

# News from the IT Department and Cluster Computing

## PI IT Team

David Berghaus, *Oliver Freyermuth*, Frank Frommberger, *Michael Hübner*<sup>1</sup>,  
Katrin Kohl, Ernst-Michail Limbach-Gorny<sup>2</sup>, Andreas Wißkirchen & more helping  
hands in projects and from the HISKP IT Team

[it-support@physik.uni-bonn.de](mailto:it-support@physik.uni-bonn.de)

19<sup>th</sup> October, 2023

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<sup>1</sup> started April 2023

<sup>2</sup> started June 2023

# Outline

- 1 News
- 2 Funded IT R&D projects on Research Data Infrastructures
- 3 Behind the scenes: Queuing jobs on the BAF cluster



# Personnel Changes

- since 2020: FTD IT position not filled

- successor for Helmut Kortmann: Ernst-Michail Limbach-Gorny, started in June 2023, welcome 😊

## Project-specific helpers

- Development Team for web and database projects: Philipp König (*leaving*), Jan Heinrichs, Luka Vomberg, Oliver But
- Research data infrastructure projects: Luka Vomberg, Simon Thiele
- IT specialist trainees: 3 months every year in cooperation with HRZ

*(several personnel changes in the past years also in these projects)*

# Personnel Changes

● since 2020: FTD IT position not filled

● successor for Helmut Kortmann:  
Ernst-Michail Limbach-Gorny, started  
in June 2023, welcome 😊

## PI Web team

Ian Brock, Daniel Jacobi, Florian Kirfel, Barbara Valeriani-Kaminski  
(*coordinating also with FTD, HISKP and department web teams*)

## Flexible project developers

David Berghaus (*leaving*), Katrin Kohl

# Projects (highlights)

- still ongoing
  - Web development team: ongoing **development of HR system**
  - Joint project of PI & HSKP IT teams, secretaries, HRZ: **Indico**
  - Development of **common firewall** (HSKP, PI, FTD)
- new in 2023
  - bandwidth upgrade of Ceph file servers (for Grid storage, new workernodes)  
 $8 \times 10 \text{ Gbit/s}$
  - Hybrid Conference equipment in Conference Room II, Seminar Room I (BCTP upcoming)
  - Mostly automated, GDPR-compliant managed Windows 11 Pro deployment
  - Work behind the scenes (construction planning, upgrade preparations etc.)

# Project highlights: Indico event management and room booking

- Instance operated at HISKP, used for local events (from colloquia up to conferences and workshops)
- Successfully used for room booking at FTD, PI, HISKP  
*Common room booking system across institutes!*

## Upcoming

- Login via [eduGAIN](#) (no local accounts for non-Uni-Bonn users needed anymore)
- Discussion on faculty level: Plan to open up Indico inside MNF, attract more users (goal: centralization)

# Funded Projects: FIDIUM

## FIDIUM project

- Federated Digital Infrastructures for Research on Universe and Matter
- Financed by the BMBF, part of ErUM-Data
- Groups: elementary particle physics, hadron physics, nuclear physics and astroparticlephysics
- 10 institutions and 4 associated partners (CERN, DESY; GridKa, GSI)
- One project in a series of projects:
  - Q3/2017 → Q3/2021 ErUM-Data Pilot I: IDT-UM
  - Q3/2021 → Q3/2024 ErUM-Data Pilot II: **FIDIUM**
  - Q3/2024 → Q3/2025 **FIDIUM** extension
  - Q3/2025 → Q3/2028 ErUM-Data 'föderierte Digitalinfrastrukturen' I
  - Q3/2028 → Q3/2031 ErUM-Data 'föderierte Digitalinfrastrukturen' II

# Federating compute resources

## Tasks in Bonn

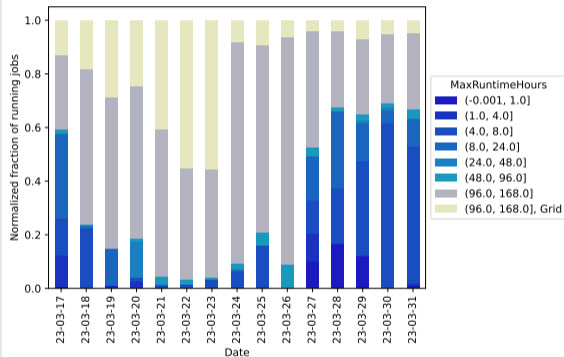
- Leverage BAF (HTC) and Uni Bonn HPC for Grid jobs via an overlay batch system operated by KIT ('Single point of Entry' for ATLAS, Belle II)
- 'Compute Site in a Box': Ease deployment for other sites



# Federating compute resources

## Results so far

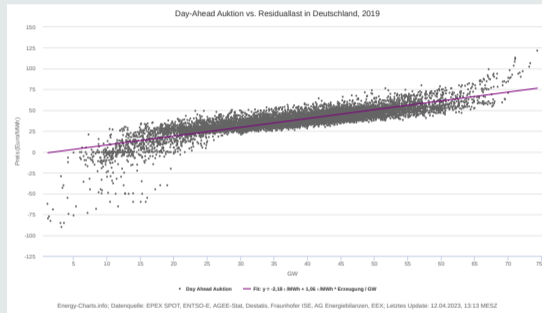
- Successfully operating backfilling since 2019
- Cluster is able to adapt quickly once users submit new jobs



# Federating compute resources

## FIDIUM successor — Planned proposal

- Premise: Heading towards an age of (renewable) energy abundance
- Consequence: Due to volatility, energy will be for free when the sun is shining & wind is blowing
- Idea: Project energy price into the future and start/stop Grid jobs accordingly



[https://www.energy-charts.info/charts/price\\_scatter/chart.htm?l=de&c=DE&year=2019&residual\\_load=1&solar=0&wind\\_onshore=0&wind\\_offshore=0](https://www.energy-charts.info/charts/price_scatter/chart.htm?l=de&c=DE&year=2019&residual_load=1&solar=0&wind_onshore=0&wind_offshore=0)

# PUNCH: On the way to a Science Data Platform

Particles, **U**niverse, **Nu**Clei and **H**adrons for the NFDI

## Goal

### Federated / FAIR 'Science Data Platform'

Provide infrastructure and interfaces for access to and working with data and compute resources of the communities, breaking community borders

## Activities in Bonn with regard to technical infrastructure

- JupyterHub frontend for federated Compute infrastructure ('Single Point of Entry')
- Including resources in Bonn in the Compute infrastructure
- Federated storage for 'small' experiments

## Other activities in Bonn

Metadata structure and definitions, Outreach activities



# IT R&D for Research Data Management

- Both projects aim to federate compute and storage resources to deal with increasing resource requirements
- Connection of federated compute and storage via federated authentication
- Leverage existing compute resources via an overlay batch system
- PUNCH Goal: break community borders & offer a FAIR Science Data Platform
  - One platform / portal to allow cross-experiment analyses
  - Usage not only for Open Data
  - Allow access to data from all communities via industry standard protocols
  - Common distributed data management infrastructure including caches



# Intermediate Summary

- Continuous modernization of existing services
- Successful R&D projects in IT (FIDIUM & PUNCH)
  - Both aim to federate compute and storage with federated authentication
  - PUNCH: break community borders & develop FAIR Science Data Platform
- Debian 12 for Desktops on the horizon
- Check out our documentation pages on Confluence!

## Ongoing future project

Common institute firewall for Physics institutes:  
More bandwidth, IPv6, less poking of firewall holes

**In case of any questions, don't hesitate to contact us!**

[it-support@physik.uni-bonn.de](mailto:it-support@physik.uni-bonn.de)

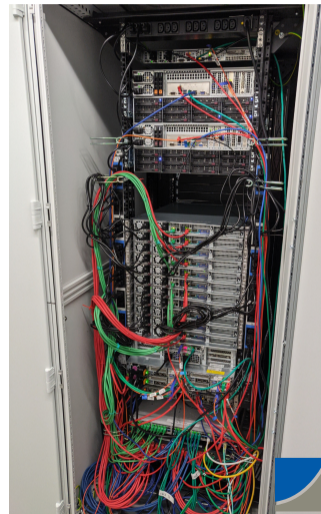
# BAF Cluster

- 2017: Started with 40 worker nodes, **2240 logical cores**
- 2019 and 2020: 3 waves of memory upgrades
- February 2020: 4 × NVIDIA GeForce GTX 1080 Ti, 11 GB VRAM
- July 2020: Integration of 56 worker nodes in HRZ institute machine room ('CephFS\_IO'), new total: **3776 logical cores**
- November 2020: Extension with 4 worker nodes, new total: **4288 logical cores**
- April 2023: Extension with 11 worker nodes, 1 high-memory node: 4 TB RAM, new total: **7104 logical cores**
  - produce significant heat (1 kW per node)
  - fileserver upgraded to  $8 \times 10 \text{ Gbit/s}$  in June 2023



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# BAF Cluster: NuBallee 12



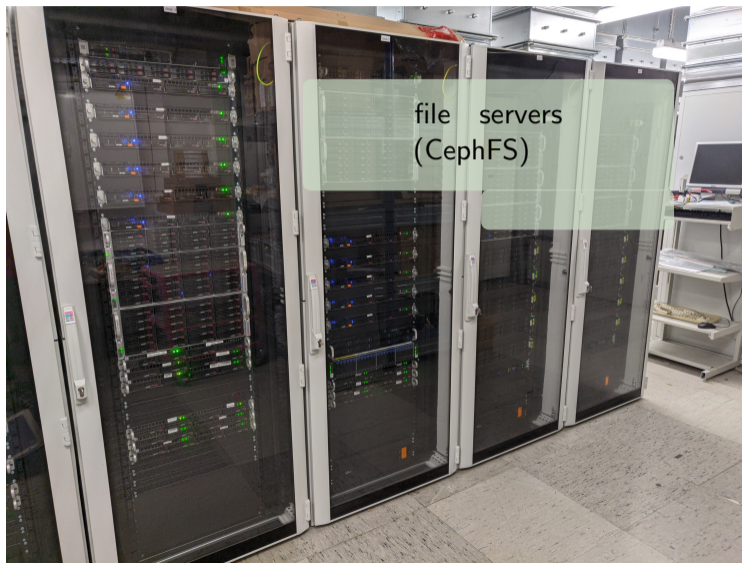


# BAF Cluster: NuBallee 12



first wave of  
worker nodes

# BAF Cluster: NuBallee 12



# BAF Cluster: NuBallee 12



# BAF Cluster: Wegelerstraße 6



- 31 racks
- 1 rack filled with 56 BAF worker nodes (on the right)

# BAF Cluster: News

## Operating System Containers on BAF

- Ubuntu 18.04 ⇒ End of Life, not offered anymore
- Ubuntu 20.04 ⇒ End of Life in April 2025
- Debian 10 ⇒ End of Life in June 2024
- Debian 11 and 12
- CentOS 7 ⇒ End of Life in June 2024
- RockyLinux 8 and 9

# BAF Cluster: News

## Organizational Developments

- Ongoing convergence to one HTC cluster for Physics Institutes
- Central HPC team: <https://www.hpc.uni-bonn.de>  
*offering courses on Linux, Python, building your own cluster,...*
- Coming soon: Large central HPC cluster 'Marvin'
  - Inauguration October 20th (tomorrow)
  - Tests with 'power users' starting up
  - likely publicly available end of 2023
- Ongoing discussions & plans to cover HTC and HPC use cases together

# HTCondor

- Workload Management system for dedicated resources, idle desktops, cloud resources, . . .
- Project exists since 1988 (named Condor until 2012)
- New naming in 2022: **HTCSS** (HTCondor Software Suite)
- Open Source, developed at UW-Madison, Center for High Throughput Computing
- Key concepts:
  - **'Submit Locally. Run globally.'** (Miron Livny)  
*One interface to any available resource.*
  - Integrated mechanisms for **file transfer** to / from the job
  - **'ClassAds'**, for submitters, jobs, resources, daemons, . . .  
*Extensible lists of attributes (expressions) — more later!*
  - Supports Linux, Windows and macOS and has a very diverse user base  
*CERN community, Dreamworks and Disney, NASA, . . .*
  - Focus on decentralized operation models (Peer-to-Peer), heterogeneous resource ownership
  - Dynamic integration of resources

# HPC vs. HTC

## High Performance Computing

tightly coupled massively parallel jobs which may span many nodes and often need low-latency interconnects, e. g.

- Climate simulations (grid cells connected to each other)
- Lattice calculations

## High Throughput Computing

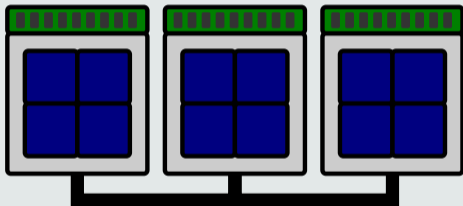
many jobs, often submitted in large batches, usually loosely coupled or independent, goal is large throughput of jobs and / or data, e. g.

- Event-based analysis (e. g. particle physics, video rendering)
- Simulation of single events
- Parameter scans



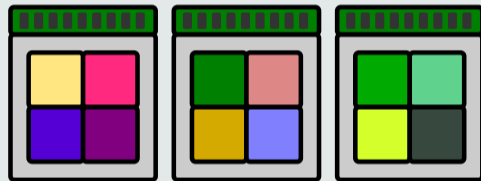
# HPC vs. HTC

## High Performance Computing



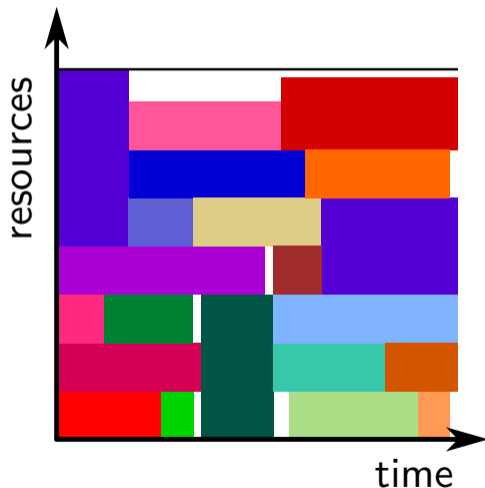
low-latency, high bandwidth interconnect  
converged memory access

## High Throughput Computing



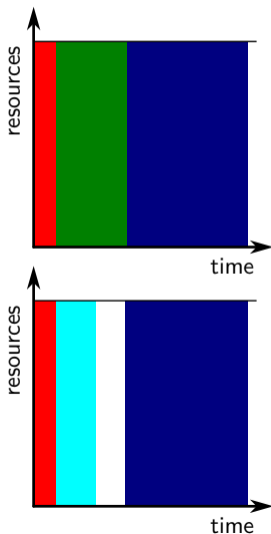
individual jobs on each CPU core,  
no memory sharing

# HTC: The tetris game



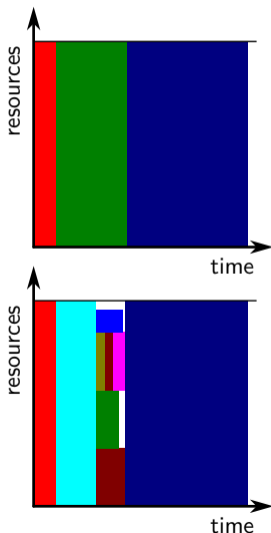
- 'Tetris' of resources: Individual, independent jobs with diverse resource requirements
- 'Fragmentation' of resources by design
- Note: The resource axis is multi-dimensional (tetris in many dimensions!)

# HPC: Priority rules



- Large interconnected chunks of resources used (up to the full cluster system)
- Priority dominates scheduling, resources left empty to prepare for large jobs

# HPC with backfilling



- Gaps in resource usage can be filled with shorter HTC jobs
- HPC schedulers are not well-suited for tetris with many jobs
- Overlay batch systems can work around this (large placeholder job submitted, 'tetris' within)

# What HTCondor needs from the user...

## A job description / Job ClassAd

Resource request, environment, executable, number of jobs,...

```
Executable = some-script.sh
Arguments  = some Arguments for our program $(ClusterId) $(Process)
Universe   = vanilla
Transfer_executable = True

Error      = logs/err.$(ClusterId).$(Process)
#Input    = input/in.$(ClusterId).$(Process)
Output    = logs/out.$(ClusterId).$(Process)
Log       = logs/log.$(ClusterId).$(Process)

+ContainerOS="Rocky8"
Request_cpus = 2
Request_memory = 2 GB
Request_disk = 100 MB

Queue
```

# What HTCondor needs from the user...

## some-script.sh

- Often, you want to use a wrapper around complex software
- This wrapper could be a shell script, python script etc.
- It should take care of:
  - Argument handling
  - Environment setup (if needed)
  - Exit status check (bash: consider `-e`)
  - Data handling (e.g. move output to shared file system)

```
#!/bin/bash
source /etc/profile
set -e
SCENE=$1

cd ${SCENE}
povray +V render.ini
mv ${SCENE}.png ..
```

# Submitting a job

```
$ condor_submit myjob.jdl
Submitting job(s)..
1 job(s) submitted to cluster 42.
```

There are many ways to check on the status of jobs:

- `condor_tail -f` can follow along stdout / stderr (or any other file in the job sandbox)
- `condor_q` can access job status information (memory usage, CPU time,...)
- log file contains updates about resource usage, exit status etc.
- `condor_history` provides information after the job is done
- `condor_ssh_to_job` may allow to connect to the running job (if cluster setup allows it)

# Advanced JDL syntax

```
Executable = /home/olifre/advanced/analysis.sh
Arguments = "-i '${file}'"
Universe = vanilla
if $(Debugging)
  slice = [:1]
  Arguments = "${Arguments} -v"
endif
Error = log/$Fn(file).stderr
Input = $(file)
Output = log/$Fn(file).stdout
Log = log/analysis.log
Queue FILE matching files $(slice) input/*.root
```

HTCondor offers macros and can queue variable lists, file names...

Can you guess what happens if you submit as follows?

```
condor_submit 'Debugging=true' analysis.jdl
```



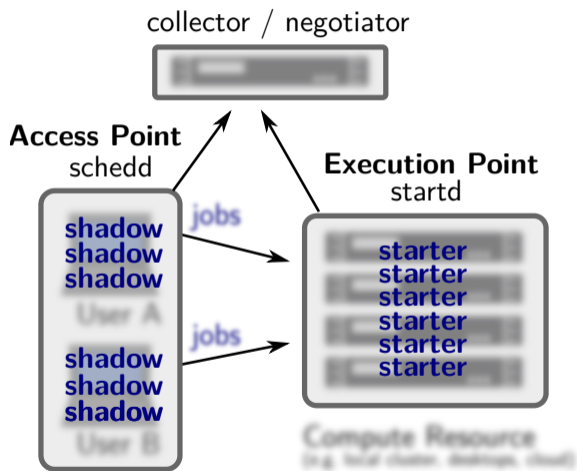
# HTCondor's commandline tools (in PATH)

```
condor_adstash condor_annex condor_check_config condor_check_password
condor_check_userlogs condor_config_val condor_continue condor_dagman
condor_docker_enter condor_drain condor_evicted_files condor_findhost condor_gather_info
condor_history condor_hold condor_job_router_info condor_now condor_nsenter condor_ping
condor_pool_job_report condor_power condor_prio condor_q condor_qedit condor_qsub
condor_release condor_remote_cluster condor_reschedule condor_rm condor_router_history
condor_router_q condor_router_rm condor_run condor_scitoken_exchange
condor_ssh_to_job condor_stats condor_status condor_submit condor_submit_dag
condor_suspend condor_tail condor_test_match condor_token_create condor_token_fetch
condor_token_list condor_token_request condor_token_request_approve
condor_token_request_auto_approve condor_token_request_list condor_top
condor_transfer_data condor_transform_ads condor_update_machine_ad condor_userlog
condor_userlog_job_counter condor_userprio condor_vacate condor_vacate_job
condor_vault_storer condor_version condor_wait condor_watch_q condor_who
```

# HTCondor's commandline tools (in PATH)

condor\_adstash condor\_annex condor\_check\_config condor\_check\_password  
condor\_check\_userlogs condor\_config\_val condor\_continue condor\_dagman  
condor\_docker\_enter condor\_drain condor\_evicted\_files condor\_findhost condor\_gather\_info  
condor\_history condor\_hold condor\_job\_router\_info condor\_now condor\_nsenter condor\_ping  
condor\_pool\_job\_report condor\_power condor\_prio condor\_q condor\_qedit condor\_qsub  
condor\_release condor\_remote\_cluster condor\_reschedule condor\_rm condor\_router\_history  
condor\_router\_q condor\_router\_rm condor\_run condor\_scitoken\_exchange  
condor\_ssh\_to\_job condor\_stats condor\_status condor\_submit condor\_submit\_dag  
condor\_suspend condor\_tail condor\_test\_match condor\_token\_create condor\_token\_fetch  
condor\_token\_list condor\_token\_request condor\_token\_request\_approve  
condor\_token\_request\_auto\_approve condor\_token\_request\_list condor\_top  
condor\_transfer\_data condor\_transform\_ads condor\_update\_machine\_ad condor\_userlog  
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# Structure of HTCondor



see also Architecture talk:

[https://htcondor.org/event\\_summary/htcondor\\_week\\_2020](https://htcondor.org/event_summary/htcondor_week_2020)

# HTCondor's processes

## on access points (where you submit jobs)

**condor\_schedd** Scheduler, keeps track of queue, spawns condor\_shadow

**condor\_shadow** Monitors a single job (plus logs etc.)

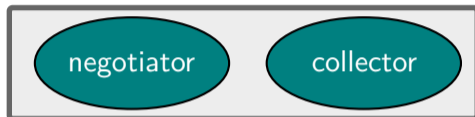
## on execute points (worker nodes)

**condor\_startd** Spawns condor\_starter

**condor\_starter** For each slot, takes care of jobs

# Structure of HTCondor

## Central Manager



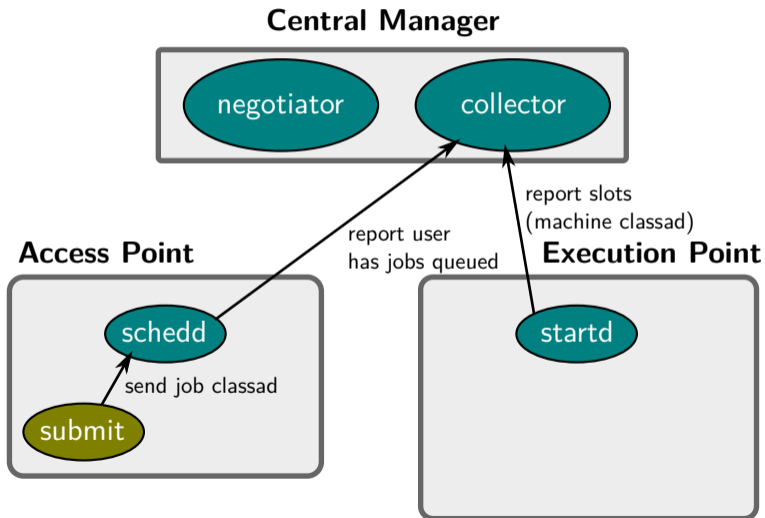
## Access Point



## Execution Point

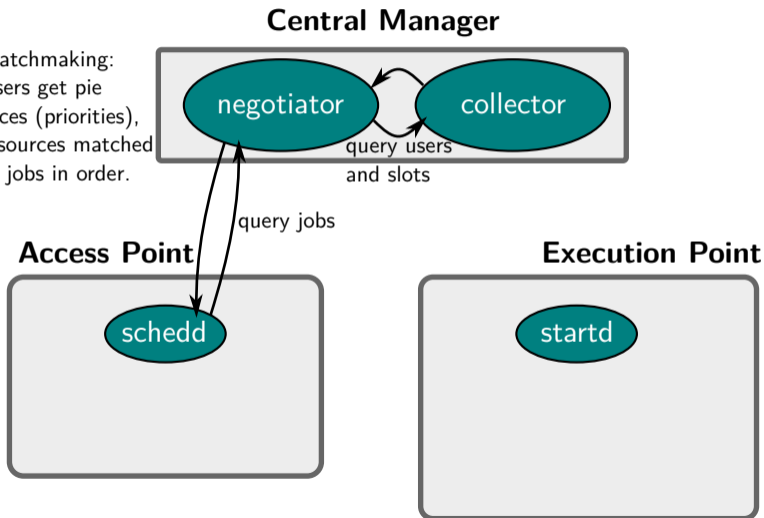


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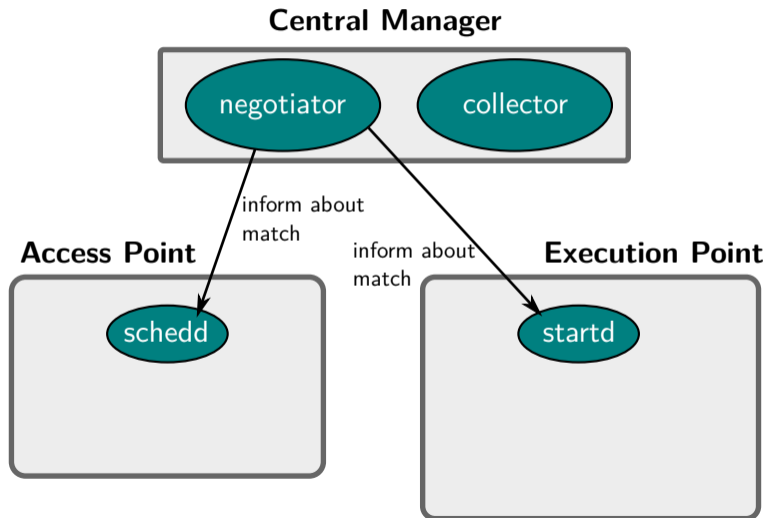


# Structure of HTCondor

Matchmaking:  
Users get pie  
slices (priorities),  
resources matched  
to jobs in order.



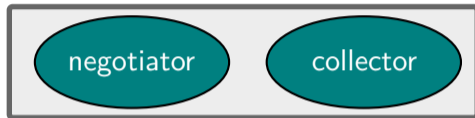
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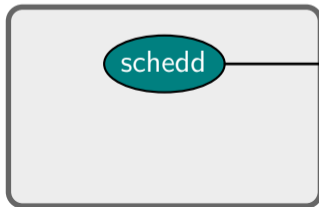


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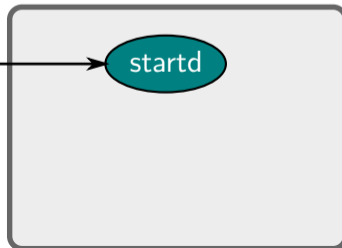
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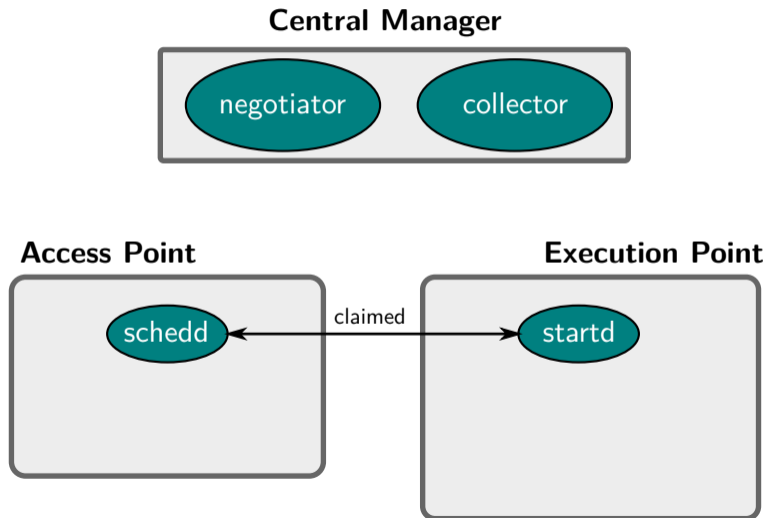
## Execution Point



claim  
resource

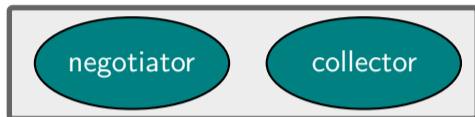


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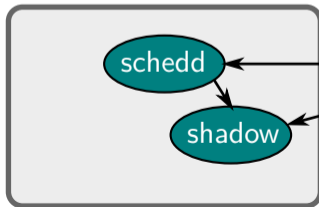


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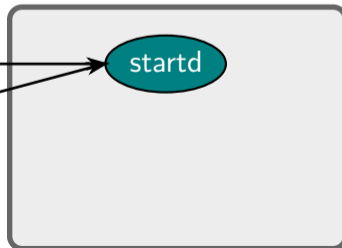
## Central Manager



## Access Point



## Execution Point

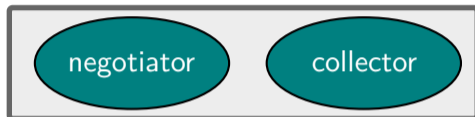


claimed

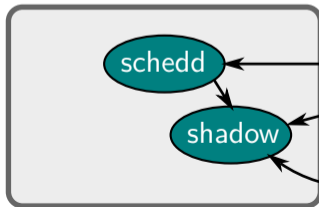
activate  
claim

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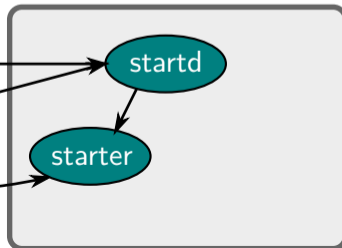
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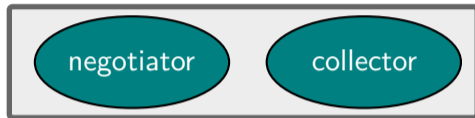
claimed

activate  
claim

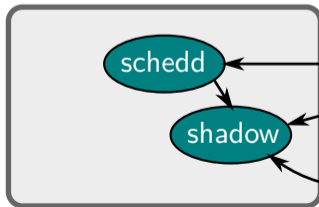
run job

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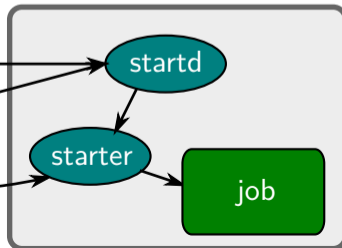
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## Access Point



## Execution Point



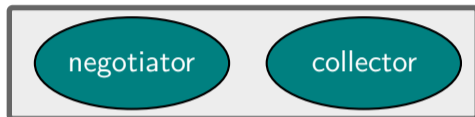
claimed

activate  
claim

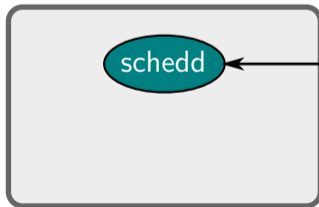
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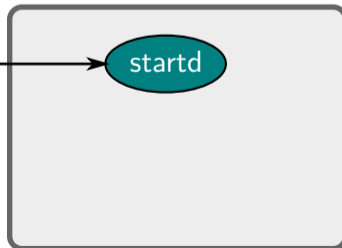
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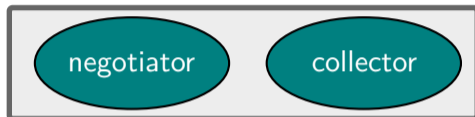
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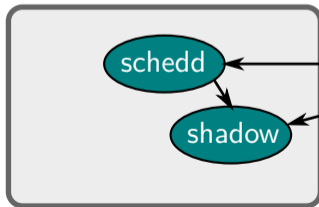
claimed

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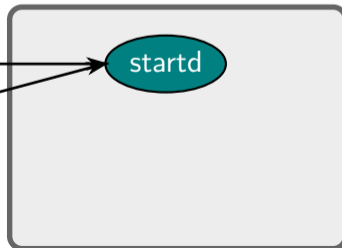
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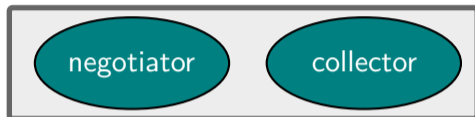


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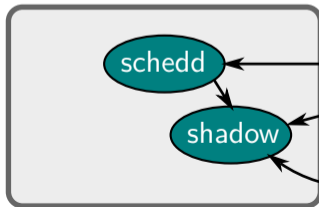
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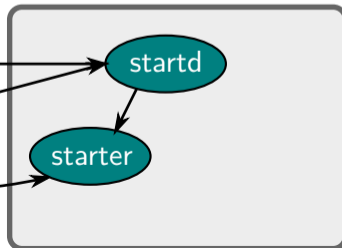
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## Execution Point



claimed

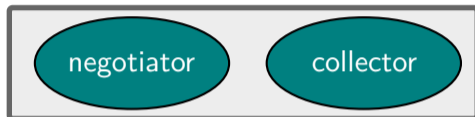
activate  
claim

run job

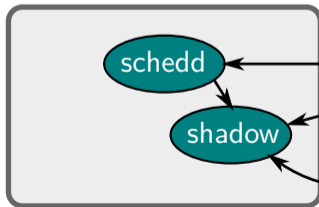


# Structure of HTCondor

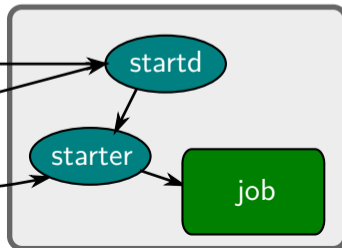
## Central Manager



## Access Point



## Execution Point



claimed

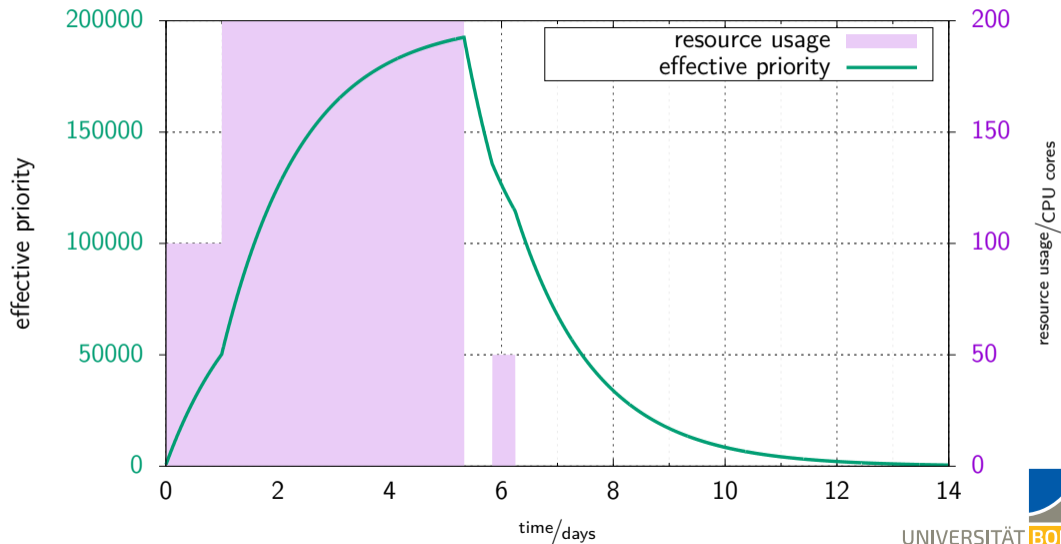
activate  
claim

run job

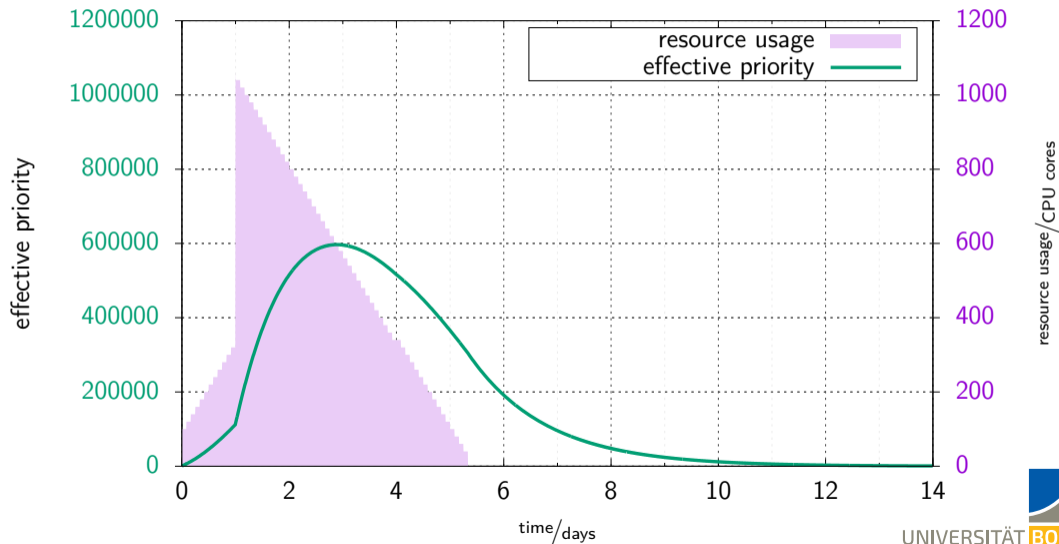
# User Priorities in HTCondor

- Every user / accounting group is given an effective priority
- Effective priority approaches weighted resource usage (cores multiplied with priority factor of 1000) in an exponential manner
- Half-life constant configurable, in our case: 24 hours
- Resources are distributed amongst accounts with queued jobs proportionally, weighted by priority ('pie slices')

# User Priorities in HTCondor



# User Priorities in HTCondor



# HTCondor's ClassAds

- Any submitter, job, resource, daemon has a ClassAd
- ClassAds are basically just expressions (key = value)
- Dynamic evaluation and merging possible

## Job ClassAd

```
Executable = some-script.sh
+ContainerOS = "Rocky8"

Request_cpus = 2
Request_memory = 2 GB
Request_disk = 100 MB
```

## Machine ClassAd

```
Activity = "Idle"
Arch = "X86_64"
Cpus = 8
DetectedMemory = 7820
Disk = 35773376
has_avx = true
has_sse4_1 = true
has_sse4_2 = true
has_ssse3 = true
KFlops = 1225161
Name = "slot1@htcondor-wn-7"
OpSys = "LINUX"
OpSysAndVer = "Rocky8"
OpSysLegacy = "LINUX"
Start = true
State = "Unclaimed"
```

# HTCondor's ClassAds

- Job and Machine ClassAd extended / modified by HTCondor configuration
- Merging these ClassAds determines if job can run on machine
- Examples for dynamic parameters:
  - Select a different binary depending on OS / architecture
  - Machine may only want to 'Start' jobs from some users
- You can always check out the ClassAds manually to extract all information (use the argument `-long` to commands!)
- To extract specific information, you can tabulate any attributes (JSON also works!):

```
$ condor_q -all -global -af:hj Cmd ResidentSetSize_RAW RequestMemory RequestCPUs
ID      Cmd      ResidentSetSize_RAW RequestMemory RequestCPUs
  2.0    /bin/sleep 91168          2048          1
```

# DAGs: Directed Acyclic Graphs

- Often, jobs of different type of an analysis chain depend on each other  
*Example:* Monte Carlo, comparison to real data, Histogram merging,...
- These dependencies can be described with a DAG
- Condor runs a special 'DAGMAN' job which takes care of submitting jobs for each 'node' of the DAG, check status, limit idle and running jobs, report status etc. (like a *Babysitter job*)
- DAGMAN comes with separate logfiles, DAGs can be stopped and resumed
- DAGs are often used behind workflow frontends (e.g. video rendering,...)

# Working with different environments

## How to compile and test code?

- Approach to access special environments or resources: **interactive jobs**
  - Advantage for admins: No separate bare metal machines
  - Advantage for users: Environment the same as in the job!
- Compile the code, pack it into a tarball, copy to shared FS / condor file transfer / CVMFS
- Can be automated with scripts / if offered, job start hooks (like `‘.bashrc’`)

## Advantages of this approach

- Portable and stable job executables
- If combined with containers and ‘mobile data’: Mostly cluster independent jobs possible



# 'Choose your OS'

- You add to the Job ClassAd:

```
+ContainerOS = "Rocky8"
```

- Jobs run in a container
- Same for interactive jobs ('login-node experience!')
- Small fractions of worker nodes exclusively for interactive jobs  
*But: Interactive jobs can go to any slot!*
- Resource-request specific tuning via `/etc/profile` possible:

```
REQUEST_CPUS=$(awk '/^RequestCpus/{print $3}' ${_CONDOR_JOB_AD})  
export NUMEXPR_NUM_THREADS=${REQUEST_CPUS}  
export MKL_NUM_THREADS=${REQUEST_CPUS}  
export OMP_NUM_THREADS=${REQUEST_CPUS}  
export CUBACORES=${REQUEST_CPUS}  
export JULIA_NUM_THREADS=${REQUEST_CPUS}
```

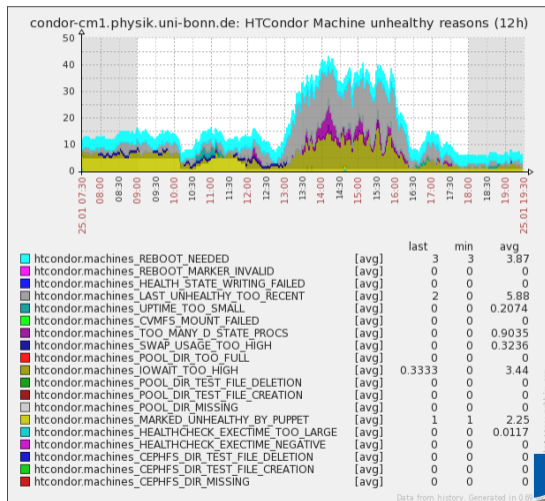
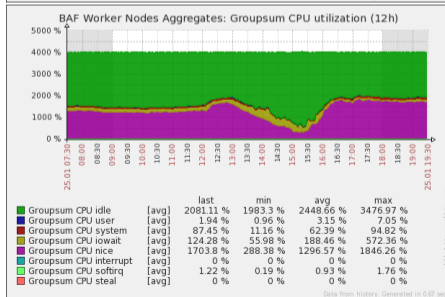
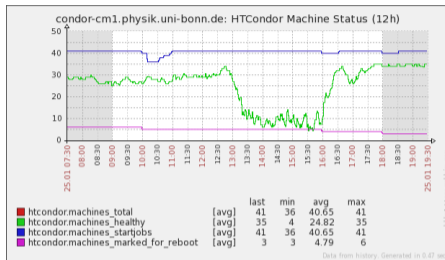
# Noteworthy tools in and around HTCondor

- Well-maintained Python API to directly talk to HTCondor daemons
- [HTMap](#) allows to scale map-reduce like algorithms from Python into HTC clusters
- HTCondor Adstash allows to push ClassAds from jobs / workers into ElasticSearch
- [HEP-Puppet/htcondor](#) for managed deployment and configuration of HTCondor
- MPI possible via `parallel` universe, even with containers, but manually tweaked start script and dedicated schedd required, and would need to teach HTCondor about interconnect topology  
⇒ Usually not a good fit for HTC

# Node health checking: Reasons for 'unhealthiness'

- 🟡🔌 last 'UNHEALTHY' too recent (debouncing,  $\leq 10$  min)
  - writing of status files failed or syntax bad (drain configuration, reboot marker, health state)
  - failed reboot actions
  - reboot scheduled (i.e. `shutdown` command with timeout)
  - minimum uptime ( $\leq 20$  min)
  - slow network interface ( $\leq 100$  Mbit/s)
  - bad kernel command line (e.g. should contain 'console=')
  - unhealthy CVMFS mounts
- 🟡🔌 swap usage is too high ( $> 80\%$ , HTCondor does not monitor swap)
- 🟡🔌 iowait too high ( $> 15\%$ )
- 🟡🔌 number of processes in D state too large ( $> \frac{\#logical\ cores}{2}$ )
  - read / write of execute directory or  $> 80\%$  used (don't limit disk use yet)
  - administrative 'UNHEALTHY' marker
  - read / write of cluster file system, check if mount healthy
  - execution time of health check ( $> 10$  s)

# Node health checking



# Node health checking

- All health information accessible via ClassAds of the machines:

```
$ condor_status -compact -af:h Machine NODE_REBOOT_REASONS
Machine                               NODE_REBOOT_REASONS
wn000.baf.physik.uni-bonn.de
wn001.baf.physik.uni-bonn.de
wn002.baf.physik.uni-bonn.de
↪ UPTIME_TOO_LARGE:39d_7h_27m_11s,NEEDS_RESTARTING_REBOOTHINT
wn003.baf.physik.uni-bonn.de
↪ UPTIME_TOO_LARGE:38d_23h_27m_19s,NEEDS_RESTARTING_REBOOTHINT
```

- Used also for monitoring, transparent for the users
- Similarly done for draining, planned reboots, node reservations, maintenances, backfilling etc.

# Conclusion

- Key features of HTCondor
  - Decentralized operation model / Peer-to-Peer design
  - ClassAd system
  - Exponential evolution of user priority when fairshare is used
  - Potentially heterogeneous machine ownership supported
  - Opportunistic resources can be integrated dynamically
  - File transfer possible

Quite some documentation on Confluence, online, passed down through PhD generations,... **How to get started?**

# User Tutorial

## User tutorial



<https://unibonn.github.io/htcondor-bonn/>

## The examples teach...

- Interactive jobs and basic job submission
- Submitting job arrays
- Submitting DAGs
- Checking on your jobs status, output, and acting on errors

**Game-like** (playing lottery with random numbers, rendering a video),  
all examples produce visible output, but still cover features used in physics analysis.

Thank you  
for your attention!





# FIDIUM Structure & Goals

## Topic Area I Development of tools to leverage heterogeneous resources

*Coordinators: Oliver Freyermuth, Manuel Giffels*

## Topic Area II Data Lakes, Distributed Data, Caching

*Coordinators: André Brinkmann, Kilian Schwarz*

## Topic Area III Testing, tuning & optimization in production & analysis environments

*Coordinators: Christian Zeitnitz, Günter Duckeck*

### Goals

- Enable transparent use of HPCs & Cloud infrastructures
- Flexible use of resources which are only available temporarily (e.g. backfilling)
- Concentration of most production data on large centres with local caches:  
⇒ Concept of data lakes

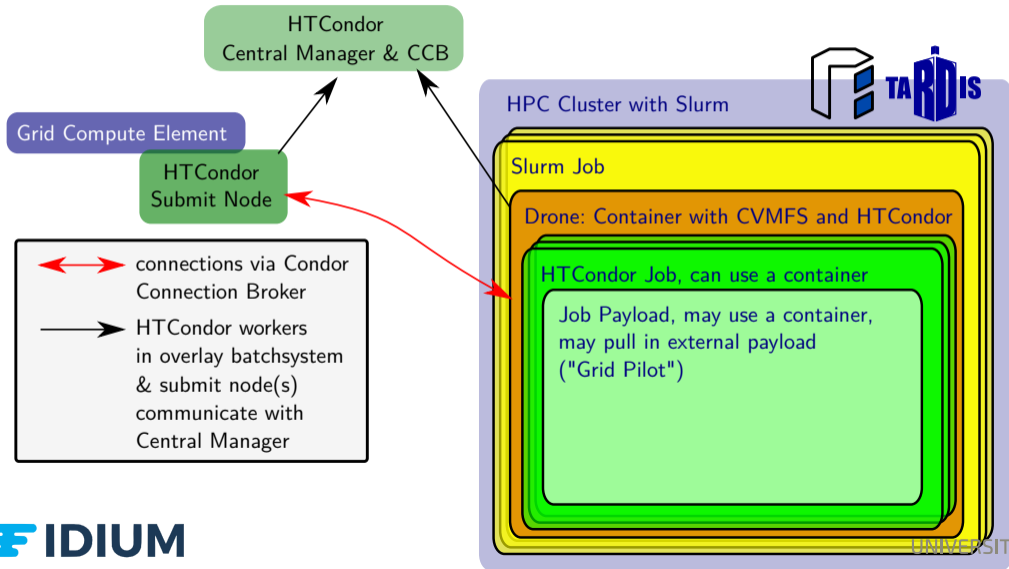
# FIDIUM Activities in Bonn

- Project 'Compute Site in a Box'
  - Usage of [COBaID/TARDIS](#) (tools developed at KIT for opportunistic computing)
  - Opening and extending existing Puppet configuration, test deployment with partners
  - Generalize unprivileged container workflows for COBaID/TARDIS resources
  - Leverage publicly accessible container infrastructure
  - Partners Mainz and GSI Darmstadt as 'testbeds'
  - Documentation and workshops for inside and outside particle physics community
- Funding: 1 FTE for three years, equal own contribution
- Close integration with developments in other topic areas (Accounting, Caching, Monitoring)

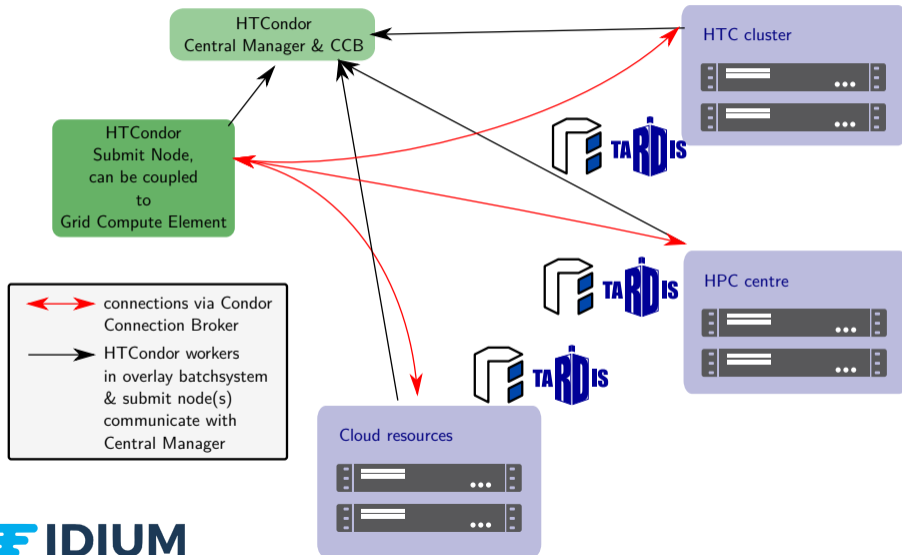
## Future

Application for the successor of FIDIUM in preparation (sustainability, checkpointing compute jobs)

# Federating compute resources



# Federating compute resources



# Transparent integration of Compute resources

## Main steps

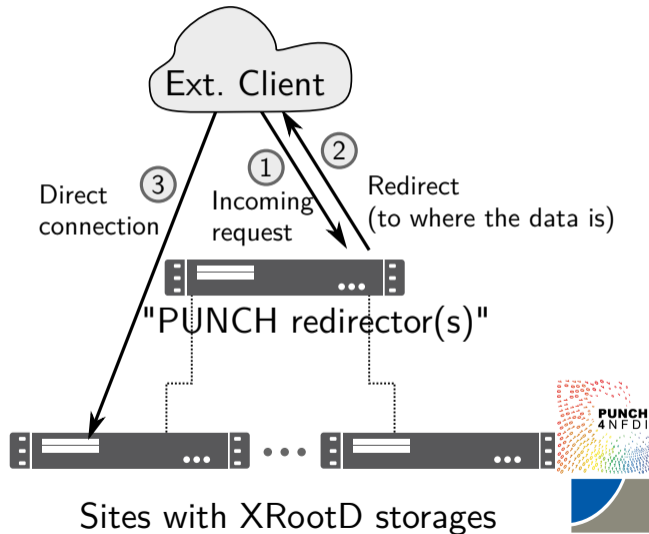
- Jobs submitted locally  $\Rightarrow$  Execution on **Overlay Batch System**
- Software stack as container (shipped via Cern-VM FS)
- Unprivileged containers started as jobs on site: Leverage User Namespaces
- Inside, an HTCondor startd (execute node) is started  $\Rightarrow$  'Drone'
- Drone registers with Central Manager of the Overlay Batch System
- Jobs inside Overlay Batch system can use containers themselves

## Scaling of number of 'Drones' based on resource usage

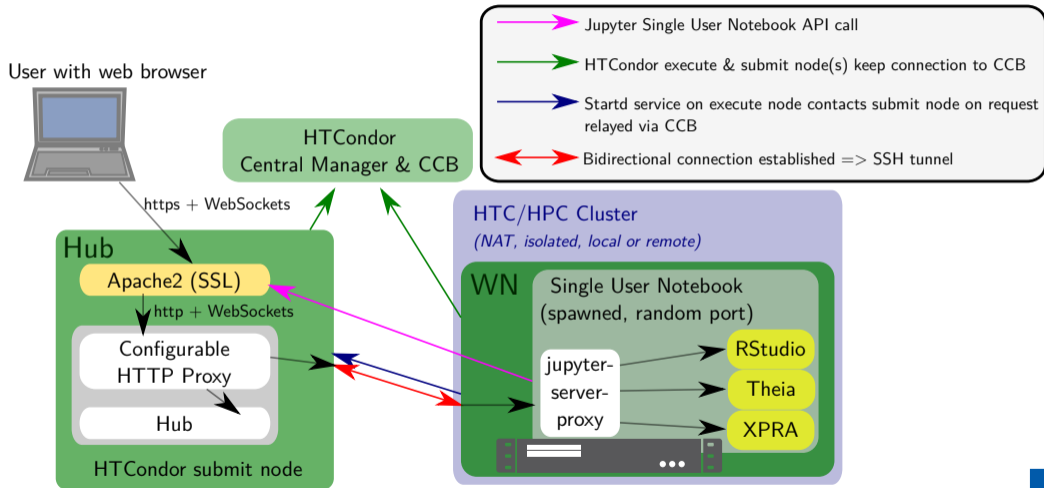
- COBalD — the Opportunistic Balancing Daemon
- TARDIS — The Transparent Adaptive Resource Dynamic Integration System

# XRootD: Federating data access across sites

- XRootD storage provides HTTPS / WebDAV and XRootD protocols
- Global namespace: Use **g**lobal **L**ogical **F**ile **N**ames
- Redirection from central redirector to site with physical files ('merge' sites)
- Compute jobs can be routed to sites with data, or close to them
- Concept also works with caches



# HTCondor Networking: JupyterHub



# HTCondor Networking

HTCondor  
Central Manager & CCB

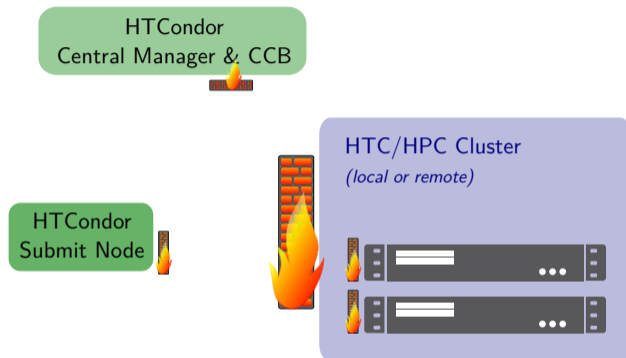
HTCondor  
Submit Node

HTC/HPC Cluster  
*(local or remote)*





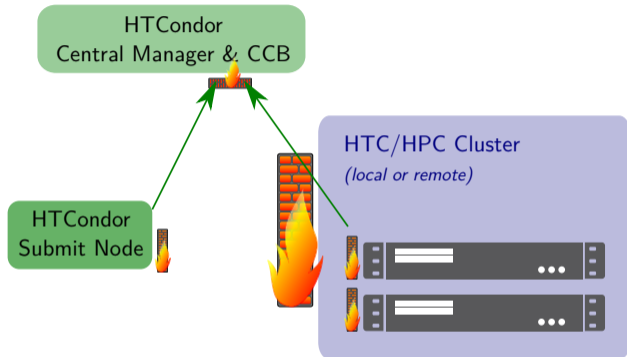
# HTCondor Networking



## Firewalling & NAT

- FW on each node (HTCondor port open)
- NAT(s), router(s), FWs in front of cluster networks

# HTCondor Networking



## Firewalling & NAT

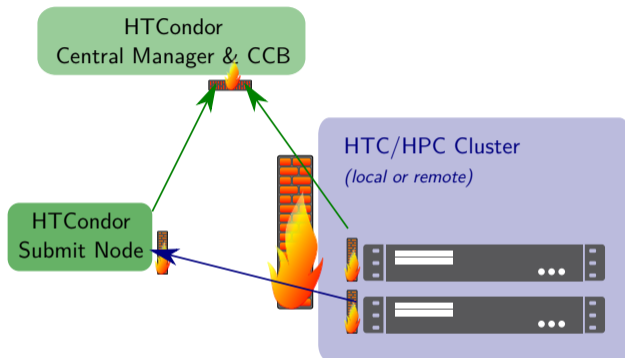
- FW on each node (HTCondor port open)
- NAT(s), router(s), FWs in front of cluster networks

→ HTCondor execute & submit node(s) keep connection to CCB

## Note:

Via the shared port daemon, only a single port needs to be open on the submit node and CCB node

# HTCondor Networking



## Firewalling & NAT

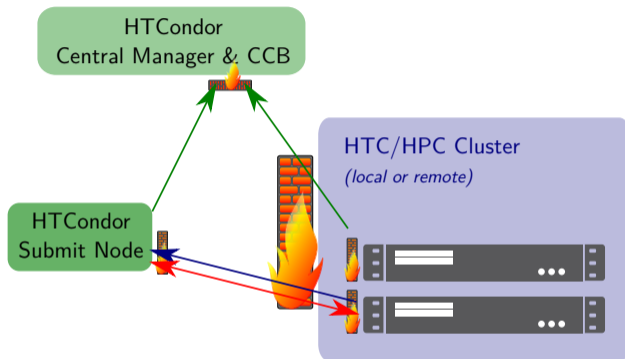
- FW on each node (HTCondor port open)
- NAT(s), router(s), FWs in front of cluster networks

- HTCondor execute & submit node(s) keep connection to CCB
- Startd service on execute node contacts submit node on request relayed via CCB

## Note:

Via the shared port daemon, only a single port needs to be open on the submit node and CCB node

# HTCondor Networking



## Firewalling & NAT

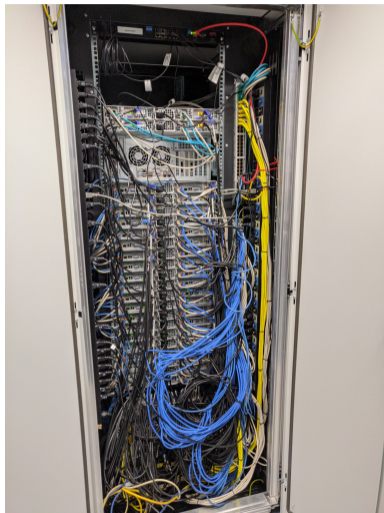
- FW on each node (HTCondor port open)
- NAT(s), router(s), FWs in front of cluster networks

- HTCondor execute & submit node(s) keep connection to CCB
- Startd service on execute node contacts submit node on request relayed via CCB
- ↔ Bidirectional connection established

## Note:

Via the shared port daemon, only a single port needs to be open on the submit node and CCB node

# Server Rooms: HRZ Institute Machine Room



- 56 worker nodes ('rear view')
- 1 Gbit/s ethernet, switches with 10 Gbit/s uplink  
⇒ CephFS\_IO 'medium'
- Nodes have to be drained (starting 7 days before!) if outside temperature exceeds  $\approx 35^\circ\text{C}$
- Relying on DWD MOSMIX (Model Output Statistics-MIX) calculations, quite reliable (with error bands!)

# Server Rooms: FTD



- 6 racks:
  - 2 network distribution and file servers
  - 2 service machines
  - 2 phone infrastructure
- central 60 kW UPS

# Server Rooms

HRZ machine room

HISKP

PI

FTD

**BAF Cluster: Compute Nodes**

(location HISKP coming soon)

BAF Cluster:  
Storage

**Virtualization infrastructure**

almost 120 VMs, hypervisors and storage  
redundant, Ceph RADOS Block devices, 3 copies

# Overview

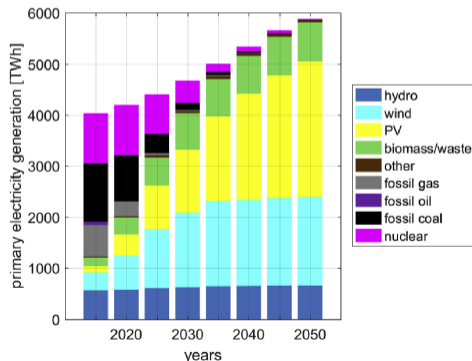
- Continue toolbox around COBaID/TARDIS to enable opportunistic computing everywhere
- Finalize connected older ideas on Compute Site in a Box
- Catchy new project (in collaboration with others?):  
**Computing in the age of strong sector coupling**
- Premise: We are headed towards a 100 % Renewable Energy (RE) based power infrastructure
- Transition has to take place in  $\mathcal{O}(10-20)$  years, and there are no alternative technologies at even remotely reasonable price available on that timescale
- Volatility of RE sources has far reaching implications



# The 2 Key Paradigms of the New Age Of Energy Abundance

## Paradigm 1

There will never be a cheaper source of energy again than solar (and to a certain extent, for a limited time, wind).

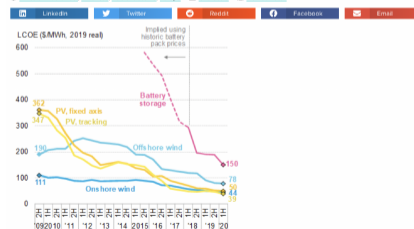


## BloombergNEF: 'Already cheaper to install new-build battery storage than peaking plants'

By Andy Colthorpe

April 30, 2020

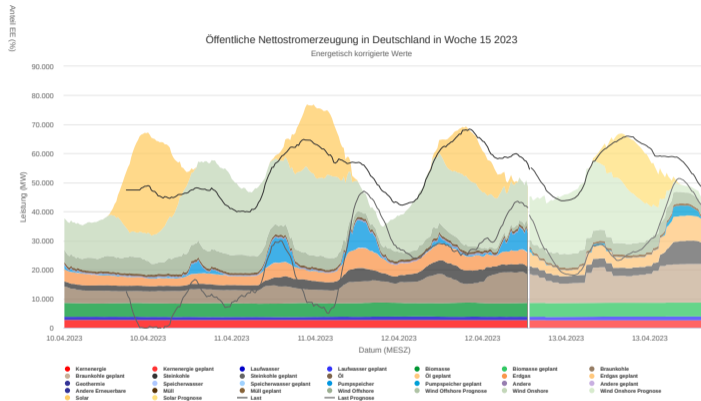
Africa & Middle East, Americas, Asia & Oceania, Europe Grid Scale Market Watch



# The 2 Key Paradigms of the New Age Of Energy Abundance

## Paradigm 2

Volatility of source availability will (probably — with caveats depending on the cost & price of Power-to-X) mean that *energy is for free when the sun is shining and the wind is blowing.*



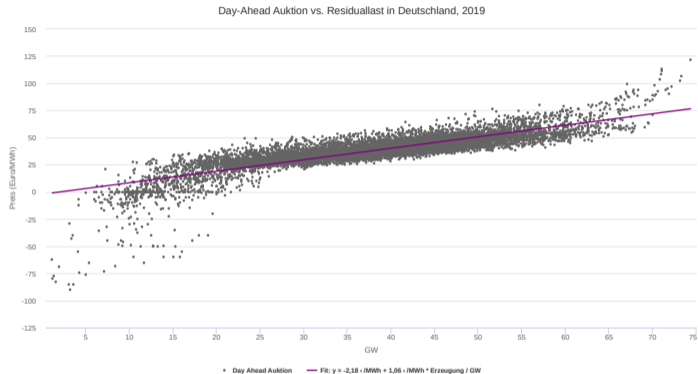
Energy-Charts.info; Datenquelle: ENTSO-E, AGEE-Stat, Destatis, Fraunhofer ISE, AG Energiebilanzen, EEX; Letztes Update: 12.04.2023, 22:34 MESZ

<https://www.energy-charts.info/charts/power/chart.htm?l=de&c=DE>

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## Paradigm 2

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[https://www.energy-charts.info/charts/price\\_scatter/chart.htm?l=de&c=DE&year=2019&residual\\_load=1&solar=0&wind\\_onshore=0&wind\\_offshore=0](https://www.energy-charts.info/charts/price_scatter/chart.htm?l=de&c=DE&year=2019&residual_load=1&solar=0&wind_onshore=0&wind_offshore=0)

# Project Idea

- Get long-term real fluctuations of renewables from <https://energy-charts.info/>
- Parametrize energy price dependents of RE power on wind/sunshine from [https://www.energy-charts.info/charts/price\\_scatter/chart.htm?l=de&c=DE&wind\\_onshore=1&wind\\_offshore=1&hydro\\_run-of-river=1&biomass=1&geothermal=1&hydro\\_water\\_reservoir=1&hydro\\_pumped\\_storage=1](https://www.energy-charts.info/charts/price_scatter/chart.htm?l=de&c=DE&wind_onshore=1&wind_offshore=1&hydro_run-of-river=1&biomass=1&geothermal=1&hydro_water_reservoir=1&hydro_pumped_storage=1)
- Get energy price projections e.g. from <https://ieeexplore.ieee.org/document/9837910>
- Project computing hardware price from past experience
- Optimize 'Computing Overcapacity' as a function of the duty cycle
- 'If we want to have a duty cycle of  $X\%$ , we will save  $Y$  k€ on electricity and have to spend  $Z$  k€ more on hardware to make up for lost time'
- Regulation of COBaID/TARDIS drone count, feedback from AUDITOR possible
- Key ingredient: 'Checkpoint and restore' of compute jobs such that jobs can be started, stopped or moved without loss, ideally on the container level.