Containerized services for FEL data processing

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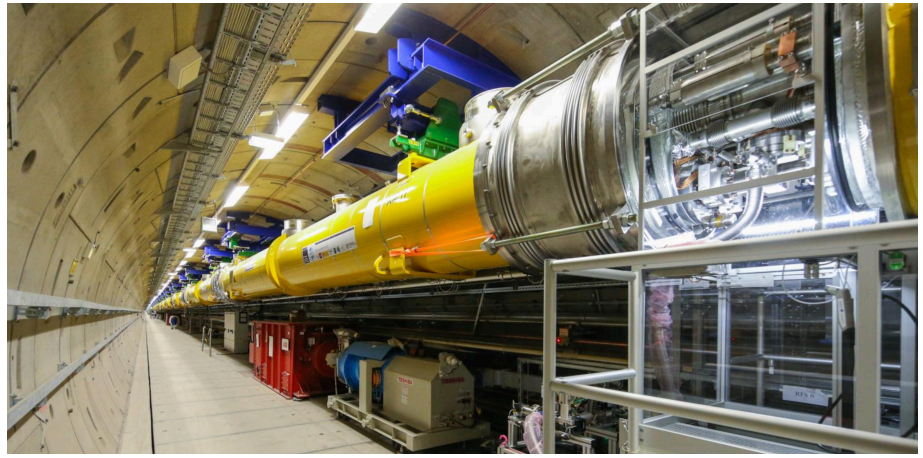
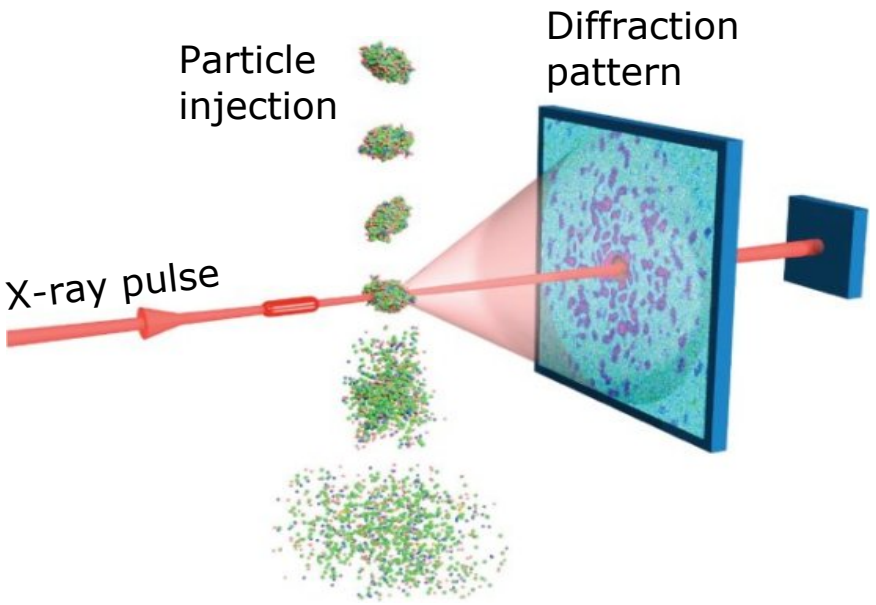
European XFEL

- X-Ray Free-Electron Laser - mega science research facility
  - High brilliance (10^9 times more than conventional X-ray source)
  - High frequency: up to 27000 flashes per second
  - Wavelength range: 0.05-4.7 nm
  - Short pulses: less than 100 fs
- Construction start – Jan 2009
- First experiments – Sep 2017



SPI Experiments

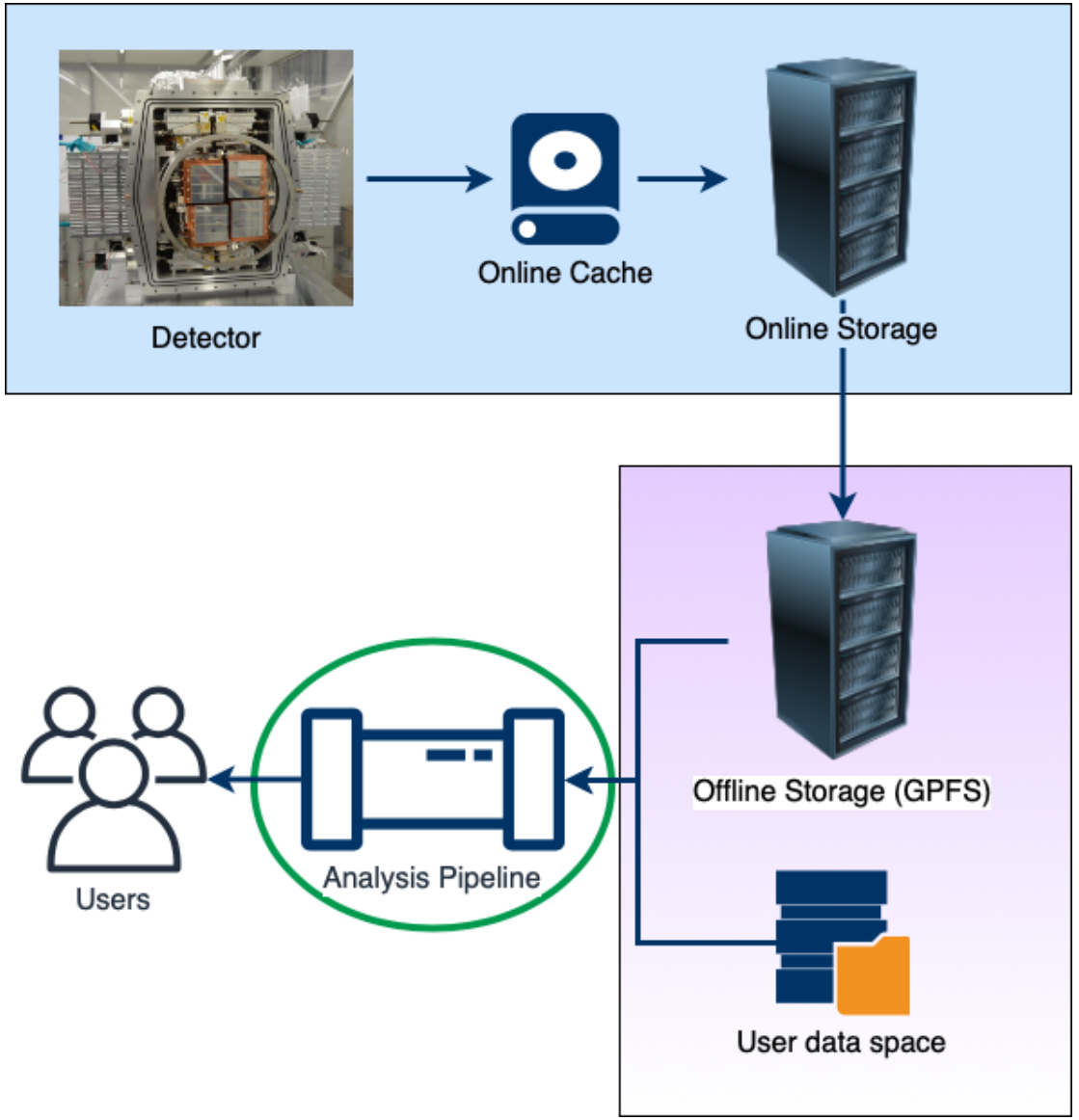
- The goal: Molecule structure at atomic level (1A)
- Big data:
  - 120 Tb per experiment (Dec 2017)
  - 360 Tb per experiment (May 2019)
  - expected to be increased **100x** times!
- Experiments evolve rapidly
- Data Analysis is also under intensive development:
  - Algorithms
  - Software
  - IT services



*Gaffney K. J. & Chapman H. N.// *Science*, 2007.

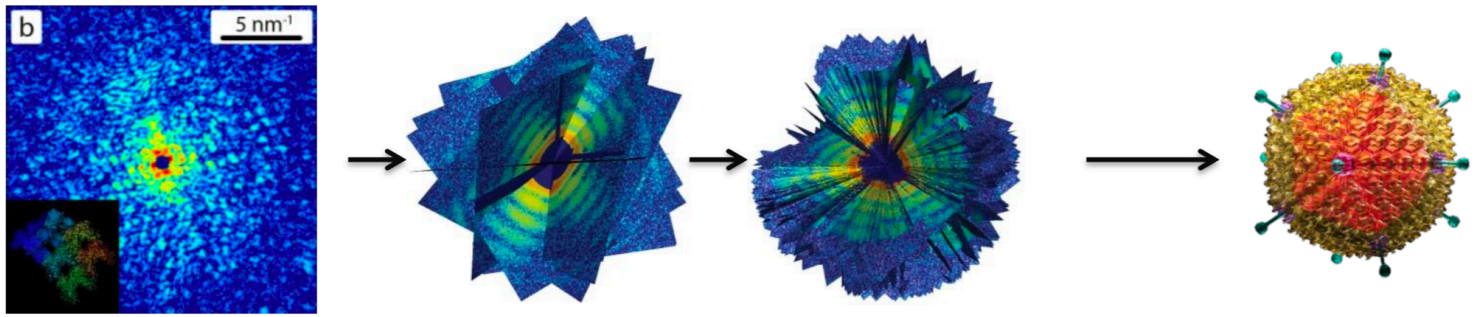
The Goal of the Project

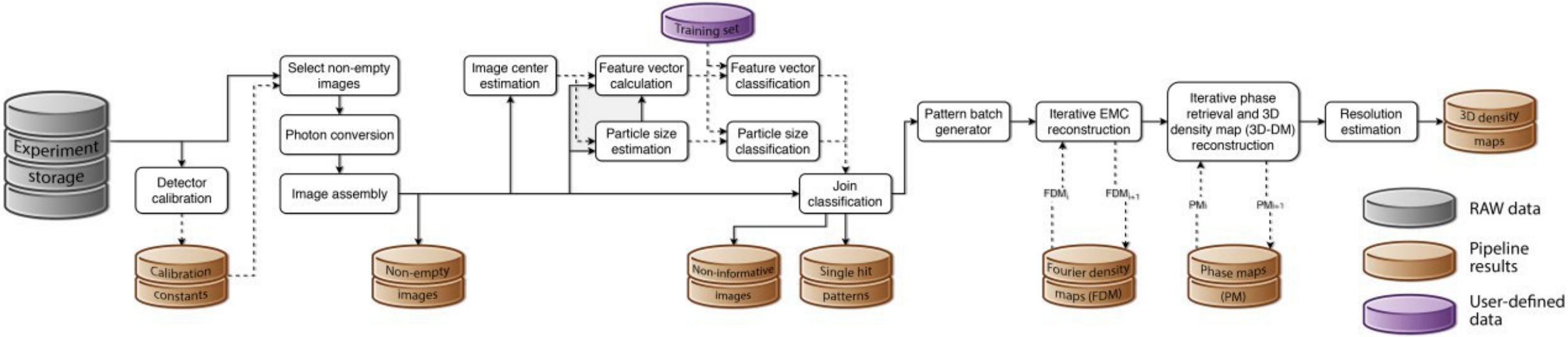
- Software Pipeline for automated data processing
- From diffraction patterns to 3D structure in near real-time
- Core Ideas:
  - Integration of software packages for various stages of data analysis in analysis pipeline
  - Simple configuration and deployment
  - Scalability
  - Extensibility, modular architecture
  - Various workflows



Structure Reconstruction Pipeline

Briefly

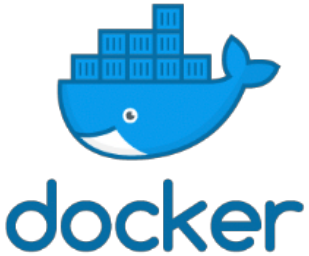


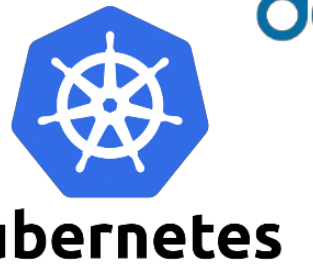


A little bit more detailed

Realization Strategy

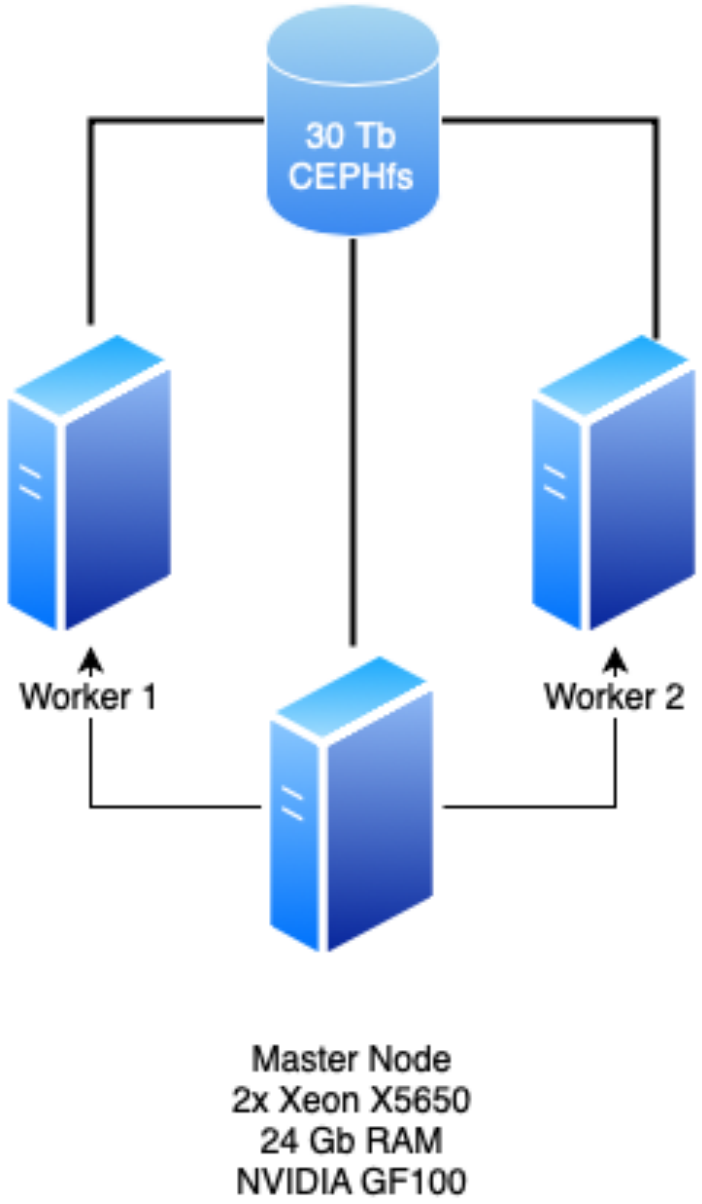
- Container technology for easy deployment
- Microservices for individual stages of analysis
- Container orchestration for scalability and management
- Shared network filesystem to reduce data transfers



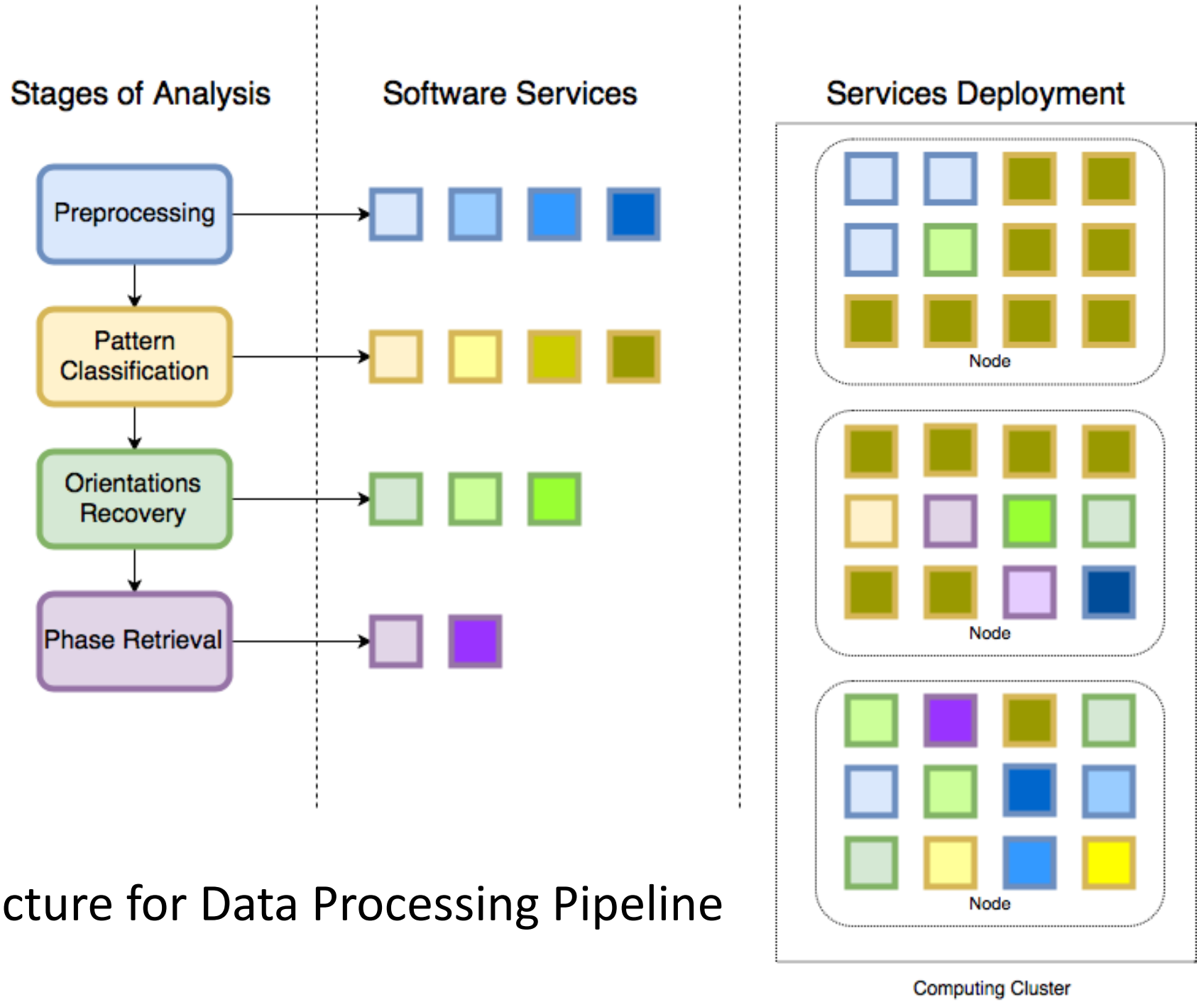


Testbed

- Dedicated K8s cluster (version v1.15.3) with three nodes
- Dedicated CEPHfs storage
- 1Gbps interconnect



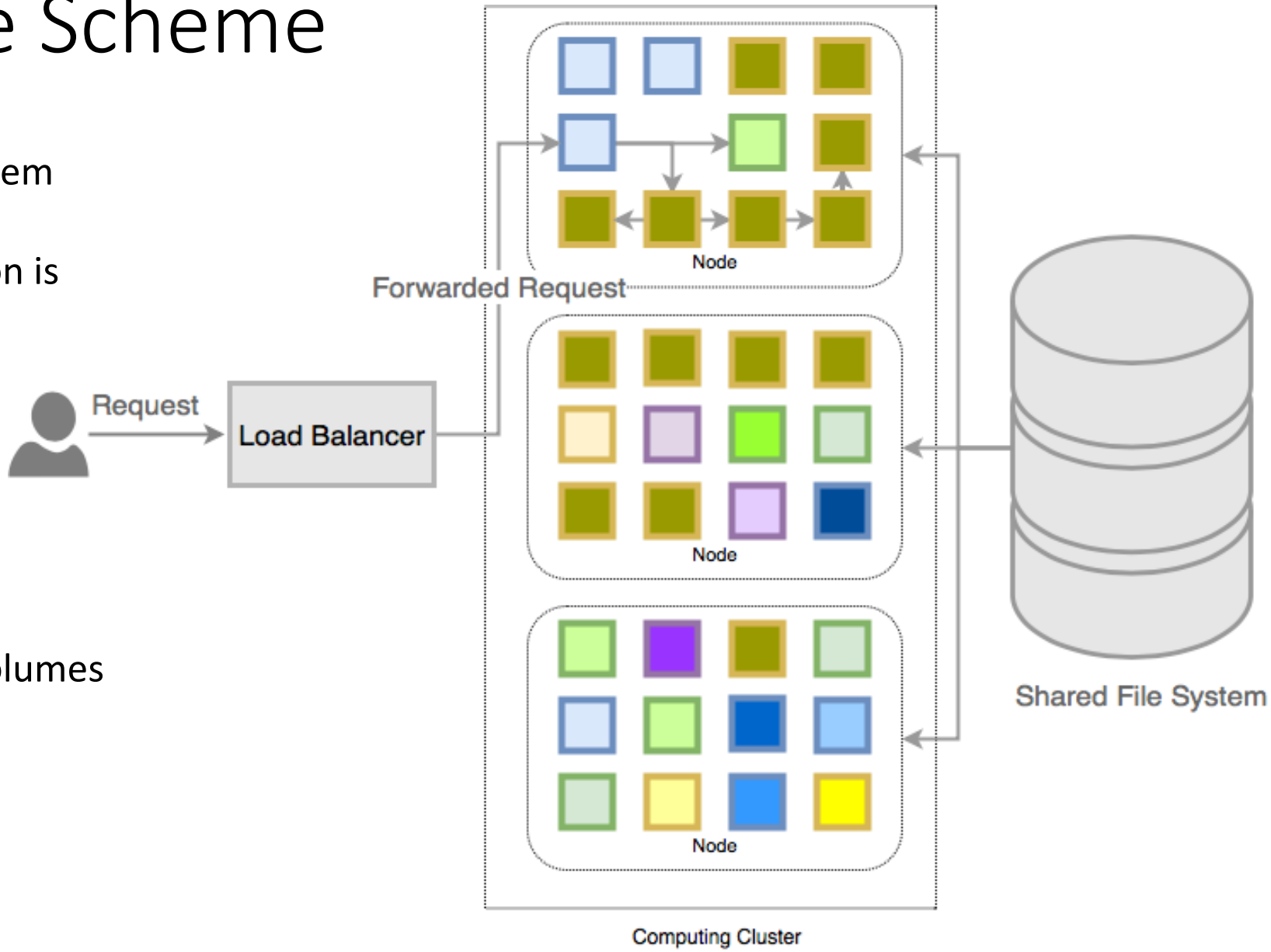
- Split analysis pipeline into small components
- Pack components into containers
- Use container orchestration infrastructure to distribute containers across computing cluster



Microservices Architecture for Data Processing Pipeline

Data Exchange Scheme

- Data is stored in a shared filesystem (GPFS, Lustre, CEPH) in HDF5
- K8s based container orchestration is used for:
  - containers deployment
  - load balancing
  - internal and external communications
  - services monitoring and management
- Native K8s support for CEPHfs volumes



Services and Jobs in K8s

Services model of operation

```
{
    "srand": 1,
    "data": "data/sample.bin",
    "data_dim": "2d",
    "number_of_outputs_images": 10,
    "number_of_outputs_scores": 10,
    "support_algo": "static",
    "support_size": 30,
    "algo": [
        { "name": "hio", "number_of_iterations": 500, "beta_init": 0.9, "beta_final": 0.9},
        { "name": "er", "number_of_iterations": 100}
    ],
    "out_file": "data/sample_out.h5"
}
```

```
root@c003f610f7a5:/opt/wsgi_app# curl  -H "Content-Type: application/json" -d @test.json localhost/phase
[8.3701095581054688, 0.090004101395606995, 0.049716383218765259, 0.12340822815895081, 0.084595672786235809, 0.077844396233558655,
0.065120011568069458, 0.068547621369361877, 0.024556649848818779, 0.024488534778356552]
```

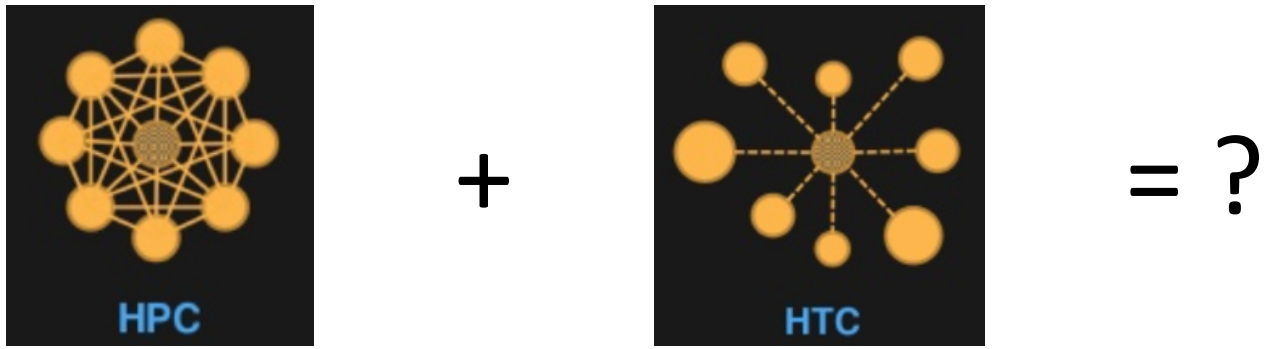
Jobs

```
root@c003f610f7a5:/opt#  kubectl create -f phaser-job.yaml
```

Use Cases: Orientations Determination

- Dragonfly
  - EMC algorithm for orientations reconstruction
  - High quality code
  - MPI
  - GUI interface

- It is the bright case where HPC application meets HTC (Cloud)!



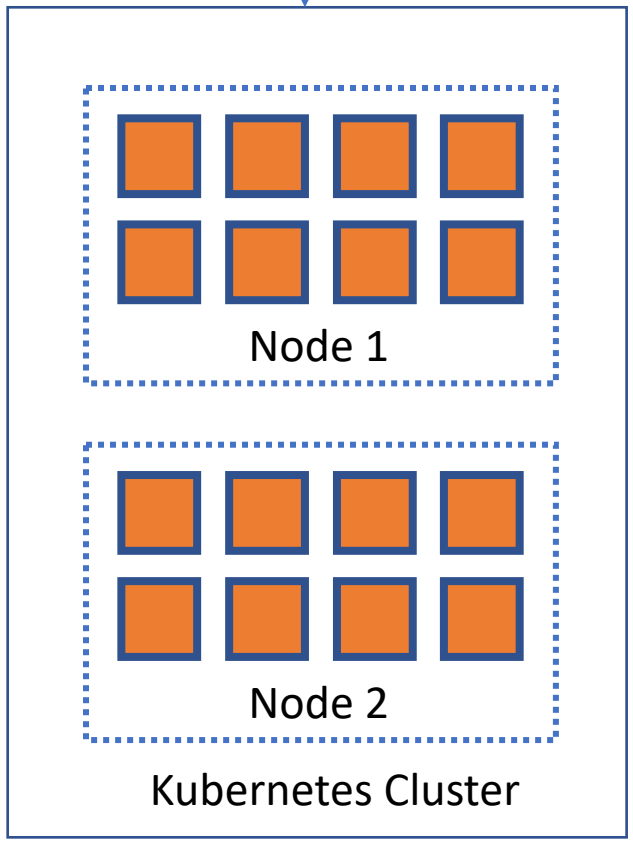
HPC vs HTC

- Different focus, history, architecture, ecosystem
  - HPC – parallel computing. Intensive communications between nodes
  - HTC – data and services centric. Loosely coupled services
- Possible scenarios of combined usage
  - application code refactoring
  - run HTC workloads in HPC systems (Singularity, Shifter)
  - virtualize HPC infrastructure in HTC systems
  - maintain separate infrastructures

Our realization

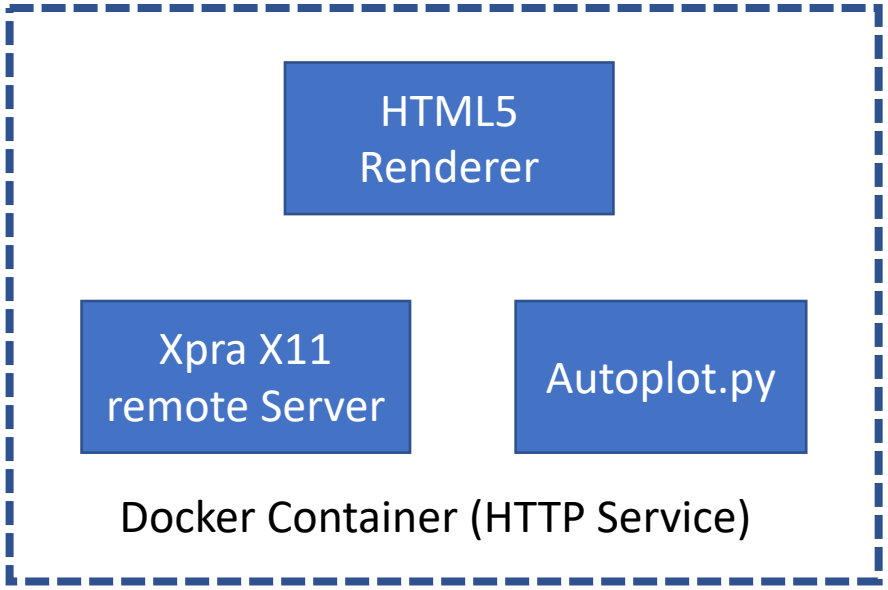
- Kube-openmpi, MPI infrastructure for Kubernetes
  - MPI nodes as Docker containers
  - OpenMPI 2.1.2
- Run Dragonfly as a native MPI application inside virtualized HPC cluster

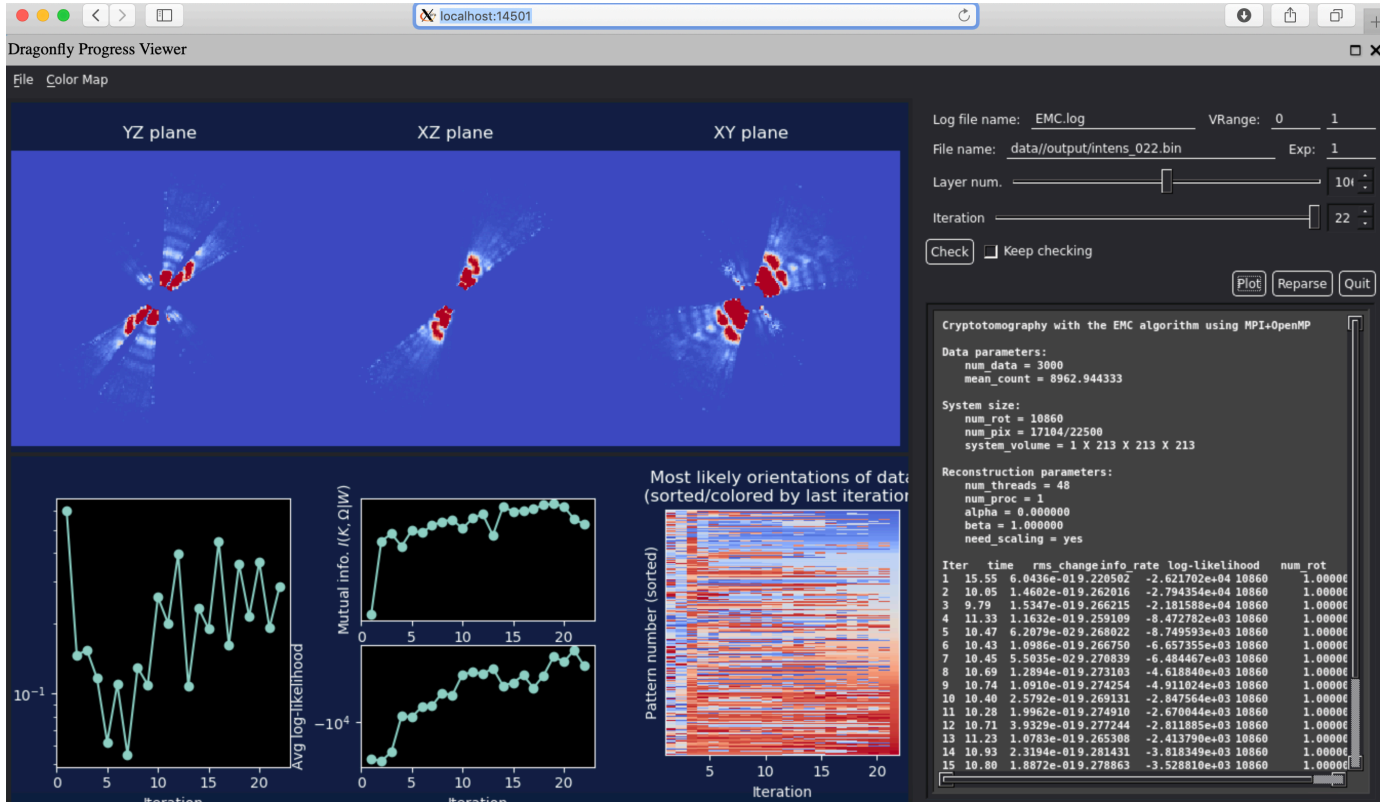
kubectl mpiexec –n 16
./run_emc.py –f emc.ini



GUI applications inside services

- autoplot.py as a HTTP service
- realtime EMC monitoring from browser



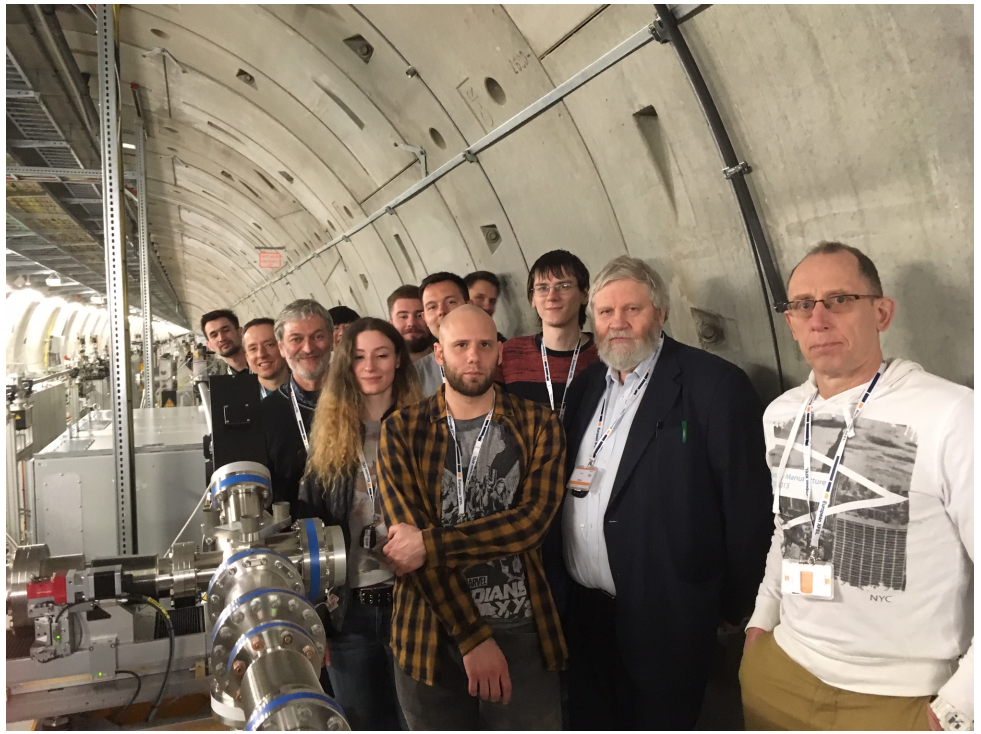


Conclusions and current status

- We have tested existing FEL data analysis software to work in containerized Docker infrastructure. Container technology looks to be effective to integrate heterogenous software with different environment requirements.
- Various patterns of software usage in K8s infrastructure were analyzed and tested: loosely coupled parallel computations, GPU-computing, HPC (MPI) workloads, GUI applications.
- Next step: arrange individual microservices into data analysis pipeline

Acknowledgements

Joined Team from
KI and DESY



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Thank you for your attention