CERN

Migrating Engineering Windows HPC applications to Linux HTCondor and SLURM Clusters

CHEP 2019

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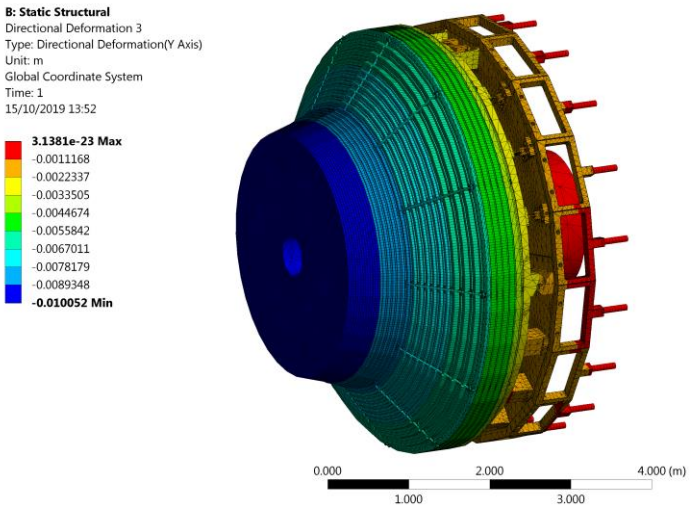
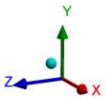
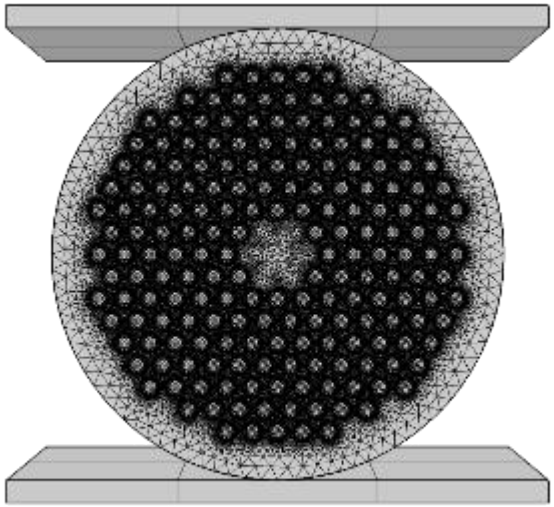
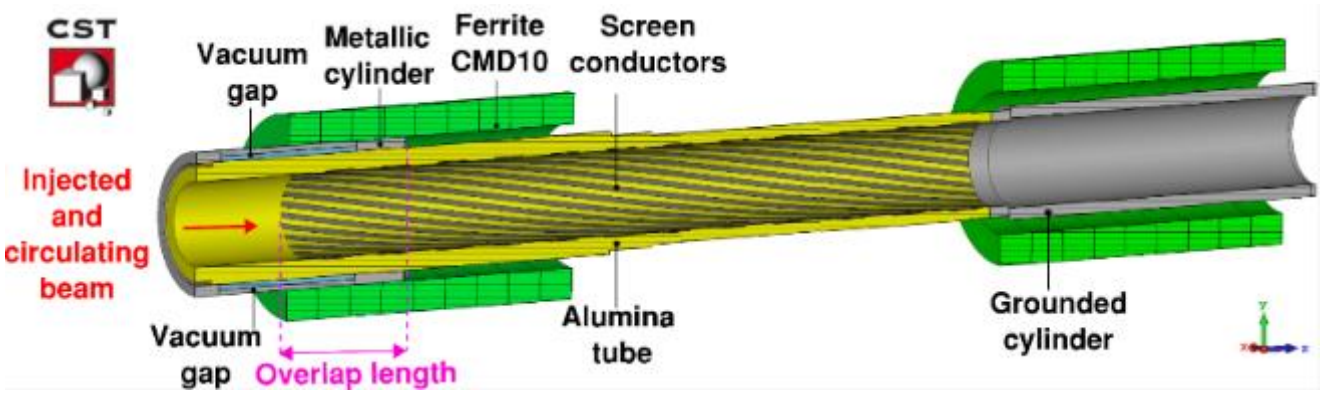
Engineering Use Cases





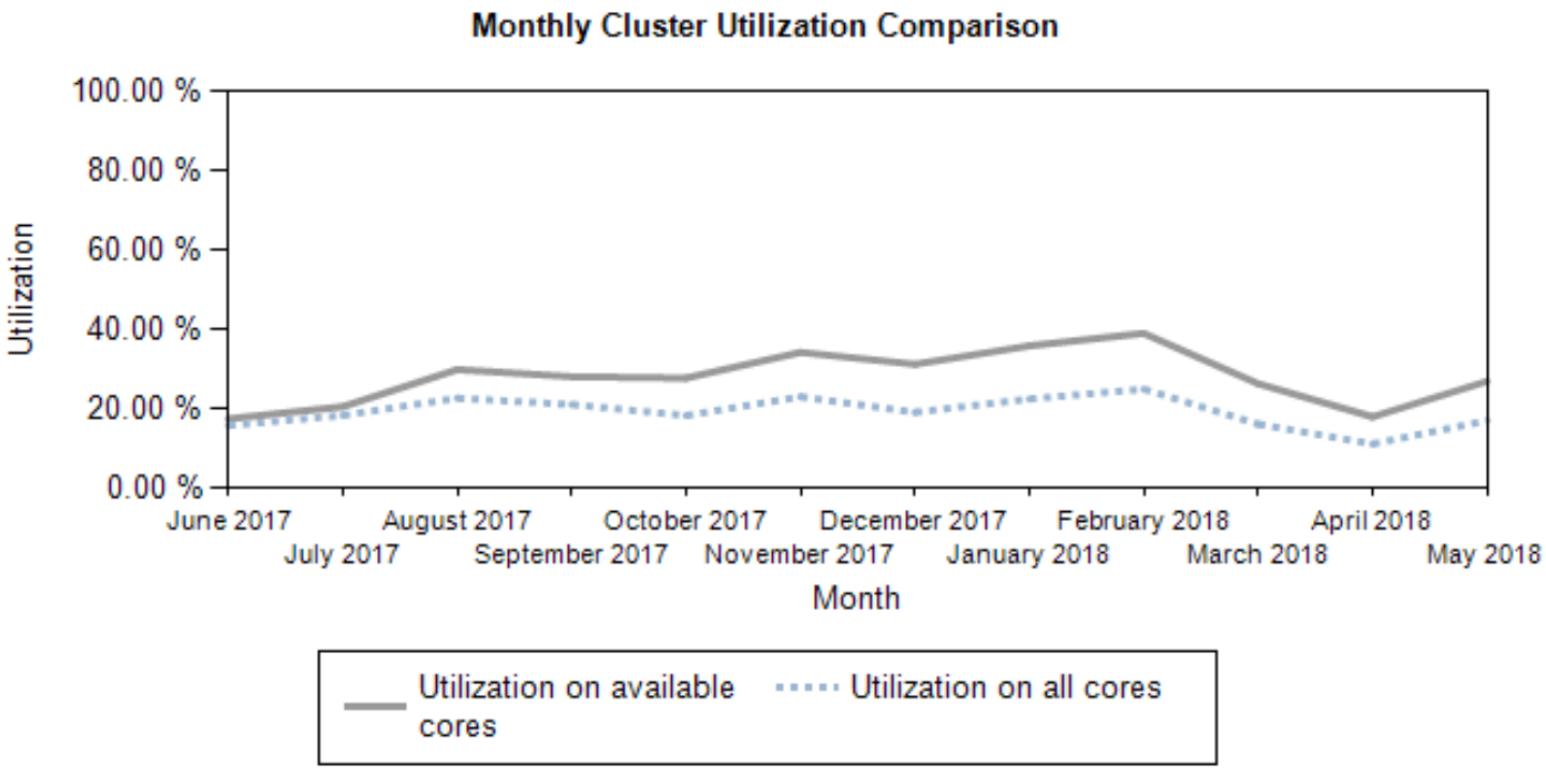




Background

- Two HPC services used to coexist in the past in CERN IT
  - Windows HPC service managed by IT-CDA
  - Linux clusters in HTCondor and SLURM managed by IT-CM
- IT Strategy is to consolidate compute intensive jobs in Linux
  - Making a better use of resources
  - Moreover…
    - This is also in line with CERN IT strategy to reduce its dependencies on MS products

Windows HPC Utilisation



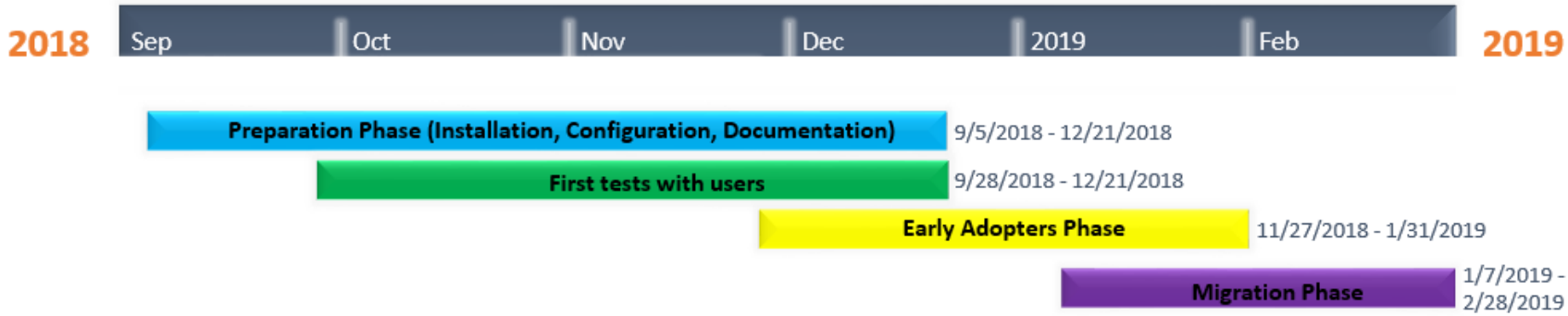
Some other constraints

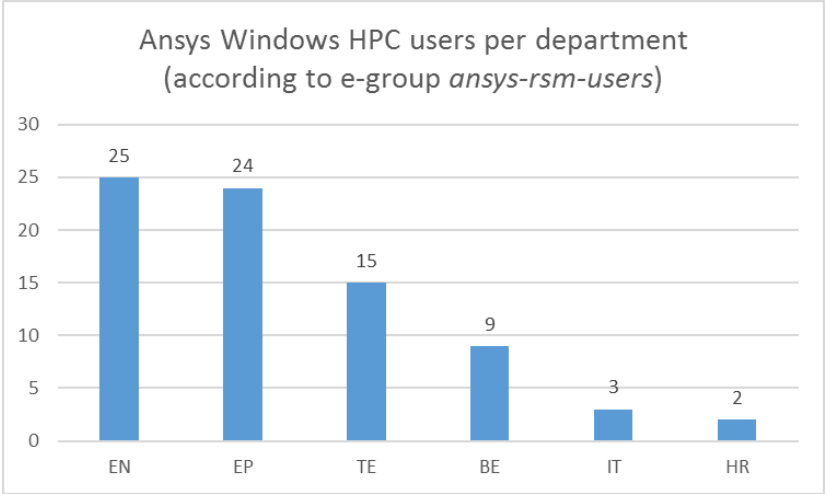
- End of warranty period for Windows HPC HW in 2019
  - Legal warranty period for systems in the CERN Data Center is 3 years; extendable to 5 years
  - Windows HPC machines were around 5 years
  - Many nodes were already giving memory errors since August 2018
- Departure of Windows HPC service manager

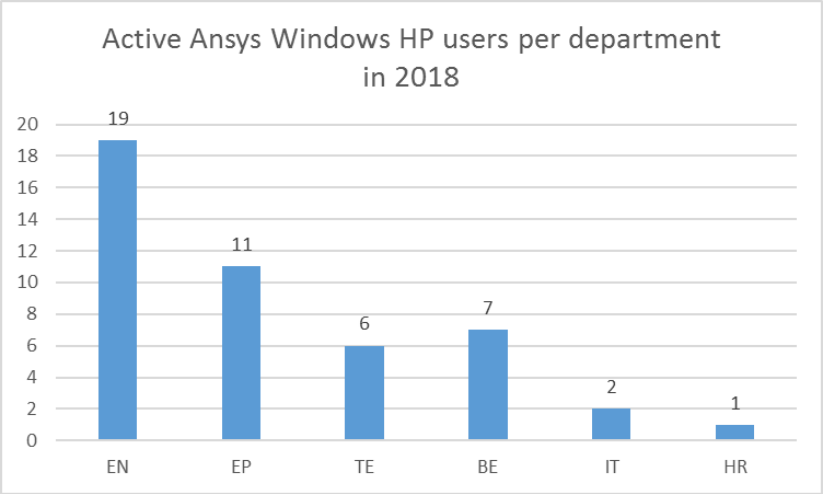
Migration Plan COMSOL and CST

- 13 COMSOL users
- 15 CST users

Migration Plan Ansys







Challenges 1

- Lack of Linux expertise among engineers
  - Steep learning curve
    - A lot of effort in user support going to solve “easy” Linux issues
  - Big change for Windows HPC users
  - Big effort to prepare tutorials and detailed documentation

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KB0005869: Preliminary steps to run Engineering Application on Linux Clusters View in tool

SE Mechanical Design Software Service
FE HPC Engineering Applications
Category: HPC

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The following instructions explain how to get access to the Linux clusters to run simulations for the following engineering applications:

- Ansys
- COMSOL
- CST
- LS-DYNA

IMPORTANT: Note that basic Linux knowledge is required except for those Ansys users who will work from RSM. All the other users, please, make sure you are able to do basic file management operations via the command line, like creating a new folder, copying files, etc. Also, editing files is needed, so please, learn some basics for tools like vi or any other Linux editor.

Register to LXPLUS

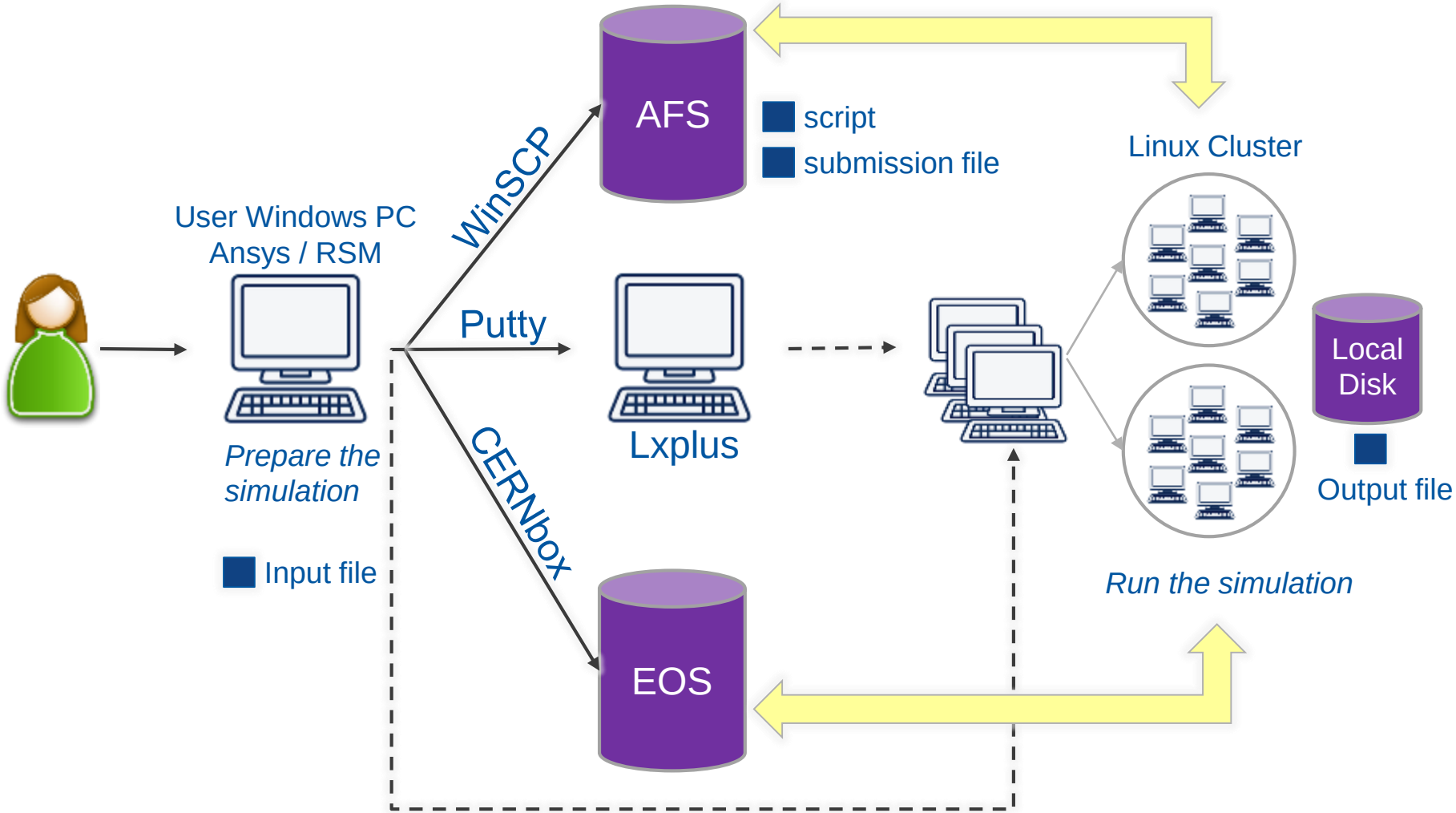
In order to work with Linux clusters, you need to have access to LXPLUS. Please, follow the instructions in this KB to know how to activate this.

You can log in to LXPLUS from a Windows machine using a program like Putty (available in CMF).

Register to EOS

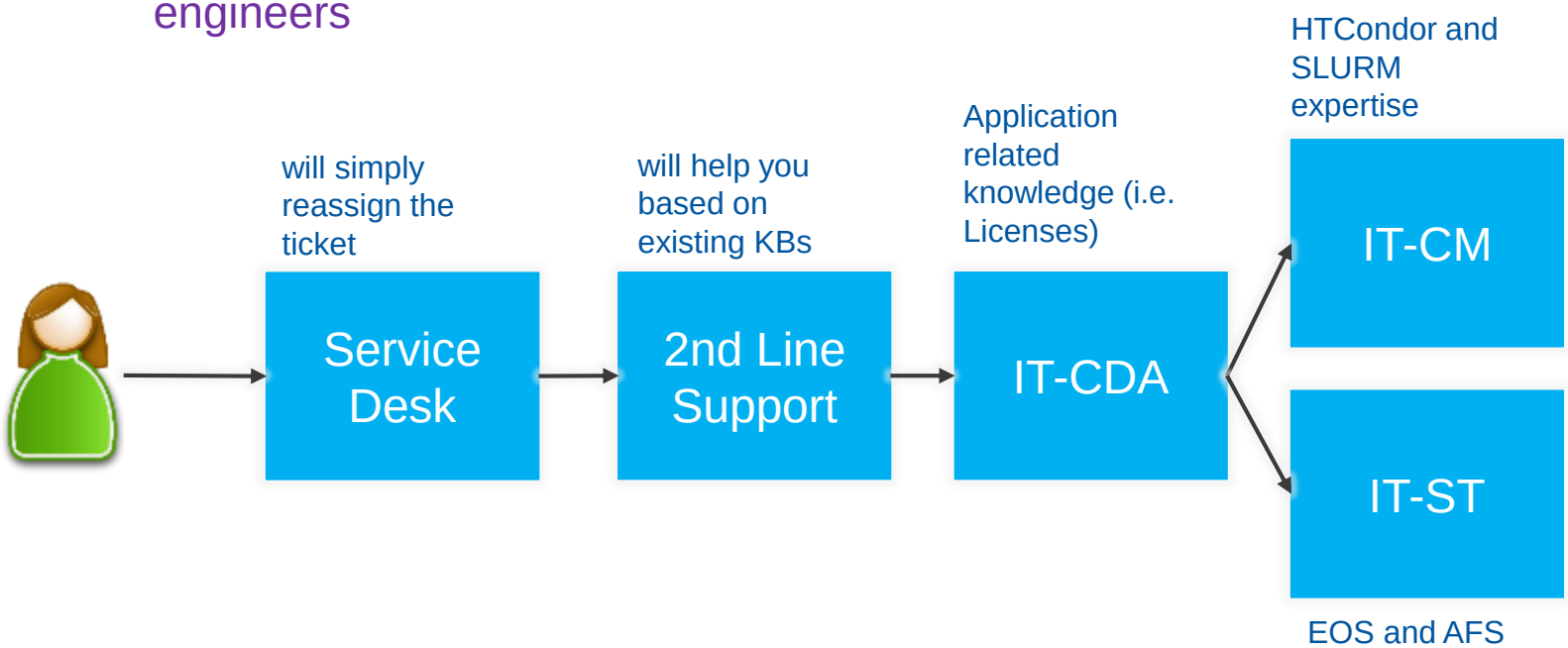
When working with Linux, your simulation and results are stored in EOS. Note that for the time being, Ansys RSM users can´t work with EOS, so you can skip this step.

Infrastructure overview



Challenges 2

- Strong collaboration among heterogeneous groups to succeed
  - Knowledge and expertise wide spread across departments and groups
  - IT support involves storage, computing and application
  - Application expertise is sitting with the engineers
    - Performance tuning requires several iterations among IT experts and engineers



Challenges 3

- Lack of HTCondor and SLURM support in CST, COMSOL and Ansys
  - Difficult to debug technical issues with vendor support teams at the beginning
  - Not possible yet to submit jobs from Windows GUI for COMSOL and CST
  - For Ansys
    - HTCondor plugin developed in-house for RSM submission
      - Still gaining experience and understanding some performance issues
    - Interaction with SLURM via PBS commands

Ansys plugin for HTCondor

A

Ansys-RSM-HTCondor

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HTCondor plugin for Ansys RSM.

Auto DevOps

It will automatically build, test, and deploy your application based on a predefined CI/CD configuration.

Learn more in the Auto DevOps documentation

Enable in settings

master | ansys-rsm-htcondor / | History | Find file | Web IDE

fix method call

Pablo Llopis Sanmillan authored 1 month ago

62417226

README | Add CHANGELOG | Add CONTRIBUTING | Add Kubernetes cluster | Set up CI/CD

Name	Last commit	Last update
scripts	fix method call	1 month ago
xml	Use +WCKey=Ansys	4 months ago

Conclusions

- Consolidating computing resources in a single infrastructure has proven to be a successful strategy:
  - Allows to share existing resources
  - Uses powerful hardware in an efficient manner
  - Benefits from a team of IT experts
- A good collaboration among engineers and IT was key to ensure a smooth migration
- Detailed documentation and clear procedures are critical to let engineers concentrate in their simulations
- Further work on batch submission from Windows for COMSOL and CST, and better performance for Ansys RSM are still needed
  - To allow engineers work from Windows
  - To benefit the most from the existing computing capacity

Acknowledgements

- Markus Tapani Jylhankangas, our technical student, who did a great job and wrote the HTCondor plugin for Ansys RSM

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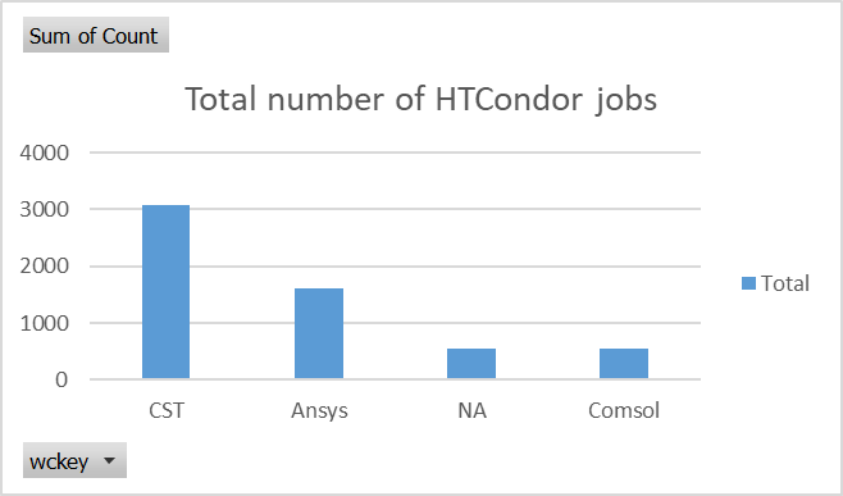
  - Ricardo Filipe Pereira
  - Eduardo Cano
  - Alessandro Cattabiani
  - Alexandre Amorim

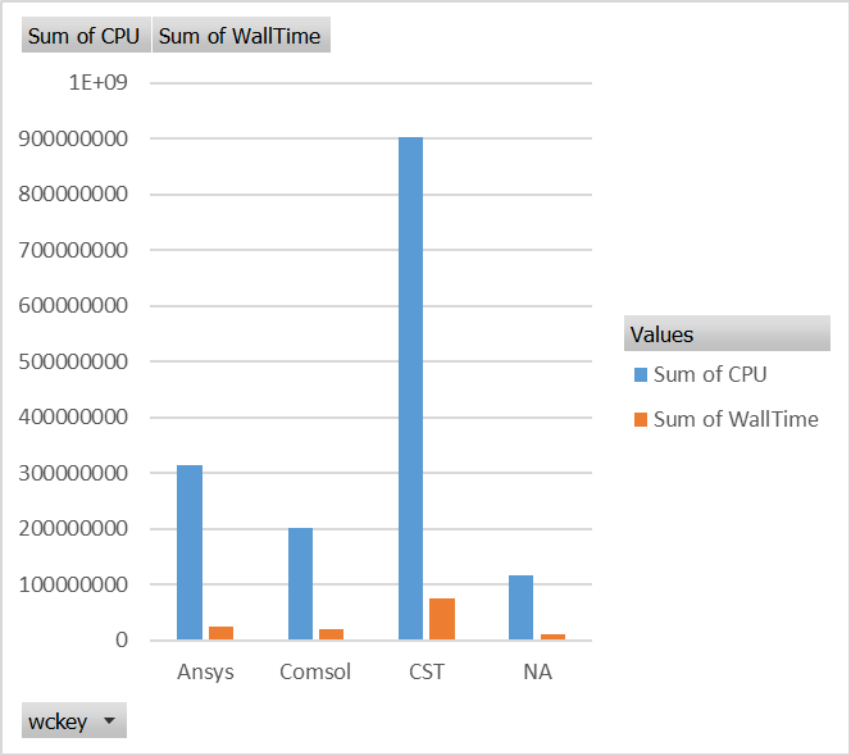
Extra slides

Linux HPC

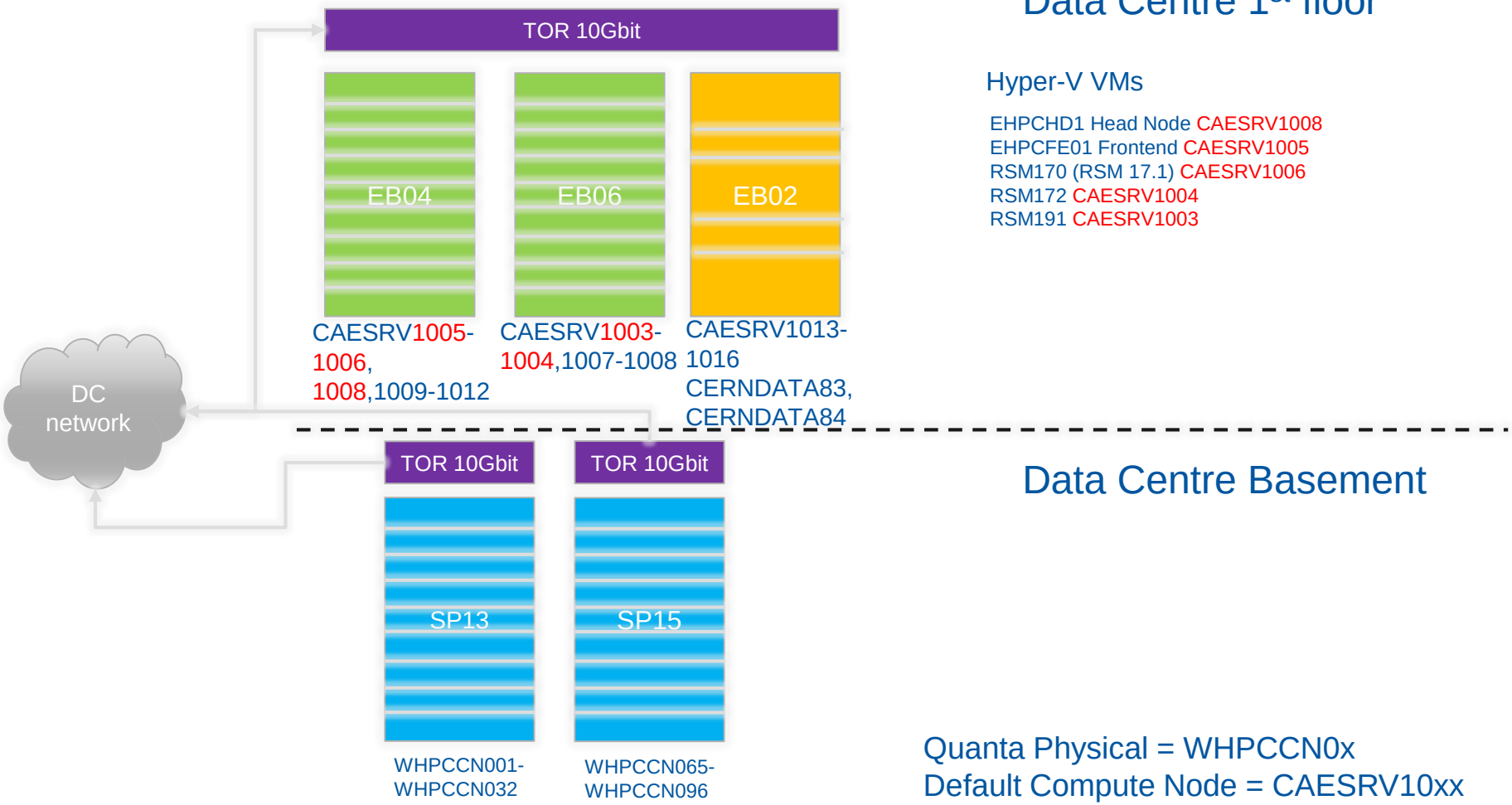
	Cores	RAM	OS	Comments
HTCondor	8 cores	16 GB	CC7	Open access
	16/32 cores	500 GB		
	24 cores	1 TB		Big Memory nodes. Access needs to be granted
	48 cores	500 GB		
SLURM	16 cores with HT	128 GB		Low-latency 10Gbit Ethernet
	20 cores	128 GB		Infiniband. Access needs to be granted

Stats in 2019





Windows HPC



Quanta Physical = WHPCCN0x
Default Compute Node = CAESRV10xx

Node Template	Cores	Sockets	Memory	Nodes
Quanta Physical	16	2	128	61
Default Compute Node	32	4	512	8

Windows HPC Statistics per job template 2018