University of York

# Advanced Research Computing at York

IT Services

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*twitter.com/UoYITServices*

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IT Services website: *www.york.ac.uk/it-services*

Research and High Performance Computing wiki: *wiki.york.ac.uk/display/RHPC*

# INTRODUCTION

**HEIDI FRASER-KRAUSS**

*Director of Information Services*

## Research is at the heart of what we do at York and fundamental to our success. IT Services is determined to support and strengthen the University's research activities by providing facilities and services that make doing research easier, faster and more productive.

Advanced computing is a major driver for innovation, allowing researchers to accelerate and develop their work. As Nobel Prize winning chemists Michael Levitt, Martin Karplus and Arieh Warshel note, "today the computer is just as important a tool for chemists as the test tube." Indeed, over the last year, we have helped researchers to solve genetic puzzles using fossil records, predict the likely locations of HIV outbreaks and investigate the perfect LED for your TV screens.

We provide a broad range of services for researchers, from increased storage space, to high performance computing facilities. Our resources are available to researchers from any discipline and we provide support for those who need it.

We hope this guide will help you to explore what is on offer to you and showcase some fantastic examples of the work already carried out using our facilities.

"

The services and staff in IT have genuinely revolutionised the way the Archaeology Data Service works, and delivered support and efficiency gains that have greatly improved the ADS and what we offer to the archaeological community."

*Michael Charno, Archaeology Data Service*

# ADVANCED RESEARCH COMPUTING

## Advanced Research Computing offers far more than even the most specialised desktop or laptop computer can achieve, cutting down the time it takes to process data and allowing for more complex analysis.

### Why use Advanced Research Computing?

We provide facilities for researchers whose desktop PC is no longer suitable for their requirements. Advanced Research Computing can help you with **faster computation and data analysis**. For example, a researcher with 3,000 sets of data to process was able to reduce the processing time from 41 days using a desktop PC to two hours using our research HPC (High Performance Computing) cluster. Our facilities can also help you to perform more complicated analysis on your data, for example:

- Genome and protein sequencing
- Spatial data analysis
- Fluid dynamics
- Large scale modelling
- Sound recognition and processing
- Language analysis

### How it works

To help you process and analyse your data, we use a technique called cluster computing, which involves a set of connected computers that work together as one system. Cluster computing offers much greater performance and reliability over a standard PC, particularly when working with complex programs or large datasets.

We operate local clusters for smaller jobs and testing. Members of the University also have access to the regional N8-HPC facility and the national ARCHER facility, for running larger jobs that would benefit from even greater computing power.

We operate a fair-share system, to ensure all users have equal access to resources.

### What support is available?

We provide training and one-to-one support so that you can make the most of our systems and resources. Whatever your level of experience, help is on hand to get you started and choose the right tools for your research or project.

Our systems and resources could be of use to all researchers, regardless of discipline. To discuss what help we can provide, email: *itsupport@york.ac.uk*

Additional information can also be found on our website: *www.york.ac.uk/it-services/research-computing*.

> I would not have been able to produce results without it, particularly for memory intensive analysis."
>
> *Rob Critchlow, Department of Biology*

# Research Computing facilities


## research0

### What it is

research0 is a large AMD based Linux server. It is an interactive service that allows you to run programs that are too large for a standard computer.

| research0 |
| --- |
| One server with four processors and a total of 64 cores |
| 512 GB of memory |

### How to access

research0 is available for all staff and postgraduate researchers. For access, email itsupport@york.ac.uk.

Final year undergraduates and taught postgraduate students can also apply for access via their supervisor or tutor.

> “I’ve found the facility to be really useful and the staff extremely helpful. I managed to get two years’ worth of CPU time done in a week.”

*Simon Hickinbotham, York Centre for Complex Systems Analysis*

# York Advanced Research Computing Cluster (YARCC)

## What it is

YARCC is a 'Tier 3' High Performance Computing (HPC) facility. It is a small cluster aimed at those who require a platform for development and the execution of small compute jobs. YARCC has been used for processing very large datasets within hours rather than days, and computational modelling.

The configuration of YARCC is designed to be a mirror of the regional N8 HPC facility (see p.7). This will enable you to move your applications and program code to the larger resource with ease.

Jobs running on the cluster can access the University's shared filestore to allow use of large datasets. Many software packages are already pre-installed and configured to work on YARCC.

| YARCC |
| --- |
| 28 computer nodes with a total of 528 cores |
| 4 terabytes of memory |
| Peak performance of 10 teraFLOPS |

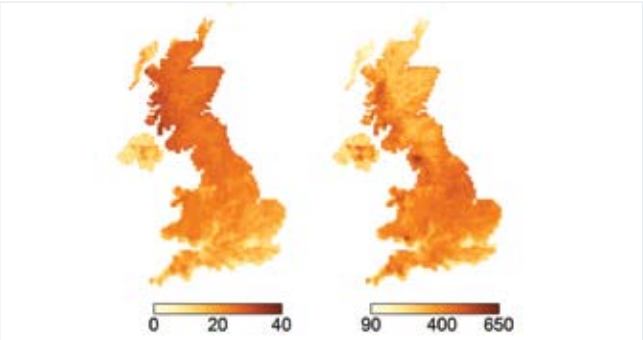
## How to access

YARCC is available to all staff and postgraduate researchers. For access, email *itsupport@york.ac.uk*.

Final year undergraduates and taught postgraduates may also apply for access.

"YARCC is wonderful! I primarily use YARCC to run quantum chemical calculations using Gaussian09 and have found it to work very well for me."

*Esther Johnston, Department of Chemistry*




## Assessing climate change impacts on UK biodiversity

*Rob Critchlow and Colin Beale – Beale Group. Department of Biology.*

The University of York has been involved in analysing data on wildlife as part of the UK's Committee on Climate Change report into the impact of climate change on natural assets.

We have undertaken a risk assessment of climate change impacts on more than 4,000 species from 17 taxonomic groups, such as birds, plants and bees. This has provided a broad spatial assessment of the potential impacts of changing climate on biodiversity across Great Britain and Northern Ireland. To perform this risk assessment, we used state-of-the-art species distribution models that account for recording effort and can quantify impacts of unknown variables, for example, land-use change, as well as assessing the importance of bioclimatic variables such as rainfall and temperature that are used to predict species distributions.

We used the York Advanced Research Computing Cluster (YARCC) to run more than 4,000 individual models. The processing of model outputs were memory intensive and time consuming. We estimated that 833 days of modelling and processing using my desktop would be required. YARCC completed the work in about five days.

"YARCC is a fundamental service for statistical modelling of large datasets and generating results quickly."

# N8 HPC

## What it is

N8 HPC offers a shared 'Tier 2' HPC facility. N8 HPC has a greater capability than YARCC and is typically used by researchers who have very large datasets or require an increased computational capacity.

N8 HPC currently operates two facilities, the Farr machine and Polaris.

We provide support for the facility in the form of technical advice, software installation and help with user applications.

| **Polaris** (SGI High Performance Computing cluster) |
|---|
| 332 computer nodes with a total of 5,312 cores |
| Fast InfiniBand interconnect between nodes |
| 24 terabytes of memory |
| Two file systems with a total of 283 terabytes of storage |
| Peak performance of 110 teraFLOPS |

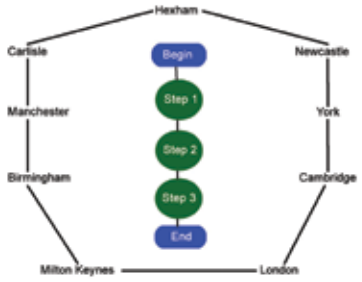
| **The Farr Machine**<br>(SGI UV2000 shared memory computer) |
|---|
| 256 cores |
| 4 terabytes of memory |
| 44 terabyte file storage system |

## How to access

Access to N8 HPC is by application. Applications should be made by the Principal Investigator of a project. If you would like to discuss your application before submission, please email: *itsupport@york.ac.uk*.

Researchers associated with projects that have access to N8 HPC may also have user access.

More information on N8 HPC, including details on how to apply for access, can be found at: *http://n8hpc.org.uk*.




## Applying Cartesian Genetic Programming to classic problems in Computer Science via functions that incorporate domain knowledge

*Patricia Ryser-Welch, Bio-inspired group. Department of Electronics.*

Hyper-heuristics is a branch of artificial intelligence that can design computer programs automatically, reproducing the method applied by programmers. Before solving a chosen problem, a sequence of instructions are written in a specific order. The program is then run and the quality of the problem solutions define how well the program works; a bad solution would indicate a bad algorithm and vice versa. Hyper-heuristics automatically applies this process and can find new programs that have yet to be thought of.

We are using the N8 HPC service to develop Hyper-heuristic algorithms. These algorithms take a long time to run, use large amounts of memory and cannot be run effectively on a PC or laptop. It is more productive to use a large cluster of computers, like the N8 HPC facility. Each node in the cluster is used to represent one simulated computer and consequently we can run several experiments simultaneously on many nodes. As a result, more computer programs are written automatically. It has helped our research immensely as we have been able to obtain more programs than we had expected.

"The N8 and the excellent services provided by IT are playing a huge part in the success of our research."

# ARCHER HPC Service

## What it is

ARCHER is a 'Tier 1' UK National Supercomputing Service. ARCHER provides a capability resource to allow researchers to run simulations and calculations that require a large number of processing cores working in a tightly-coupled, parallel fashion.

The ARCHER hardware consists of the Cray XC30 MPP supercomputer, external login nodes, post processing nodes, and the associated file systems.

| ARCHER (Cray XC30 MPP) |
| --- |
| 4,920 computer nodes, a total of 118,080 cores |
| 64/128 GB of memory per node |
| High-performance Lustre storage system |
| 1.6 petaFLOPS |

## How to access

For more information on ARCHER, see: *www.archer.ac.uk*
To enquire about access, please email: *itsupport@york.ac.uk*

> The single largest area of science that ARCHER will be used for is the realm of chemistry and materials science. The larger computing power available is enabling researchers in this area to actually explore the chemical properties of materials in physically realistic environments rather than making approximations and using idealised systems. This step-change in modelling ability allows the scientific research to have a direct impact on our day-to-day lives much more quickly than was possible previously."

*Alan Simpson and Andrew Turner "So supercomputers are mega-powerful, but what can they actually do?" The Conversation, 1 April 2014*

Time taken to process 3,000 sets of data

LAPTOP

984 hours

41 days

HPC CLUSTER

2 hours

# STORAGE, VIRTUAL MACHINES, DATA

## We can provide you with the computing facilities you require for your research, whether that's additional storage space, virtual machines or databases.

### Storage

All staff and students are automatically allocated space on the central filestore; if this no longer meets your requirements, we can provide you with additional storage.

Up to two terabytes of storage can be allocated to you by your Departmental Computing Officer (*www.york.ac.uk/it-services/dco*). If you require more space than this, or if you have specialist requirements, (eg long term archiving or high speed storage for High Performance Computing) please contact us. We can also provide you with information on storage options for inclusion in grant and funding applications.

### Virtual Machines

The Virtual Machines (VM) hosting service provides you with a server running either a Windows or Linux operating system. They offer a number of advantages to researchers and can be useful for:

- providing an application to multiple people, and allowing them to work on the same data simultaneously
- running a service that needs to be online 24/7
- running applications that can only be installed on a specific operating system
- tailoring the operating system, memory or CPU size to package requirements

We also provide Bare-metal virtualisation. This is a highly specialised service that provides a VM without any operating system or application software. The specification of the VM can be varied to meet specific requirements you might have. These will be discussed on a case-by-case basis.

### Databases

If you need to manage large amounts of data as part of your research, we offer the following centrally hosted and managed databases that are secure and regularly backed up:

- MySQL Database Service
- Microsoft SQL database
- PostgreSQL
- Oracle

For more information on these services, please see the IT Services website:

***www.york.ac.uk/it-services***

## Dissemination and preservation of archaeological data

*Michael Charno. Archaeology Data Service.*

The Archaeology Data Service (ADS) is the UK's national digital data archive for Archaeology and the cultural heritage sector. We run a number of services to disseminate archaeological data and provide guidance to the community, which include various web applications, wikis, and web services. Traditionally this had been done by building monolithic servers for production every few years which had a sandwich of Java, Apache, ColdFusion and Oracle services. While this worked in the early days of the ADS, this didn't scale well and became more unsustainable over the years.

The offer to use VMs hosted by IT Services was presented to us and this has led to a much more sustainable and sane system architecture for the ADS. We currently have 20 VMs hosted by IT – 18 Linux Ubuntu servers and two Windows servers. Each VM is extremely focused and lightweight (usually only one CPU and under 2Gb of RAM), and serves a dedicated function.

Data storage has all been rolled into the IT filestore, that provides ample space, robust backups, and enables NFS shares to the various VMs. Storage is obviously very important to a digital archive, and the IT offering has removed most of the concerns related to scalability, reliability and accessibility. Our Oracle database instance is also hosted by IT, which has allowed us to leverage the expertise of their database team; this has immediately improved our database performance and security.

> "The benefit of moving to IT Services hosted services has been a noticeable improvement in up-time and performance of our applications and services."

# SOFTWARE

## We provide access to a wide range of software to support your research. The following packages are just some of those you might find helpful.

### MATLAB

MATLAB is a programming environment for algorithm development, data analysis, visualisation and numerical computation. It is installed on all IT Services classroom PCs and is also available for staff and students to install on unmanaged University owned PCs and personally owned devices.

### Mathematica

Mathematica is a computational software program used in scientific, engineering and mathematical fields and other areas of technical computing.

It is installed on IT Services classroom PCs, and is available for staff and research graduates to install on unmanaged University owned PCs and personally owned devices. The Mathematica Learning Centre provides an extensive range of learning resources including videos, demonstration and documentation.

### Stata

Stata is a general purpose statistical software package for data management, statistical analysis, graphics, simulations, regression analysis (linear and multiple), and custom programming. Stata is available on all IT Services classroom PCs and can be installed on managed office PCs.

### Qualtrics

Qualtrics is a survey tool that makes it quick and easy to collect and analyse data. You can select and add pre-written questions to your survey from a large question library or write your own. You can host your survey through Qualtrics and also analyse results on the fly. Qualtrics is available to all staff and students.

### NVivo

NVivo is a qualitative data analysis (QDA) software package. It has been designed for qualitative researchers working with very rich text-based and/or multimedia information, where deep levels of analysis on small or large volumes of data are required.

### SPSS

SPSS is used for statistical analysis. The add-on module, SPSS Amos, also enables structural equation modelling. Staff and students can install SPSS for free on home or office computers, and it is also available on IT classroom PCs.

For a full list of available software, visit:

***www.york.ac.uk/it-services/software***

## Qualtrics case study

*Rachel McAllister. Social Policy Research Unit.*

The Social Policy Research Unit (SPRU) sends out a lot of surveys. In the past these were on paper, but more often now we want to provide people with an online survey. We have used Survey Monkey and Jotform in the past, until a particular need and an international collaboration brought us to Qualtrics.

Back in 2013 we were working with colleagues in Melbourne, Australia to deliver a tool to measure stress in people who worked in paediatric oncology units. It was a very carefully produced scientific measure and part of it needed to be in a particular format; a central column of statements flanked on either side by a scale of frequency and a scale of stress. None of the online survey systems could reproduce this format until we found Qualtrics, which had a great amount of flexibility in its design interface. Another great benefit is that all the data warehousing for Qualtrics is in Ireland and so within the European Economic Area. This is an important requirement of many of our research funders and ethics committees.

In SPRU, we have now used Qualtrics to survey NHS providers about their services for people with dementia, social services practitioners about their reablement services, local authorities about how they allocate services to support carers, as well as to register people for conferences and events. One very useful facet is that it allows you to share the survey that you are creating with anyone (they do not need to have an account) which is excellent for collaborative working with other research institutions.

As well as very sophisticated piping, looping, and merging functions within surveys, it also allows you to distribute individual surveys to named people within panels of survey recipients. Responses are tracked and notifications sent to your email inbox if required. There are options to export the survey results into CSV, SPSS, Fixed Field Text, XML, HTML and zipped files which helps enormously with the further analysis of results.

As you use it, and the further into it you explore, it tends to reveal ever greater abilities, whilst remaining a very quick and easy way to do a plain, simple form. We at SPRU wouldn't be without it!

# SUPPORT AND TRAINING

## IT Services provide training, support and information, so that you can make the best use of our Research Computing services and facilities.

### Training

We provide training in the use of our advanced research computing facilities and courses on the use of regional and national facilities are delivered periodically. The training is provided via classroom based courses and online training modules. One-to-one support is also available.

Courses include:

- Introduction to the Linux Shell
- Introduction to YARCC (York Advanced Research Computing Cluster)
- Introduction to programming with Python
- High Performance programming with "R"
- MATLAB online tutorials

The IT website contains more information on training and details of how to book: *www.york.ac.uk/it-services/training*

### IT Security

If you are developing web systems and writing programs, we would advise you to complete our IT Security training. The training focuses on secure development and how to write secure code. It aims to educate people in developing systems that not only control access to data but also do not include weaknesses enabling the server running the code, or others, to be compromised.

Please email *itsupport@york.ac.uk* if you would like to find out more about IT security training.

### Further information

Additional information on research computing can be found on our website: *www.york.ac.uk/it-services/research-computing* and the Research and High Performance Computing wiki: *wiki.york.ac.uk/display/RHPC*

"The documentation on the YARCC website, the YARCC courses, and contact with staff in IT Services, have all meant that I've been able to understand and use the facilities pretty quickly."

*Georgina Palmer, Department of Biology*

# RESEARCH DATA MANAGEMENT

## Research data is a valuable asset and is sufficiently important that the University has requirements for how it is managed. This section gives you a brief overview of the services and support we provide, so you can manage your data with ease.

### Good Practice in Managing Research Data

To ensure good research practice (and to meet funder, ethical, legal and other responsibilities) the University has a Research Data Management Policy (*www.york.ac.uk/rdm-policy*) that you will need to adhere to. To meet your research data management responsibilities you will need to look after and effectively manage the data you create or collect during the course of your research. The following webpage provides guidance on good practice in managing research data and links to established tools and sources of advice: *www.york.ac.uk/rdm*

### Library Research Support Team

The Library's Research Support Team has been established to support the research activities of the University. They can help with:

- Open Access, including University policy, funder mandates, and REF Open Access requirements
- Research Data Management, including guidance and advocacy for good practice
- Copyright legislation and related licences
- ORCID (Open Researcher and Contributor Identifier) IDs
- Citation analysis and bibliometrics

Find out more at: *www.york.ac.uk/library/info-for/researchers/support*

### Research Data MANTRA

MANTRA is a free online RDM training course created by the University of Edinburgh. If you need to know more about specific aspects of good data management practice (eg file formats and transformation, storage and security) you can complete the appropriate MANTRA module.

*http://datalib.edina.ac.uk/mantra*

### DMPonline

The key to successfully managing data is to plan ahead – writing a data management plan will help you do this. Created by the Digital Curation Centre (DCC), DMPonline is designed to help researchers create personalised data management plans to meet specific funder requirements. The tool provides examples of guidance and best practice from the DCC, research funders and the University of York.

*https://dmponline.dcc.ac.uk*

# OTHER RESOURCES

## The following IT resources and facilities may also be of use for researchers.

### Linux desktop

Ubuntu LTS Linux is available for installation on staff PCs and accessed using your University account. The installation is configured and maintained with security updates and can be set up to access your University filestore. It is available as single-boot, or dual-boot with an IT Services Windows desktop.

Core scientific and programming applications are available, and departments and research groups may add their own software or resources to the standard build.

To request access, please email *itsupport@york.ac.uk*.

A Linux desktop is also available to students on classroom PCs in G/N/022, G/N/169, and some department-managed classrooms.

### Managed laptops

A managed laptop provides you with a fully supported system, so there is no need to worry about security or software updates. Laptops come with Microsoft Office pre-installed and other core applications are available via the Software Center. McAfee Encryption is also installed and configured.

Managed laptops have on-site warranty for a minimum of three years so, in the unlikely event something goes wrong with the hardware, we will arrange for it to be fixed.

Managed laptops are available to staff only. Please email requests to *itsupport@york.ac.uk*.

### Google Apps

The University provides access to Google Apps for Education. Apps including Google Sites, Google Hangouts and Google Groups can be of particular use for researchers who wish to work collaboratively, whether on or off campus.

### DropOff

The DropOff Service allows you to easily and securely exchange files up to 20Gb with University staff and students, or external people.

It is a handy service to use when your file is too big to send as an email attachment.

For more information on all the services and facilities we provide, visit our website:

**www.york.ac.uk/it-services**

# CASE STUDIES

## Analysis of ancient proteins

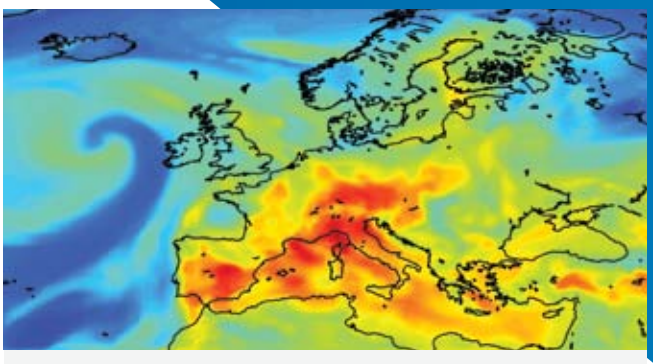
*Matthew Collins, Frido Welker, Beatrice Demarchi and Jessica Hendy. BioArCh, Department of Archaeology.*

The BioArCh group at the University of York is exploring the recovery and application of ancient proteins and proteomes. To do this, we use analytical software to help analyse and interpret data from fossil records. The software requires that we have one single installation and, by using the VM, multiple users can access the software remotely.

Having dedicated VMs for each software instance removes the need to use PCs in the lab and the associated problems of where to site them and who should be given access to the office or lab. It is also easier to check a VM from any location – including from home.

Initially there were some setup issues, but the IT team were very helpful and resolved these for us. Using the VMs solved a problem for us and saved us the cost of two PCs and the space to locate them. The software we use on them has helped us to solve the sequence of a range of South American fossil bone samples.

The results of this research have been published in issue 522, number 7554, of the journal Nature.



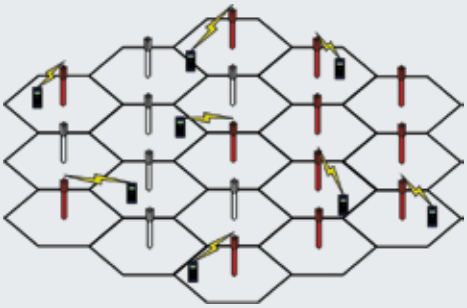
## Simulating the composition of the Earth's atmosphere

*Mathew Evans. Wolfson Atmospheric Chemistry Laboratories, Department of Chemistry.*

We try to simulate the composition of the atmosphere using computer models. Although compounds like ozone and methane and aerosols are at low concentrations in the atmosphere they can have a profound impact on climate and human health. Our simulations take our best understanding of the important chemistry, physics and biology occurring and make a prediction of the concentration of key gases and aerosols in the atmosphere. We work in collaboration with groups that make observations of the composition of the atmosphere to allow us to test our models. This allows us to go to some exciting places around the world. Recently we have been involved in making observations in the Pacific, Atlantic, Africa and Borneo.

We secured £210,000 from NERC to invest in new computer hardware to support our activities. The IT Services Research Computing team helped us to procure the correct system, install it and they now manage the system for us. This has freed up my group's time to concentrate on doing the research, rather than managing the computers.

> "The research computing service has been fantastic in managing our system. They've been really responsive to our needs and have completely removed the burden of system administration for us, allowing us to concentrate on our science."



## Artificial intelligence in cognitive communications

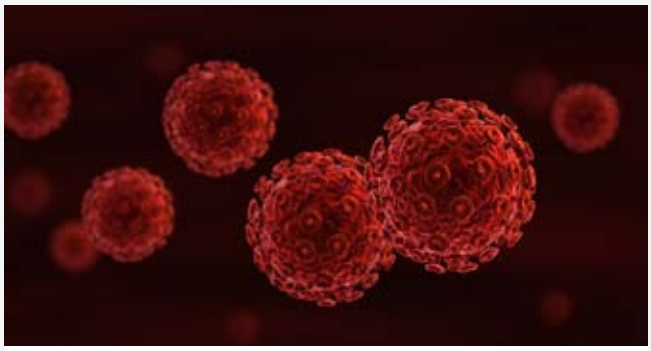
*Nils Morozs. Intelligent Systems and Communications and Signal Processing Research Groups, Department of Electronics.*

The main aim of the project I'm working on is to establish a strong link between mobile communications and artificial intelligence (AI). The application areas of primary concern are dynamic radio resource and topology management. The results of investigating these particular areas contribute to the EU FP7 ABSOLUTE project, which is working to develop intelligent, rapidly deployable, mobile networks for large coverage areas affected by unexpected events (for example, natural disasters) and for large scale temporary events (for example, the Olympic Games).

I use YARCC for large scale simulations of mobile networks in temporary stadium event scenarios. These typically have 11,000 mobile subscribers, and 82 base stations covering a wide suburban area with a densely populated stadium in the middle. YARCC allows for hundreds of independent simulations in parallel for algorithm testing and statistical analysis of results.

"

YARCC is an excellent easy-to-use service which keeps improving and expanding."



## Optimal budgetary policies in the face of uncertainty: a case study in HIV

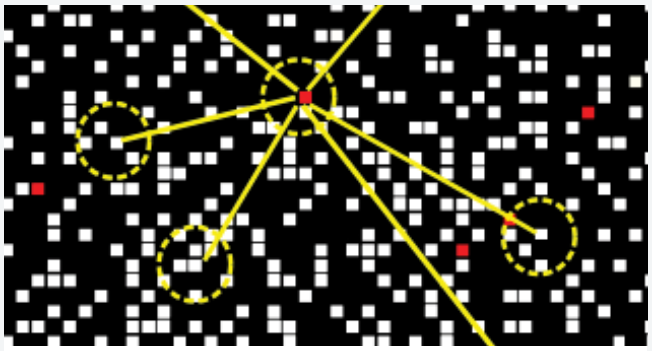
*Beth Woods, Claire Rothery, and Karl Claxton, Centre for Health Economics, University of York. Sarah-Jane Anderson, Jeffrey W Eaton, and Timothy B Hallett, Department of Infectious Disease Epidemiology, Imperial College London.*

There is growing recognition that to maximise the health gains achieved by a HIV prevention programme, funding should be focused on the people and locations at greatest risk of infection. Targeted health care spending plans should therefore be developed based on our current knowledge of where, and in whom, HIV infection risks are expected to be highest. However, this current knowledge about the epidemic is subject to uncertainty. Our research focuses on how this uncertainty impacts on the health that can be generated from HIV prevention programmes (for example, if programmes miss key unanticipated HIV "hotspots") and how alternative resource allocation approaches can be used to improve decision making under uncertainty.

The project has been highly demanding in terms of computation. To explore the impact of uncertainty we needed to simulate a wide range of possible eventualities in each location. We needed to model the possibility that, in some locations, insufficient funds were allocated due to an underestimate of HIV infections. We therefore explored the health outcomes these areas could generate via partial provision of their planned programmes. This entailed using YARCC to run the model for many different levels of partial provision.

"

The YARCC service has made aspects of our research possible which would not have been using standard computing approaches. It has also improved our workflow, allowing us to review and react to results quickly and progress the project accordingly."



## Cell Branch: exploring stem cell differentiation and pluripotency with Branching Process Theory

*Dr. Richard B. Greaves, Dr. Julianne D. Halley, Professor Susan Stepney. Non-standard computation group, Department of Computer Science and York Centre for Complex Systems Analysis (YCCSA).*

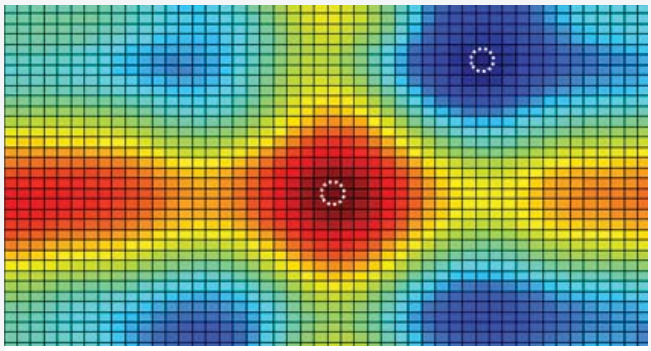
Our research centres on simulating gene regulatory networks in pluripotent embryonic stem cells. Pluripotent stem cells are capable of indefinite self-renewal and of differentiation into any cell lineage in the body. We are interested in modelling these cells because they offer huge potential for regenerative medicine, but the mechanisms used by the stem cells to compute their fate are not precisely understood.

A fuller understanding of the factors that influence stem cell fate computation would potentially facilitate greater precision in the use of stem cell-based therapies for existing medical conditions, for example, neurological damage such as that encountered in Alzheimer's disease or Multiple Sclerosis.

Our simulation is based on a theoretical, branching process model of the gene regulatory network that was developed by Dr. Julianne Halley. During the previous year we have developed a working agent-based simulation and characterised it in terms of changes in system behaviour in response to changes in the four alterable system parameters.

YARCC was of immense value to our research effort, enabling us to carry out these simulations.

"The IT team in charge of the cluster were extremely helpful, with particular thanks being due to Dr. Andrew Smith who co-ordinates the cluster facility. Dr. Smith quickly helped me to get our simulation running on the cluster."



## Self-Organisation and Self-Assembly in Aliphatic Liquid Crystals

*Dr. Richard J. Mandle. Advanced Materials Group, Department of Chemistry.*

Liquid crystals have become the dominant display technology in the past decade, however, there is a constant need for new and improved liquid crystalline materials for use in the next generation of displays. The properties of an LCD such as the time taken to turn each pixel on/off, the maximum viewing angle of the display, and ultimately the device lifetime are dependent on the actual chemical composition of the liquid crystal itself. In order for LCDs to be able to out-perform alternative display technology, significant improvements are needed in the chemical makeup of the liquid crystal. Our EPSRC funded research program focused on two main display types; ultra-fast switching materials for use in large LCDs such as monitors and TVs and so-called scattering LCDs that work without a backlight and so offer vastly reduced power consumption and could therefore be highly desirable for use in tablet and e-reader devices.

Calculations performed on YARCC allow us to predict the properties of new liquid crystals before preparing them in the laboratory. In a few hours we can get a predicted result, whereas undertaking chemical synthesis and subsequent materials evaluation can take months. Thus, we can focus our efforts where they are likely to yield the best results.

This process also works in reverse – when new phenomena arise we can use calculations from YARCC to help understand our experimental results. To this end, we have used YARCC to gain an insight into how changes to the molecular structure can yield increased device performance.

"The computational resources offered by YARCC have allowed us to perform calculations on much more complicated molecular systems than we were previously able to and so has significantly enhanced our research."