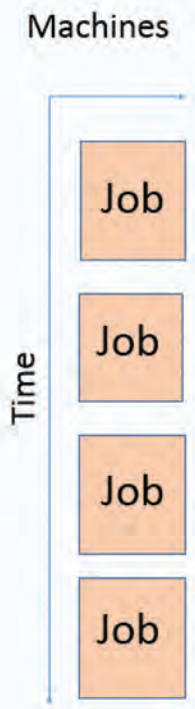
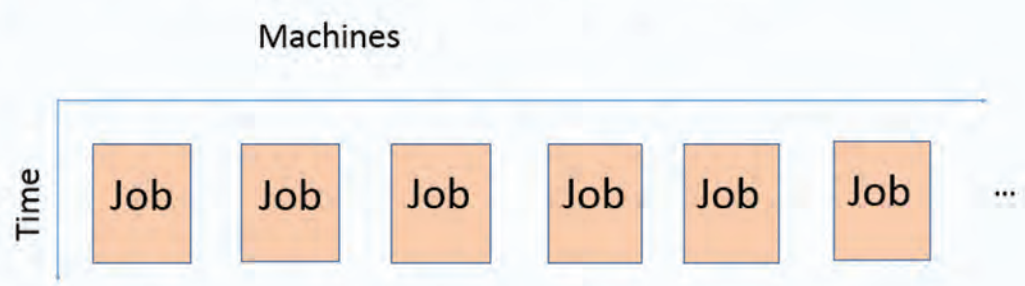
Surface Scanning with High Throughput Computing

HTCondor
High Throughput Computing

Suppose you want to run 50 simulations that take an hour at a time. Instead of running them on 1 machine for 50 hours, why don't you run them on 50 machines for 1 hour?





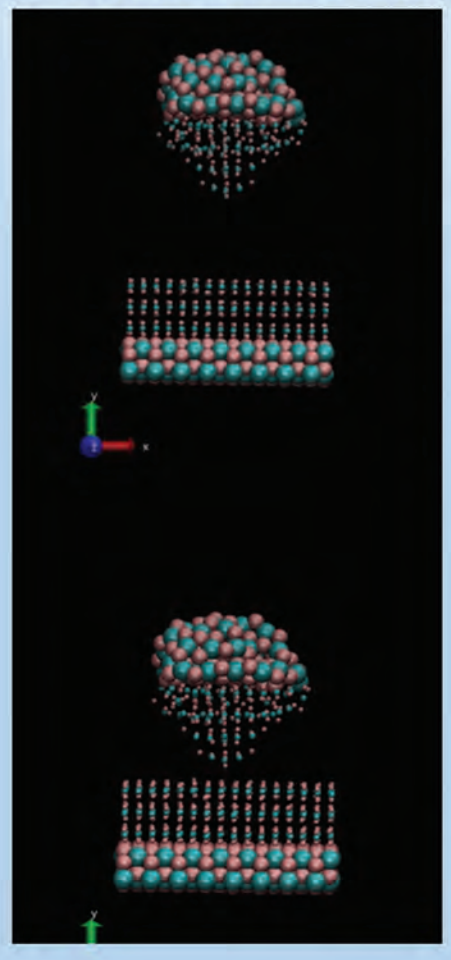
To pool together the machines we looked to HTCondor, a high-throughput computing software. Using HTCondor we can group any number of machines together to run jobs simultaneously. Instead of back to back on one machine, as the left image shows.

This can save an enormous amount of computation time.

There are 3 roles a machine can take in a pool. Submit hosts send the job, the central manager finds available execute hosts and oversees the running and transfer of files, and the execute hosts simply run said job.

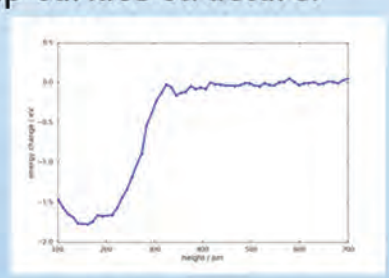
GROMACS
FAST. FLEXIBLE. FREE.

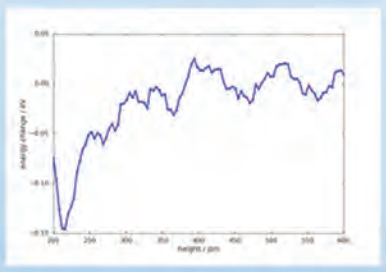
GROMACS is a molecular dynamics software, normally used for protein simulations. But in our case, we simulated clusters of calcium and fluoride ions in a tip-surface structure.



The simulations we wanted to run aimed to analyse the interactions between the tip and surface ions as they move closer together. So the x and y co-ordinates were fixed and we shifted the tip ions down the z axis with each simulation.

Therefore with HTCondor we could queue 100 of these simulations where each run the tip was slightly closer to the surface.





The images above show an approach curve at different temperatures. They both show the variation in potential energy as the tip moves closer to the surface. On the left curve we see that around 300pm from the surface the potential energy begins to become more negative as the ions are feeling attractive forces, but at 150pm energy starts to be gained again due to the repulsive forces acting between the ions as they're too close together.

The right image displays the same concepts but due to insufficient sampling our plot appears a lot noisier.

However it was acquired on spare local resources rather than the national supercomputer and can readily be extended.

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