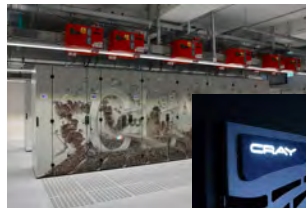


HOW A CLUSTER CAN BE USED IN PRACTICE:

Laptop or Desktop Computer



HPC Systems



CLAIX18, Aachen



Noctua1, Paderborn

Performance: 0.05-0.5 TFLOP/s
(FLOP=floating-point operations)

Storage: 0.2-2 TB

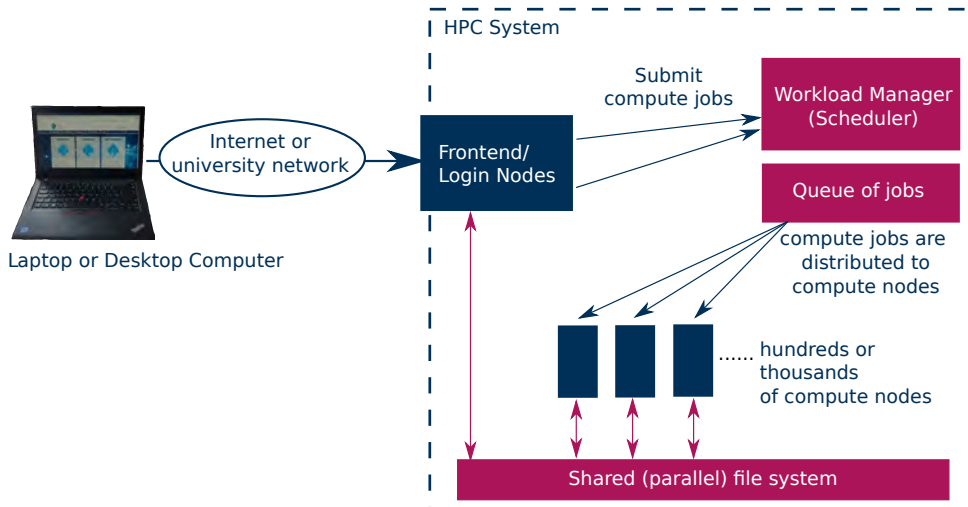
1.000-10.000 TFLOP/s

1.000-10.000 TB

Factor ~20.000-100.000 more

- HPC systems are usually use **Linux** and not Microsoft Windows.
 - ⇒ HPC.NRW offers Linux introduction courses
- HPC systems are **shared** between a large number of users
- HPC systems are **expensive** (1-15 Mio. Euro for HPC.NRW systems)
 - ⇒ have to operated efficiently
 - ⇒ compute centers try to avoid idle time

HOW A CLUSTER CAN BE USED IN PRACTICE:

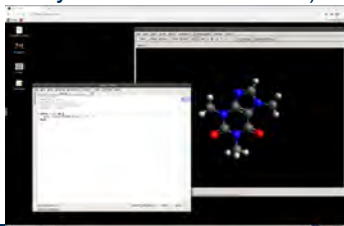


Access to the Cluster:

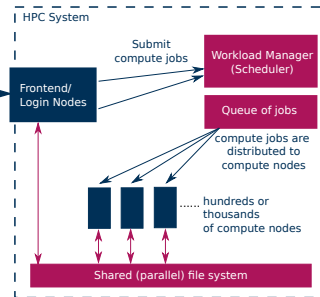
- usually with **SSH** (remote text terminal)

```
[rschade@john:~]$ ssh rschade@fe.pc2.uni-paderborn.de
rschade@fe.pc2.uni-paderborn.de's password:
[rschade@fe1 ~]$
```

- some HPC systems offer **remote desktop access** (basically a desktop that runs virtually on the HPC cluster)



Internet or
university network



Submission of Compute Jobs:

- Compute Jobs are usually formulated in terms of so called **job scripts**:

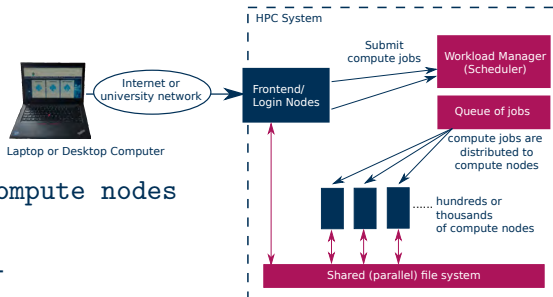
```
#!/bin/bash
```

```
#SBATCH --nodes=2
```

```
#SBATCH --time=00:30:00
```

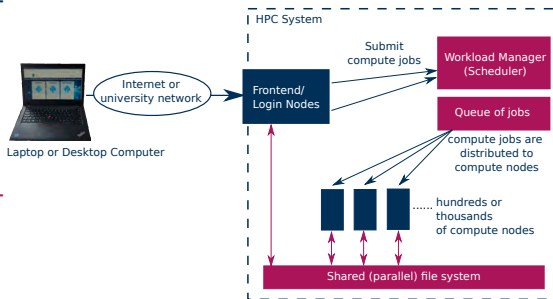
```
#commands to be executed on the compute nodes  
srun cp2k.psmf molecule.inp
```

- many **examples** are available on the support web pages of the cluster system
- taught in **Cluster/HPC introduction courses**



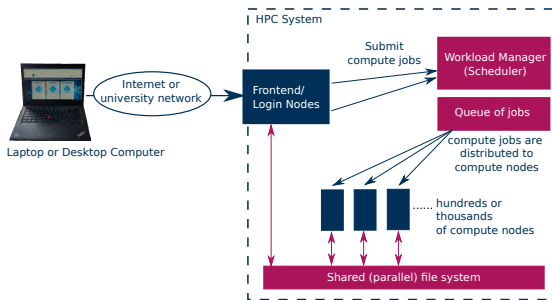
Scheduling of Jobs:

- Workload manager on the cluster schedules the jobs
- The waiting time might depend on:
 - the requested resources
 - the priority of your user or your group
 - the overall utilization of the HPC system
- ⇒ jobs usually don't start directly
- but you can submit and run **many jobs** at once!



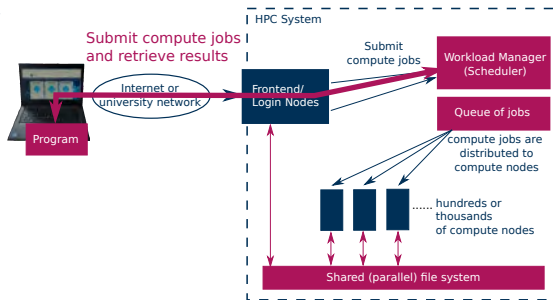
Scheduling of Jobs:

- not that useful for **interactive uses**
- \Rightarrow but some HPC systems offer separate compute nodes for interactive use



Alternative way for programs that support it:

- some programs on your laptop can directly use the cluster
 - submit jobs and data for computation
 - wait for calculation to be scheduled and finish
 - retrieve results
- examples: ANSYS, MATLAB and Python
- **caveat:** has to be supported by the HPC system, contact support



1. Before you start a proposal: Contact and ask support of the HPC systems.
2. In the proposal: List the software you plan to use or need.
 - **Attention:**
Listing software in the proposal doesn't mean it will be installed or purchased **automatically!**
(i.e., usually only the compatibility is checked in the proposal!)

- Basic software is always available:
 - compilers,
 - MPI-libraries,
 - basic numerical libraries,
 - text editors,
- Other software depends on the HPC system:
 - consult documentation of the HPC system
(usually there are huge lists of installed software)
 - and/or contact support of the HPC system

HOW CAN I GET THE SOFTWARE I NEED INSTALLED?

- Open-Source software with a free license:
 - just contact support and ask, installation usually only takes a few days
 - or install yourself
 - or bring a software container (Singularity, Docker or similar depending on the HPC system)
- Licensed software:
 - free-to-use but licensed software (examples: ORCA, GAMESS-US,...):
 - if already installed, then you have to agree to license (via web form or mail) and then access to software is enabled
 - commercial licensed software: complicated, more on next slide

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 - commercial licensed software: complicated, more on next slide

WHAT ABOUT COMMERICAL SOFTWARE?

Different situations:

- HPC system has a license that covers your case:
 - you have to apply (via web form or mail) for usage so that the applicability of the license conditions can be checked
 - you have to agree to license and then access to software is enabled
- You already have a license that covers use on an HPC system:
 - Often you can use your license also on the HPC system (examples: VASP, WIEN2K)
 - Contact support of HPC system for help
- No-one has a license that is applicable:
 - you might have some funding,
 - HPC.NRW has some funding for software licenses,
 - or the HPC center may have some funding for software licences.

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