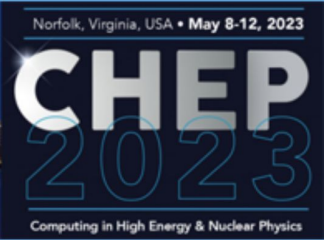


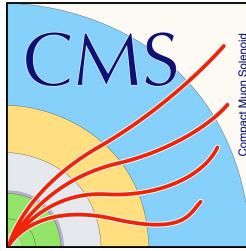


# The integration of heterogeneous resources in the CMS Submission Infrastructure for the LHC Run 3 and beyond

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1. CIEMAT and PIC (ES), 2. (US), 3. National Center for Physics (PK), 4. CERN, 5. Fermi National Accelerator Lab. (US)

**CHEP 2023, May 11th 2023**

# Outline of the talk

- Intro to using heterogeneous resources
- GPUs integration in SI
  - GPUs in FE and pilot factories, first matchmaking
  - GPUs in the Global Pool, second matchmaking
  - Using GPUs in WM and CRAB
- GPUs already available to CMS
- Non-x86 CPU architectures
- Conclusion and next steps

# Interest on heterogeneous resources

- **The availability of compute power in non CPU, non x86 processor types is abundant and increasing**
  - For example, looking at the examples from the top500.org list, it's clear that:
    - A significant fraction of the processing power in HPCs is provided by accelerators.
    - Many top positions include non-x86 CPU architectures (e.g. IBM Power systems:Summit, Sierra, Marconi-100)
  - Not only at HPC facilities, but also among traditional WLCG computing sites as well

- **HEP experiments must be prepared to run substantial part of their processing tasks at HPCs**

- CMS internal study (**ECoM2x, 2020**) of the computing model and resource needs looking into the LHC Run 3, but specially at the HL-LHC phase, includes in its recommendations:
  - *"CMS should continue to **aggressively expand the resources** accessible to it for production processing at facilities beyond those dedicated to the LHC"*
  - *"**CMS should strive towards using HPC resources effectively**"*
  - *"Use of on board **accelerators** as much as possible during reconstruction"*
  - *"Work towards enabling CMS software on CPUs, GPUs, FPGAs and TPUs as primary targets for its software stack"*
  - *"**Support non x86_64 CPU architectures**"*
- The CMS Phase-2 Computing model update document (**CMS-NOTE-2022-008**) also advises to **abandon the assumption of uniformity of our compute resources**, **evolving our WM and SI systems to embrace heterogeneity**

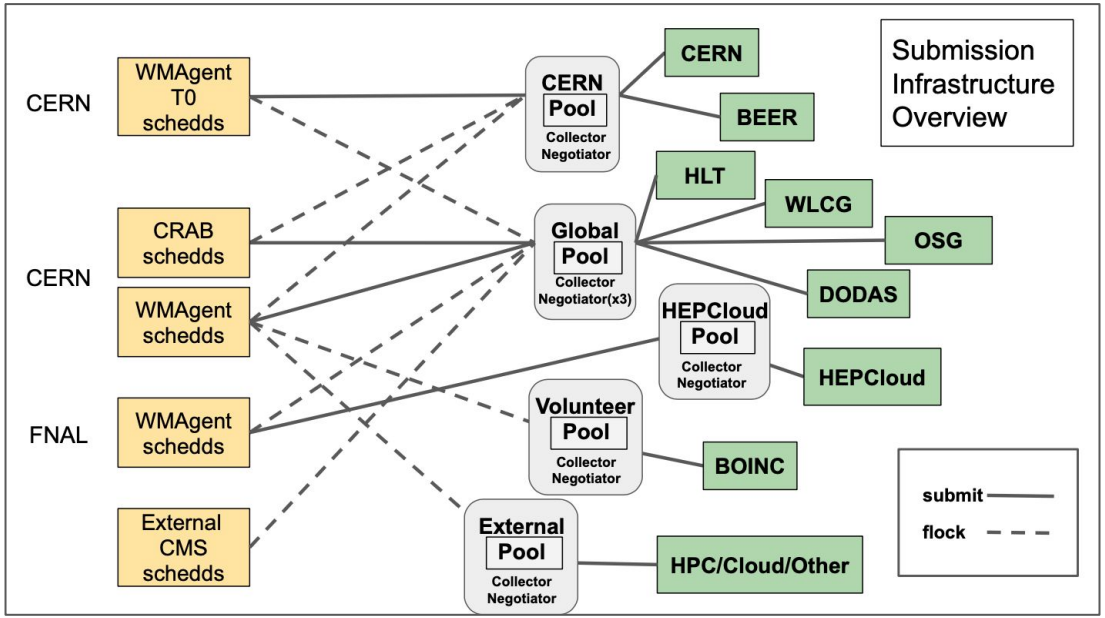
# The CMS Submission Infrastructure

**The CMS Submission Infrastructure** team in CMS Offline and Computing is in **charge** of operating a set of federated HTCondor pools which aggregates **resources from 70 Grid sites, plus non-Grid resources, where reconstruction, simulation, and analysis of physics data takes place**

**The challenges:**

- Operate our infrastructure managing an ever growing collection of computing resources
- Use all of our resources efficiently, maximizing data processing throughput
- Enforce task priorities according to CMS research programme
- Connecting new and more diverse resource types (including non-x86 architectures and GPUs) and sources (WLCG and OSG, HPC, Cloud, volunteer)

The topic of this talk



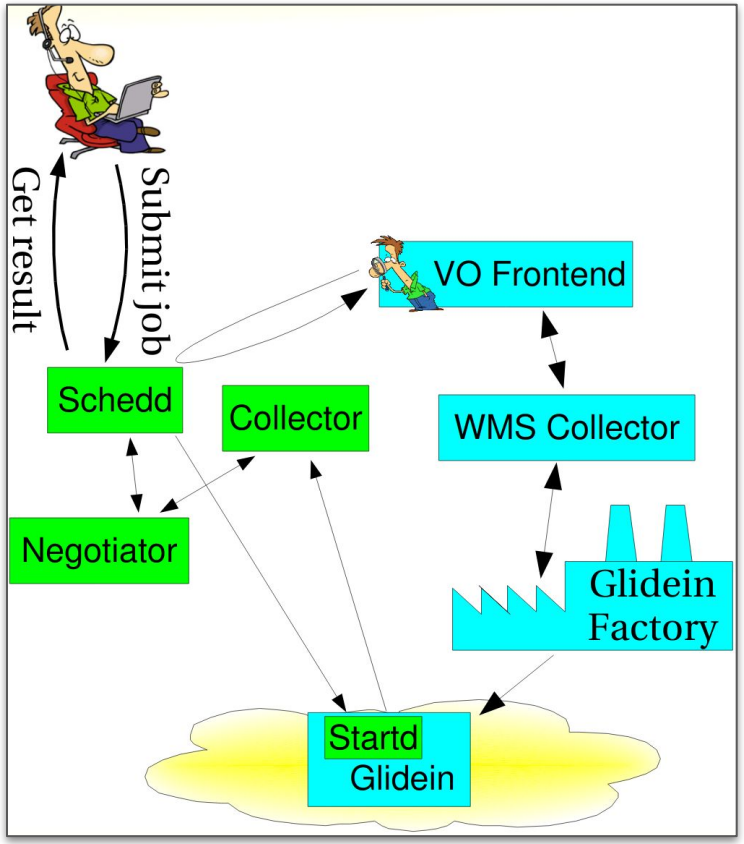
# GPUs integration to CMS SI

# Non-pledged heterogeneous resources

In relation to the use of GPUs in CMS offline computing, we need to consider that all GPUs available and in use by CMS today are still opportunistic, not pledged:

- **Pledged CPUs: agreed upon standard job execution slot**
  - **8-core slots, 48h of runtime, Minimum of 2 GB/core, etc**
- **No equivalent to "standard job slot" for GPUs**. This affects:
  - How to approach sites on what GPU resources CMS can use: how do we even know there are GPUs available for CMS? What CEs, queues and other parameters to use?
  - What is the correct GPU type?
  - How to configure the execution of tasks on these resources: no predefined rules on e.g. slot size, max execution time, memory, etc
- **Deeply affects how we use the resources**: no generic slot, requires more careful and detailed job and slot description in order to select the correct slot and avoid wastage

# Using resources in our dynamic HTCondor pools




**Two matchmaking stages** in Submission Infrastructure: resource allocation (GlideinWMS) and job to slot matchmaking (HTCondor)

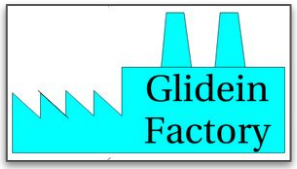
1. GlideinWMS and pilot jobs
   - Submit resource requests on sites CEs in order to join them into the Global HTCondor Pool

2. HTCondor matchmaking
   - Slot joins the Global Pool, then resources are negotiated and assigned to payload jobs

**GPU resources just follow the same general logic**

# GPU resource description in GWMS Factories

- **GPU resource description for first matchmaking in pilot factory entries**
  - **Limited information about the available GPUs:**
    - **CEs that allow access to GPUs, queue names, etc**
    - Slot attributes agreed upon with the site admins, (e.g. GPU slot lifetime 24h? 48h?)
    - **Statically configured, with most GPU specs only available at pilot runtime**
  - Typically, GPU slots are configured along with standard pilot features (8 CPU cores, 2 GB/core RAM)



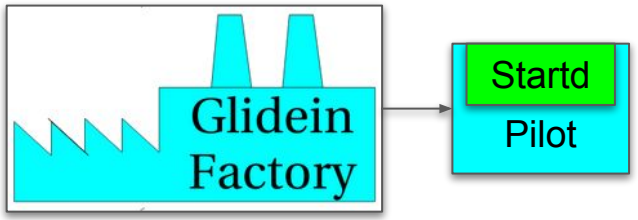

```
<entry name="CMSHTPC_T2_US_Wisconsin_cmsgrid01_gpu" auth_method="grid_proxy"
gatekeeper="cmsgrid01.hep.wisc.edu cmsgrid01.hep.wisc.edu:9619" gridtype="condor" ...>
   <config>
        (...)
        <submit_attrs>
               <submit_attr name="+maxMemory" value="20000"/>
               <submit_attr name="+xcount" value="8"/>
               <submit_attr name="Request_GPUs" value="1"/>
        </submit_attrs>
        </submit>
   </config>
   <attrs>
        <attr name="GLIDEIN_CMSSite" ... type="string" value="T2_US_Wisconsin"/>
        <attr name="GLIDEIN_CPUS" ... type="string" value="8"/>
        <attr name="GLIDEIN_MaxMemMBs" ... type="int" value="20240"/>
        <attr name="GLIDEIN_Max_Walltime" ... type="int" value="216000"/>
        <attr name="GLIDEIN_Resource_Slots" ... type="string" value="GPUs,1,type=main"/>
        (...)
   </attrs>
</entry>
```

# First Matchmaking (GWMS Front End)

- First matchmaking:
  - Only jobs with ***RequiresGPU*** will trigger GPU pilot job submission
  - Slot description very limited (“slot has some kind of GPU”), runtime parameters are not available at this stage yet
  - But of course other parameters, such as site whitelist, still apply here
  - Upon successful match, pilots are submitted to all corresponding CEs

- Being opportunistic, we implemented site preferences concerning how to use their GPUs, **reserving the slot for GPU-like workloads**:
  - No CPU jobs will start for the first 30 mins
  - Then either open for all jobs, or return the slot back to site (site preference)
  - Once GPU is in use, try to saturate the remainder CPU part

- Given late-binding, to minimize waste, **avoid pilots landing on a GPU node once the GPU workload is done**
  - Remove stale pilots still queued at sites CEs
    - Common practice for CPU pilots, but even more critical for GPUs



# Resource description in the Global Pool

- **Once a pilot starts** execution on remote resources, **GPU properties** are updated to the slot classad:
  - **condor_gpu_discovery** retrieves most of the relevant matchmaking attributes
  - CMS_CUDA_SUPPORTED_RUNTIMES from CMS script in cvmfs

## GPU slot attributes

```
CPUs = 8
TotalSlotMemory = 20000
GPUs = 2
CUDACapability = 8.0
CUDAClockMhz = 1410.0
CUDAComputeUnits = 108
CUDACoresPerCU = 64
CUDADeviceName = "NVIDIA A100-PCIE-40GB"
CUDADriverVersion = 11.3
CUDAECCEnabled = true
CUDAGlobalMemoryMB = 40536
CUDAMaxSupportedVersion = 11030
CMS_CUDA_SUPPORTED_RUNTIMES = 10.1,10.2,11.0,11.1,...
CMS_NVIDIA_DRIVER_VERSION = 515.48.07
```

# Second matchmaking in HTCondor

- For each properly configured GPU slot that joins the Global Pool, the HTCondor *negotiator* will compare **job requirements** with machine attributes (**second matchmaking**)
  - **Any dynamically retrieved GPU property can now be used to filter suitable slots in relation to a given workflow**

**Job requirements**

```
RequestGPUs = 1
RequiresGPU = 1
...
Requirements =
CUDACapability >= 3 &&
CUDARuntime = "11.4" &&
GPUMemoryMB = 8000 && …
...
```

**Collector + Negotiator**

```
...
Machine.CUDACapability in Job.CUDACapability
Job.CUDARuntime in Machine.CMS_CUDA_SUPPORTED_RUNTIMES
Job.GPUs <= Machine.GPUs
...
```

**Machine attributes**

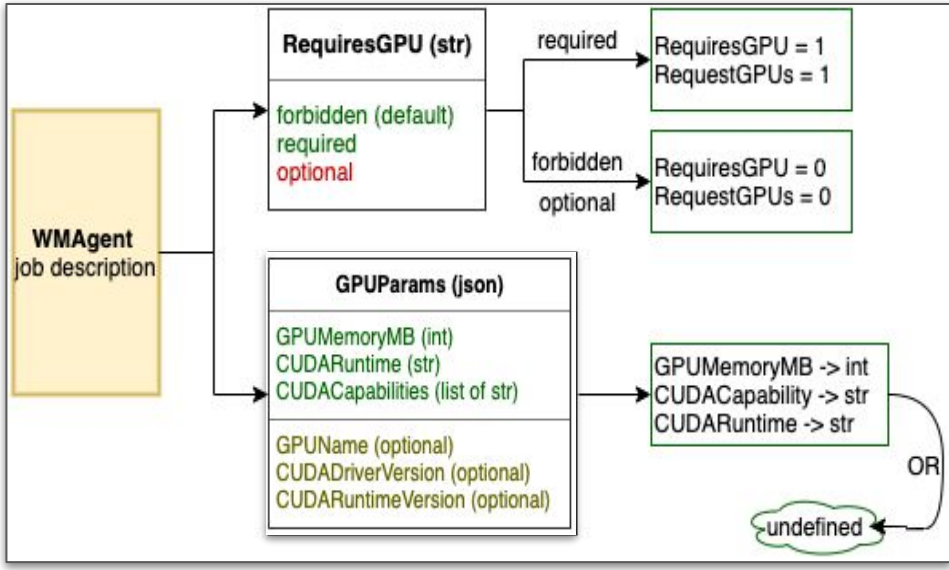
```
CPUs = 8
GPUs = 2
CUDACapability = 8.0
CUDAClockMhz = 1410.0
CUDAComputeUnits = 108
CUDACoresPerCU = 64
CUDADeviceName = "NVIDIA A100-PCIE-40GB"
CUDADriverVersion = 11.3
CUDAECCEnabled = true
CUDAGlobalMemoryMb = 40536
CUDAMaxSupportedVersion = 11030
CMS_CUDA_SUPPORTED_RUNTIMES =
10.1,10.2,11.0,11.1,...

...
```

# GPU support in the WM system

- WM layer acts as interface between user requests and the actual **job creation** into the HTCondor *schedd* queues
  - Map user request into a job jdl with attributes to be used in both matchmaking stages

- Agreement on the introduction of a new set of key/value pairs to be employed by any GPU workflow
  - mapped into **a total of 5 htcondor job attributes (plus 3 optional)**




GPU support in WMCore and CRAB

# GPU use cases and matchmaking stages

- With regards to how CMS jobs relate to GPUs, while the situation is evolving, three use cases are considered:
  - Job must use GPUs
  - Job can use GPUs
  - Job can only use CPUs

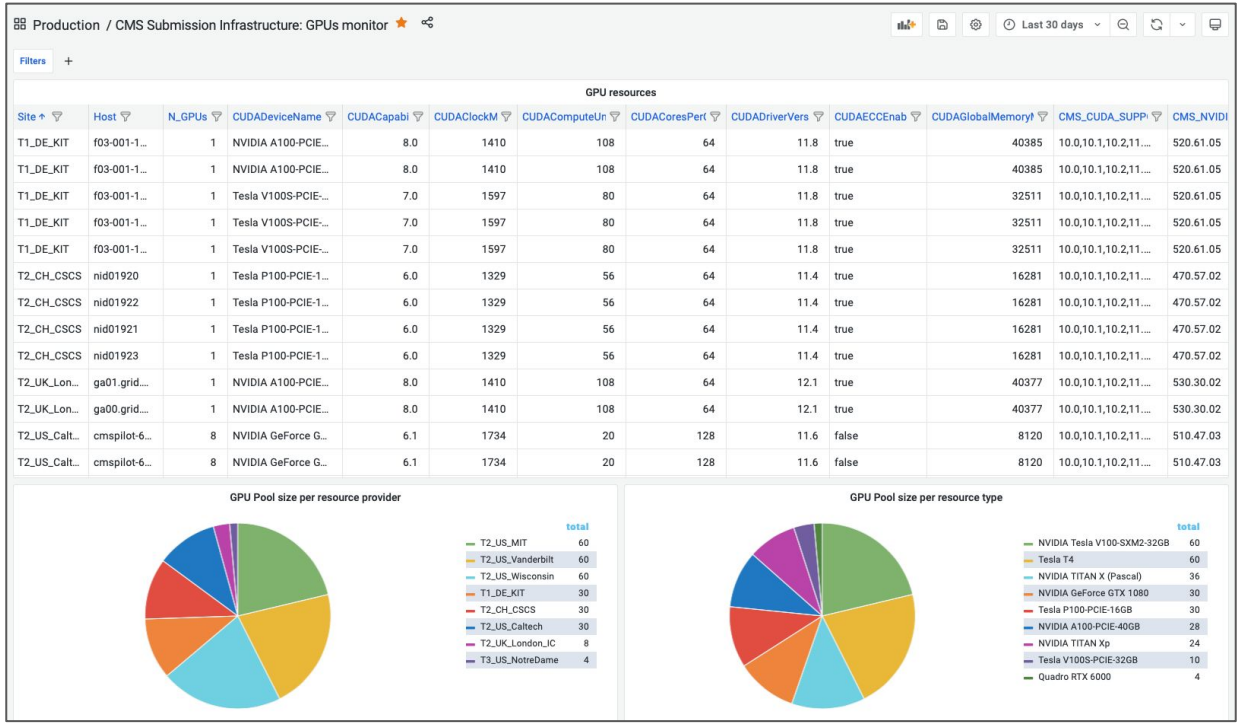
- Access and use of GPUs under control of two main attributes in the job jdl:
  - `RequiresGPU`: Defines whether or not GPU pilots will be requested by the first (GlideinWMS FE) matchmaking
  - `RequestGPUs`: Number of GPU resources to be matched in the second (HTCondor) matchmaking

- The three use cases are covered:
  - `RequiresGPU = 1 && RequestGPUs>0` will trigger GPU pilot, then match the slot
  - `RequiresGPU = 0 && RequestGPUs>0` will not trigger GPU pilots but CAN match already available GPU slots.
    - Need to discuss preference for CPU+GPU over CPU slots
  - `RequiresGPU = False && RequestGPUs=0` for purely CPU task

# Availability of GPUs in CMS SI

# Advertising GPUs already available to CMS

- **Multiple CMS WLCG sites already kindly making their GPU resources available for CMS use**
- **GPU inventory:** SI regularly scanning the Global Pool for GPU resources**, collecting their availability** and **properties**, then **published in the GPU monitoring table**
  - Recent (e.g. last 30d) results should inform users about “what is available and where”

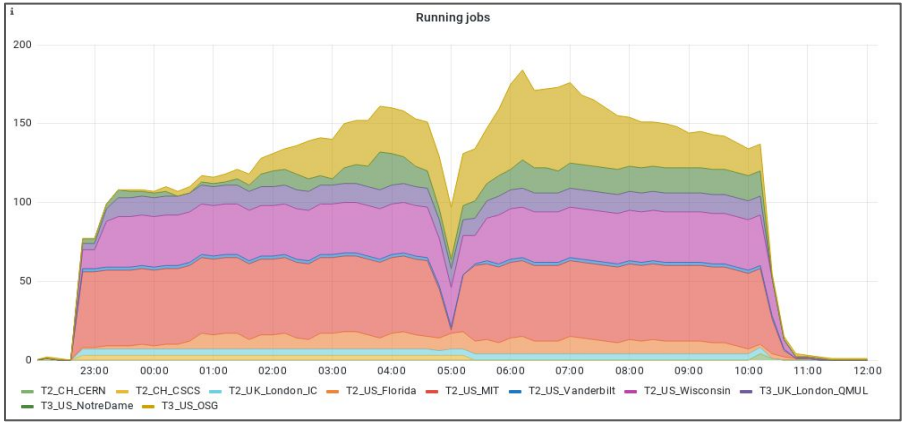


# Scale test for GPUs in CMS SI

**Executed a scale and performance test on GPUs in the CMS Global Pool**

- Injected about 15k test jobs on the Global Pool, targeting any available GPU for 24h: **match as many GPUs as possible**, check how many and where they are and what type, etc
- Used a simple TensorFlow multiple (10k x 10k, float16) **random matrix multiplication** script as GPU payload
- Recorded total **execution time**, correlated to accelerator performance

**Results**: Achieved a peak allocation of over **150 GPUs in parallel** in the Global Pool




## About 230 distinct opportunistic GPUs discovered during the test

| Site | GPU_Type | N_GPUs |
|---|---|---|
| T2_CH_CERN | Tesla V100S-PCIE-32GB | 8 |
| T2_CH_CERN | Tesla T4 | 8 |
| T2_CH_CERN | Tesla V100-PCIE-32GB | 5 |
| T2_CH_CSCS | Tesla P100-PCIE-16GB | 4 |
| T2_UK_London_IC | NVIDIA A100-PCIE-40GB | 4 |
| T2_US_Florida | NVIDIA GeForce RTX 2080 Ti | 72 |
| T2_US_MIT | NVIDIA Tesla V100-SXM2-32GB | 3 |
| T2_US_Purdue | NVIDIA Tesla T4 | 4 |
| T2_US_Vanderbilt | NVIDIA TITAN Xp | 3 |
| T2_US_Wisconsin | Tesla T4 | 32 |
| T3_UK_London_QMUL | NVIDIA A100-PCIE-40GB | 12 |
| T3_US_NotreDame | Quadro RTX 6000 | 15 |
| T3_US_NotreDame | Tesla V100-PCIE-32GB | 2 |
| T3_US_OSG | Tesla V100-PCIE-32GB | 31 |
| T3_US_OSG | Tesla P100-PCIE-16GB | 9 |
| T3_US_OSG | Quadro RTX 5000 | 8 |
| T3_US_OSG | Tesla V100-PCIE-16GB | 3 |
| T3_US_OSG | Tesla P100-PCIE-12GB | 2 |
| T3_US_OSG | NVIDIA GeForce GTX 1080 Ti | 2 |
| T3_US_OSG | Quadro RTX 8000 | 2 |
| T3_US_OSG | NVIDIA GeForce GTX 1060 6GB | 1 |

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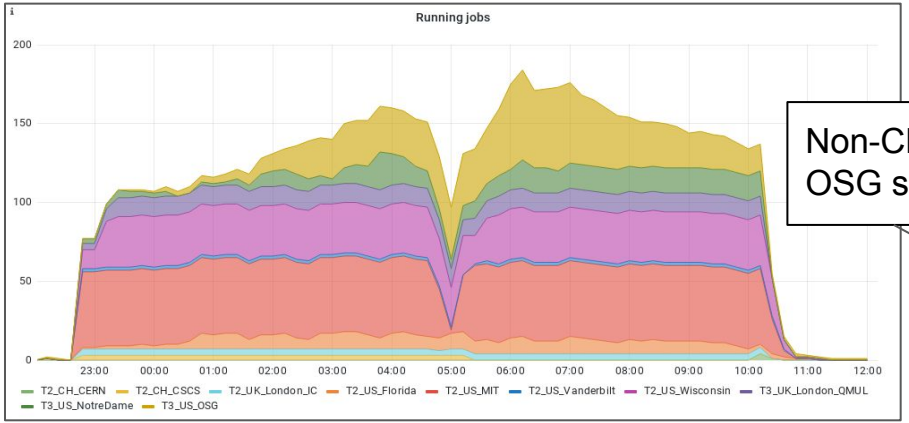


Non-CMS OSG sites!

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| T2_US_Purdue | NVIDIA Tesla T4 | 4 |
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| T2_US_Wisconsin | Tesla T4 | 32 |
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| T3_US_OSG | Quadro RTX 5000 | 8 |
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| T3_US_OSG | NVIDIA GeForce GTX 1080 Ti | 2 |
| T3_US_OSG | Quadro RTX 8000 | 2 |
| T3_US_OSG | NVIDIA GeForce GTX 1060 6GB | 1 |

# Integration of non-x86 architectures

# Multi-architecture matchmaking (I)

The CMS SI and WM systems were originally built and deployed assuming the x86_64 standard

- The WM and SI underwent adaptation to allow access and use of other architectures
  - Power9 was the first non-x86 platform available at scale for CMS (at CNAF/CINECA)
  - Initially tested with manually launched pilots (ad-hoc compiled HTCondor startd), no singularity container
  - By mid 2022, HTCondor support for ARM (aarch64) and Power PC (ppc64le) CPU architectures available
    - Startds added to the GideinWMS pilot factory, can now access these resource types with GlideinWMS pilots

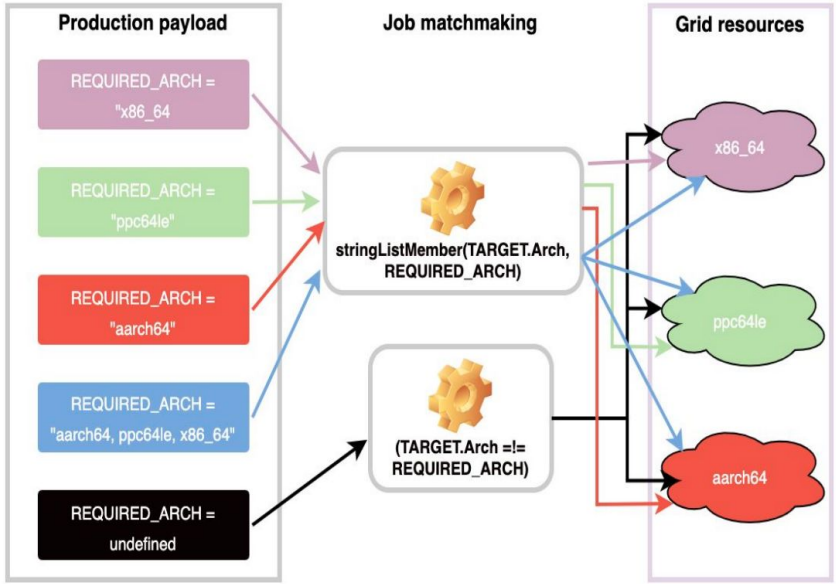
- Power9 arch is now fully commissioned and its CMSSW has been physics-validated. **Next is ARM:**
  - CERN granted access to a few ARM machines to be accessed as Grid resources, and again at CNAF
  - Ongoing integration and physics validation tests

- RISC-V architecture by the HL-LHC era?

# Multi-architecture matchmaking (II)

Resource architecture has been turned into a configurable parameter, to be used in the two CMS SI matchmaking phases:

- Payload jobs describe their resource requirements, which may include matching a specific or multiple architectures
- Provisioning of the corresponding resources via the HTCondor Global Pool
- HTCondor second matchmaking step




```
Requirements = (stringListMember(TARGET.Arch,"ppc64le,X86_64")) && (TARGET.OpSys
== "LINUX") && (TARGET.Disk >= RequestDisk) && (TARGET.Memory >= RequestMemory) &&
(TARGET.Cpus >= RequestCpus) && (TARGET.HasFileTransfer)
```

# Conclusions

# Conclusions

- **Resource heterogeneity** in HEP computing is a **key element** moving forward
  - CMS is adapting its WM and SI systems to properly manage new resource types and providers and put them to good use
- Heterogeneous collection of resources: **no standard slot definition exists**
  - Workload scheduling requires careful description of slot properties and workload requirements for effective matchmaking
- With regards to **GPUs**, still **opportunistic** but a sizable number and variety **already available** in the CMS Global Pool
  - Detailed inventory of available GPUs produced to promote GPU resource exploitation by CMS users
  - **CMS scientists and central production can now easily use GPUs for their workflows on the Grid**
- Non x86 CPU architectures **integration** to CMS computing is **ongoing**
  - Power9 fully integrated and validated
  - ARM being commissioned
- Challenges ahead
  - Efficient execution of CMS multi-steps jobs on CPU/GPU heterogeneous resources
  - Benchmarking and accounting required for realistic usage at scale in the WLCG context

# Acknowledgements

Projects FPA2016-80994-C2-1-R, PID2019-110942RB-C21, BES-2017-082665 and PID2020-113807RA-I00 funded by: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US National Science Foundation under Grant No. 2121686

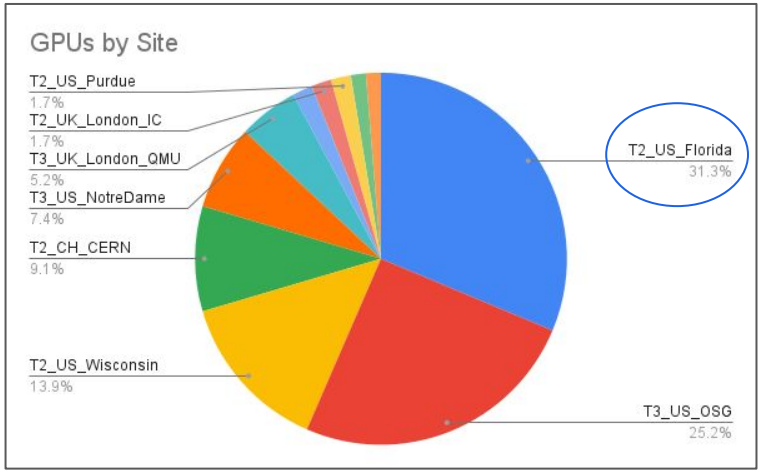
UC San Diego

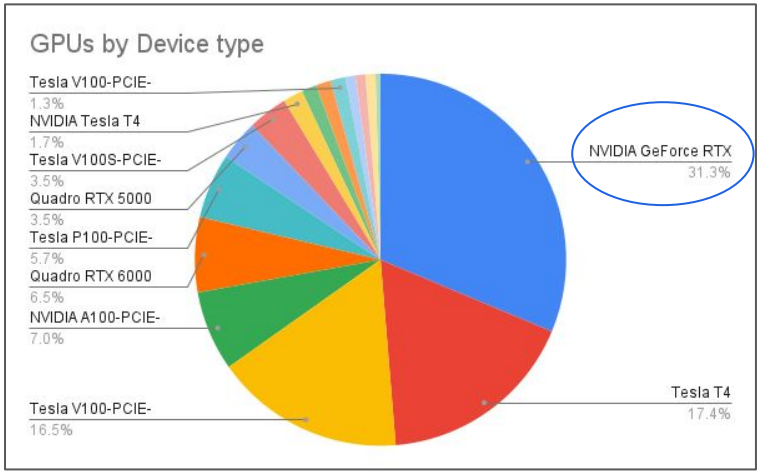
# Backup Slides

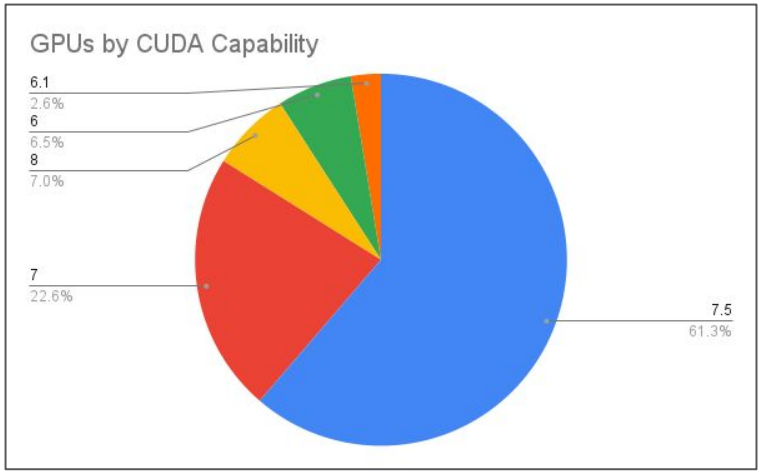
# Abstract

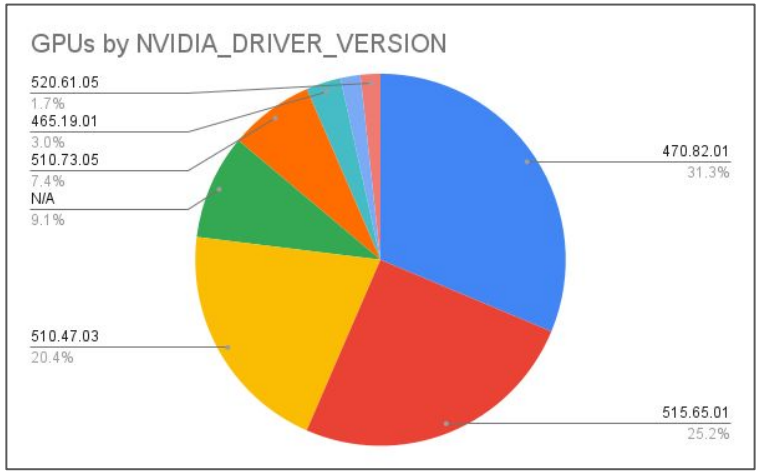
The computing resources supporting the LHC experiments research programmes are still dominated by x86 processors deployed at WLCG sites. This will however evolve in the coming years, as a growing number of HPC and Cloud facilities will be employed by the collaborations in order to process the vast amounts of data to be collected in the LHC Run 3 and into the HL-LHC phase. Compute power in these facilities typically includes a significant (or even dominant) fraction of non-x86 components, such as alternative CPU architectures (ARM, Power) and a variety of GPU specifications. Using these heterogeneous resources efficiently will be therefore essential for the LHC collaborations reaching their scientific goals. The Submission Infrastructure (SI) is a central element in the CMS Offline Computing model, enabling resource acquisition and exploitation by CMS data processing, simulation and analysis tasks. The SI is implemented as a set of federated HTCondor dynamic pools, which must therefore be adapted to ensure access and optimal usage of alternative processors and coprocessors such as GPUs. Resource provisioning and workload management tools and strategies in use by the CMS SI team must take into account questions such as the optimal level of granularity in the description of the resources and how to prioritize CMS diversity of workflows in relation to the new resource mix. Some steps in this evolution towards profiting from this higher resource heterogeneity have been already taken. For example, CMS is already opportunistically using a pool of GPU slots provided mainly at the CMS WLCG sites. Additionally, Power processors have been validated for CMS production at the Marconi100 cluster at CINECA. This contribution will describe the updated capabilities of the SI to continue ensuring the efficient allocation and use of computing resources by CMS, despite their increasing diversity. The next steps towards a full integration and support of heterogeneous resources according to CMS needs will also be reported.

# GPU scale and performance test



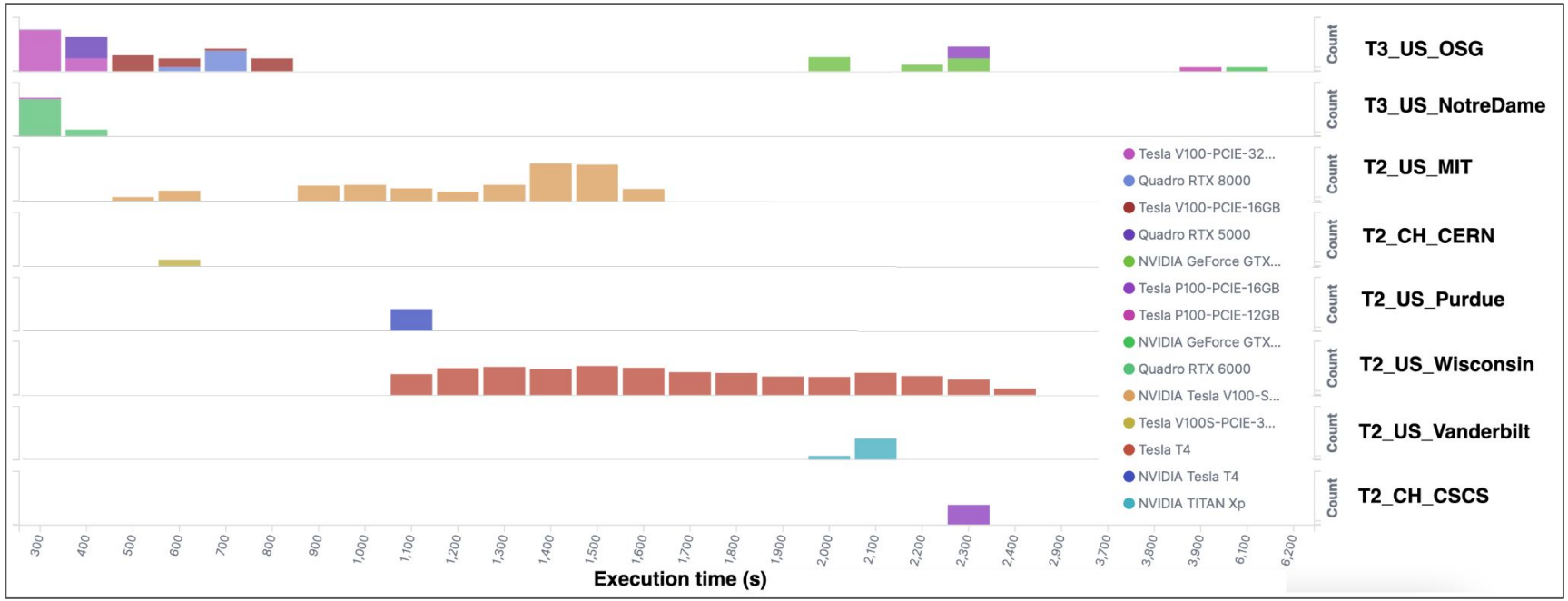



# GPU scale and performance test

- Execution time as a function of site and GPU type: a factor 10x variance in results observed overall



# Remaining challenges in the use of GPUs

# Further Challenges in the use of GPUs

- Policy for GPUs in **StepChain workflows**?
  - Multi-step jobs (multiple cmsRun with different settings), not all of them capable of making use of the GPUs
- **Benchmarking** of GPUs (as soon as HEPScore is available)
  - A requirement for **pledge definition** and **resource acquisition**
  - **Predictable** workflow **runtimes**, a key parameter for an efficient matchmaking of jobs to slots
    - Hard now because of high heterogeneity among GPUs
    - Even our simple script found a 10x factor in execution time!
- GPU usage **accounting**
  - Also requires GPU resource benchmarking
  - Could use HTCondor's GPUsAverageUsage as proxy
    - Cron job uses the NVIDIA driver and tools libraries to query statistics on all of the GPUs
    - Generate usage **report** back to the slot info and **payload job classad**