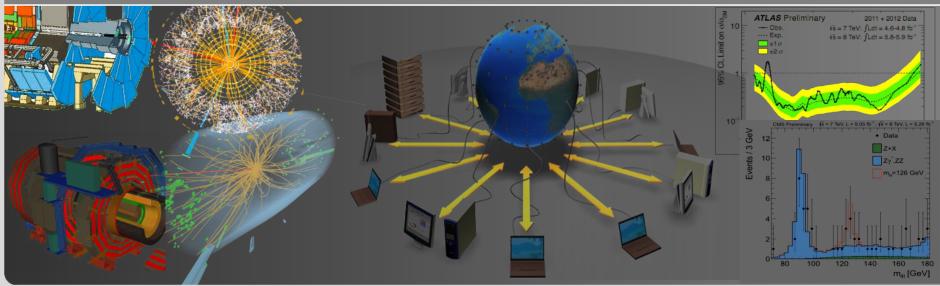


Integration of Clouds in HEP Grid

Günter Quast

Fakultät für Physik Institut für Experimentelle Teilchenphysik

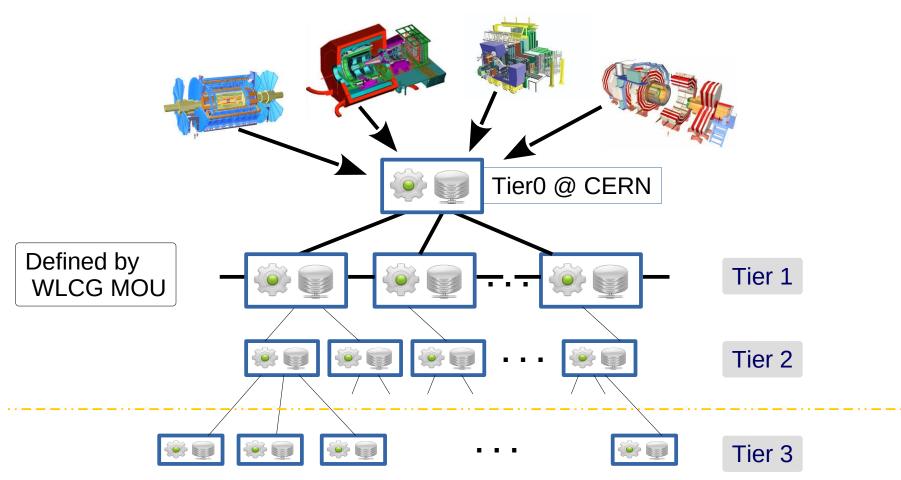
KET Workshop Software & Computing



www.kit.edu

Grid to Cloud

The original hierarchical World Wide LHC Computing Grid

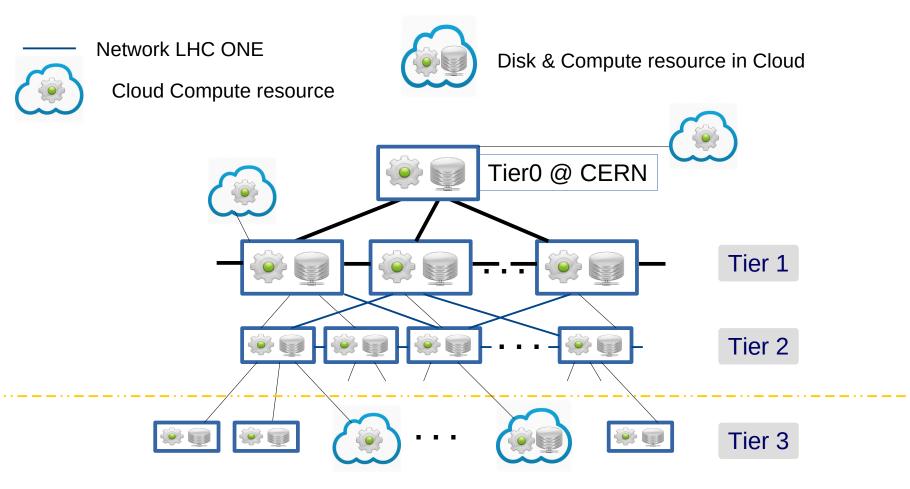


All centers "owned" by particle physics groups

- common operating system (scientific linux)
- common services, in particular grid middleware
- common software stack

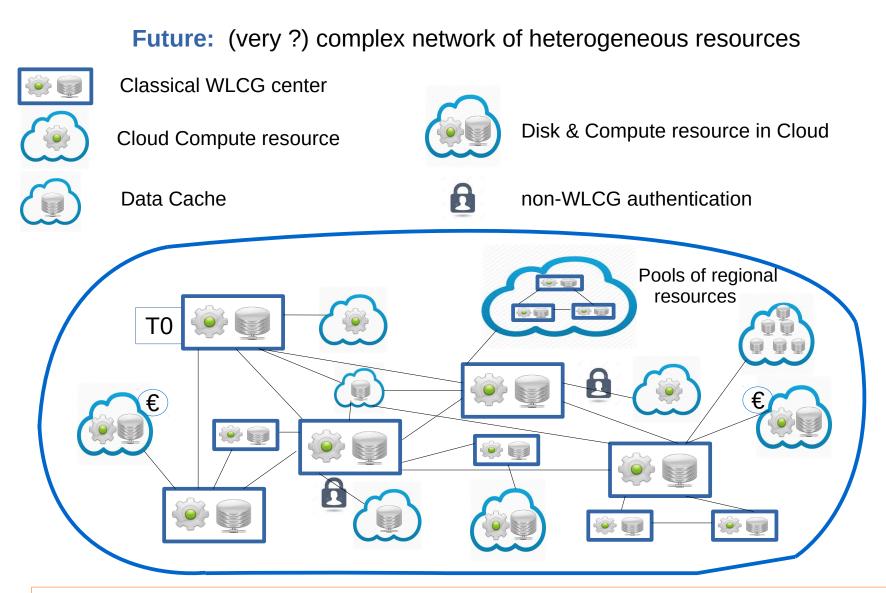
Grid to Cloud

Today with many more network connections (Grid \rightarrow Mesh) and first cloud additions



- LHC One Network connecting Tier2 / Tier2
- Data federations with remote access
- addition of "diskless Tier3", and of Cloud Resources

Grid to Cloud



Challenges: (dynamic) workflow management and scheduling, optimisation of data placement, (dynamic) resource provisioning, authentication, billing, ...

Cloud-enabling Technologies in HEP

CernVM:

- Virtual machine based on Scientific Linux (maintained by CERN)
- Very lightweight, can be directly deployed on various cloud sites

Container: Docker or Singularity

encapsulates services, experiment software and user code

CernVM-FS:

- On-demand HTTP based file system (Caching via HTTP Proxy)
- Many big experiments use it to deploy software to WLCG compute centres
- works excellently also on cloud sites

HTCondor:

- Free and open-source batch system commonly used in HEP
- Excellent with integrating dynamic worker nodes (even behind NATed networks)

<u>xRootD</u> and **data federations** for remote access

Cloud Management Interface, e.g. ROCED [KIT]:

- Cloud scheduler that supports multiple cloud APIs (OpenStack, Amazon EC2 and other commercial providers, special HPC site adapters)
- Easily extendable thanks to modular design Parses HTCondor ClassAds and boots VMs on cloud sites depending on the number of queued jobs





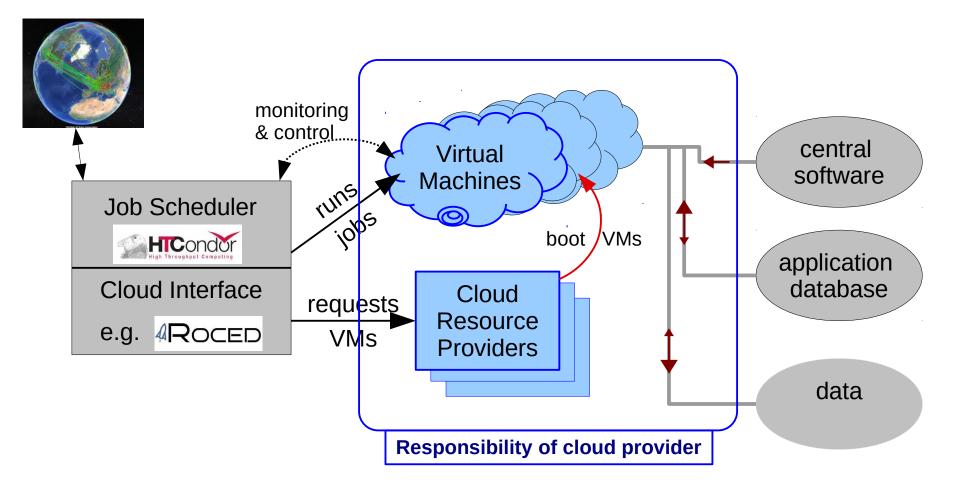






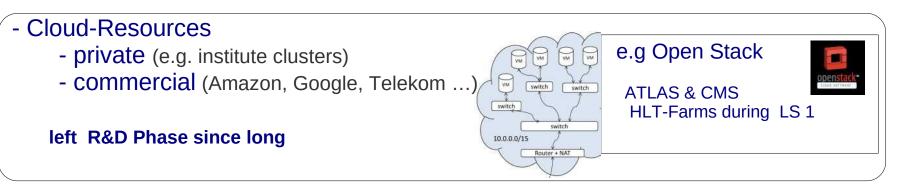


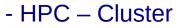
Principle of including external resources



automated, dynamic provisioning of cloud resources for suitable classes of jobs

Existing Examples





- many HEP applications run
- MPI interfaces and SAN not needed for HEP
 - \rightarrow an expensive way!



e.g. Super-MUC at LRZ in Munich, SDCC at CMS or the new bwHPC Cluster in Freiburg (ATLAS/CMS/LHCb)

- no Grid services / authentication
- fast, but small and expensive disk
- often small WAN bandwidth
- different "Site Policies"

special solutions for every single case → personnel !

- Commercial providers,



IaaS provided by two commercial consortia in final project phase







- working with industry is different
- must define requirements precisely & monitor results

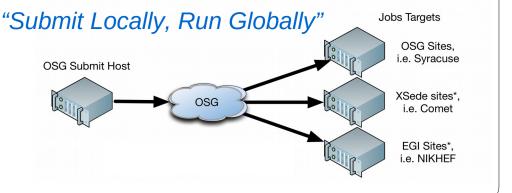
feeling of project participant: "spent far more (unfunded) time than initially estimated"

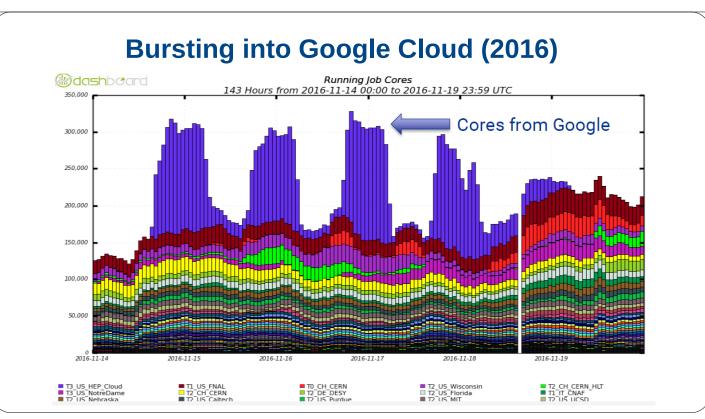
Existing Examples (2)



Open Science Grid (OSG) in the US

drive development of Science Clouds, centered around HTCondor, provide full software stack & documentation, organize schools and support





Existing Examples (3)

Amazon Cloud (Amazon Web Services)

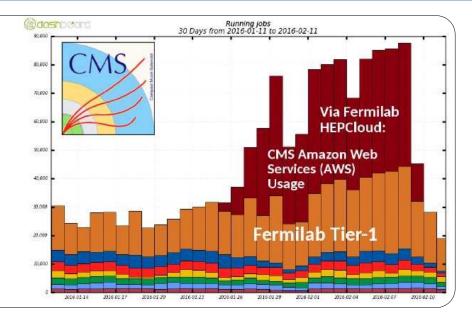
- provided to CMS via FNAL Tier1 – more than doubled available CPU at
 - Tier Ones
- sponsored by provider, but cost on spot market approaching reasonable levels: (FNAL: 0.9 Cent/ CPU hour, Amazon: 1.4 Cent/CPU hour)

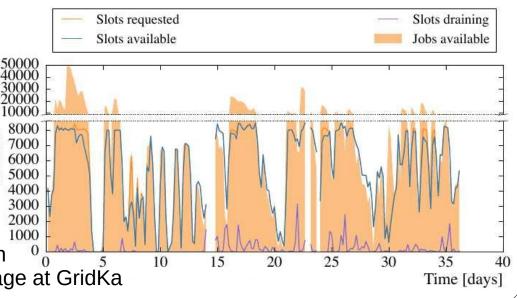
a similar project with Amazon also by ATLAS via BNL

bwFOR cluster NEMO in Freiburg:

(for Neuro-Science, Elementary Particle Physics and Microsystems Engineering)

- fully virtualised set-up; controlled by ROCED (KIT) and HTCondor
- Production system scaled up to 11k
 virtualised cores, more than 7 million of USE
 CPU hours of user jobs processed in four months
- saturating 20 GBit/s BelWü link between 0 Karlsruhe Freiburg and NRG Grid storage at GridKa





a word on Opportunistic Resources

Opportunistic Resource: Any resources not permanently dedicated to, but temporarily available for a specific task, user or group.

- very common in university environments:
 - university clusters shared by many groups and communities
 - DFG-funded resources,
 - typically allocated on approved request only for given time or *#* of CPU hours, only temporary storage as long as project runs
 - "empty" cycles on HPC systems
 - in the future:
 - cheap commercial CPU cycles
 - to cover peak loads or to benefit from special offers on the "spot market"
 - dedicated "Science Clouds"
- Challenges:
 - often not at all corresponding to "typical" HEP setups need easy and light-weight access methods
 - must be dynamically managed and integrated into workflows need automatic cloud and batch interfaces
 - need careful monitoring of remote resource usage
 e.g. to avoid expensive network traffic from/to commercial cloud sites
 - "every such site is special"
 can only be integrated by "local" personnel
 - may require special access rights and authentication may need local "proxy" to submit jobs

Opportunistic Resources @ KIT

Longtime experience @ KIT with virtualisation, opportunistic resources and containers:

- Software development
 ViBatch, Roced (now → CBOalD), NaviX
- Virtualisation with Xen, kvm, OpenStack
- Containers Docker and Singularity
- Opportunistic Resources
 - Test systems (incl. Desktops) with OpenStack and Docker
 - HPC Clusters

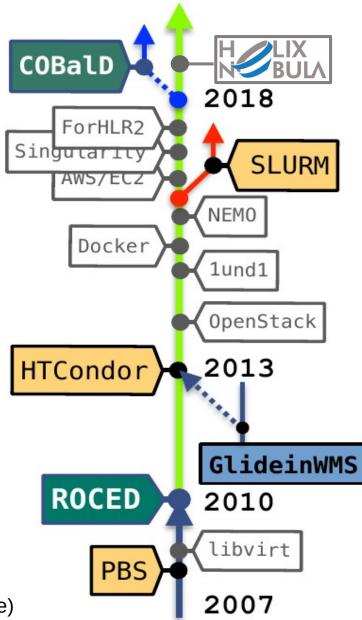
Ic1 @Uni Ka (ViBatch), ForHLR @KIT (Singularity), bwFORcluster NEMO @Uni Fr (OpenStack)

 commercial Cloud providers AWS, 1&1 Cloud Services, OTC, ExoScale

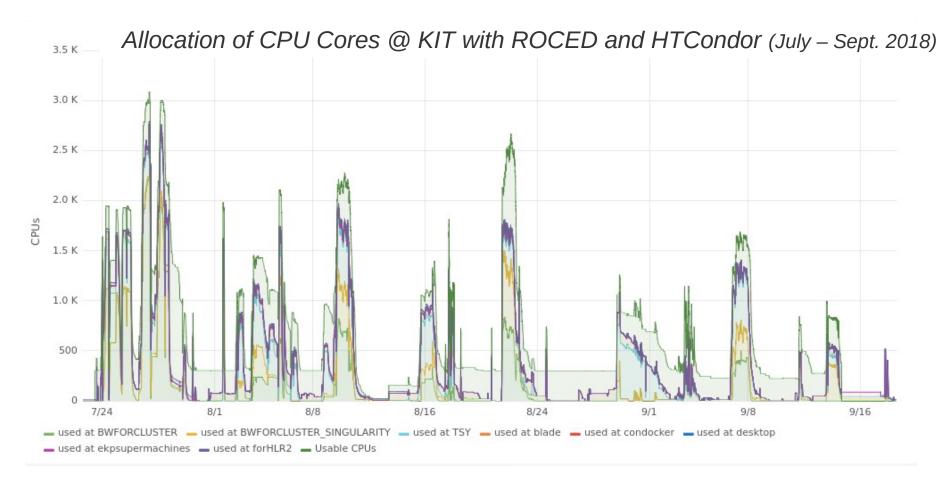
All controlled via a single HTCondor instance and cloud interface AROCED

many of them simultaneously and in production mode

(see next slide)



Usage of Opportunistic Resources @ KIT



- ~3000 cores, dynamically allocated, at fives sites: bwFor NEMO (Fr), forHLR2 (Ka), TSystems (HelixNebula), local desktops & blade center
- low to medium I/O jobs, e.g. NNLO Calculations, Monte Carlo production, or generation of hybrid events by embedding MC in data
- Job scheduling is still partly "hand work"

Could Interface, here AROCED

ROCED (Responsive On-Demand Cloud-enabled Deployment):

Interface between batch system (Torque, HTCondor) and cloud sites.

- monitoring of computing needs (jobs in queue) and resources
- dynamic management of remote cloud resources: starting/stopping of virtualized remote worker nodes
- site adapters "know" how to provide vitualized or containerized resources

Integration Adapters		Requirement Adapters
integrates booted compute nodes into existing batch server		supplies information about needed compute nodes, e.g. queue size
HTCondor Torque Grid Engine 	ROCED Core	HTCondor Torque Grid Engine
	decides which machines to boot or shutdown	https://github.com/roced-scheduler/ROCED
	Site Adapters	ROCED has grown over time
	boot machines on various Cloud Computing sites	 – easy to integrate new providers
	Hybrid HPC Cluster Commercial Providers OpenStack Eucalyptus OpenNebula	 difficult to manage many providers for many users needs refactoring and further modularization successor: CObalD
		- the opportunistic balancing Demon

new development @ KIT for GridKa

Caching is common solution for repeated access to the same data. Cache data as close as possible to the CPU !

- Suitable for
 - HEP workflows that process the same datasets frequently
 - CPU resources without permanent storage

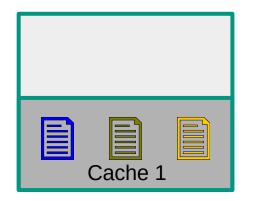
Problematic on distributed resources with multiple caches:

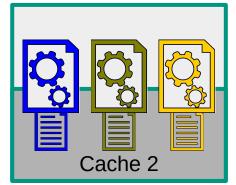


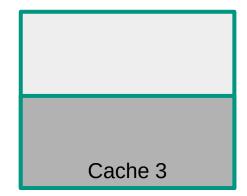
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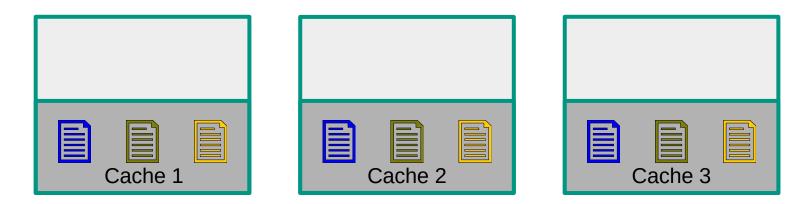




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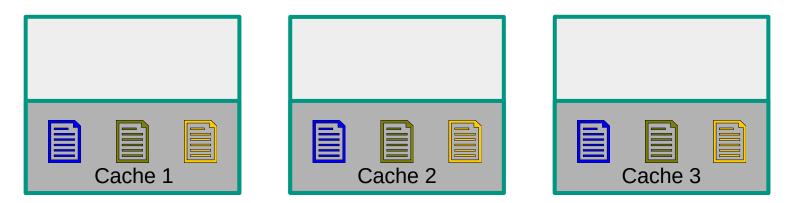
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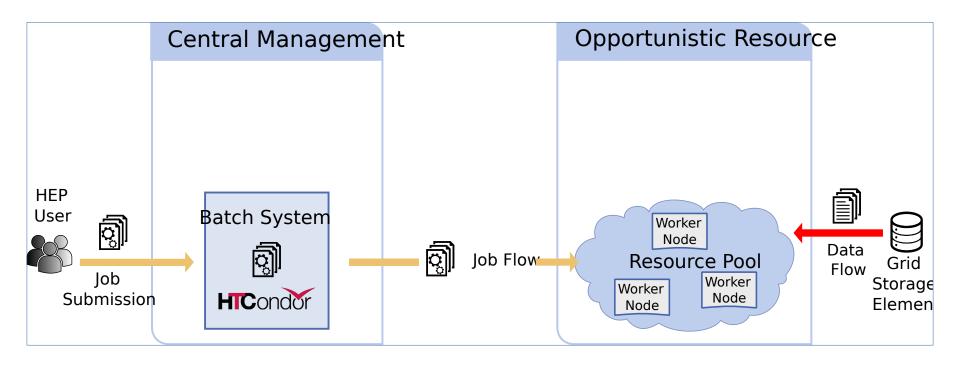
Waste of storage capacity due to replication of data!

⇒ Caches must be "coordinated" !

Coordinated Caching

Basic features for caching are provided by XRootD

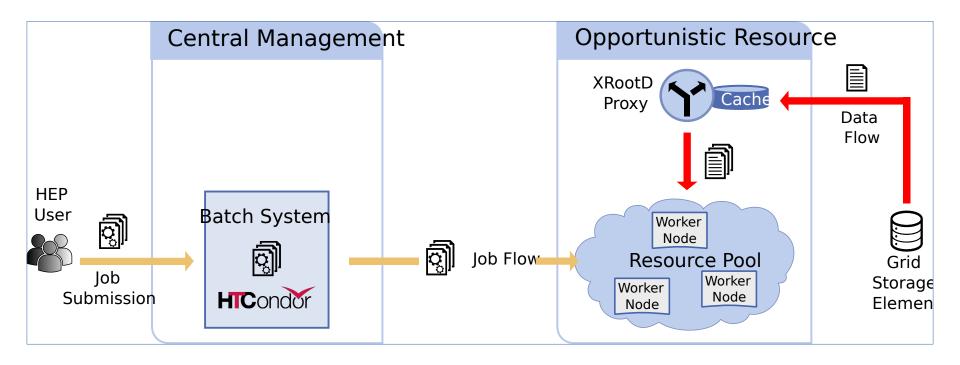
HICONDUT can handle job-to-resource scheduling



Coordinated Caching

Basic features for caching are provided by XRootD

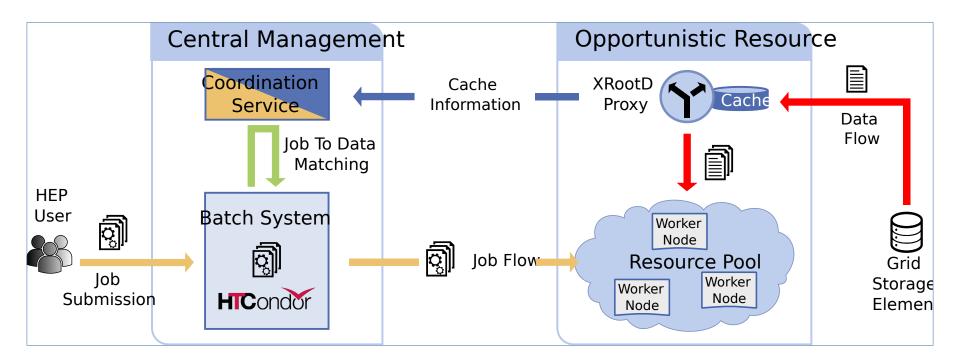
HICONDUR can handle job-to-resource scheduling



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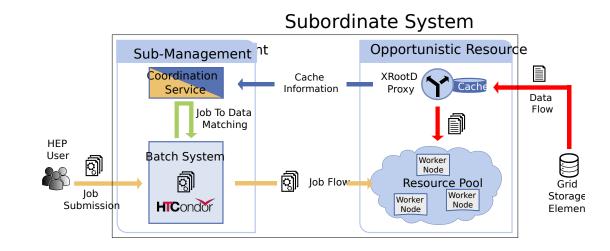
HICONDUT can handle job-to-resource scheduling



Coordination Service NaviX under development at KIT based on long-term experience: "Data Locality via Coordinated Caching for Distributed Processing", M. Fischer et al., J. Phys.: Conf. Ser.762 012011 (2016)

Scalability as a design feature of NaviX

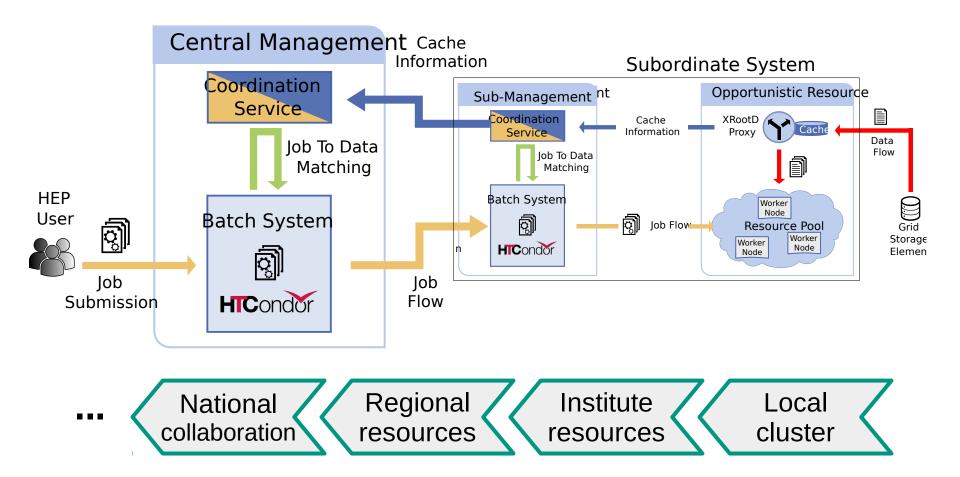
ideally, use the same components for local, site and regional caching



Scalability as a design feature of NaviX

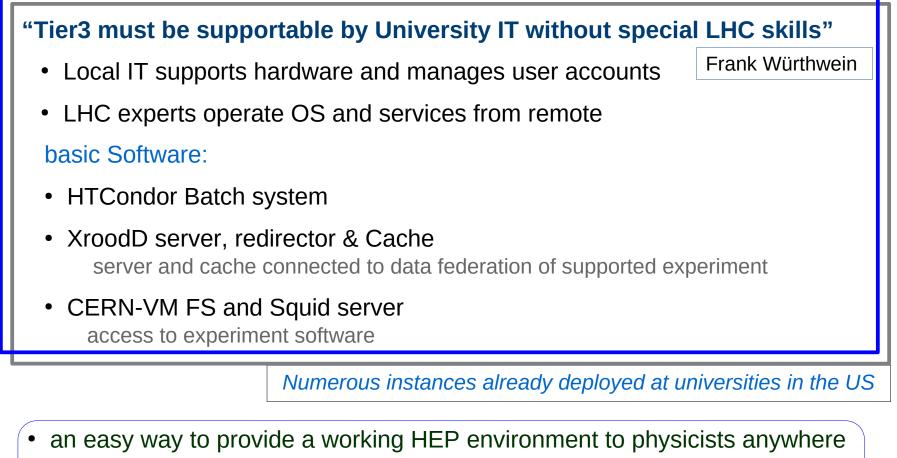
ideally, use the same components for local, site and regional caching

- XRootD and HTCondor take care of hierarchical upscaling
- Job-to-Cache coordination can be performed at all levels with regard to the data location information of the subsystems.



Easy Setup of a working HEP-Site

"Tier3 in a Box"



- concept can (and should be !) extended to "Tier2 in a Box"
- can also set up remote production sites in cloud environments
- provide "opportunistic resources" to WLCG when not (fully) used locally

however: Need sufficient network bandwidth (≥100 Gb/sec) to benefit

Setting up the "Box"

- VM-image(s) or container(s) set-up by (small) group of experts

can be very lean, as most of the required software comes via CERN-VM FS however, some providers require using their own images, allowing only moderate modifications

in such cases: can run HEP applications in a container

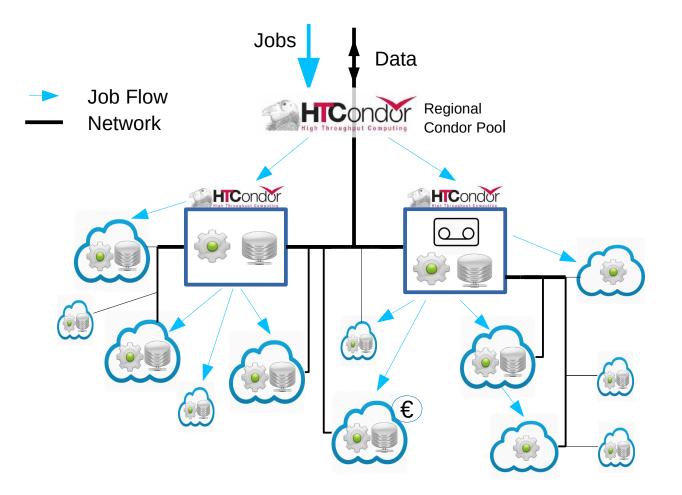
- permanent services (Squid server, XrootD, ...) also provided in virtual machines or containers, but sometimes difficult to guarantee presence of these services at a given site (requires permanently running instances)
- images may contain site-specific configurations (require automated) image and configuration management

Containers are much easier than virtual machines !

Provisioning of VM-images (in particular) and containers requires **additional R&D** and funding for **long-term support**

btw: since every one can contribute, this approach is **very beneficial for the training of young physicists !**

Blueprint (?) for the German contribution to LHC computing >2025 ?



Conclusions

Cloud technologies for HEP sites

- have proven to work well and reliably
- allow for sharing of resources between groups, institutes and scientific communities
- give access to resources not available otherwise, incl. commercial providers
- set-up of the scientific compute environment may happen "@home": educational benefit for young people !
- operate HEP sites with less effort: "Tier 2 / 3 out of the Box"
- Data Caching enables "diskless sites" (i.e. sites without centrally managed data store): temporary resources in clouds, institute clusters, ...
- Coordinated Caches in distributed environments reduce required disk space and increase bandwidth for data access

Cloud technologies are relevant future German contributions to LHC computing:

- Virtualised T2 and T3 ?
- bundle access to all national resources in one HTCondor pool?
- Disk Space @ T2 and T3 as (coordinated) caches ?

