HPC Use and Requirements
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ESRF: European Synchrotron Radiation Facility

- international institute for research with (hard) X-rays

- molecular biology, physics, chemistry, archaeology, …

- electron storage ring with 6 GeV, 844 m circumference

- X-ray spectrum: 10 to 120 KeV (0.10 to 0.01 nm wavelength)

- 42 experimental stations

- 6500 scientific users and $\approx$ 2000 publications / year

Data processing at ESRF

Want to use cloud for **offloading peak-load** computing requests

Two quite different types of tasks:

1) analysis of experimental data
   - processing time / dataset typically short (seconds)
   - but large amounts of data (10 TB / day)
   - **difficult** to transfer required data to cloud

2) theoretical calculations and modeling
   - small amounts of data (a few GB max)
   - but long processing times (80 cores for 5 days not uncommon)
   - **not difficult** to get processing power on cloud

$\Rightarrow$ move theoretical calculations and modeling to cloud

HPC tests for HNSci Cloud

Test case FDMNES: calculation of X-ray spectra

Very CPU and memory intensive calculations:
- up to 64 parallel processes
- runtimes up to several days
- up to 45 GB RAM per process

Run successfully at both provider clouds for calculations of varying complexity. First results:

- for equal total number of cores, distribution over a few big nodes is better (up to factor 2) than many small ones
- selection of "most suitable node type" is strongly dependent on memory requirements of calculation to perform

$\Rightarrow$ need large choice of node configurations (cores, RAM, ...)