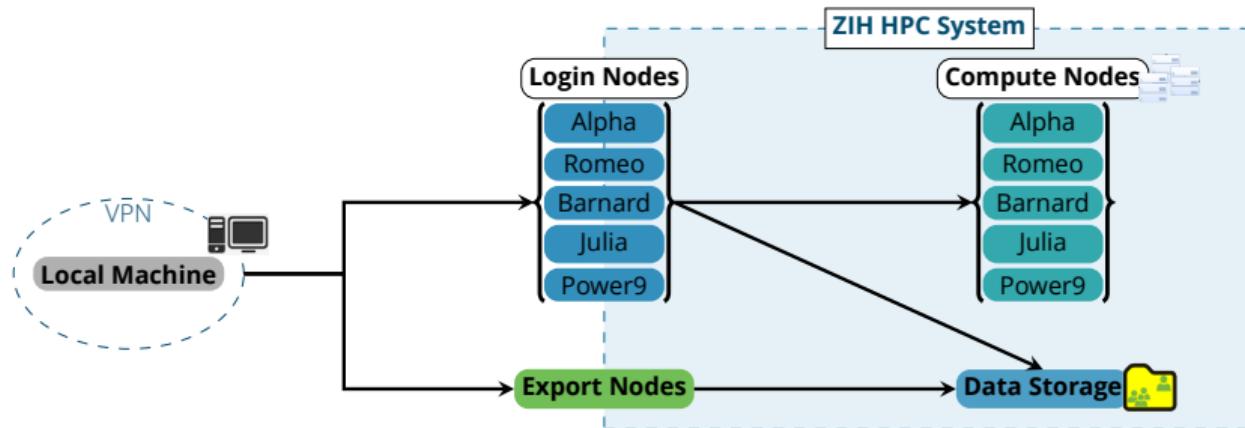
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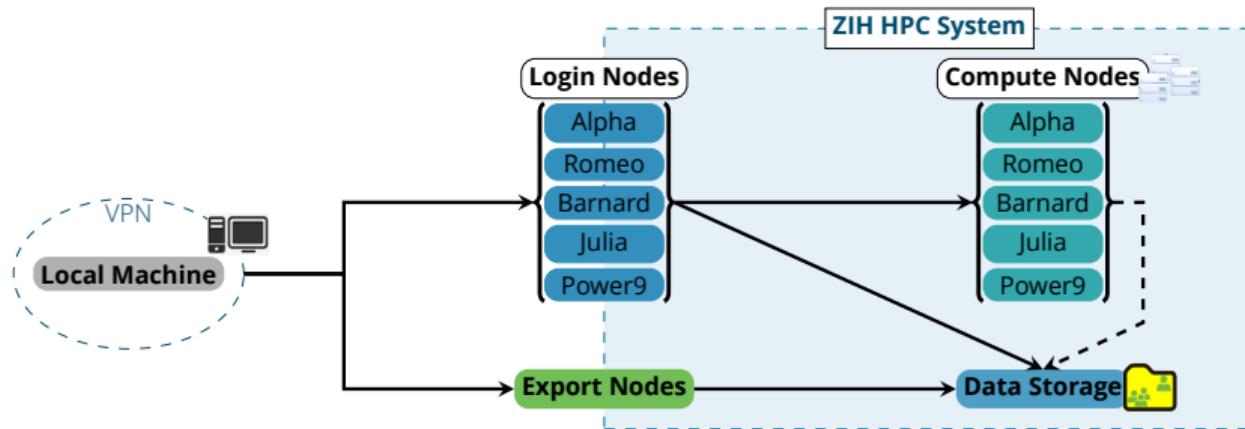
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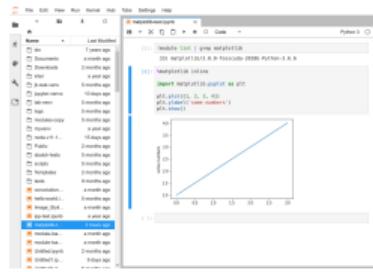
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# Recap: Access the ZIH HPC System

## JupyterHub

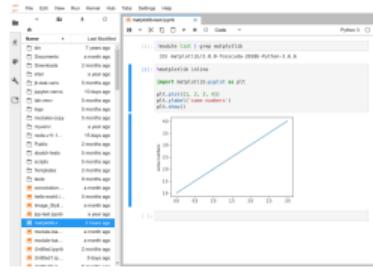
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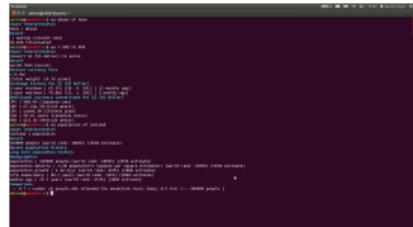
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## SSH connection (CLI)

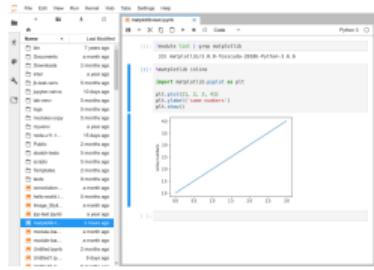
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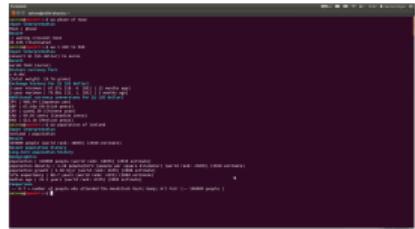
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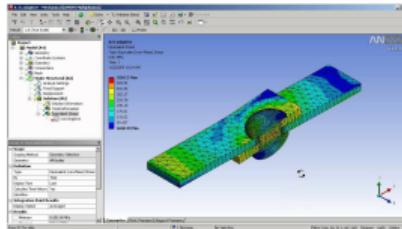
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## Desktop visualization

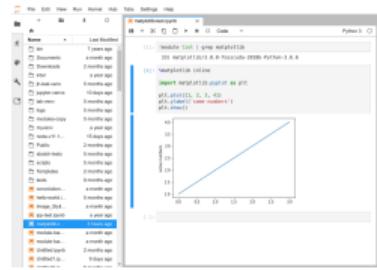
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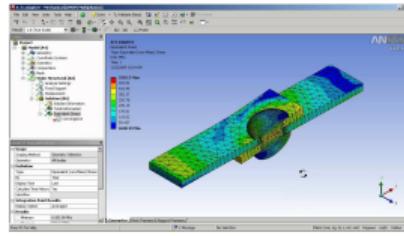
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A screenshot of a terminal window. It shows Python code being run, including imports and a plot command. Below the code, a plot of a linear relationship between two variables is displayed.

```
import matplotlib.pyplot as plt
plt.plot([1, 2, 3, 4], [1, 4, 9, 16])
plt.show()
```

## Desktop visualization

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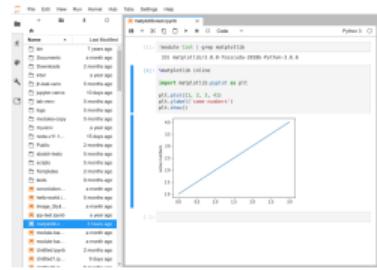
## Note

- When working from **outside of the university network**, the ZIH HPC system can be accessed **only via Virtual Private Network (VPN)**
- Please use **provided** login information for this training

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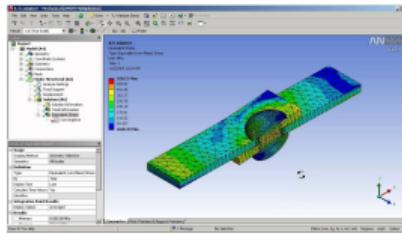
In [1]: import matplotlib.pyplot as plt
        plt.plot([1, 2, 3, 4], [1, 4, 9, 16])
        plt.ylabel('Square')
        plt.xlabel('Number')

Out[1]:
<Figure>

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## Hint

More info on VPN: [↗](#)

# HPC system

- **Facility:** Center for Information Services and High Performance Computing (ZIH)



# HPC system

- **Facility:** Center for Information Services and High Performance Computing (ZIH)
- **Details:**
  - ▶ More than 60,000 cores,
  - ▶ 720 GPUs,
  - ▶ Flexible storage hierarchy with about 16 PB total capacity,
  - ▶ Linux, shared login nodes, filesystems, batchsystem Slurm,
  - ▶ Perfect platform for highly scalable, data-intensive and compute-intensive applications.



# HPC and Big Data Processing - Why it Fits

## Big Data Processing Engines:

- Software designed to make scaling of big data processing easy across node boundaries
- Handle a huge amount of available and distributed compute resources
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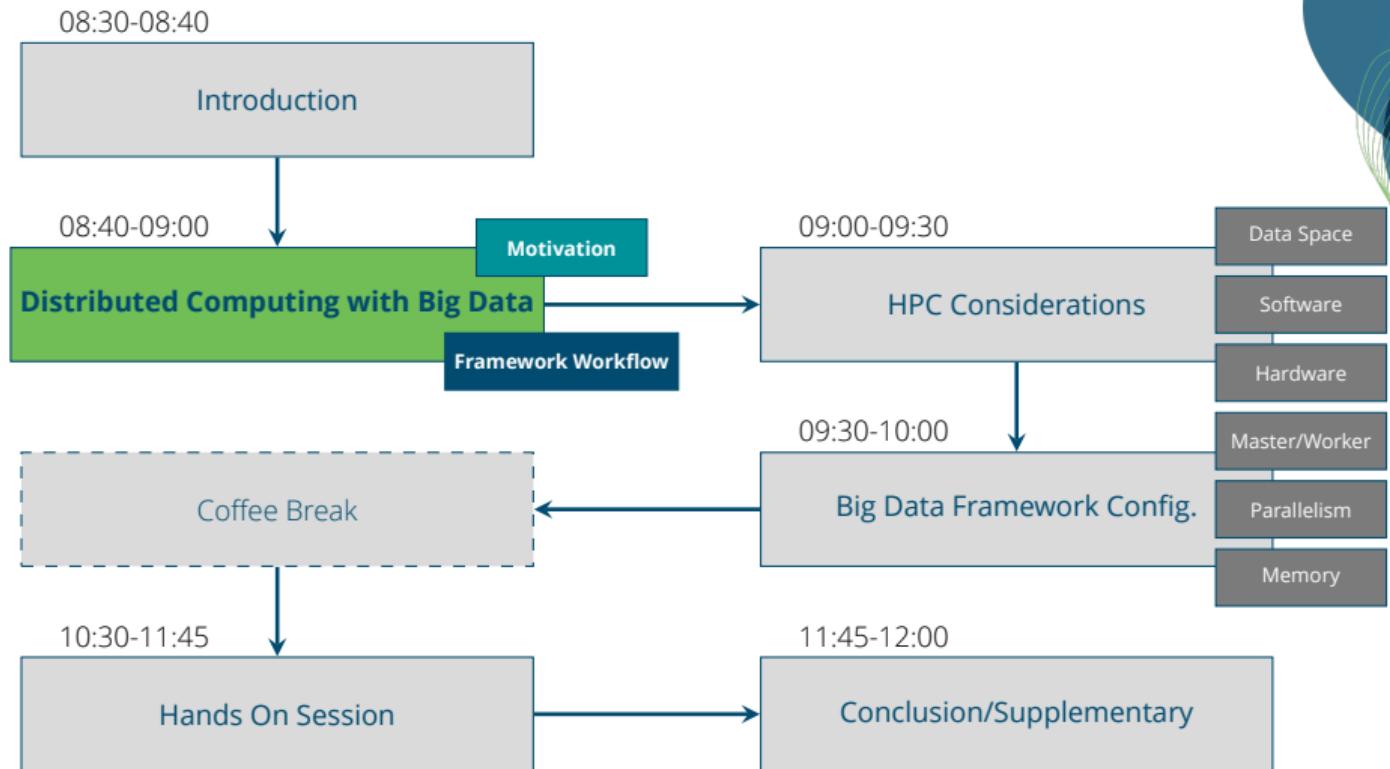
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**Big data processing engines unleash the potentially sheer infinite scalability of HPC clusters.**



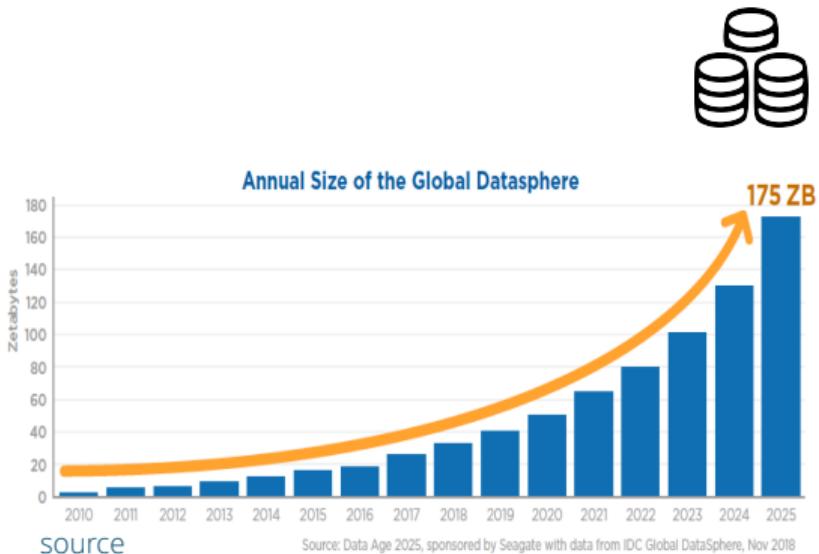


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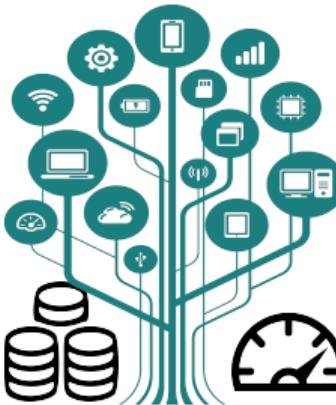
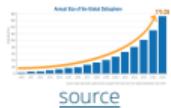
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milisecond latency

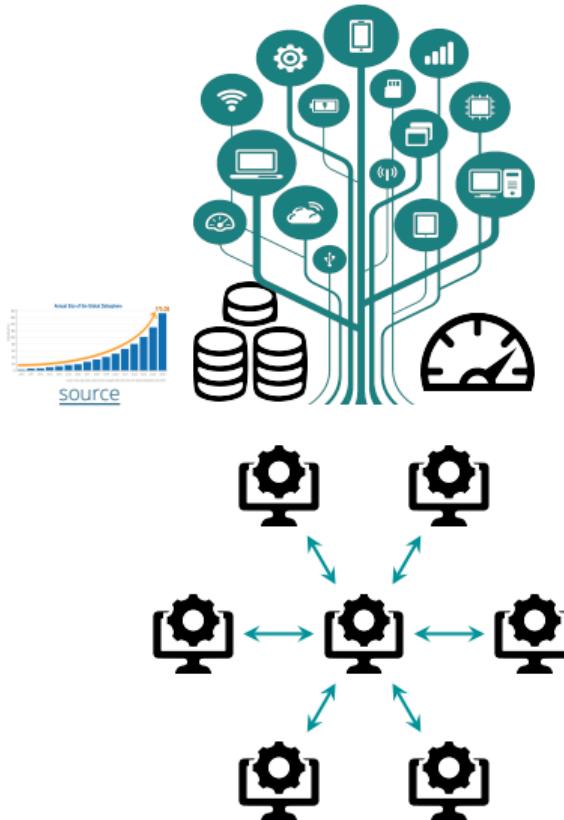
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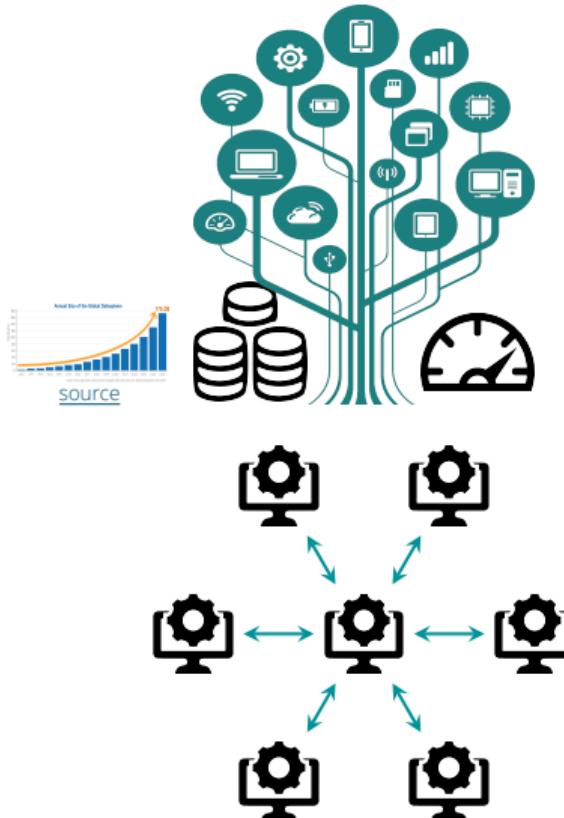
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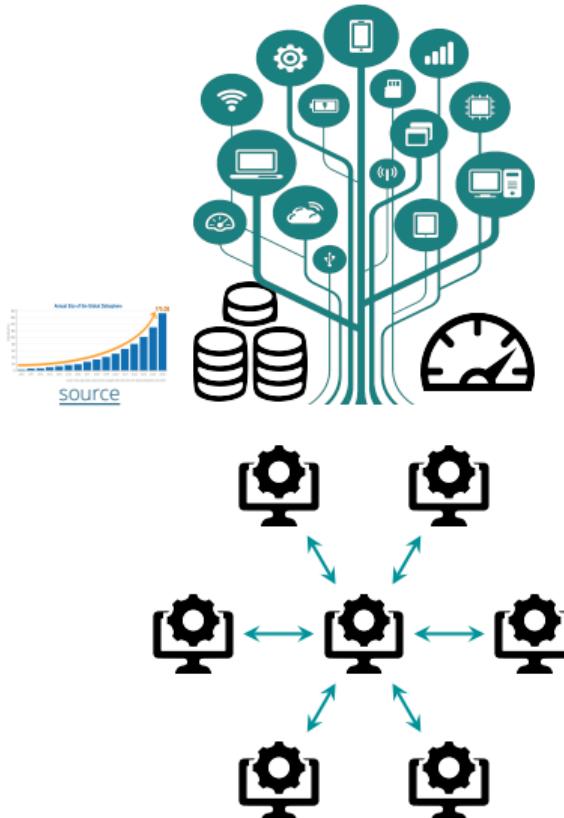
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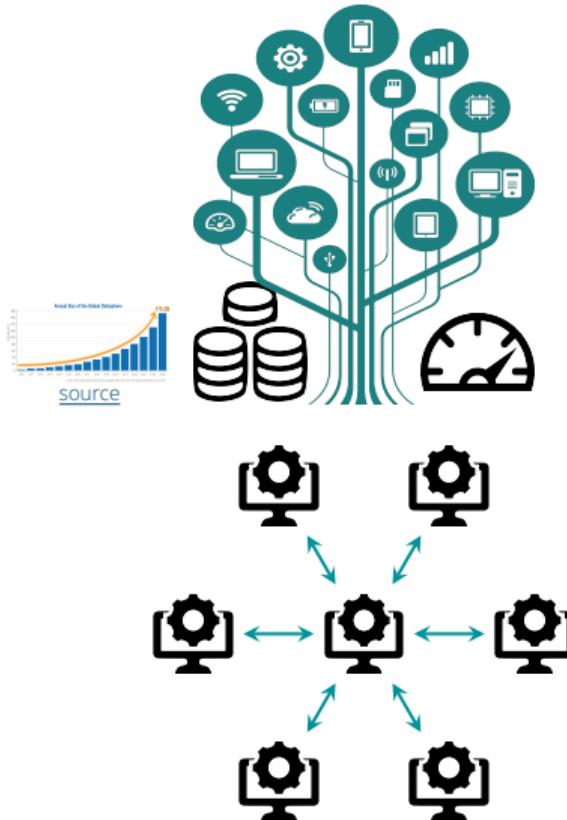
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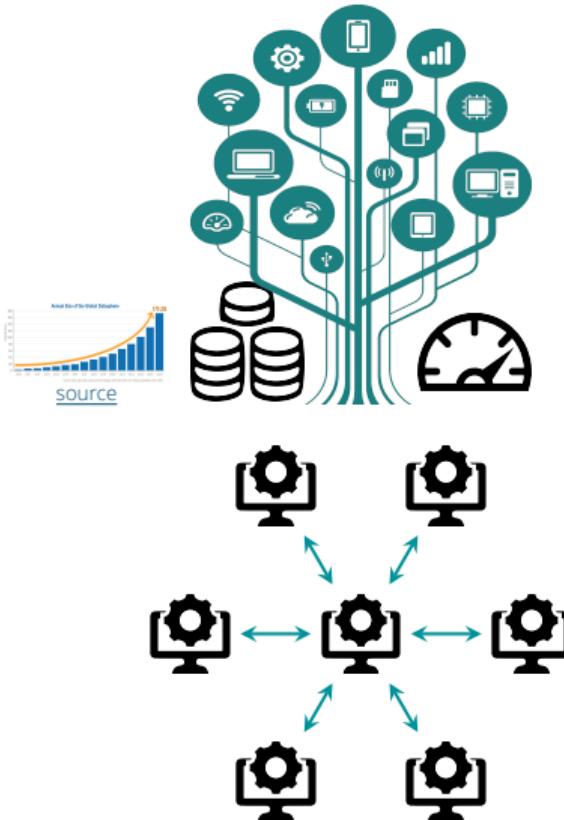
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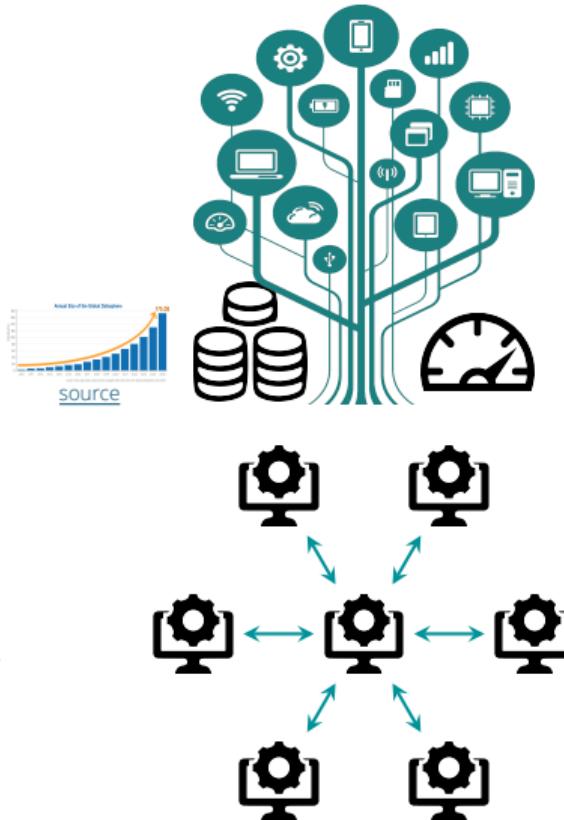
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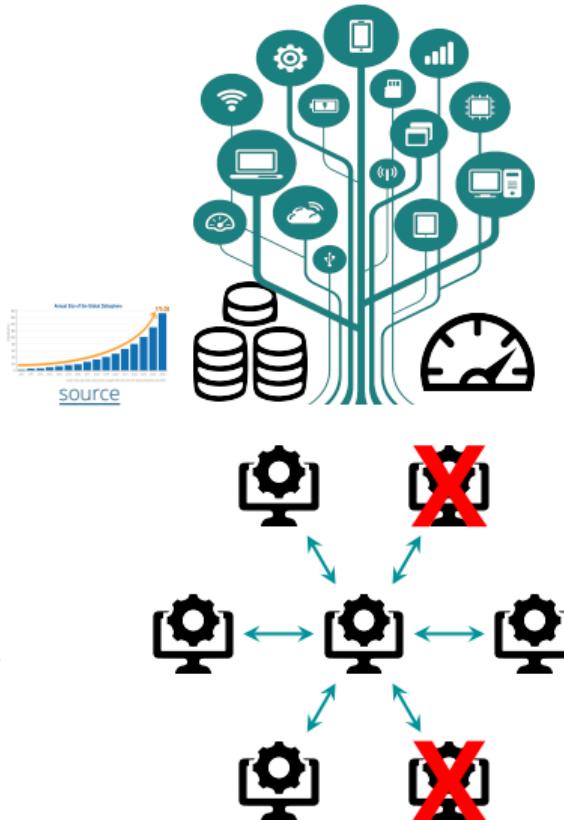
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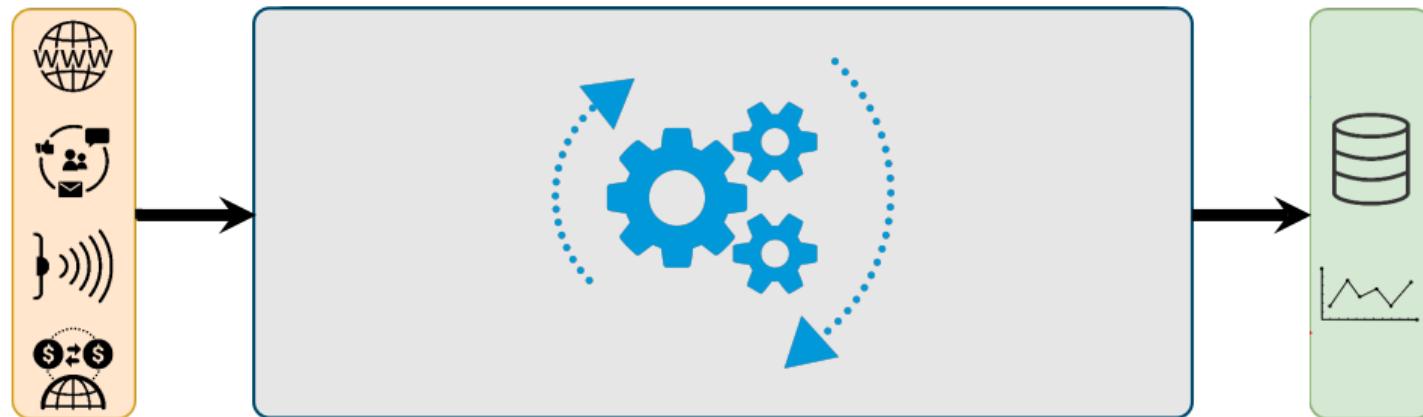


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- Robust and resilient against failure



# Processing Patterns

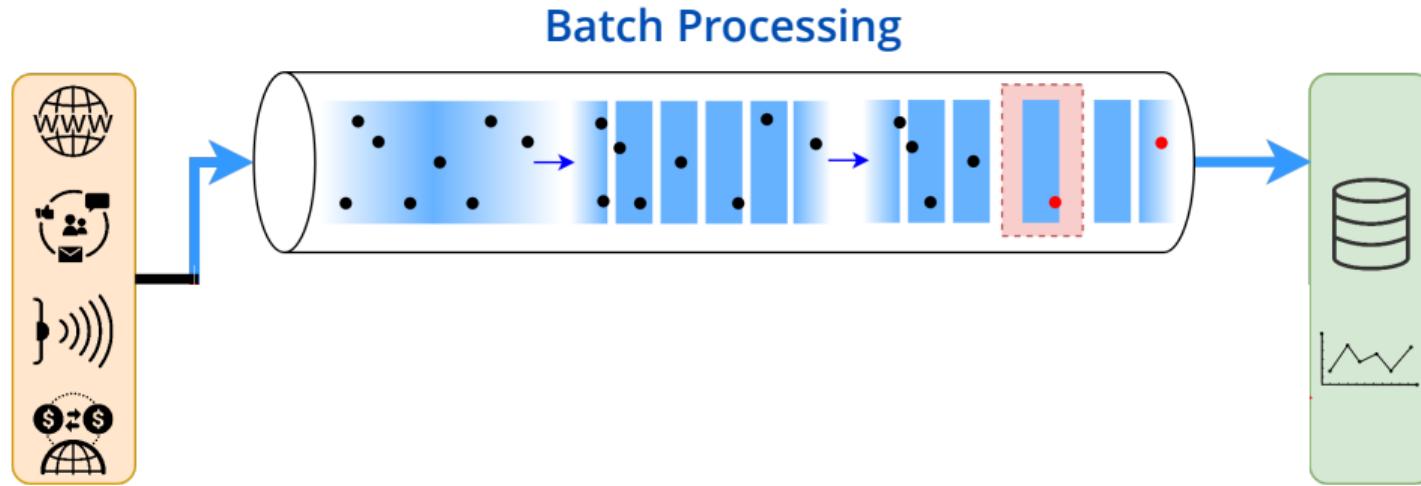


Data Source

Data Processing

Dashboards,  
Storage

# Processing Patterns

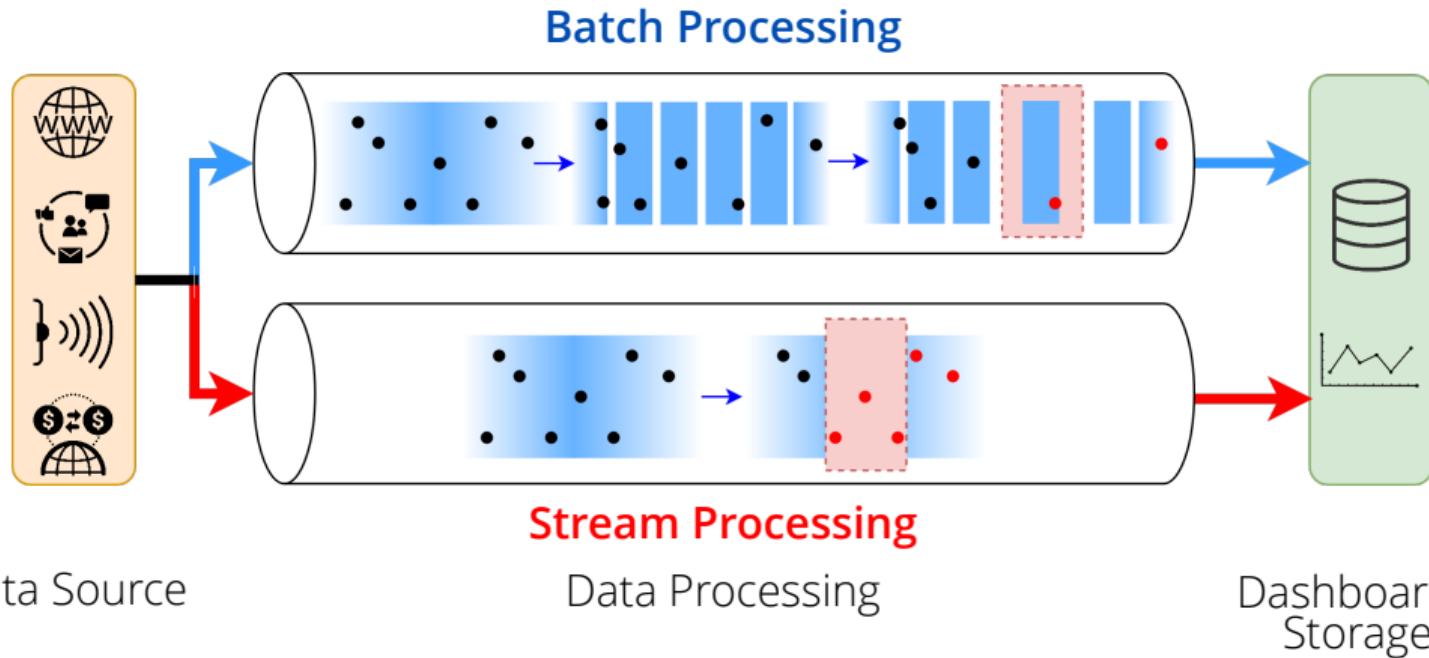


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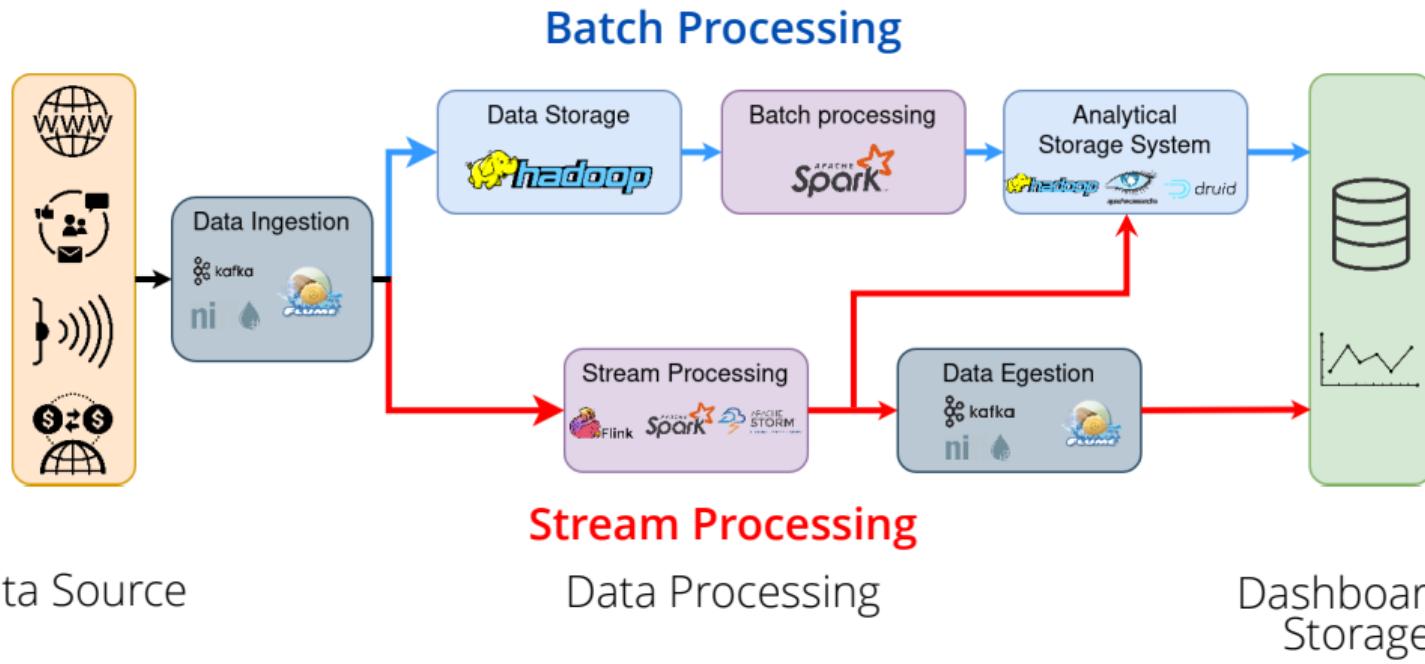
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Components of a typical Big Data Framework:

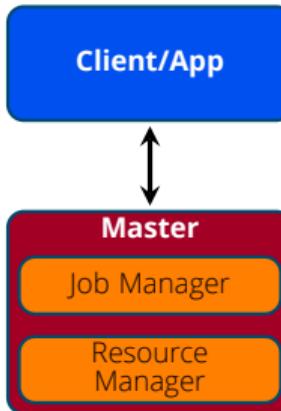
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Entry point of any big data process.

Client/App

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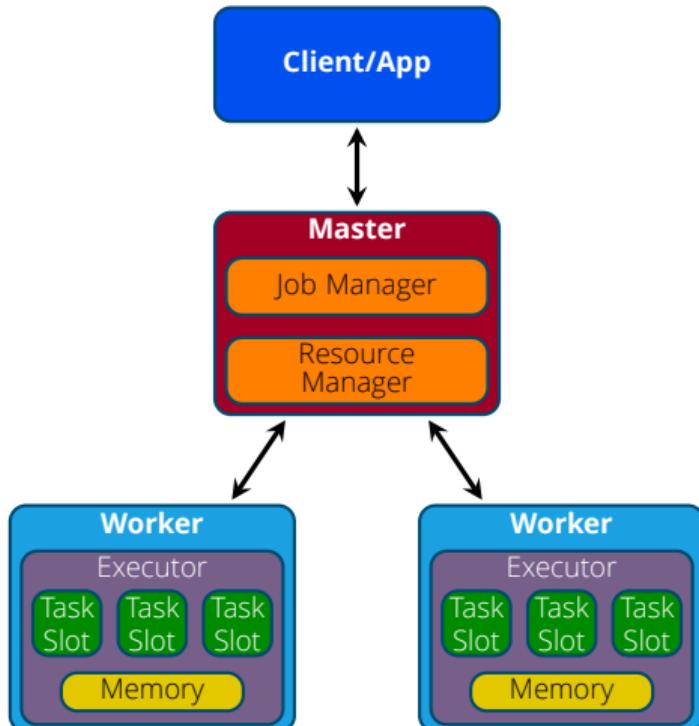
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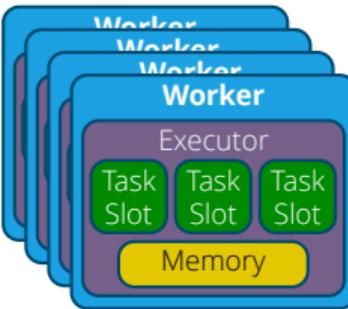
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- **Worker:**
  - ▶ **Executors/Taskmanagers:** These are worker processes consisting of a certain number of task slots.
  - ▶ **Task Slot:** Each task slot contains a single executable task.  
A task is a part of the application.



# General Workflow

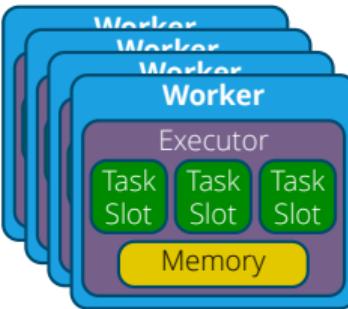
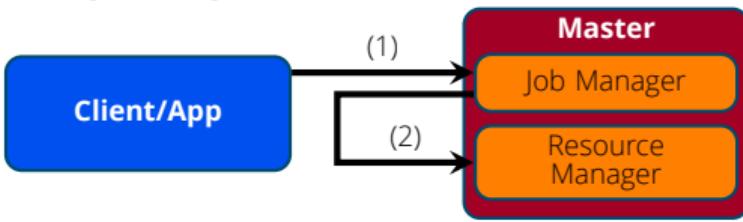


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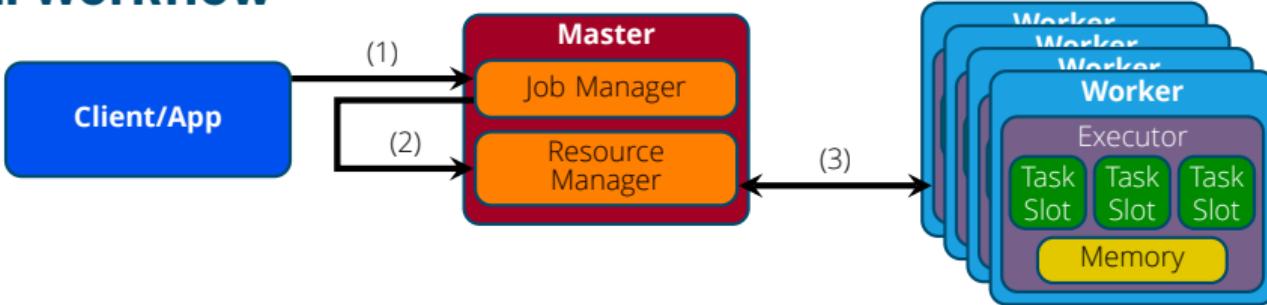
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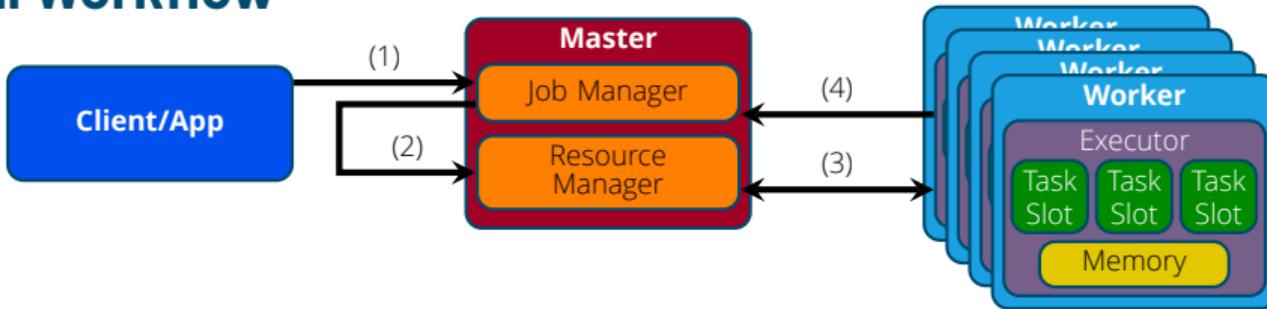
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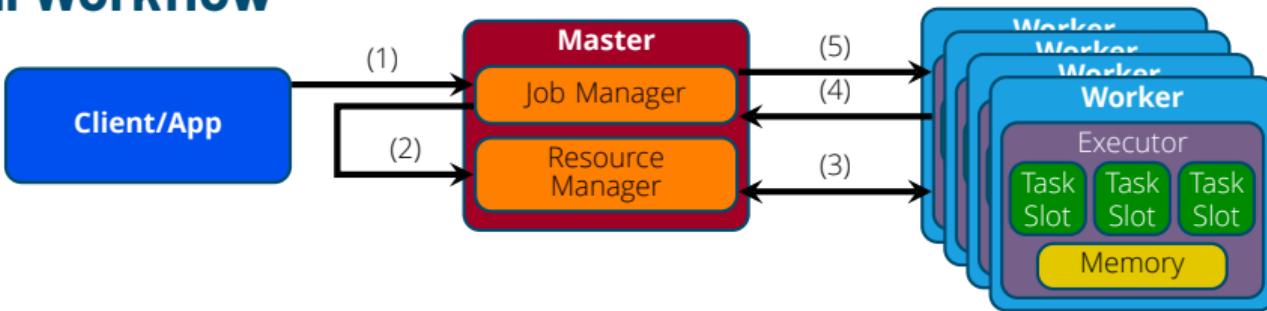
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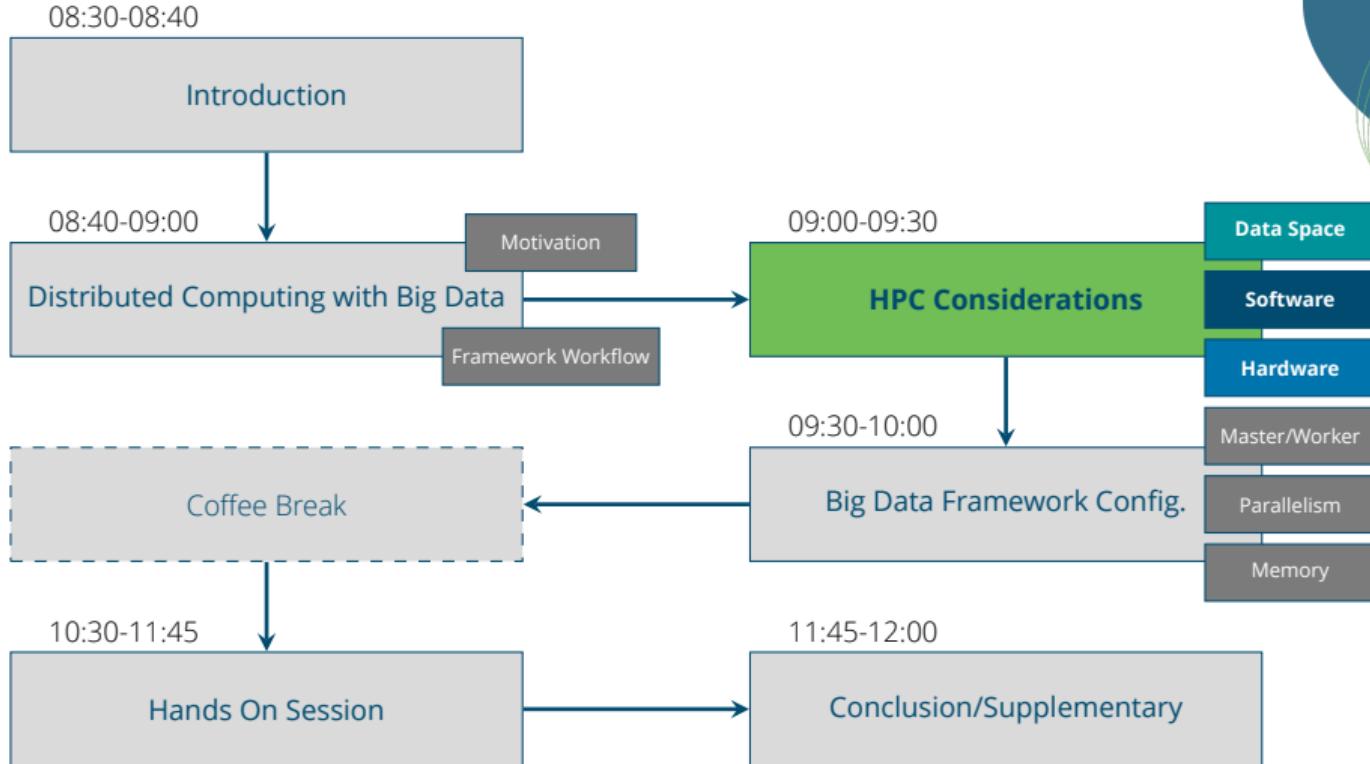


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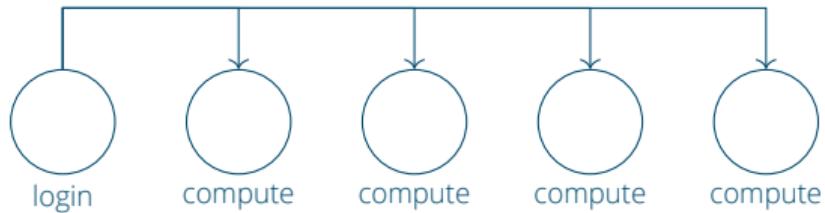
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5. The job manager deploys the tasks to the executors present on the worker nodes.



# Workflow for working with Big Data Frameworks on HPC



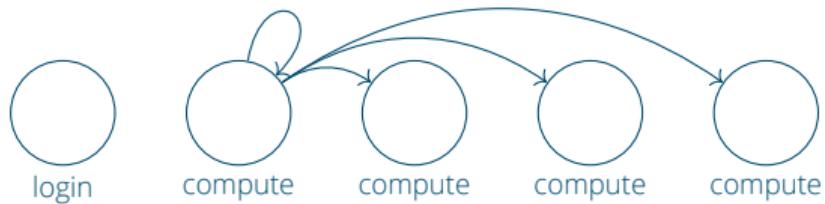
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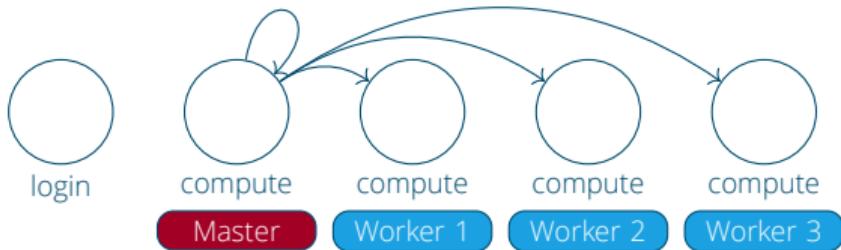
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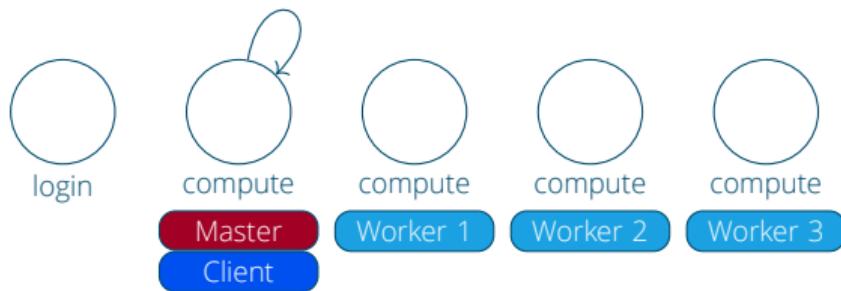
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3. Configure framework on the allocated resources

# Workflow for working with Big Data Frameworks on HPC



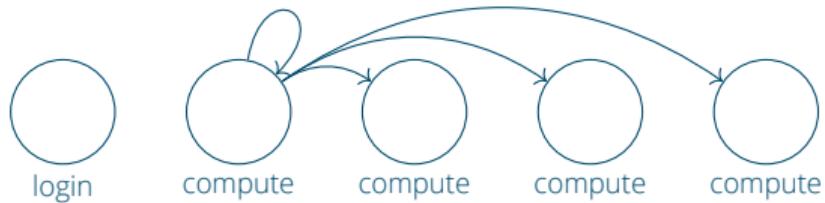
1. Allocate resources from Slurm
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# Workflow for working with Big Data Frameworks on HPC



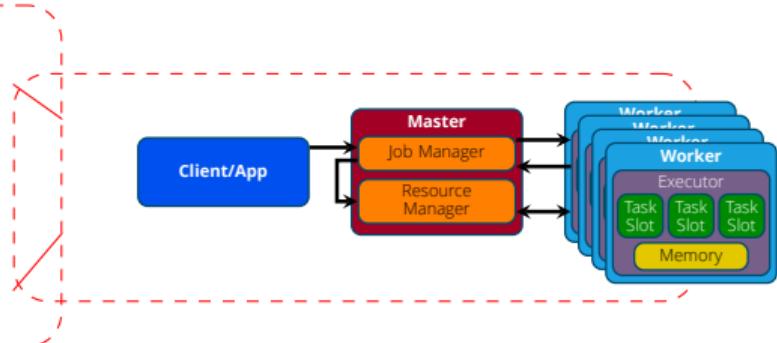
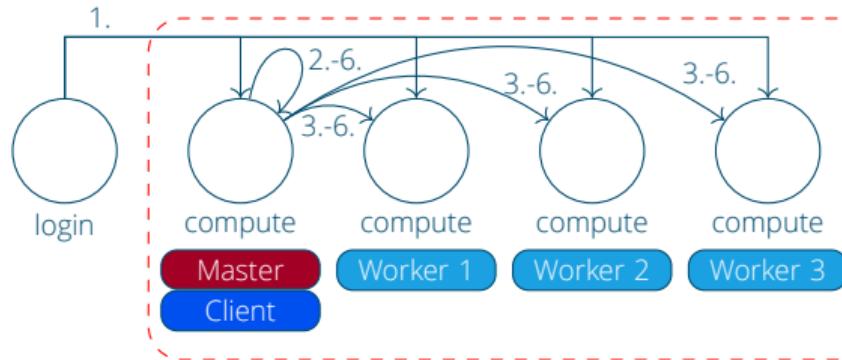
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# Workflow for working with Big Data Frameworks on HPC



1. Allocate resources from Slurm
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6. Tear down the cluster after the pipeline finishes

# Workflow for working with Big Data Frameworks on HPC



1. Allocate resources from Slurm
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# Data Management on HPC System

- Various data storage systems differ in capacity, bandwidth, IOPS rate, etc.
- Organization of these storage systems in **file systems**
- Many file systems, users, data require mechanisms for data management (duration, size, permission)
- The concept of workspaces is used on the ZIH system for data management

## 💡 Hint

For this presentation: a file system refers to a "place" to store data and a **workspace** refers to the "access" to that place.

# Filesystem Storage Overview

- Each filesystem serves a respective capacity, performance, duration, lifetime.
- User creates a workspace with defined expiration date.
- A workspace can be extended multiple times, depending on the filesystem.
- Following is the overview of the filesystem available at ZIH:

Filesystem	Scope	Type	Mount Point	Size	Duration (extensions)
Temporary	Local	Ext4	/tmp or /dev/shm	95 GB	Job Duration
horse	Global temporary	Lustre	/data/horse	20 PB	100 days (x9)
walrus	Global temporary	Lustre	/data/walrus	20 PB	365 days (x2)
weasel	Global temporary	WEKAio	/data/weasel	1 PB	-
User Space	Global permanent	Lustre	/home/<user-id>	50 GB	unlimited
Project Space	Global permanent	NFS	/project/<project-id>	on demand	unlimited
Archive	Inter./ Long term	Tapes	/data/archiv	on demand	3 years

# Workspaces

- On the ZIH system, data has a limited lifetime depending on the filesystem;
- Users create a workspace on filesystems with defined expiration date;
- Data is deleted automatically after expiration.

Some commands to manage workspaces on the ZIH system:

Command	Description
<code>ws_find --list</code>	Find available workspace filesystems
<code>ws_allocate -F &lt;filesystem&gt; &lt;name&gt; &lt;duration&gt;</code>	Allocate workspace
<code>ws_list</code>	List your workspaces and get information
<code>ws_extend -F &lt;filesystem&gt; &lt;name&gt; &lt;duration&gt;</code>	Extend workspace

## 💡 Hint

[https://compendium.../data\\_lifecycle/workspaces/](https://compendium.../data_lifecycle/workspaces/) ↗

# Data Transfer: To/From HPC System

- Using `scp`, `rsync` and `sftp` at:
  - ▶ `dataport1.hpc.tu-dresden.de` or,
  - ▶ `dataport2.hpc.tu-dresden.de`

## Example

```
1 # Copy a file from your workstation to ZIH systems
2 marie@local$ scp !*<file> dataport1.hpc.tu-dresden.de:<target-location>*!
3 # Add -r to copy the whole directory
4 marie@local$ scp !*\{\color{blue}-r\} <directory> dataport1.hpc.tu-dresden.de:<target-location>*!
5 # Copy a file from ZIH systems to your workstation
6 marie@local$ scp !*dataport1.hpc.tu-dresden.de:<file> <target-location>*!
```

## Hint

[https://compendium.../data\\_transfer/dataport\\_nodes/](https://compendium.../data_transfer/dataport_nodes/) ↗

# Data Transfer: Within HPC System

- Linux commands like `cp` and `mv` can be used transfer small data

## Example

```
1 # Copy the training data into horse workspace directory
2 marie@login$ cp <my-file> /data/horse/ws/marie-myworkspace/
```

# Data Transfer: Within HPC System

- Linux commands like `cp` and `mv` can be used transfer small data

## Example

```
1 # Copy the training data into horse workspace directory
2 marie@login$ cp <my-file> /data/horse/ws/marie-myworkspace/
```

- Datamovers are used to move data faster within the ZIH HPC system.

- ▶ For using such datamover machines, you have to use commands prefixed with `dt`: `dtcp` , `dtrsync` , `dttar` , `dtls`
- ▶ `dtqueue --me` to check the status of the data transfer
- ▶ These commands create a Slurm job with dedicated resources to conduct the data handling/transfer.

## Example

```
1 # dtcp for copying data from one filesystem/location to another filesystem/location
2 marie@login$ dtcp !*<\color{blue}-r*>! !*<fs\_origin>/results <fs\_destination>/*
3
4 # dtrsync for moving data from one filesystem/location to another filesystem/location
5 marie@login$ dtrsync !*<fs\_origin>/ws/results <fs\_destination>/ws/ws-archive/*
6
7 # dttar for archive data "results.gz" from one filesystem/location to another filesystem/location
8 marie@login$ dttar !*\color{blue}-czf*! !*<fs\_destination>/results.tgz <fs\_origin>/ws/results*
```

# Compute Hardware at ZIH

ZIH HPC System consists of heterogeneous compute resources:

- CPU-based (of different manufactures)
- GPU-based (of different manufactures)
- Large shared memory nodes

Name	System	Nodes	Cores/Node	Threads/Core	Memory/Node [in MB]	GPUs/Node
Barnard	CPU	630	104	2	515,000	0
Romeo	CPU	192	128	2	505,000	0
Capella	GPU	144	64	1	768,000	-
Alpha	GPU	37	48	2	990,000	8
Power	GPU	30	44	4	254,000	6
Julia	SMP system	1	896	1	48,390,000	-

## 💡 Hint

[https://compendium.../jobs\\_and\\_resources/hardware\\_overview/](https://compendium.../jobs_and_resources/hardware_overview/) ↗

# Running Programs on an HPC Machine

- user-defined calculations, programs etc. are not run directly and interactively on an HPC system (as commonly on a personal workstation or laptop)
- running some program on an HPC machine means running it within a temporary resource allocation
- the definition of a program and a resource allocation is a **job**

On the ZIH system: job scheduling and workload management with **slurm**

- manages jobs and provides an interface for the users to submit their jobs
- evaluates resource requirements and priorities, distributes jobs to suitable compute nodes -> "job queue"

## Note

Most crucial issue esp. for HPC beginners: You need to specify in advance compute, memory, and time resources according to your program's needs. We will refer to this later.

More details about job schedulers can be found at: [https://hpc-wiki.info/hpc/Scheduling\\_Basics](https://hpc-wiki.info/hpc/Scheduling_Basics)

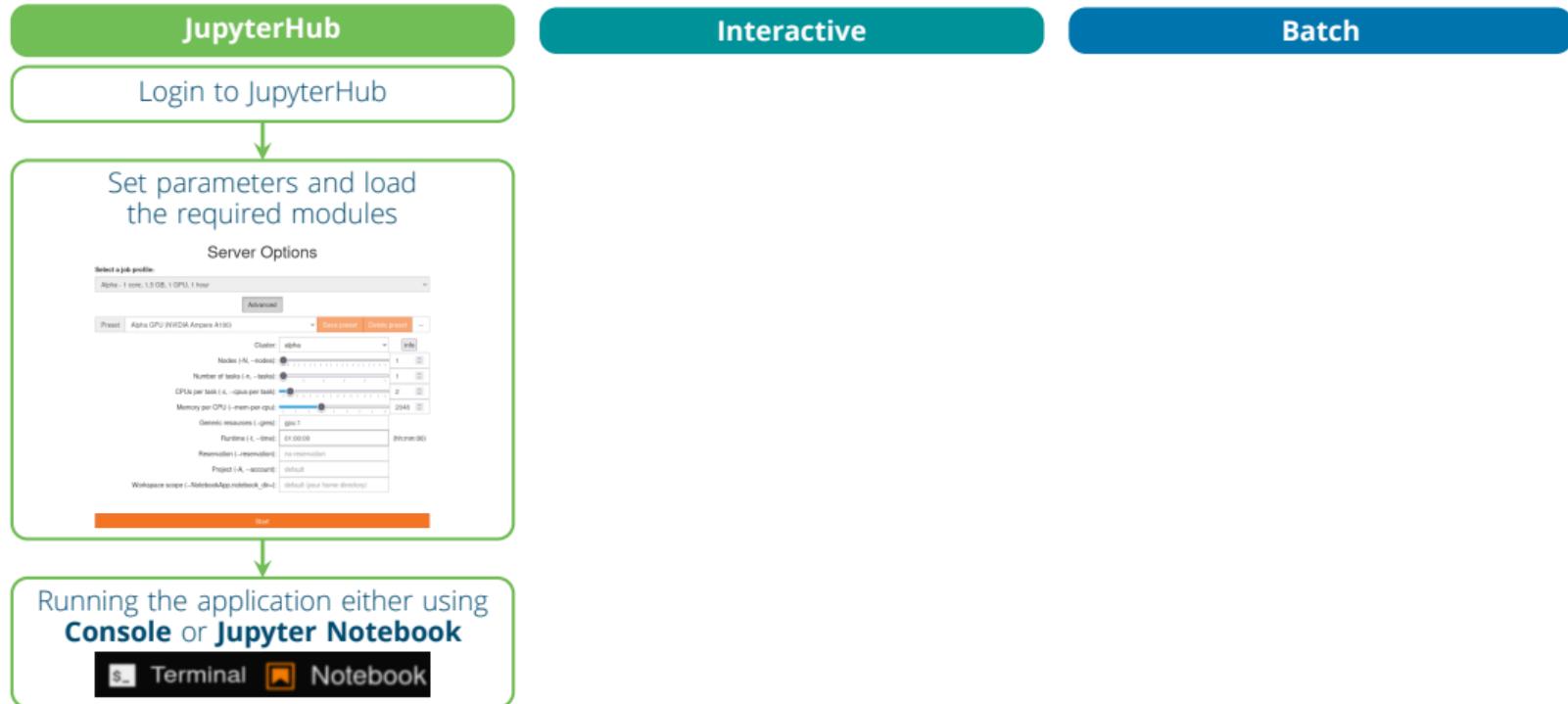
# Job Scheduler Basics: Running Jobs

JupyterHub

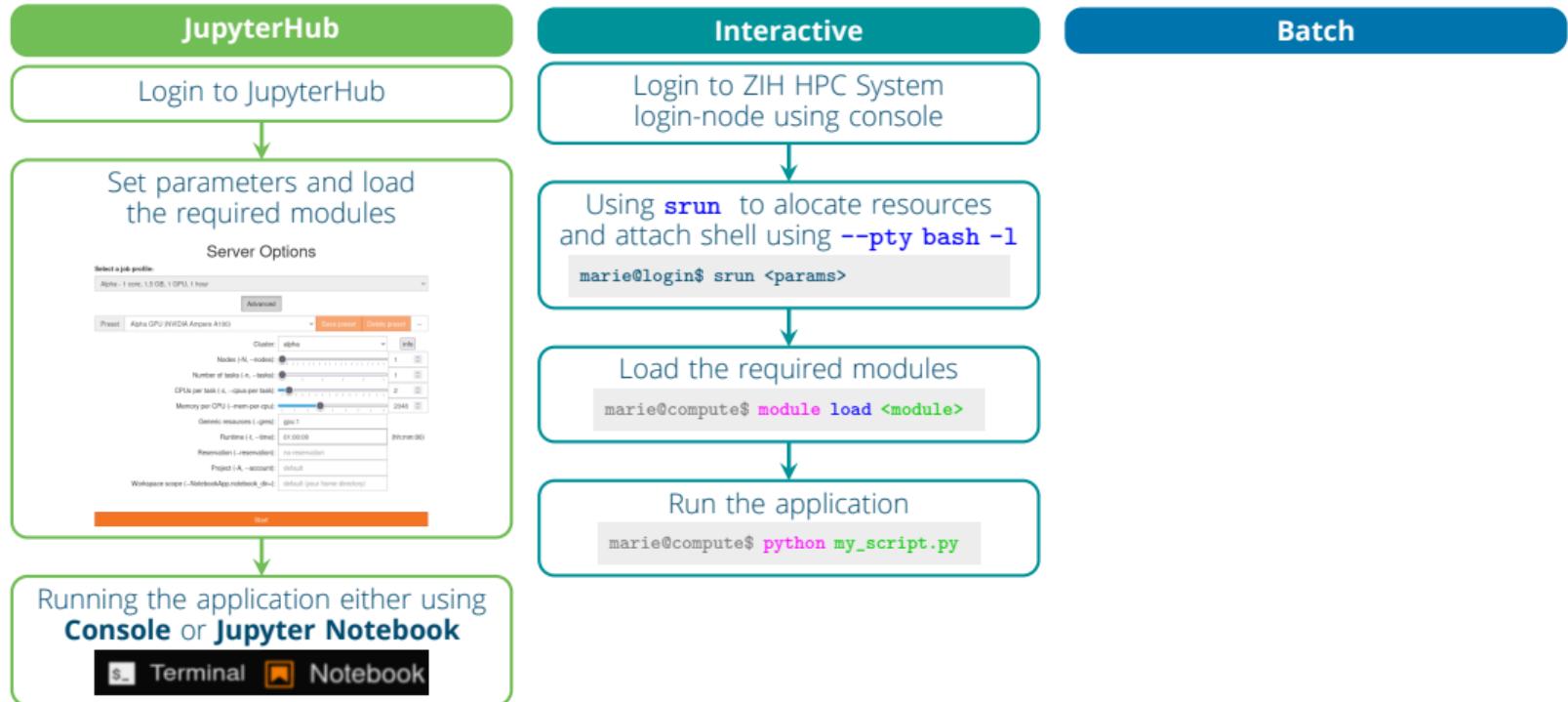
Interactive

Batch

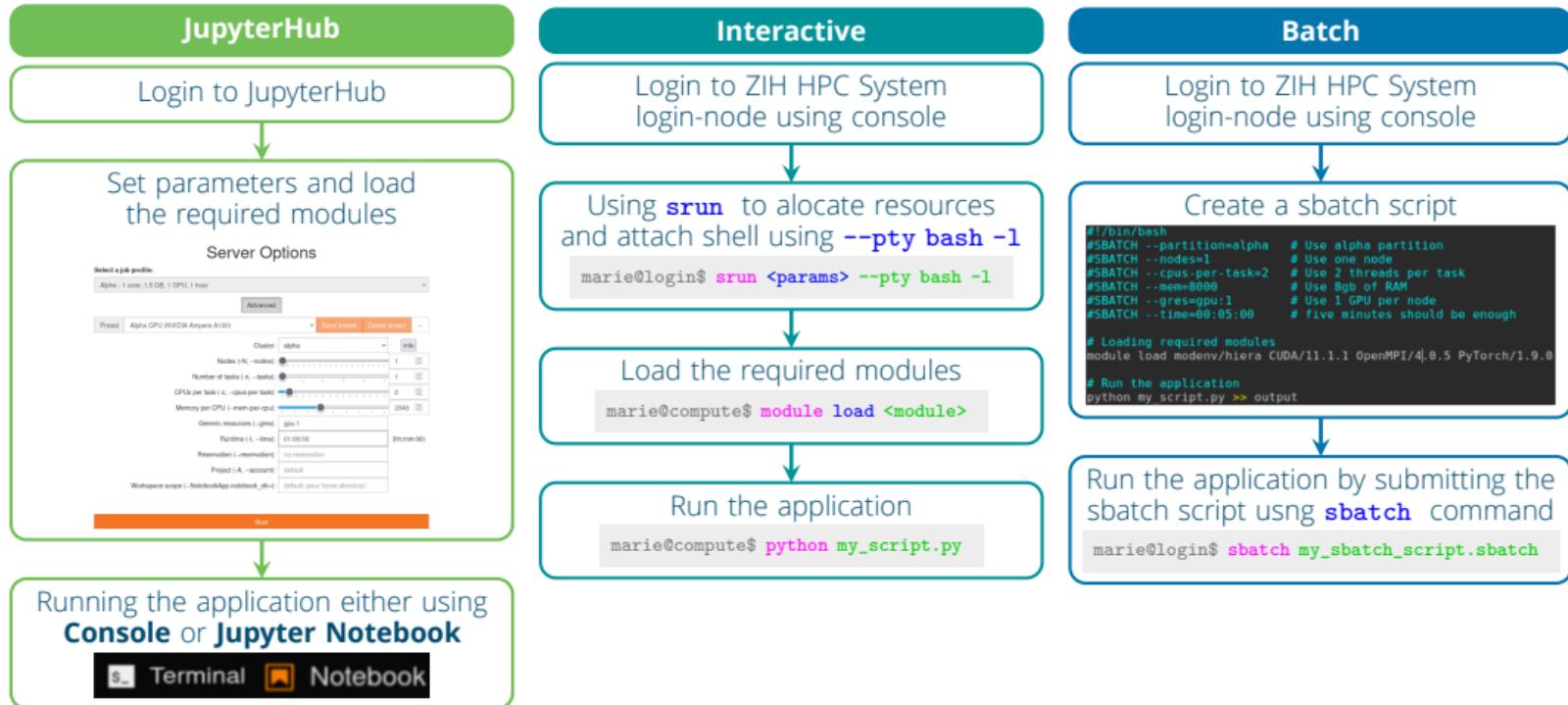
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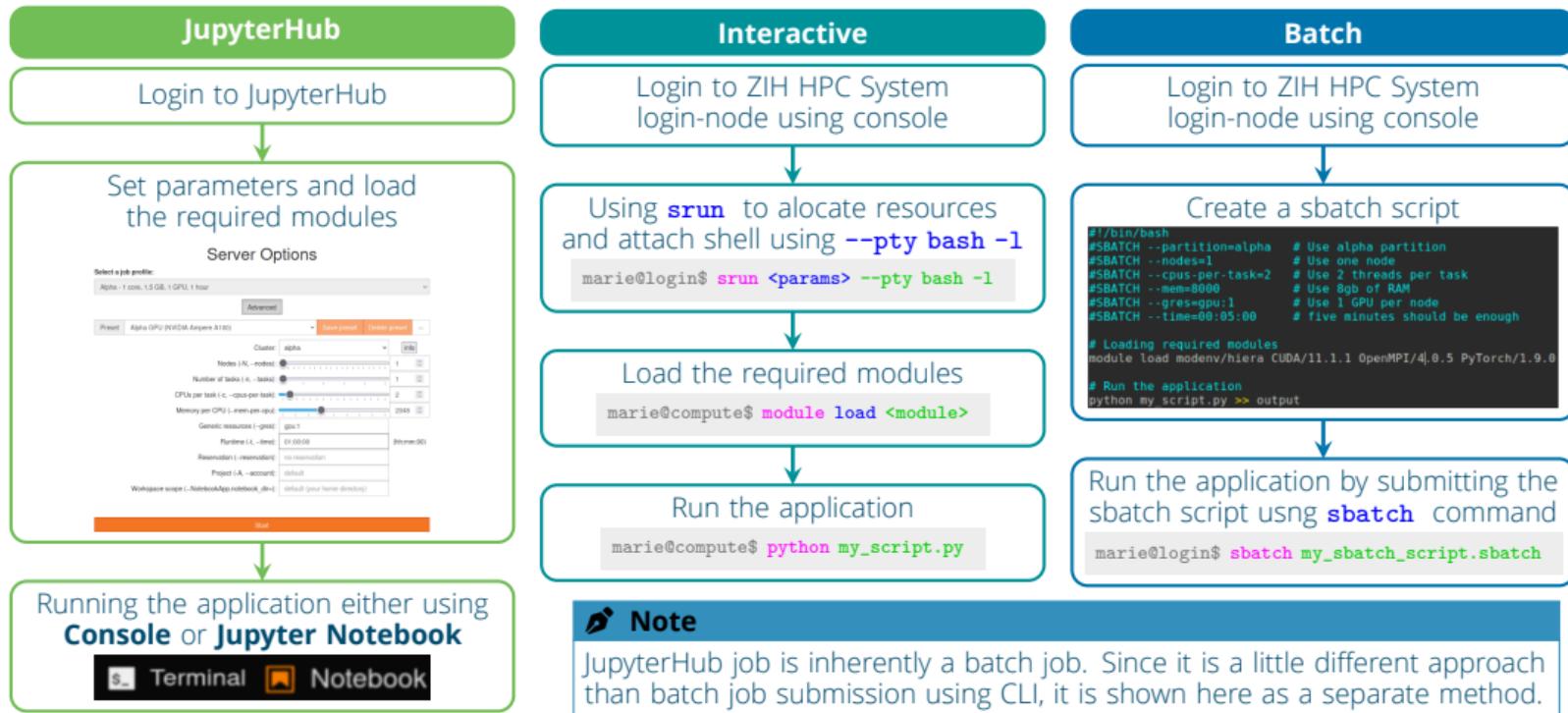
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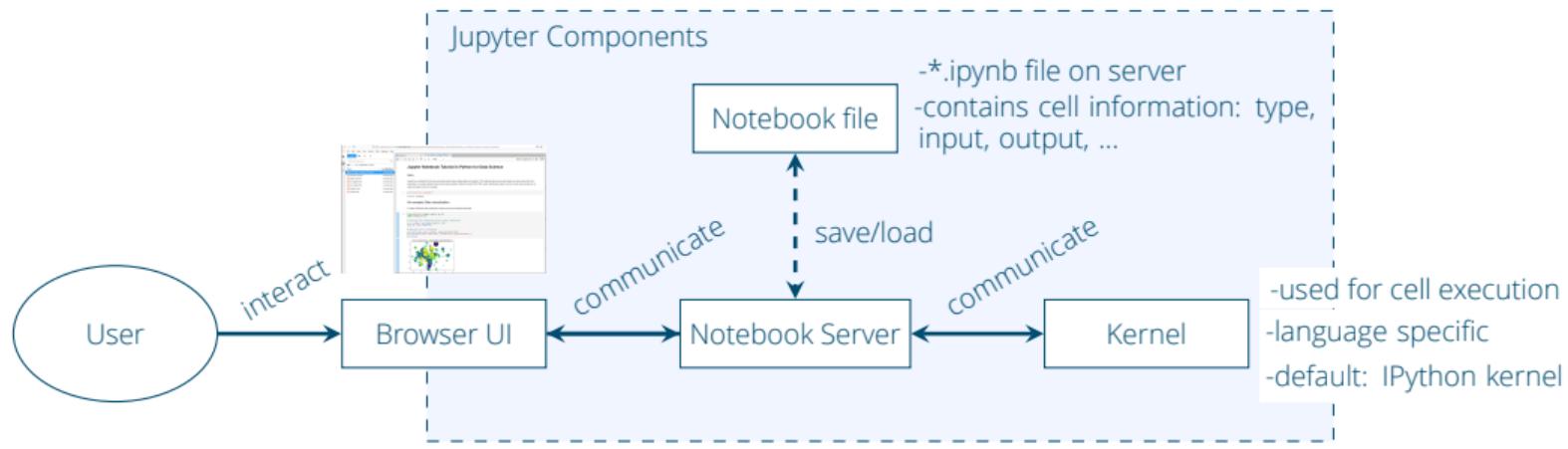
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# Job Scheduler Basics: Running Jobs

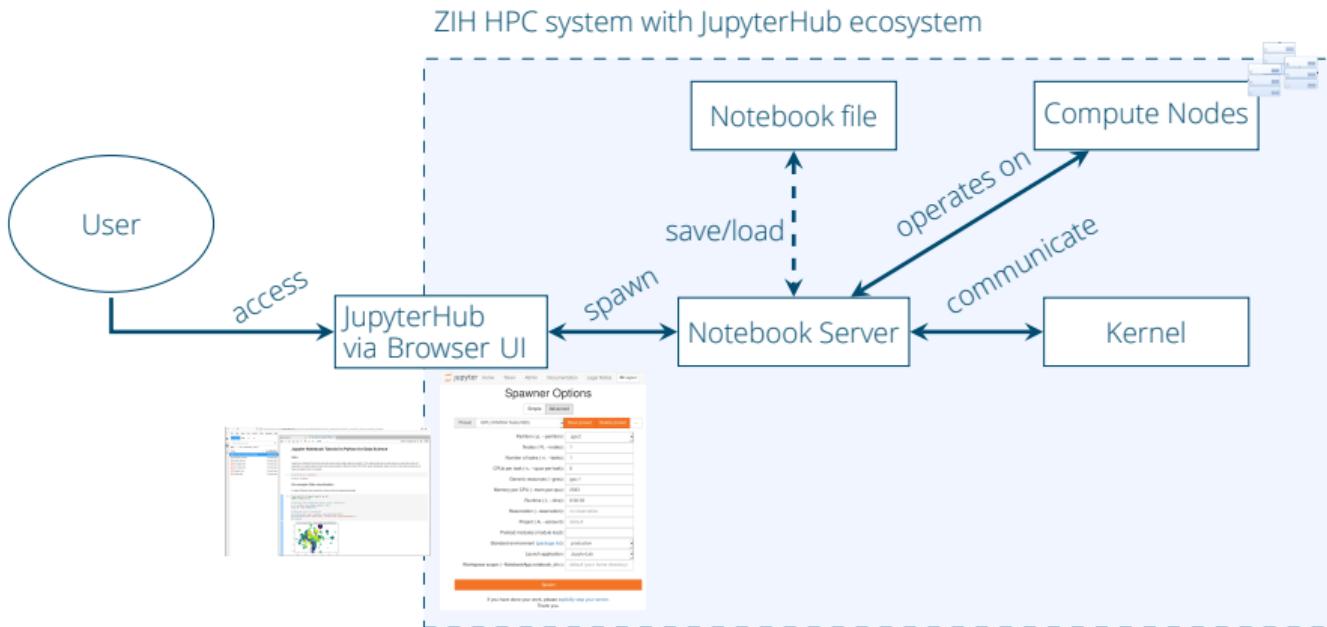


# Jupyter Overview - Behind the Scenes

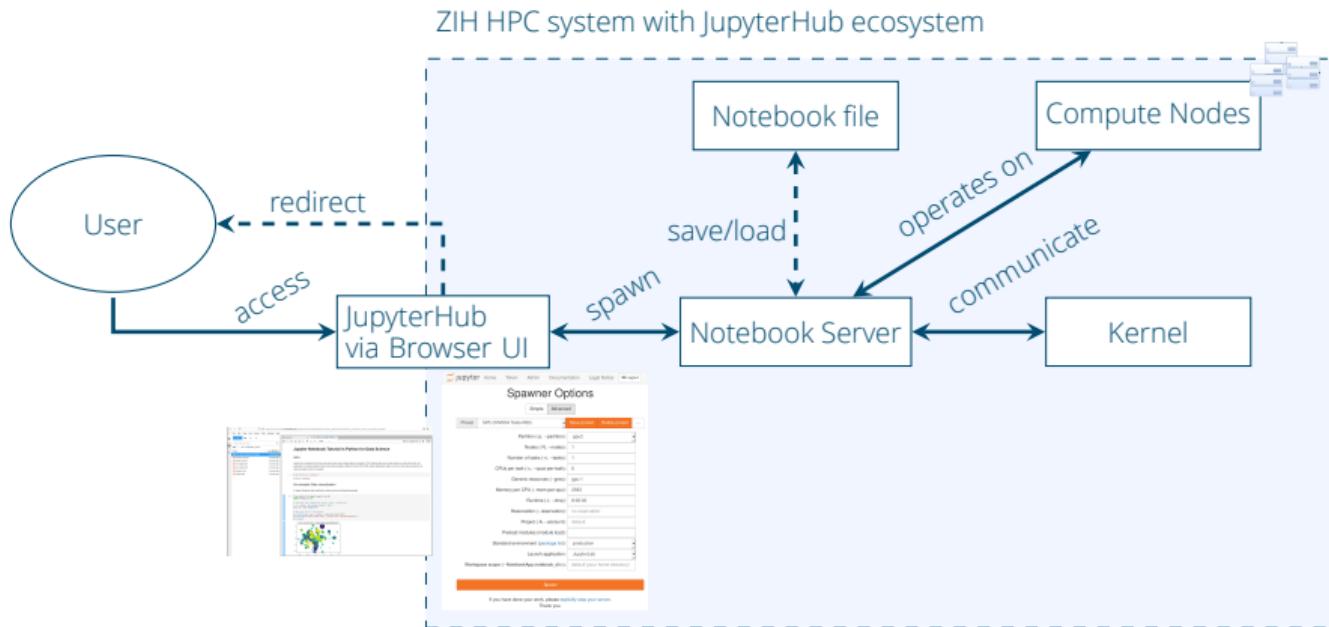


structure according to: [jupyter.readthedocs.io/.../content-architecture](https://jupyter.readthedocs.io/.../content-architecture)

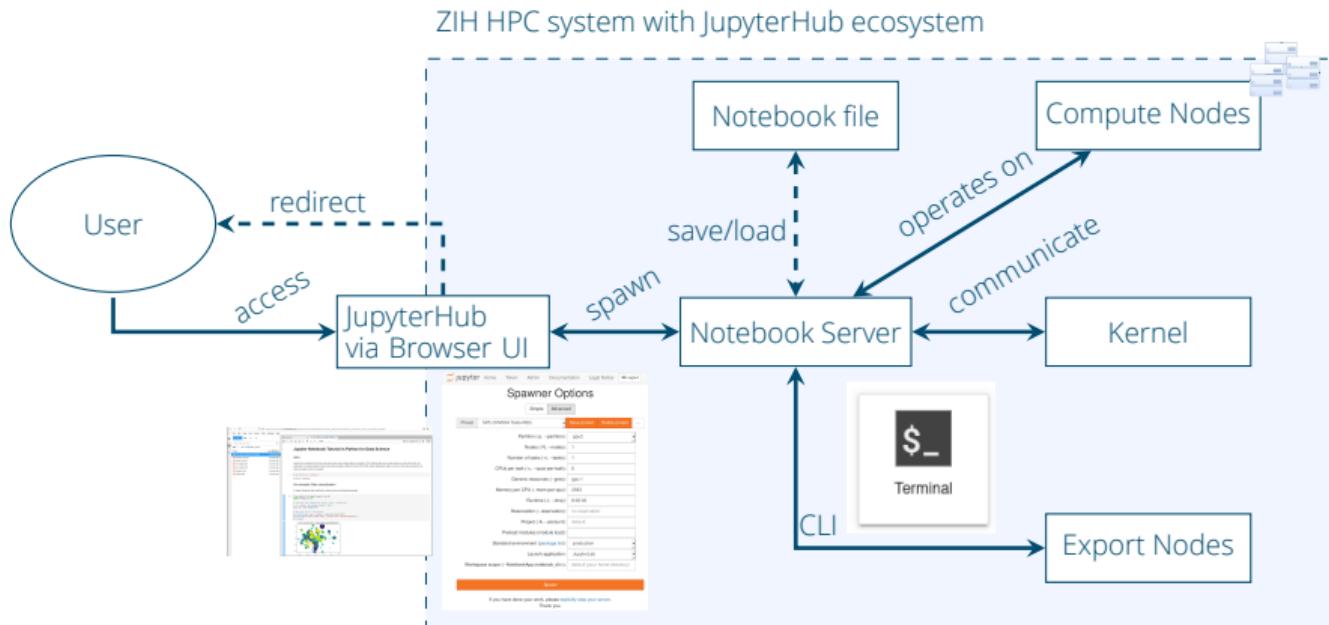
# Access the ZIH System via JupyterHub

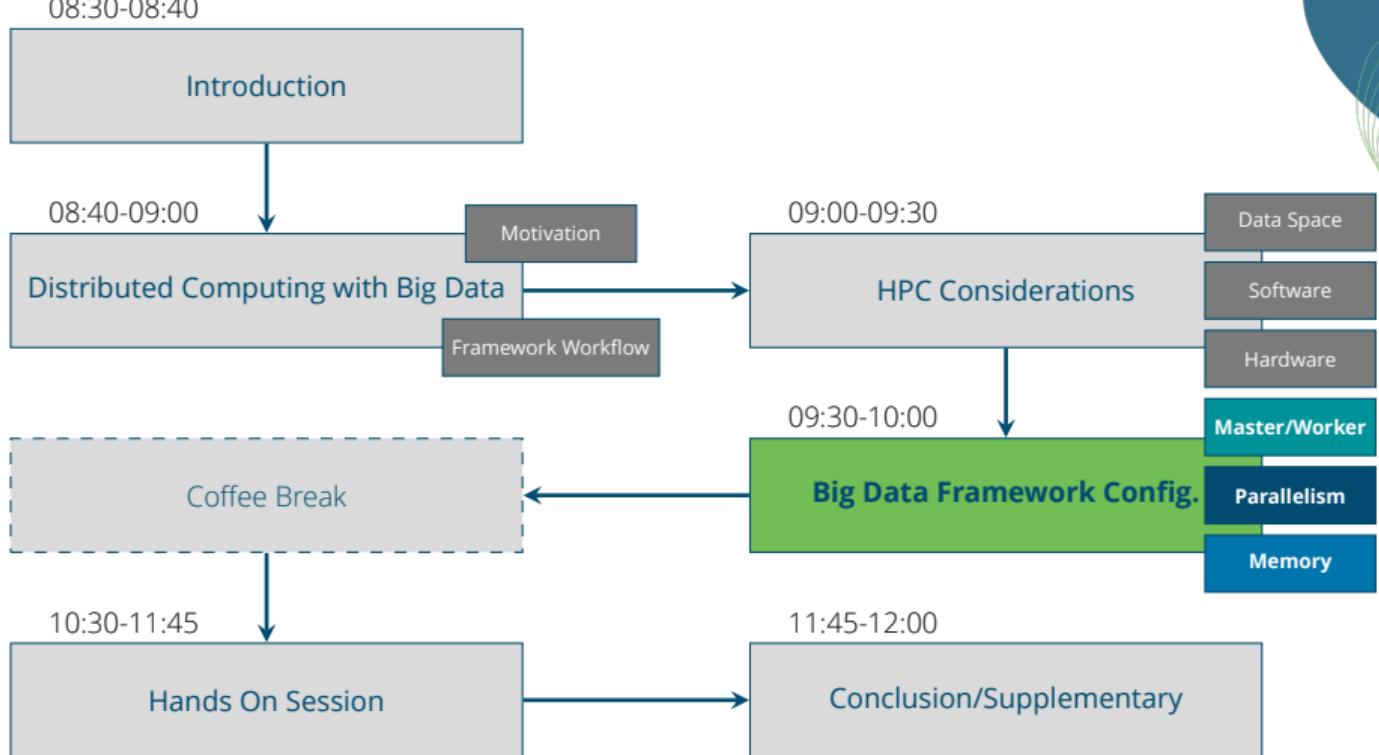


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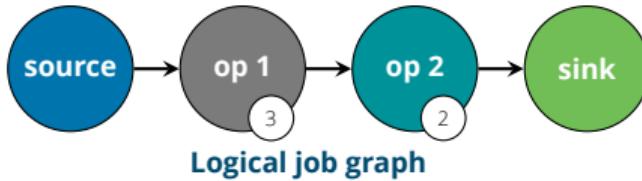


# Parallelism: Job Graphs

- Any big data processing job can be represented using a job graph (also known as a data flow graph), which shows how data flows.

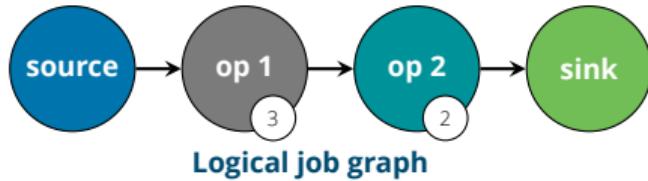
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- Any big data processing job can be represented using a job graph (also known as a data flow graph), which shows how data flows.
- **Logical job graph** depicts a high-level overview of a job. A node in a logical job graph represents the processes or operations, while edges show where the data flows between these operators.

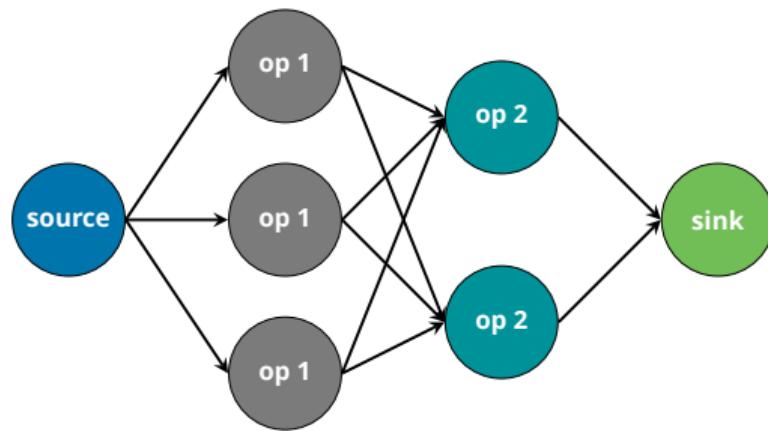


# Parallelism: Job Graphs

- Any big data processing job can be represented using a job graph (also known as a data flow graph), which shows how data flows.
- Logical job graph** depicts a high-level overview of a job. A node in a logical job graph represents the processes or operations, while edges show where the data flows between these operators.
- Physical job graph**, which is derived from the logical job graph, shows how the processes are actually implemented on a system. It considers parallelism, where each node represents a task.

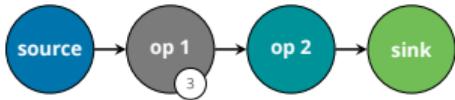


Logical job graph

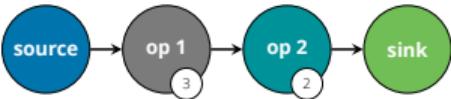


Physical job graph

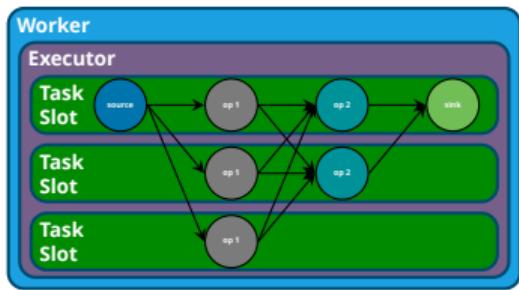
# Parallelism: Job Graphs (cont..)



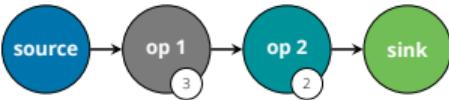
# Parallelism: Job Graphs (cont..)



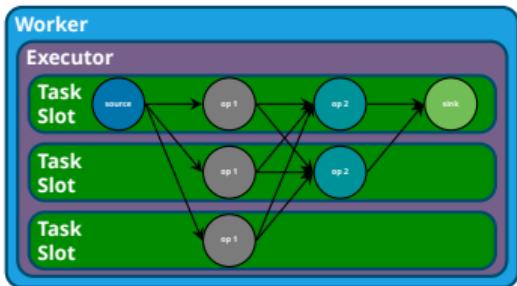
1 Worker, 1 Executor/Worker,  
3 Task-Slots/Executor



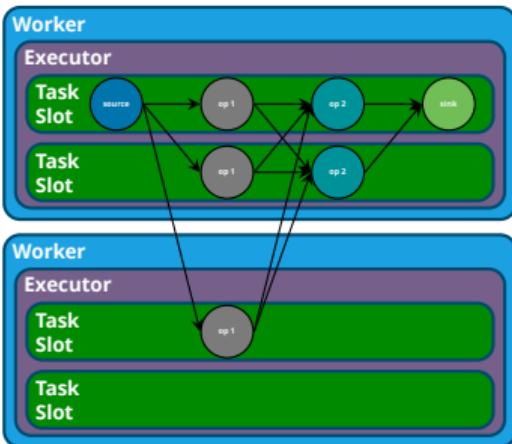
# Parallelism: Job Graphs (cont..)



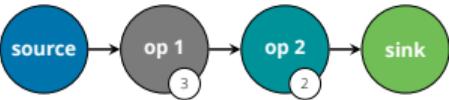
1 Worker, 1 Executor/Worker,  
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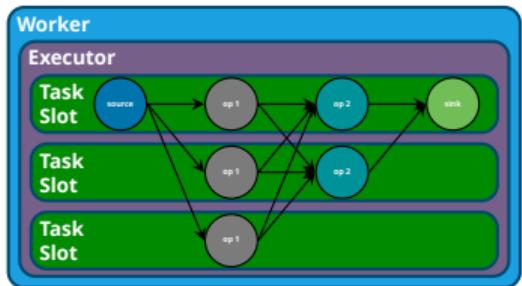
2 Workers, 1 Executor/Worker,  
2 Task-Slots/Executor



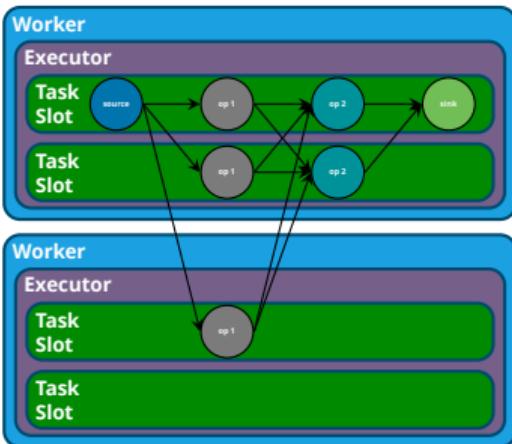
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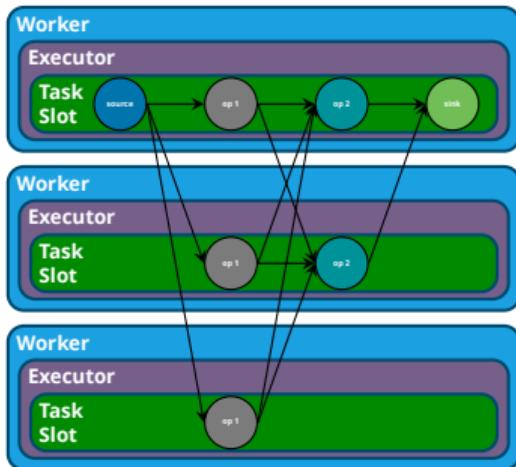
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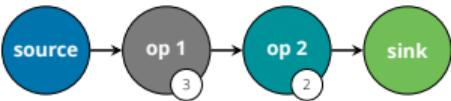
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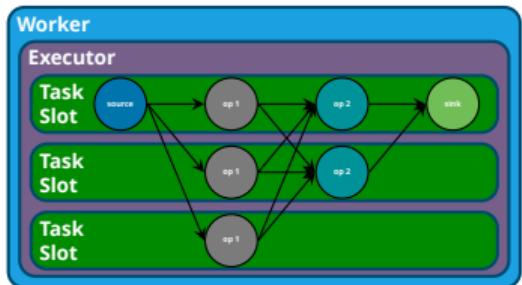
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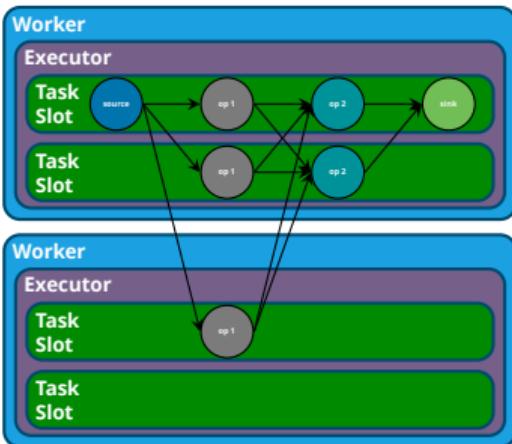
# Parallelism: Job Graphs (cont..)



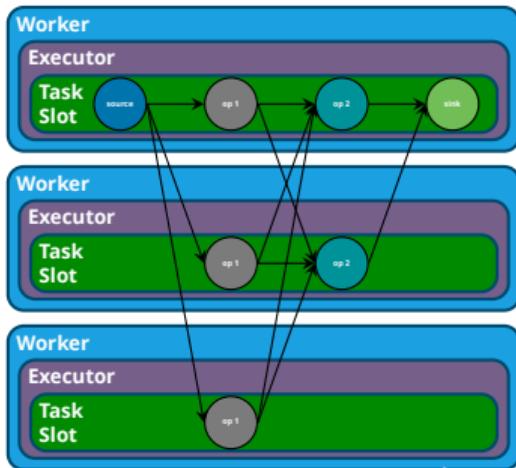
1 Worker, 1 Executor/Worker,  
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2 Workers, 1 Executor/Worker,  
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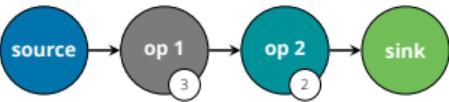


3 Workers, 1 Executor/Worker,  
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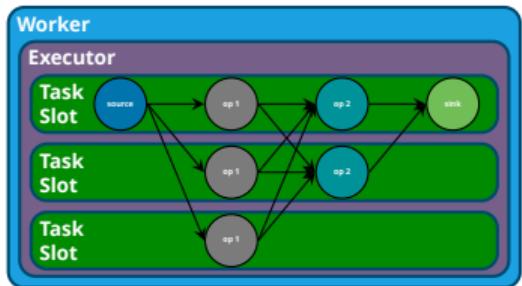


Communication overhead increases

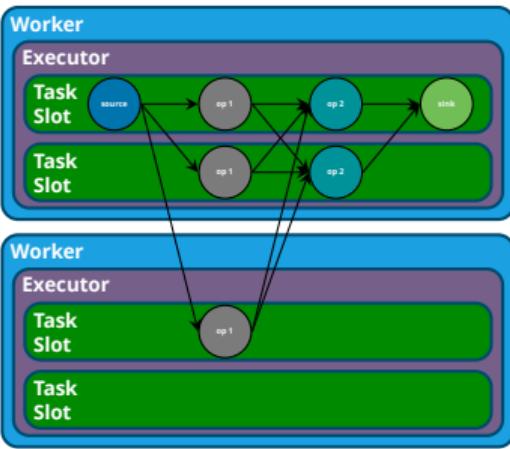
# Parallelism: Job Graphs (cont..)



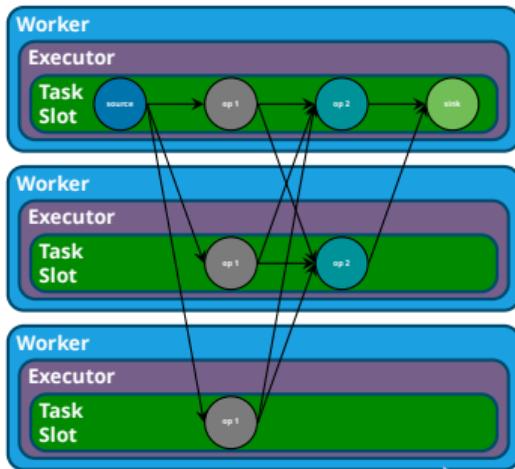
1 Worker, 1 Executor/Worker,  
3 Task-Slots/Executor



2 Workers, 1 Executor/Worker,  
2 Task-Slots/Executor



3 Workers, 1 Executor/Worker,  
1 Task-Slot/Executor



Communication overhead increases

The CPU and memory requirements of each worker node increase

# Parallelism

Apache Flink (v1.15.0) 

Apache Spark (v3.3.0) 

Tskmgr=Taskmanager

# Parallelism

Apache Flink (v1.15.0) 

- Configuring task slots per taskmanager:

►  $\#Slots/Tskmgr = \frac{\#CPU/Node}{\#Tskmgr/Node} = \#CPU/Node$

► **flink-conf.yaml**

```
taskmanager.numberOfTaskSlots: <INTEGER>
```

- Configuring default parallelism:

►  $Parallelism_{max} = \#Slots/Tskmgr \times \#Nodes =$

$\#CPU/Node \times \#Nodes$

► **flink-conf.yaml**: Default=1

```
parallelism.default: <INTEGER>
```

Apache Spark (v3.3.0) 

Tskmgr=Taskmanager

# Parallelism

## Apache Flink (v1.15.0)



- Configuring task slots per taskmanager:

►  $\#Slots/Tskmgr = \frac{\#CPU/Node}{\#Tskmgr/Node} = \#CPU/Node$

► **flink-conf.yaml**

```
taskmanager.numberOfTaskSlots: <INTEGER>
```

- Configuring default parallelism:

►  $Parallelism_{max} = \#Slots/Tskmgr \times \#Nodes = \#CPU/Node \times \#Nodes$

► **flink-conf.yaml**: Default=1

```
parallelism.default: <INTEGER>
```

## Apache Spark (v3.3.0)



- Configuring executor cores:

►  $\#Cores/Executor = \#CPUs/\#Node$

► **spark-env.sh**

```
export SPARK_WORKERS_CORES=<INTEGER>
export SPARK_EXECUTOR_CORES=<INTEGER>
```

- Configuring default parallelism:

►  $Parallelism_{max} = \#Cores/Executor \times \#Nodes$

► **spark-default.conf**: Default = total number of cores allocated to all executors.

```
spark.default.parallelism
```

Tskmgr=Taskmanager

# Aspects of Parallel Programming

- **Applicability:** Not all methods/algorithms are parallelizable, i.e. to be divided into independent sub tasks.
  - ▶ not possible: sequential algorithms (e.g. stochastic gradient descent for machine learning training)
- **Load Balancing and Data Partitioning:** Split data into chunks of comparable size that can be processed in parallel.
- **Communication/Aggregation Overhead:** Running something in parallel needs communication and aggregation of results. Choose a reasonable level of parallelism, but not the max level.

Note that parallel programming is a vast field, and in this workshop, we are only scratching the surface.

# Crucial Aspects When Using Spark

## 1. Lazy Evaluation

- ▶ Transformations like `filter()`, `select()`, are lazy and no execution until an action (e.g., `count()`, `show()`) is triggered.
- ▶ See docs for transformations vs. actions:  
<https://spark.apache.org/docs/latest/rdd-programming-guide.html#transformations>

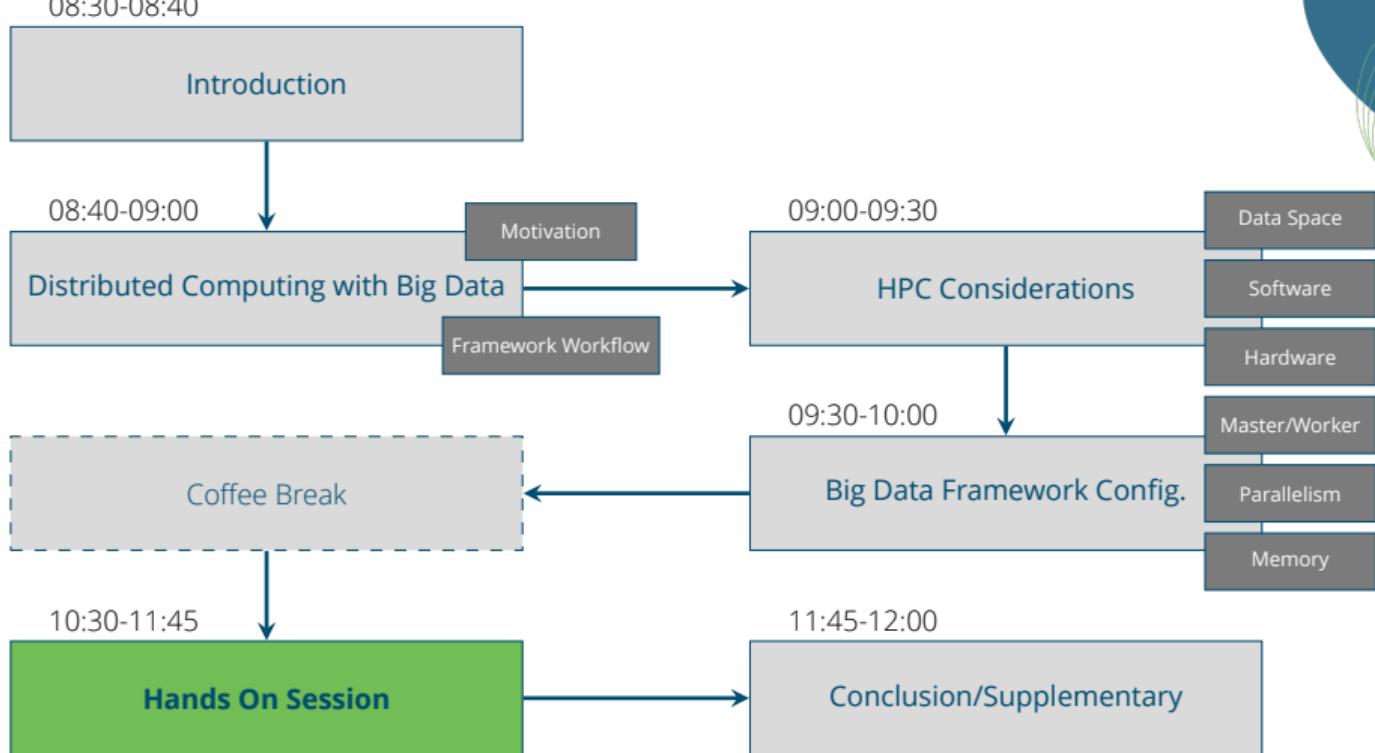
## 2. Shuffling & Partitioning

- ▶ Spark works with distributed data (RDD = resilient distributed dataset)
- ▶ Shuffling is the process of (re-)distributing data chunks among the cluster (caused e.g. by `groupBy`, `join`, `repartition`).
- ▶ Repartition only when needed; use `coalesce()` to reduce partitions without full shuffle.
- ▶ Spark controls the number of partitions internally, but this also can be set by user

### 💡 Hint

Spark has a lot of configurable parameters that need to be considered within development of a concrete application.

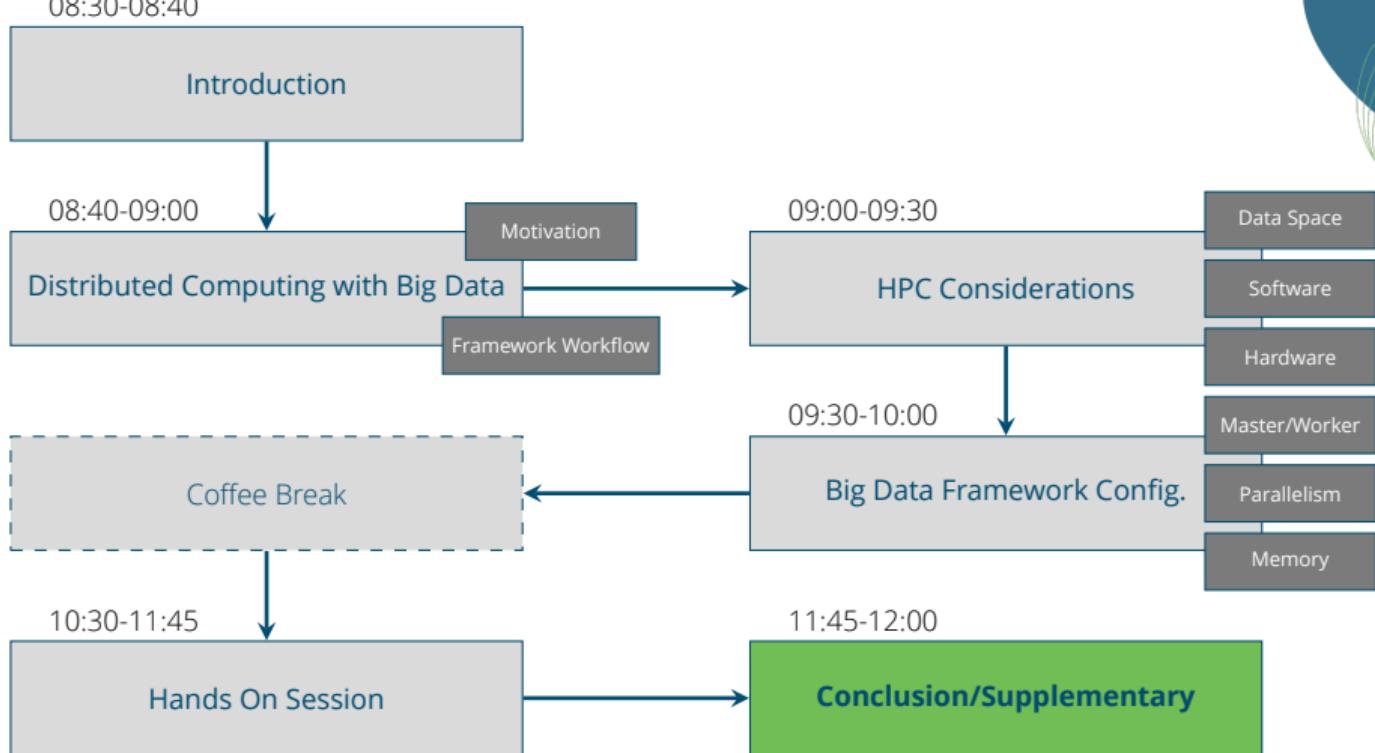
# Big Data Processing on HPC - Demo



# Hands-on session: Overview

Assume, we want to analyse the New York City taxi dataset. Here are some information:

- New York City taxi dataset
  - ▶ contains taxi trips within NYC with many details:
    - Start/end times
    - Locations
    - Cost
    - Number of persons
    - ...
  - ▶ Original source: <https://www1.nyc.gov/site/tlc/about/tlc-trip-record-data.page>
  - ▶ Exercise is stored at [/data/horse/ws/s4122485-ai4seismology/big\\_data](#).
- Analysis aims:
  - ▶ Use Jupyter as frontend with a small Apache Spark cluster as backend.
  - ▶ Follow the tasks in the Jupyter notebook.
  - ▶ (for details, see next slide)



# Conclusions

- Big Data Processing works on HPC, but is more complex (no fixed resources, but SLURM scheduling)
- HPC and Big Data Processing are also complex individual tasks, that need time to learn about
- Leveraging HPC infrastructure by Big Data frameworks can lead to efficient distribution of data intensive tasks
- For effective deployment of Big Data frameworks in HPC, HPC principles need to be considered
- On ZIH HPC system:
  - ▶ Apache Flink and Apache Spark are available via the module system
  - ▶ A useful basic configuration of Big Data frameworks is provided via `BigDataFrameworkConfigure` module and `framework-configure.sh` script
  - ▶ JupyterHub can leverage Big Data clusters and compute visual outputs (e.g. maps)

# Conclusions

- In case of questions start at the official docs for the ZIH system:  
<https://compendium.hpc.tu-dresden.de/>
- Software ecosystems are changing dynamically, esp. in Big Data and ML: with HPC systems it is hard to react immediately
- Contact us with your own ideas, experiences and wishes!

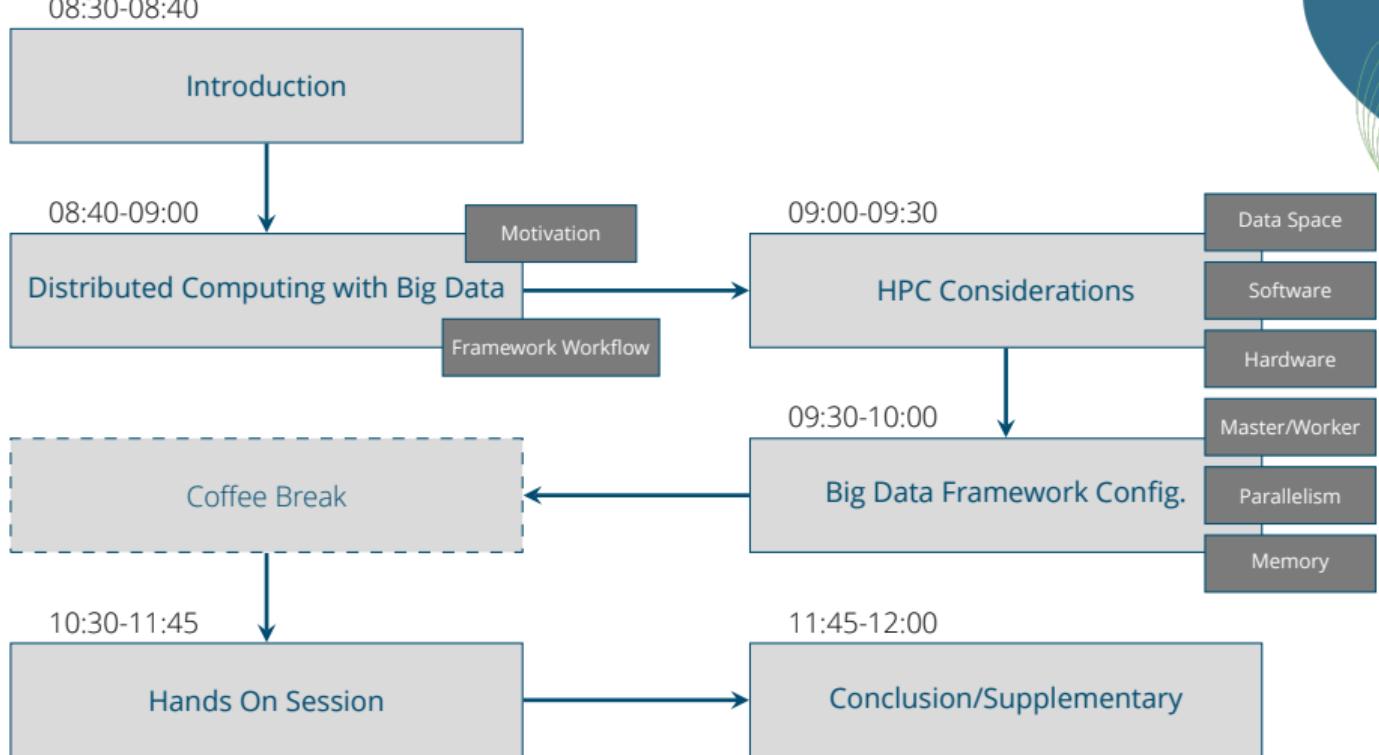
## Note

- Logins (scadsxxx) will work for further 10 days
- If you are interested afterwards please apply for your own HPC project. More information can be found at:  
<https://compendium.../application/overview/> ↗



Thank you

Contact us at:  
transferscads.ai@tu-dresden.de



# Flink Taskmanager Memory Model

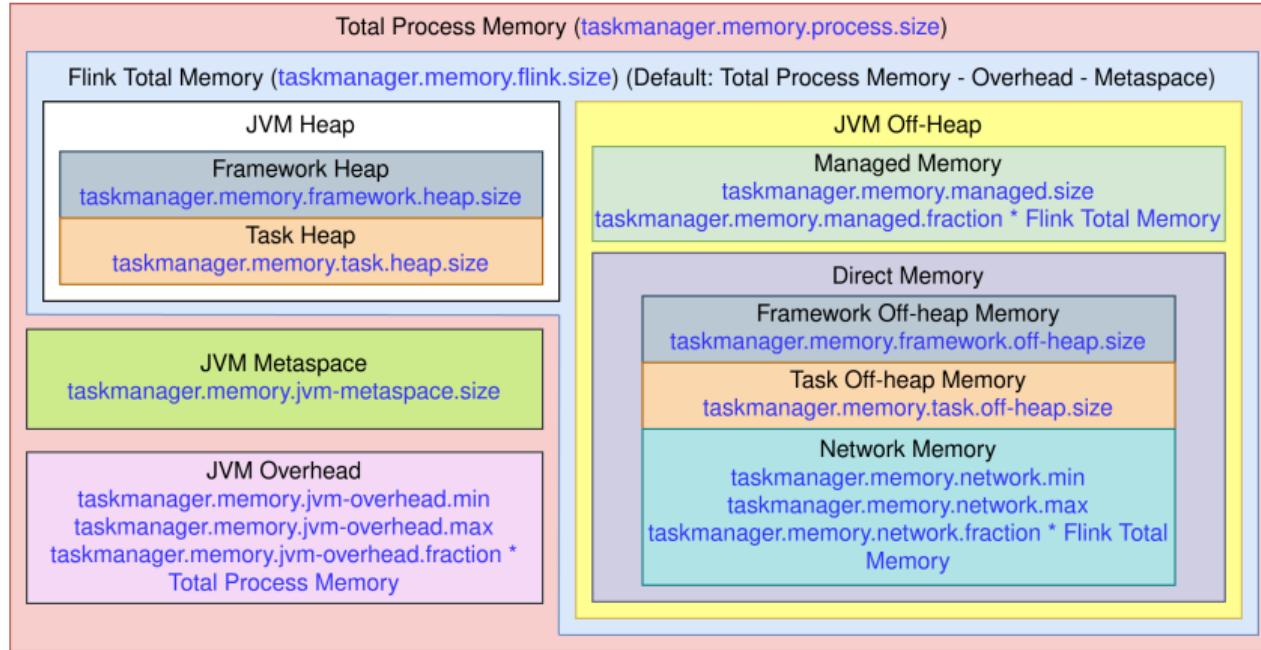


Figure 1: Executor memory model

# Flink Taskmanager Memory Model (cont..)

- Framework Heap/Off-Heap Memory: Memory dedicated to flink framework and its internal data structures
- Task Heap/Off-Heap Memory: Used to run tasks (operators) and user code.
- Managed Memory: Used for RocksDB state backend, sorting, hashtable, caching of intermediate results.
- Network Memory: Used for data exchange between tasks and acts as network buffer.
- JVM Metaspace: Used for storing metadata for classes.
- JVM Overhead: Used for JVM overheads like code cache, GC collection space, etc.

# Spark Executor Memory Model

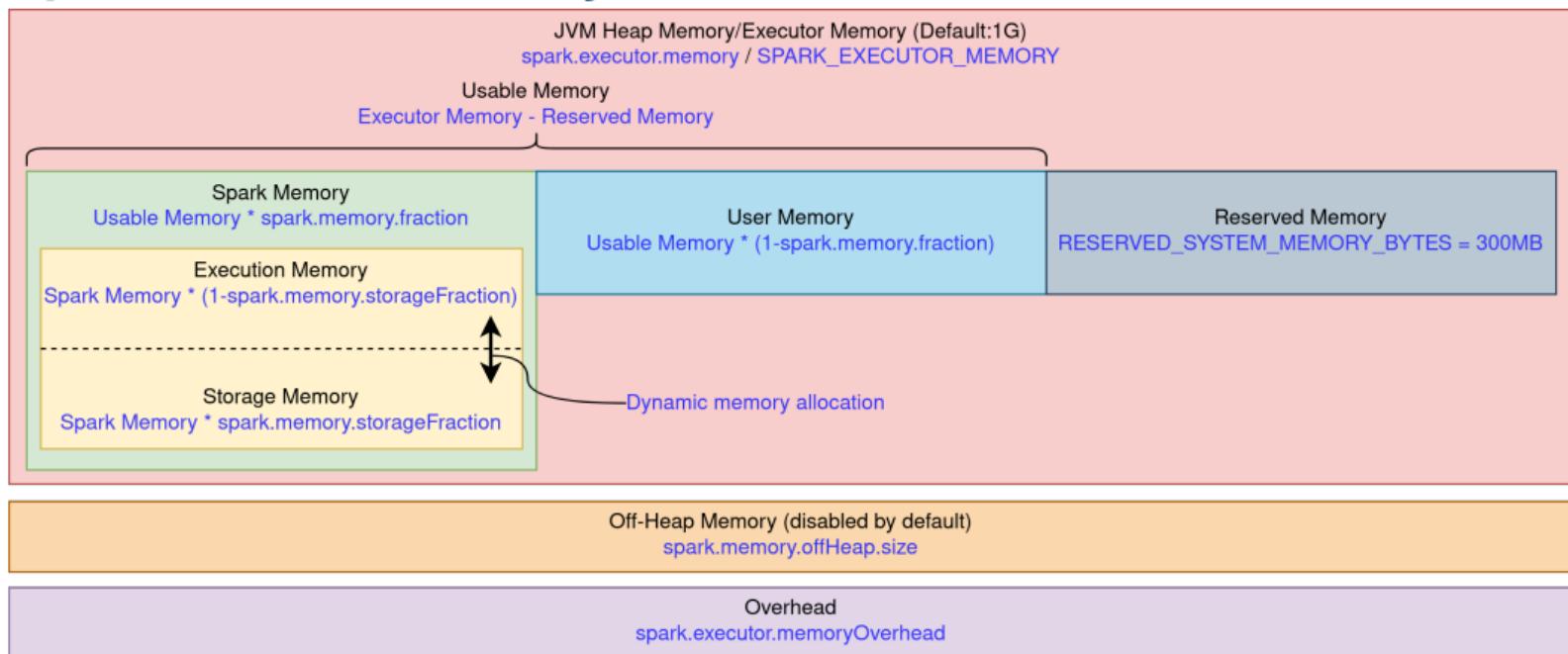


Figure 2: Executor memory model

# Spark Executor Memory Model (cont..)

- Executor Memory: Maximum JVM memory where objects are also bounded by garbage collector
- Execution Memory: Used for storing temporary data created during execution of the task like shuffle, join, sort, aggregation etc.
- Storage Memory: Used for storing cached and broadcasting data.
- User Memory: Used for storing UDFs and user defined data structures.
- Reserved Memory: Hard-coded memory used for storing spark internal objects.
- Off-Heap memory: Additional memory that accounts for operations like VM overheads, interned strings, other native overheads, etc.

# Performance Analysis - Job Monitoring with PIKA

- Simple approach for overview and to check used resources for a job: PIKA (hardware performance monitoring stack)
- monitoring during and after runtime: access PIKA web interface at  
[https://selfservice.zih.tu-dresden.de/l/index.php/hpcportal/jobmonitoring/z./jobs\\_and\\_resources](https://selfservice.zih.tu-dresden.de/l/index.php/hpcportal/jobmonitoring/z./jobs_and_resources)
- Choose between "Live" (for running jobs) and "Jobs" (finished jobs with filtering by date/time if needed)



## Hint

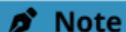
More info about PIKA at: <https://compendium.../software/pika/>

# Workflow: Using git

Git is a version-control system, commonly used for managing source code and coordinating the work of multiple contributors on a software project.

Please consider the following basics while using git on the ZIH system:

- git is available on all cluster nodes
- can be used on HPC in the same way as in the shell of your local machine, e. g. `git clone`, `git add`, `git commit`, `git push` etc.
- every project collaborator is working on his own copy and changes are pushed to the remote repository
- no binary files are contained in the repo (this keeps the storage requirement low)
- cloned repo copies are located in user space



## Note

Using the same repo copy for different users will cause permission and access issues - DON'T DO THAT.