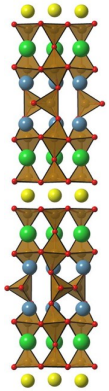
Case Study 1

Researchers in the School of Biosciences used the **ARC Condor Pool** to identify and date the genetic mutation that gave rise to the black form of the peppered moth, which spread rapidly during Britain's Industrial Revolution.

A simulation-based statistical model of the mutation was developed and implemented as an R script which was run repeatedly under Condor. A typical simulation run comprised 300,000 jobs and competed within ten days. On a single PC however, this would run for *eight years !* The results of the research where published in the June 2016 edition of *Nature* [doi:10.1038/nature17951].

Case Study 2

To discover completely new materials, chemists try to form compounds from novel combinations of elements. Searching through random arrangements is combinatorially impossible, so researchers in the Department of Chemistry have developed a new crystal building method using chemically sensible modules as the basis. Calculations employ Monte-Carlo structure sampling and Density Functional Theory requiring thousands of CPU hours on local, regional and national HPC resources. From only a choice of the elements, this method has led directly to the synthesis of two entirely new materials of previously unknown structure and composition, that have potential optical applications or uses in fuel cells. The report on this research is under consideration by Nature.



For further information, visit the ARC website at www.liv.ac.uk/csd/arc or email the team at arc-support@liverpool.ac.uk. You can register to use local HPC systems and Condor at:

www.liv.ac.uk/csd/advanced-research-computing/access/

Computing Services for Researchers

Are you a researcher whose computing requirements have outgrown your humble PC ? Maybe your programs seem to be taking forever to run or perhaps you need more memory or larger storage than a PC can provide. If this is you, then the help is at hand from the **Advanced Research Computing (ARC)** team.

We provide a variety of services and resources aimed specifically at researchers including:

- local **high performance computing (HPC)** systems;
- a **Condor Pool** for high throughput computing (HTC) applications;
- advise on how to make the most of research computing resources, locally , nationally and internationally and
- help on good software design and optimisation for users who write their own codes (e.g. FORTAN, C/C++, MATLAB, R and Python).

The **ARC** team have helped researchers across a wide range of disciplines to tackle their computing problems including physical sciences, engineering and health and life sciences.

If you are unsure of how to proceed or just want some general advice, contact the **ARC** team at: **arc-support@liverpool.ac.uk** or take a look at the ARC website at:

www.liv.ac.uk/csd/arc

High Performance Computing (HPC)

The main HPC resource, **chadwick**, is a Bull supercomputer dedicated to research use. The system is ideal for problems involving the solution of large systems of differential/integral equations found in (for example) Finite Element Modelling and many other application areas.

The hardware consists of 118 nodes , each of which are powerful computers in themselves. Nodes contain 16 cores and 64 GB of memory. A large memory node comprising 128 cores and 2 TB of memory is also available. In addition there is 48 TB of networked storage plus another 90 TB of parallel (fast access) storage available.

A wide variety of software packages are already installed on **chadwick** including VASP, CP2K, Abaqus, Fluent, MATLAB and R. Requests for additional software to be installed are viewed sympathetically, particularly if the software is free.

chadwick is widely used by researchers in fields such as engineering, computational chemistry and surface science. For more information go to:

www.liv.ac.uk/csd/arc/hpc

All Liverpool users also have free access to HPC systems provided by the N8 collaboration of Northern England universities. This includes a similar system to **chadwick** with 332 x 16 core nodes. Details can be found at: **n8hpc.org.uk**

Condor High Throughput Computing (HTC)

The **ARC Condor Pool is** not a dedicated system but comprises around 400 teaching/learning centre PCs located across the campus. Each PC has (effectively) a four core 3.3 GHz processor and 8 GB of RAM.

Users of the **Condor Pool** generally write their own codes rather than using third party applications and tools have been developed to aid in the running of codes written in MATLAB and R (both of which **ARC** have significant experience of).

The **Condor Pool** It is is especially suited to running very large numbers of independent programs (jobs) where each runs only for a short time (20-30 minutes is ideal) however, it is also possible to run programs for arbitrarily long periods using a technique called checkpointing.

Condor can process large datasets quickly and help speed up statistically-based problems such as simulations. A good example of this is problems involving Monte Carlo methods. Condor is also very effective in developing and verifying statistical models coded in R.

Researchers in the health and life sciences (amongst others) have found that Condor has reduced time-to-solution from months to days and many Condor applications start life just as simple R (or MATLAB) codes run on a PC. You can find more about Condor on the **ARC** website at: **condor.liv.ac.uk.**