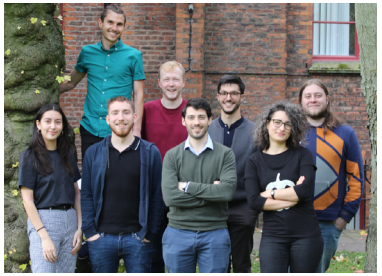
Infrastructure Case Studies
The Chilton Group



The Chilton Group, 2019

The Chilton Group at the University of Manchester are researching the properties of magnetic molecules.

The group's interests include novel metal coordination geometries and oxidation states, the link between molecular structure and magnetic anisotropy, and magnetic relaxation dynamics.

Can you give us an overview of the project?

Vast amounts of energy are currently used to power and cool data centres. It is forecast that by 2040 data centres will account for 14% of global greenhouse gas emissions.[1] Single molecule magnets could be an energy efficient way of storing data, reducing the demand for power and cooling.

Analysing the behaviour of molecules under different conditions is a parallel problem with thousands of similar calculations to be performed on each state and molecule. The group wanted to run 47,000 simulations before the 7th European Conference on Molecular Magnetism (ECMM2019) to test a new hypothesis.

Did you work with research infrastructure specialists from the start of the project?

The Chilton Group have been working with the University of Manchester's Research Infrastructure team for 5 years. They have made extensive use of the Computational Shared Facility (CSF) and on-site Condor Pool to further their research.

However, with a relatively tight deadline to the conference it was impossible to run all of the jobs using the university's on-site platforms. Being a parallel problem it was an ideal candidate to burst to the cloud with HTCondor and Amazon Web Services.

Did you encounter specific problems or challenges?

Research IT had already been developing a workflow to allow computational jobs to burst in to the cloud. The work undertaken included a range of modifications to the submission scripts:

- Identify idle compute nodes in the Amazon Spot Market to reduce cost
- Submit jobs to the cheapest Amazon region
- Submit the jobs in small batches to prevent being flagged as malicious activity by Amazon
- Ensure the most demanding jobs are routed to high performance instances
- Provide accurate costs to enable accurate internal re-charging

Despite this comprehensive set of instructions there is very little difference to a researcher submitting jobs. They simply add the line **MayUseAWS=True** to their script and the jobs will run in the cloud.

Did working with RIT help to solve these issues?

The simple answer is yes. Even using the School of Chemistry's entire computational resource allocation the work would have still taken 8 months to complete. Bursting to the cloud with AWS saw the work completed in two weeks at a cost of around $1,500.

Although this cost, met by the University of Manchester as a scoping exercise, is significant, the speed with which the work was completed makes it extremely good value.

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COMPUTATIONALLY INTENSIVE RESEARCH

1 - '2015 international technology roadmap for semiconductors itrs' page 12 and The Guardian, Dec. 2017. "tsunami of data could consume fifth of global electricity by 2025".