Science & Technology Facilities Council

UK Research and Innovation

SCIENCE HIGHLIGHTS 2018

SCIENTIFIC COMPUTING DEPARTMENT

Contents

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Welcome

Welcome to the STFC Scientific Computing Department (SCD) scientific highlights for 2018.

In July I was delighted to be appointed as Director of SCD and have now been in post for three months. I've spent time learning about the work of the department and I have been truly impressed by the range and quality of the work SCD staff carry out to support the STFC science programme, and our national and international communities. Supporting such a range of science communities can mean some areas only see a fraction of our work – this year's highlights are a great opportunity to celebrate some of the excellent work across these communities with a wider audience.

Towards the end of 2017, we launched CoSeC - the Computational Science Centre for Research Communities – to bring together the existing investments from three UK Research Councils: the Engineering and Physical Sciences Research Council (EPSRC), the Medical Research Council (MRC) and the Biotechnology and Biological Sciences Research Council (BBSRC). CoSeC is bringing together our activities in these areas to support the advancement of scientific research by developing and strengthening software to analyse and solve increasingly complex problems in multiple disciplines - physics, chemistry, life sciences, engineering, and more. This year's review contains several highlights from developments within CoSeC.

As part of the IRIS Collaboration (formerly UKT0) we were successful in our bid to BEIS for £16m over 4 years to support the eInfrastructure requirements of our particle physics, astronomy, and large facilities communities. This additional funding is enabling us to work with new parts of the Particle Physics, Astronomy and Nuclear (PPAN) communities, and to ensure efficient use of resources in a very tight funding environment.

Our programme of work with the STFC Facilities continues to grow – leveraging our expertise in computational science for new communities and helping ensure maximum impact from the experiments the facilities support. The Ada Lovelace Centre, which brings together SCD, the ISIS Neutron and Muon Source, Central Laser Facility, Diamond Light Source, and the Culham Centre for Fusion Energy, has also received funding as part of IRIS project, to deliver the essential eInfrastructure to support these facilities.

When people think of SCD they tend to focus on the tens of thousands of compute cores we manage, the petabytes of data we store, or the scientific codes we develop. This is of course important, but our key asset is the highly skilled and dedicated people that make all this happen.

Finally, I'd like to thank David Corney for his dedicated leadership of the department over the last four years – I inherit a department in excellent shape to face the challenges ahead.

Tom Griffin

Director, Scientific Computing Department

Scientific Computing Department Strategy

During 2016-17 we launched our new 5 year strategy to help us to achieve our mission:

"to maximize the impact of scientific computing through our expertise, leadership and collaboration."

Our mission is fully aligned to support and enable the STFC Corporate Strategy and the STFC e-infrastructure Strategy.

The Scientific Computing Department fulfils its mission by:

- Designing, deploying and operating large and complex computing and data systems
- Supporting the research life-cycle by extracting insights and value from data
- Creating algorithms and software to exploit future research computing infrastructure
- Providing cross-domain expertise to develop, innovate, and sustain software, and related digital assets for research
- Leading and participating in the national and international collaborations working to achieve these aims
- Committing to STFC's corporate theme of Inspiring and Involving to deliver a vibrant programme of public engagement
- Actively supporting and contributing to the developing skills agenda in Scientific Computing

Delivering our mission

SCD is one of the largest scientific computing departments in Europe and comprises around one hundred and fifty staff. We deliver expertise in computational science and professional large-scale scientific and data management and computing systems, services and expertise to our STFC, national, and international scientific user communities, and to our collaborators and stakeholders in other Research Councils – particularly the Engineering and Physical Sciences Research Council (EPSRC), the Natural Environment Research Council (NERC), the Biotechnology and Biological Sciences Research Council (BBSRC), and the Medical Research Council (MRC).

Delivering our mission builds on our core strengths and is described in the following sections.

Theme 1

- SCD will build and strengthen our existing capability of providing enabling computational expertise and e-infrastructure to support STFC in fulfilling its strategic goals: "world class research, world class innovation, and world class skills."

Theme 2

- SCD is committed to deliver and further develop its expertise in scientific analysis, data science, modelling and simulation, to support STFC's commitment to: Establish the Ada Lovelace Centre, an integrated, cross disciplinary, data-intensive science centre, to transform the use of real time data processing, computer simulation and data analytics to deliver more effective research at our national facilities.

Theme 3

- SCD delivers a comprehensive programme of computational and data science services, research and development to underpin STFC's Data Intensive Science ambition: to develop and deliver cutting edge solutions for academia and industry to advance data intensive science and innovation.

Theme 4

- In order to ensure that the UK's e-infrastructure supports the country's leading international research status and delivers the data capabilities essential for academia, industry and STFC's science program, SCD will collaborate with our Research Council UK partners and stakeholders, and with Innovate UK, and JISC, as part of the emerging UK Research and Innovation (UKRI), to shape and build an efficient and effective UK e-infrastructure for UK science and industry.

More details can be found in the SCD 5 year Strategy 2017-2021 document which can be downloaded here: https://www.scd.stfc.ac.uk/Pages/SCD-Strategy.aspx

SCD is continuing on the journey to implement the five year plan. The articles in this report give a spotlight on activities so far.

Strategic Theme 1

SCD will build and strengthen our existing capability of providing enabling computational expertise and e-infrastructure to support STFC in fulfilling its strategic goals: "world class research, world class innovation, and world class skills."

Using Multiphysics simulations to assess frozen wall technology in Molten Salt Fast Reactors

Credit: Pixabay

Our scientists, working with colleagues from the University of Liverpool, used advanced simulations to carry out a feasibility study examining the formation of frozen salt films in molten salt fast reactors, with a view to reducing the amount of corrosion of the reactor walls. Molten salt fast reactors use liquid fuel instead of the solid fuel rods used in conventional nuclear reactors. They are seen as a safe, reliable, environmentally and economically sustainable way of generating energy. The fuel is dissolved in the salts and is circulated through a vessel with no internal structures. Such structures can moderate or slow down the neutrons. The faster neutrons capture, scatter and react with the fuel and any fission products present, converting the fission products to lighter elements. These reactions and the slower neutrons heat the liquid fuel. This heat can then be extracted to generate power. Operating the reactor in this way allows us, over the longer term, to burn separated plutonium and spent nuclear fuel, and this can lead to smaller quantities of waste being sent for deep geological disposal.

A problem limiting the development of these reactors is that the molten salts corrode the vessels in which they are contained, leading to shortened operational lifetimes. Frozen salt film technology has the potential to reduce vessel wall corrosion by preventing the direct contact of highly reactive hot molten salt with the structural materials. Our simulations showed that it is possible to create a frozen film, which could reduce corrosion. However, this film is thin and it could be difficult to maintain under the nominal operating conditions of the selected molten salt fast reactor. Further studies are being prepared to better understand the behaviour of the salt as it freezes and melts.

Background

Molten salt fast reactors (MSFRs) are a novel application of nuclear fission reactors and are seen as an economically and environmentally sustainable low carbon option that can tackle the issue of reliable and safe energy production. MSFRs are inherently safer than Generation III reactors (i.e. the current generation being built) since the nuclear fuel is dissolved in the molten salt (i.e. they cannot melt down) and they are operated at atmospheric pressure. They can be operated with a continuous feed or small quantities of "fresh" nuclear fuel and a small quantity of the undesired fission products can be separated from the reactor.

The environmental sustainability is bolstered by the use of alternative fuel cycles burning mixtures of either uranium and thorium or spent nuclear fuel and separated plutonium (SNF-Pu). Burning SNF-Pu has the potential to make significant reductions in the quantities of high level radioactive waste being sent to a deep geological disposal repository with only the undesired fission products being removed from the fuel-salt mixture.

Nevertheless, there are a number of engineering and safety case issues that need to be dealt with in the development of the reactor concept. Two of the issues regard the vessel wall, which in current concepts specifies a nickel alloy that has been shown to be resistant to the chemical attack from the fluoride based salts used. It is expected that the operating temperature of the reactor would be between 600ºC (873K) and 750ºC (1023K). This has the consequence of increased rates of corrosion and helium void embrittlement due to the high neutron flux in a fast reactor.

It is envisaged that freezing the salt at the vessel wall may reduce the corrosion of the vessel wall and reduce the impact of helium void embrittlement (bubbles of helium that evolve from the interactions of neutrons with the structural material). Frozen salt films (a crust of salt formed on a wall which is cooled to lower than the melting point of the salt) have been investigated by both the UK Atomic Energy Authority and Oak Ridge National Laboratory (US) in the 1960's and 70's. These studies demonstrated the formation of the salt film experiencing a significant heat flux.

Modelling approach

The modelling approach is based on multi-physics simulations where the open source computational fluid dynamics (CFD) solver called Code_Saturne (www.code-saturne.org) is coupled with the neutronics code DYN3D-MG. The coupling has been enabled by using the Multiscale Universal Interface (MUI) library, where the interface passes interpolated point clouds between the coupled codes. The coupling is required to account for the response of the scattering, reaction and leakage of neutrons in the MSFR to the local change in temperature and the change in salt density.

A porous medium approach has been used to model the solid-liquid phase change. The model is based on a permeability source term, which is proportional to the liquid volume fraction used to identify the solid region in the CFD domain. An additional source term is also included in the energy equation to take into account the latent heat of fusion of the phase from solid to liquid phase and vice versa.

Full variation of the physical properties has also been considered as function of the local temperature with relationships based on those found in the available literature (Rouch et al. 2014).

Simulation

The simulated molten salt fast reactor (Figure 1) is based on a vessel with toroidal side walls. The fluid is pumped through sixteen cooling circuit loops, which contain heat exchangers that cool the salt and extract the heat to generate power via a Rankine cycle (Rouch et al. 2014). The fuel is dissolved in the salt and no other internals are present that can moderate the neutron flux. Half of the volume of the reactor is located in the core, while the other half is in the cooling circuit loops. The molten salt enters through the inlet ducts at the base of the reactor core and flows up through the vessel and out at the top and down through the heat exchangers.

Figure 1: Reactor configuration with streamlines indicating the flow direction. Half of reactor geometry is shown.

Figure 2 presents streamlines indicating some of the turbulent flow features in the MSFR core and the frozen salt film formed at the vessel wall. The frozen salt film is coloured by the temperature of the salt between the wall temperature (colder colours) and just above the melting point. The effect of the flow structures such as jets and eddies can be linked between their occurrence to changes in the temperature field observed on the fluid side of the frozen salt film. For example the jet from the second inlet just below the temperature scale affects the temperature field below it, as well as the whirlpool-eddy nearby generating a circular pattern of hotter and cooler salt on the surface of the salt film of cool salt. Hotter molten salt also impacts on the salt film frozen onto the vessel side wall near to the outlet where large vortices form as the fluid enters the outlet ducts. This is indicated by the ridge of hotter salt temperatures at the edge of the salt film, which occurs where the flow stagnates between flow structures.

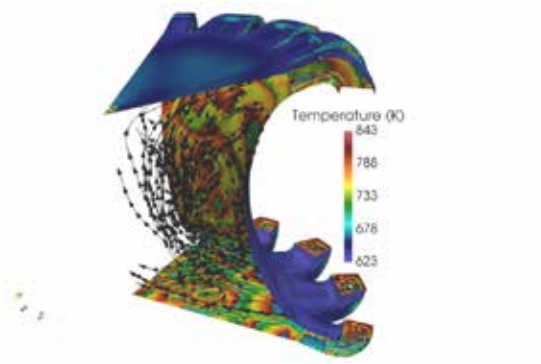

Figure 2: Contours of temperature applied to both sides of the frozen salt film formed at the vessel wall. Streamlines indicate the turbulent nature of the flow. A quarter of reactor geometry is depicted.

At each inlet a thicker salt film is formed (Figure 2 and 3a), where the temperature gradient is guided by the inlet conditions (Figure 3b) and not by the heat generated from the nuclear reactions (Figure 3c). The narrowing of the duct by the salt film accelerates the flow and directs it to the lower wall of the reactor vessel. Hot fluid is observed next to the wall in almost all parts of the reactor (Figure 3b), which leads to strong changes in the temperature over short distances. The changes to the physical properties of the fluid also influences these temperature gradients in the formation of a very thin layer next to the wall (Figure 3a), where the properties control the transport of heat and fluid and turbulence has little effect. It is in these regions that the frozen salt formation is observed. Therefore, the heat flux from the nuclear reactions that result in the sharp temperature gradients and the turbulent flow in the reactor hinder the formation of the frozen salt film.

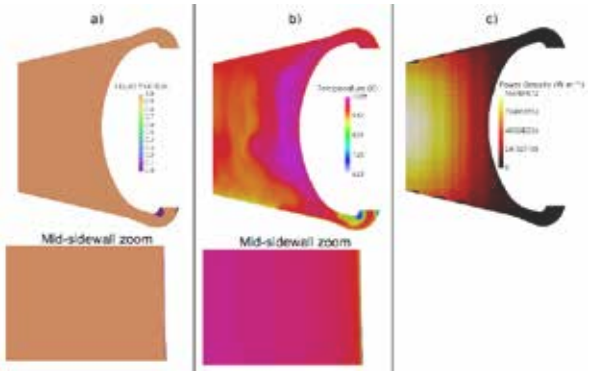

Figure 3: Contour plots of the fraction of liquid in the MSFR (a), temperature (b), and the power density (c) derived from the nuclear reactions. The zooms of the liquid fraction and temperature fields at the midpoint of the core vessel side show the thin salt film (blue line on the inclined side wall) and the strong temperature gradient at the wall.

Conclusions

Coupled numerical simulations of the neutronic and thermal fluid dynamic behaviour of a molten salt fast reactor have been performed. These simulations investigated the feasibility of the formation of frozen salt films on the core vessel. The reactor was fuelled by plutonium and spent nuclear fuel.

We found that the variation of the Prandtl number of the fluid plays a key role in the thickness of the sublayers of the boundary layer next to the wall, where the salt films form. The thickness of the salt film was limited to less than 1 mm in the reactor vessel without accounting for the transfer of heat through the vessel wall. The thinness of the salt film was due to two effects, the heat flux from the nuclear reactions and the high levels of turbulence near to the vessel walls.

We can conclude that for the numerical models, the operating conditions and the physical properties applied here, the application of frozen wall technology to the MSFRs do not currently look as though they are a feasible approach to corrosion control. However, there is a significant lack of knowledge of the change in the physical properties of any salt selected to carry the fuel, particularly around the melting point. The physical properties used in this study were extrapolated over most of the temperature range considered in this study. Therefore, further studies are being developed to examine the physical properties of the salts as they melt and solidify and the effect that the combination of the internal heat flux and turbulence has on the stability of the salt films formed.

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Research Outputs: Publications/Presentations

A. Skillen, S.M. Longshaw, G. Cartland-Glover, C. Moulinec, D.R. Emerson Profiling and application of the multi-scale universal interface (MUI). Proceedings of the 6th European Conference on Computational Mechanics (ECCM 6) 7th European Conference on Computational Fluid Dynamics (ECFD 7), Glasgow, UK, 11-15 June 2018.

G. M. Cartland-Glover, S. Rolfo, A. Skillen, D. R. Emerson, C. Moulinec, D. Litskevich, B. Merk, Modelling frozen salt films in a molten salt fast reactor. Proceedings of the 26th International Conference on Nuclear Engineering (ICONE26) July 22-26, 2018, London, UK, Paper ICONE26-82210.

G. M. Cartland-Glover, S. Rolfo, A. Skillen, D. R. Emerson, C. Moulinec, D. Litskevich, B. Merk, Modelling the neutronics of a molten salt fast reactor using DYN3D-MG for the investigation of the application of frozen wall technology. Proceedings of the 26th International Conference on Nuclear Engineering (ICONE26) July 22-26, 2018, London, UK, Paper ICONE26-82170.

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G. Cartland-Glover, S. Rolfo, A. Skillen, D. Emerson, C. Moulinec, D. Litskevich, B. Merk, Modelling frozen salt films in a Molten Salt Fast Reactor, Proceeding of the International Nuclear Engineering Conference, Manchester, UK, 4-5 October, 2018.

G. Cartland-Glover, A. Skillen, S. Rolfo, D. R. Emerson, C. Moulinec, D. Litskevich, B. Merk, On the feasibility of the application of frozen walls to a molten salt fast reactor. Proceedings of the 12th International Topical Meeting on Nuclear Reactor Thermal-Hydraulics, Operation and Safety (NUTHOS-12) Qingdao, China, October 14-18, 2018.

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H. Rouch, O. Geoffroy, P. Rubiolo, A. Laureau, M. Brovchenko, D. Heuer, E. Merle-Lucotte, (2014). Preliminary thermal–hydraulic core design of the Molten Salt Fast Reactor (MSFR), Annals of Nuclear Energy 64, 449-456.

Strategic Theme 1

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Many Interacting Worlds: a new computational approach to nuclear quantum effects

Credit: Pixabay

What does it mean for a particle to behave like a wave?

This was a question that the first pioneers of quantum mechanics had to struggle with. The equations were clear in describing matter waves that propagated through space. Their predictions were excellent; yet, their meaning was elusive. Waves represented spread out probability distributions, but localised particle hits could still be measured. At what point lies the boundary - when and how does the probability distribution turn into an actual measurement - was and is still unclear, and constitutes the so-called measurement problem of quantum mechanics.

Many interpretations have been suggested to address this problem - none of which seems to be able to ever settle the matter, since they mostly change the meaning of the same equations while making no distinct falsifiable predictions. One of these, advanced by Louis de Broglie first and David Bohm later[1], tried to restore the classical nature of the world by bringing back point-like particles into the wavy field of quantum mechanics. We are not any closer to deciding whether it represents the true underlying reality of quantum mechanics than its authors were; but a modern offshoot of this theory might have unexpected applications in ab-initio atomistic simulations.

Pilot waves or multiple worlds?

The de Broglie-Bohm theory, also known as Pilot Wave theory or Bohmian mechanics, is an interpretation of Quantum Mechanics (QM) that does away with the notion of randomness. It posits that there exist both wave functions and particles. The former evolve in time with the Schrödinger equation that we know, while the latter follow a so-called guiding equation that determines their velocity at all times from the wave function. In this way, particles move in a deterministic fashion, and due to the choice of the form of the guiding equation the probabilities given by traditional quantum mechanics are respected at all times, while at the same time a 'true' value of the particle positions exists, removing any ambiguity. This interpretation, while being effectively a hidden variable theory, gets away with the constraints imposed by the Bell theorem by being non-local, through the wave function. For computational purposes, however, it is not very useful in this form. It does nothing to simplify the formalism of QM - in fact, it complicates it, by adding another entity, the particles, on top of it. The wave function still evolves in time according to the Schrödinger equation, and thus the computational complexity remains unchanged.

In 2014, Hall, Deckert and Wiseman suggested a novel interpretation of QM[2], or rather, a reformulation of Pilot Wave theory, that they called Many Interacting Worlds. In their paper, they argue that there is in fact no need to keep the wavefunction at all; instead of having one wavefunction and one particle surfing along, one can have a theory featuring many particles, each inhabiting its own parallel world, distributed according to the probabilities given by the Born rule, and evolving according to the laws of Newtonian mechanics with an added 'quantum potential' term. The wavefunction can then be reconstructed – for the quantum potential, we don't really need its phase, only the modulus, so that can be derived from the density of the particles themselves – and from it, one can predict how the particles should be guided. The wavefunction piloting the particles is replaced by the particles interacting with each other in a rather complex way, with the wavefunction being only a disposable intermediate step. The potential is repulsive, keeping the particles apart; together with our ignorance about which world we are in, this means we get to observe indeterminacy in position, as expected. Other dynamical phenomena (such as interference and tunnelling) emerge through the complex patterns in which particles interact and bounce off each other. Figure 1 shows in more detail how this differs from the traditional and Bohmian views.

Compared to the original pilot wave theory, this approach is much more interesting in terms of potential computational applications. It describes quantum mechanics in terms of a number of parallel classical worlds – a description that only becomes exact in the limit of infinite such worlds – linked only by a quantum potential that seems relatively simple to compute. This opens up the way to a number of possible applications for this theory as an alternative method to solve quantum problems.

1 "A Suggested Interpretation of the Quantum Theory in Terms of" Hidden …." https://link.aps.org/doi/10.1103/PhysRev.85.166. Accessed 7 Aug. 2018.

2 "Quantum Phenomena Modeled by Interactions between Many …." 23 Oct. 2014, https://link.aps.org/doi/10.1103/PhysRevX.4.041013. Accessed 7 Aug. 2018.

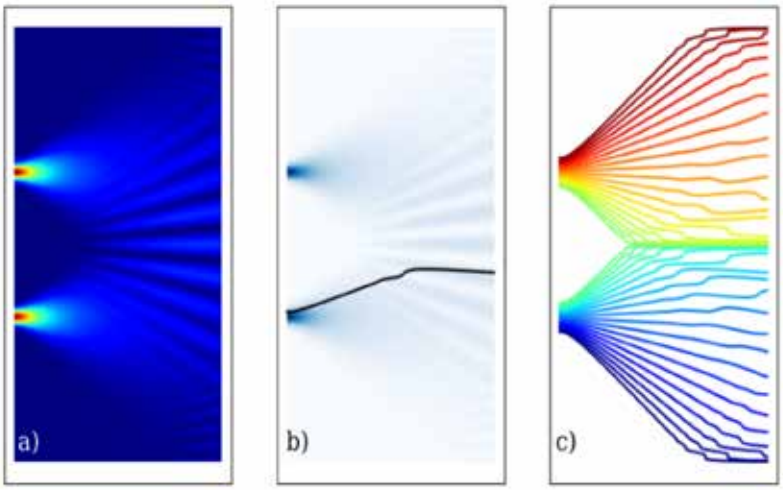

Figure 1: three alternative interpretations of the double slit experiment. a) traditional quantum mechanics: the wave function evolves in time, creating interference fringes which reflect the final probability of detection; b) Bohmian mechanics: a single particle 'rides' the wavefunction following a guiding equation; c) Many Interacting Worlds: multiple particles, each in their own world, evolve dynamically following Newton's equations with an added quantum potential.

Nuclear quantum effects and how to treat them

In atomistic ab-initio simulations it is a common approach to make use of the Born-Oppenheimer approximation[3], namely, the separation of the global wavefunction into electronic and nuclear parts, and their separate treatment. This is justified by the fact that the masses of electrons and nuclei are orders of magnitude apart, and thus their dynamics are expected to be decoupled - with the nuclei appearing essentially static compared to the electrons. In this approach, nuclei are then treated as classical particles, and the quantum description is reserved to the electrons only. We know, however, that this description is not sufficiently accurate for a number of systems. There exist nuclear quantum effects which are especially crucial for light nuclei in shallow potential wells - a typical example being protons in hydrogen bonds. Approximate methods have been developed to address these effects[4] and reintroduce the 'quantumness' to the atomic part of the system. The most common methods are variations of the Path Integral Molecular Dynamics (PIMD) algorithm[5], which reproduces the quantum thermal density matrix by simulating a chain of connected 'classical' beads in place of each nucleus.

In a recent paper[6], we proposed the Many Interacting Worlds (MIW) as a new such method. We believe the MIW interpretation holds a number of qualities that could make it a great complement to PIMD in the study of quantum nuclear effects. For example, since the MIW quantum potential is repulsive, it could allow to compute ground states by geometry optimisation, whereas PIMD only can be used for dynamical simulations. In addition, MIW seems to converge best for low temperature systems, whereas PIMD is optimal at high T. Finally, the structure of the algorithm, featuring multiple parallel classical simulations coupled by an anomalous potential, is very similar to PIMD, thus making it easier to implement in existing software.

Many Interacting Worlds with a kernel approximation

The remaining difficulty is how to effectively implement the MIW algorithm for practical use. The algorithm requires that, in order to compute the quantum potential, an expectation value for a probability distribution is built from the positions of a discrete number of point-like particles (usually, less than 100). Our proposal was to use the technique of Kernel Density Estimation , which rebuilds the total distribution as the sum of multiple kernel distributions each centred on one particle. We tested both Gaussian and Laplacian kernels for this purpose. The resulting quantum potential and forces can be computed analytically, and the cost is trivial compared to a full quantum calculation. In atomistic ab-initio optimisations and dynamical simulations, thus, the quantum calculations for the electronic state would dominate the overall computational cost. The kernel method allows an easy generalisation to any

3 "On the Quantum Theory of Molecules M Born and J R Oppenheimer ...." http://www.chm.bris.ac.uk/pt/manby/papers/bornop.pdf. Accessed 7 Aug. 2018.
4 "Nuclear quantum effects enter the mainstream | Nature Reviews ...." 28 Feb. 2018, https://www.nature.com/articles/s41570-017-0109. Accessed 7 Aug. 2018.
5 "Path integral molecular dynamics: a computational approach to ...." https://www.worldscientific.com/doi/abs/10.1142/9789812839664_0014. Accessed 8 Aug. 2018.
6 "Computational applications of the many-interacting-worlds ...." 31 May. 2018, https://link.aps.org/doi/10.1103/PhysRevE.97.053311. Accessed 7 Aug. 2018.
7 "Rosenblatt : Remarks on Some Nonparametric Estimates of a Density ...." https://projecteuclid.org/euclid.aoms/1177728190. Accessed 8 Aug. 2018.

dimensionality and only depends on one parameter, a kernel width that the user must set at the beginning of the calculation. A full exploration of how the choice of kernel width affects the results is planned for the future. Tests in multiple potentials and at different dimensionalities have shown that the method is indeed suitable to reproduce with good approximation the known theoretical solutions of the Schrödinger equation[6].

An interesting property of the MIW algorithm is that, in the exact limit, it should reproduce real time quantum dynamics in a very natural way. This also means that processes such as tunneling and thermal effects should become relatively easy to explore. An example of this is seen in Figure 2, where tunneling rates computed for a particle in a 1D double well are compared with theoretical predictions.

The MIW algorithm has been shown to be a useful new approach to quantum nuclear effects. Going forward, we plan to move on to testing it on molecular systems and comparing its results with known methods such as PIMD. Ultimately, we hope for it to be implemented in major ab-initio software packages such as CASTEP, as an easy to use alternative to approximate nuclear quantum effects in all systems that may require it.

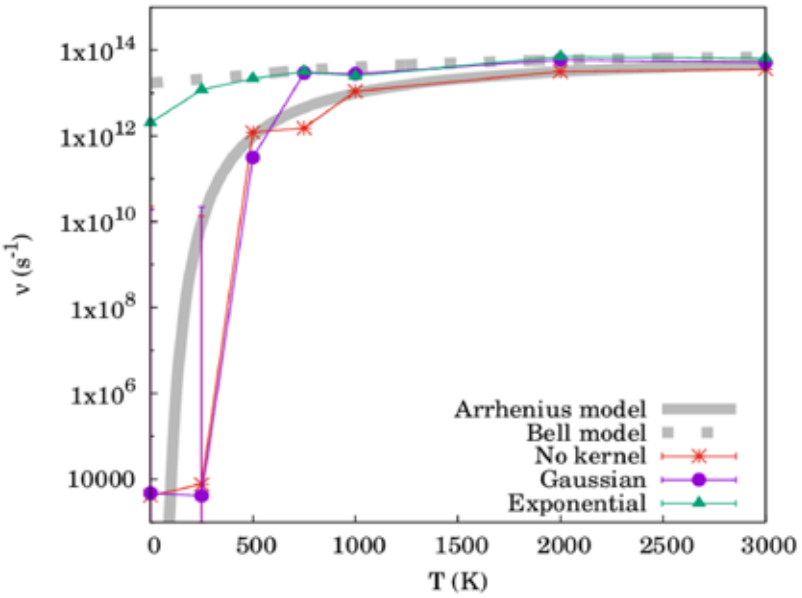

Figure 2: thermal tunneling rates for a particle in a potential double well, theoretical models with (Bell) and without (Arrhenius) quantum effects, compared with classical (No kernel) and quantum mechanical MIW simulations (Gaussian and exponential, aka Laplacian, kernels). Notice how the Laplacian kernel performs better from low temperatures, whereas the Gaussian one works best at high T.

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Strategic Theme 1

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Novel bottom-up approach to dissipative particle dynamics coarse-graining

Credit: Pixabay

Our scientists have discovered a new way of mapping and setting parameters for a class of models and computational algorithms known as dissipative particle dynamics (DPD), that were specifically developed to address mesoscale problems in complex fluids. This new approach links DPD with the important physical phenomena of condensed matter. It reduces the number of variables usually required in simulation models, making it easier to understand hydrodynamic behaviour at the atomic scale - for example, how the millions of molecules collectively move, mix together, or separate in viscous fluids such as mucus or blood. These models will contribute to a better understanding of the way biological macromolecules, like proteins, evolve in the human body, leading to better drug design.

Introduction

Computer simulations in condensed matter are typically performed using physical models pertinent to the scales of the studied phenomena. At the nanoscale, the basic unit of denomination is the atom. Modelled as a point object while still bearing the chemical identity of the element, the atom is a pawn in the statistical mechanics game of molecular dynamics. At the microscale, there is no clear candidate for this role and scientists, challenged by complex biological and hydrodynamic phenomena at this scale, often have to resort to large-scale simulations involving millions to trillions (10^9) of atoms [1,2]. Clearly, such fine resolution is excessive in describing the collective evolution of the system where even a look through 'blurred eyes' of coarse-graining should provide some insight.

Coarse graining (CG) in statistical mechanics is a powerful technique to reduce the number of variables in the equations to be solved by simulation and therefore to dramatically reduce the computing requirements. Rigorously, the approach is based on application of the projection operator method of Zwanzig and Mori [3], which in practical terms means that Newtonian equations of motion of the atomic level have to be replaced with more complex Langevin equations at the CG scale. Coarse-graining inevitably introduces a pair of new forces: a frictional force, proportional to the velocity of the CG particle, and a compensating stochastic force that covers for the eliminated degrees of freedom, i.e., for the collisions that the CG particle would experience with an atomistic subsystem. In some biological applications the structure, rather than dynamical processes, is of primary importance and by replacing a whole functional group of chemically connected atoms with a single 'bead' and retaining the Newtonian dynamics a sensible structure could be found [4].

When the dynamic processes in fluids are the object of study the additional forces introduced in Langevin dynamics can no longer be ignored, and new simulation methods are required. One such method, called Dissipative Particle Dynamics (DPD), for a recent review see [5], is particularly suitable for the study of dynamic and transport properties of the complex fluids at the mesoscale. The DPD method introduces soft dissipative particles with purely repulsive forces, representing swarms of atoms or 'lumps of fluid', but without clear definition of the DPD particle.

Here, we present a new general method of deriving the DPD model parameters from fully atomistic simulation. We start by defining a Brownian quasiparticle (BQ), which will bridge atomistic and DPD views. We then describe a new method of calculating the dissipative forces as direct statistical averages over the atomic ensemble and use BQ to translate the coarse-grained forces into DPD ansatz. Finally, we present results in a test simulation of a simple atomic system, deriving the DPD parameters, and use them in the DPD simulation to validate the method.

Brownian quasiparticles

In order to facilitate the link between the atomic and DPD levels we introduce a concept of Brownian quasiparticle (BQ). We define BQ as a CG object of constant volume, which is both immersed and consists of fluid, as illustrated in Fig. 1. This distinguishes it from the usual Brownian particle. BQ collectively represents all atoms contained at a particular moment of time in its spherical volume element and its kinematics is defined by the collective motion of all constituent atoms. This definition implies that the mass of the quasiparticle fluctuates in time according to the grand canonical conditions in the language of statistical ensembles of Gibbs. BQs are used to collect certain distribution functions from their trajectories driven by the atomic host system in atomistic simulation.

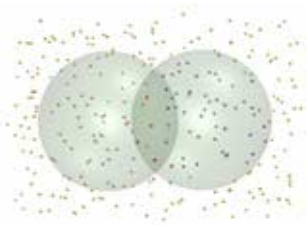

Figure 1: Two overlapping Brownian quasiparticles immersed in the host atomic fluid. Atoms, shown as small spheres, are distinguished by the colour inside each quasiparticle and in the overlap region, where two blue atoms are assigned to the right sphere, and four red atoms – to the left sphere.

In order to derive the forces between BQs, a number of quasiparticles is randomly dispersed in the atomic system. Since the DPD is not a space-filling model, the density of BQ is a free parameter that we would like to tune. Conducting a standard molecular dynamics simulation at the atomic level would drive the motion of quasiparticles but the motion of atoms is unaffected by the presence of BQ 'observers'. We define the interaction between quasiparticles in terms of the exchange of 'virtual particles', which are atoms, only virtually present at the coarse-grained level. There are two types of quasiparticle interactions depending on whether the atom leaving the BQ volume enters another BQ or goes into a 'reservoir'. While the latter describes the interaction with the environment, and is contributed to stochastic forces only, the former is a classical analogue of 'exchange repulsion'. Thus, the receiving BQ would get a momentum kick along the exchange particle velocity direction, i.e., away from the originating BQ, which simultaneously receives a recoil momentum. One may use an analogy with two boats on a lake exchanging watermelons by throwing them. Momentum conservation requires that each atom could be allocated to, at maximum, one BQ and could not be present in two BQs simultaneously. When two or more BQ beads overlap, the atoms are reassigned according to Voronoi tessellation, i.e., each atom associated with the nearest bead. This condition is sufficient to devise the interactions between BQ beads.

Estimating DPD forces in molecular dynamics

In the pairwise approximation of DPD, the force between two DPD particles is a sum of conservative, $\mathbf{f}_{ij}^{(c)}$, dissipative,$\mathbf{f}_{ij}^{(d)}$, and stochastic, $\mathbf{f}_{ij}^{(s)}$ forces

$$\mathbf{f}_{ij}(r_{ij}) = \mathbf{f}_{ij}^{(c)}(r_{ij}) + \mathbf{f}_{ij}^{(d)}(r_{ij}) + \mathbf{f}_{ij}^{(s)}(r_{ij}),$$

where the last two terms, defining collectively the Langevin forces, form a DPD thermostat [5]. Individual terms could be written as

$$\mathbf{f}_{ij}^{(c)}(r_{ij}) = \alpha(r_{ij})\mathbf{e}_{ij},$$

$$\mathbf{f}_{ij}^{(d)}(r_{ij}) = -\gamma(r_{ij})u_{ij}\mathbf{e}_{ij},$$

$$\mathbf{f}_{ij}^{(s)}(r_{ij}) = \sqrt{2k_BT\gamma(r_{ij})/\Delta t}\,\theta_{ij}\mathbf{e}_{ij}.$$

Here, k_B is the Boltzmann constant, T is the temperature, u_{ij} is the relative velocity of two DPD particles, $\mathbf{e}_{ij}$ is a unit vector in the direction of the interparticle vector $\mathbf{r}_{ij}$, i.e., $\mathbf{e}_{ij} = \mathbf{r}_{ij}/r_{ij}$, and $r_{ij} \equiv |\mathbf{r}_{ij}|$ is the interparticle separation. In the stochastic term, θ_{ij} is a random variable, independent for each pair of particles, with zero mean and unit variance.

The model thus includes two functions, $\alpha(r_{ij})$ and $\gamma(r_{ij})$, whose functional form including the required parameters we want to derive from underlying atomistic simulation rather than postulate it. These two functions define conservative and dissipative forces, respectively, and this also fixes the parameters in the stochastic force.

Conservative force does not present a problem and could be calculated by differentiation of the conservative part of the energy $U^{(c)}$ in the dilute Brownian quasiparticle limit (with only two BQ present) rigorously as

$$U^{(c)}(r) = -k_BT \ln g(r)$$

where $g(r)$ is the BQ – BQ radial distribution function.

For the dissipative force, a suitable procedure can be established by noticing that the dissipative term is the only odd term with respect to time reversal. Therefore, by multiplying it by the relative velocity and taking the statistical average, one obtains

$$\left\langle \mathbf{f}_{ij}(r_{ij})\mathbf{u}_{ij} \right\rangle = \left\langle \mathbf{f}_{ij}^{(d)}(r_{ij})\mathbf{u}_{ij} \right\rangle = -\gamma(r_{ij})\left\langle \mathbf{u}_{ij}^2 \right\rangle,$$

where we took into account that both $\left\langle \mathbf{u}_{ij} \right\rangle = 0$ and $\left\langle \theta_{ij}\mathbf{u}_{ij} \right\rangle = 0$. Thus, the dissipative force can be estimated by taking the direct ensemble average,

$$\gamma(r_{ij}) = -\frac{\left\langle \mathbf{f}_{ij}(r_{ij})\mathbf{u}_{ij} \right\rangle}{\left\langle \mathbf{u}_{ij}^2 \right\rangle}.$$

and the total force between two BQ beads is the sum of all pair forces between atoms belonging to first and second BQ. Similarly, velocity of a bead is a centroid velocity of all atoms that belong to it at that moment.

Test case and the simulation results

As a test case we considered a supercritical state of the Lennard-Jones (LJ) fluid at reduced temperature T^*=1.8 and reduced density ρ^*=0.5. The system of 13500 LJ particles was placed in a 30x30x30 cube with periodic boundary conditions in 3D, and a set of microcanonical molecular dynamics calculations was performed using the velocity Verlet scheme as implemented in DL_POLY MD code [6]. The integration time was $t^* = 5.5 \times 10^6$ using a time step $\Delta t^* = 3.73 \times 10^{-3}$.

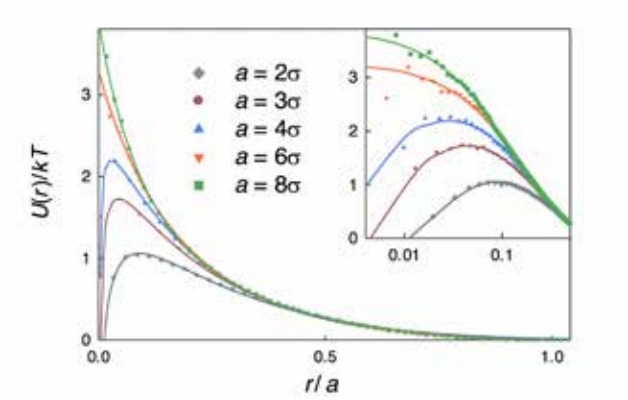

Figure 2: Potential of mean force for BQ of several dimensions. Symbols – simulation results, lines – truncated exponential fit. The inset shows initial part of the distributions at close BQ separations, note the log scale for the separations

First, we calculated the structure of the BQ subsystem for a range of quasiparticle sizes a ranging from 2σ to 8σ. Figure 2 presents the potential of meanforce results obtained from the radial distribution function in the dilute BQ density limit. At two larger BQ sizes, the potential decreases monotonically. Inversion observed for smaller sizes at short range is related to the correlated motion of BQ at short separation and due to the contribution from BQs not containing atoms. At long range, all profiles collapse on a single curve. Solid lines are the fits used to derive conservative forces.

Figure 3 shows the distance dependent viscous drag coefficient in DPD units using the method outlined above. The results, shown in the graph for BQ of size $a=2\sigma$, almost collapsed to a single line, making it possible to use a single fit independent of density of BQ, shown in Figure by the dashed line.

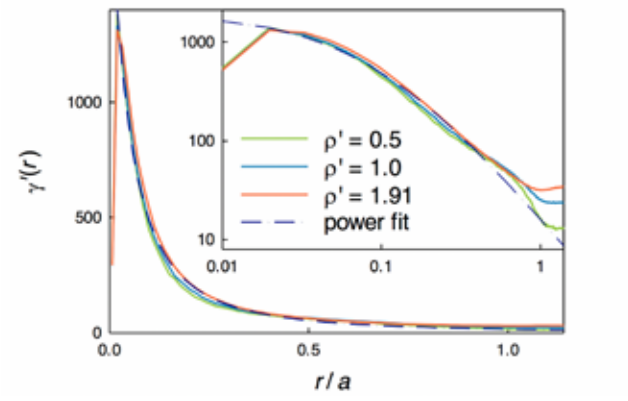

Figure 3: Viscous drag coefficient for several values of BQ density for $a=2\sigma$. Full lines, simulation results; dashed line, power fit. Inset shows the log–log plot

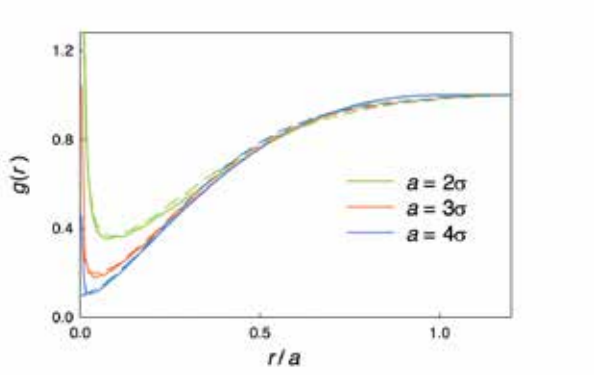

Figure 4: Radial distribution functions calculated for the matching BQ (full lines) and DPD (dashed lines) systems for three sizes of coarse-grained particles

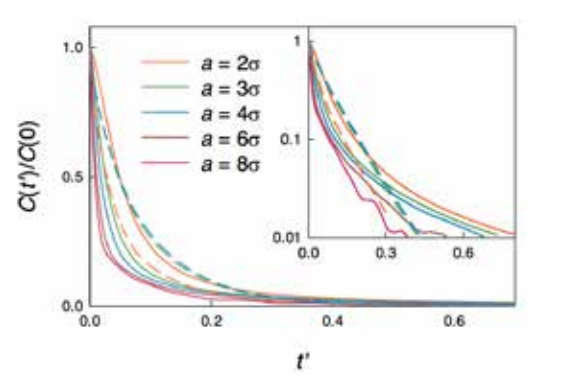

Figure 5: Velocity autocorrelation function of BQ (full lines) and DPD (dashed lines) systems for several sizes of coarse-grained particles. The inset illustrates the long-range behaviour of the same functions in the log–log plot

We then obtained parameters in DPD simulation using DL_MESO software package [7], which was modified to include the new potential forms for conservative and dissipative forces and to calculate on-the-fly radial distribution and velocity correlation functions. Using the DPD velocity Verlet integrator as implemented in the code and a system containing 1728 DPD particles in a cubic box with the side length of 12σ, which correspond to a reduced density 1.0 in DPD units, we calculated the radial distribution function of the DPD beads and compared with that of BQ used in derivation of the DPD parameters. The results, shown in Figure 4 demonstrate perfect structure mapping between BQ and DPD particles. The small differences are due to inaccuracy of the fit, done with an eye towards transferability.

Comparison of the DPD and BQ velocity autocorrelation functions for all calculated BQ sizes, shown in Figure 5, illustrate the influence of nonlocality present in BQ calculations through the correlations in atomic motion, and absent in DPD, where the velocity autocorrelation functions decay exponentially, as clear from the log–log plot in the inset. However, the functions for both models overlap in the important region and therefore the transport coefficients should be of the same order of magnitude. This is a dramatic improvement with respect to standard methods where the difference by several orders in magnitude is usual.

In summary, we have presented a new approach towards fundamental derivation of model parameters for coarse-graining the non-bonded degrees of freedom. We tackled this complex process in stages, which reflect its different strands and which require different assumptions. In the first stage, we introduced a Brownian quasiparticle as an open Lagrangian system. The atomic flux in and out of quasiparticle defines the dissipative and stochastic forces acting on it, and the condition that an atom at any time could be associated with at maximum one quasiparticle defines the conservative forces. The atomistic host system drives the dynamics of quasiparticles and gives a faithful description of the fluid motion at the coarse-grained level defined by the dimensions of quasiparticles.

The second stage involves recasting the Brownian quasiparticle dynamics in the form of DPD. This involves several approximations pertinent to the DPD ansatz, including pairwise approximation for the forces, Markovian approximation for Langevin forces (no memory), and truncation of viscous drag forces at the DPD particle size.

As shown in this work, the proposed method provides a working route to derive the DPD parameters from the underlying atomistic system and gives a quantitative agreement in the structure and qualitative describes the dynamics. The proposed concept of Brownian quasiparticle is found to be constructive in revealing the links between the host and coarse-grained description.

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Strategic Theme 1

SCD will build and strengthen our existing capability of providing enabling computational expertise and e-infrastructure to support STFC in fulfilling its strategic goals: "world class research, world class innovation, and world class skills."

The SCD 100Gb SuperSpine "Bridge" network

Credit: Pixabay

The Scientific Computing Department (SCD) has evolved and grown over more than a decade into its current form. Over that time computing infrastructure projects have come and gone but the networks they are connected to have remained , organisationally, mostly static. Here, Jonathan Churchill, Architect and Infrastructure Manager for JASMIN, a super-data-cluster which stores and analyses vast swathes of environmental data, takes us through the complexities of designing and implementing new networks to provide a robust 'backbone' of systems that work seamlessly for our users. He explains how he began this process:

The network (the IP address range) that the first cluster I worked on at STFC, over a decade ago, still exists today but hosts many different kinds of services, long after that cluster has been retired.

The thing that remains constant throughout is largely the group of people responsible for that network, in whatever organisational structure they happen to be in. So when we look at the structure of the SCD networks today, we observe a collection of several large but discrete networks each connected to the STFC Rutherford Appleton Laboratory's (RAL) central backbone network. This structure has worked very well and has the advantage of stopping issues in one part of the network affecting all the others. However, the downside to this is that when services and machines hosted on one of these discrete networks needs to transfer data to another one of the SCD discrete networks, we rely on the STFC RAL backbone network to transfer the data.

The capacity of the links to the backbone are tens of Gigabits/second (10,20,40,80 Gigabit/sec capacity) and in the past these have never been the limiting factor in data transfer rates, with servers connected at 1Gigabit/sec. However with the advent of cheap, direct-attach cabling for 10Gigabit/sec servers, around 2010/11 and with the falling costs of 10Gb networking switches more and more of the SCD servers and clusters have become connected at 10Gbps to drive the extraordinary rise in science data needing to be processed and stored (The SCD services in the RAL 'R89' data centre have capacity for approaching 100 PetaBytes on disc and 200 PetaBytes on tape). Since ~2013-15 40Gbps to the server, and more recently in 2016-2018 100Gb to the server has become economically feasible. So whereas it would take 40 or more server to server connections across the backbone network to saturate the uplinks, now it can take just two or even one. So the total bandwidth to the servers in one discrete SCD network far exceeds the practical capacity of the uplinks to the RAL backbone. This is the effect we refer to as the "trapped bandwidth" - see Figure 1.

In systems run by SCD - such as JASMIN and the Tier1 (which handles huge amounts of data from the Large Hadron Collider) is now, in orders of magnitude, larger than the uplinks. JASMIN has over 12Terabits/sec bandwidth (ie 12,000 Gigabits/sec) to servers for one 80Gigabit uplink.

The trapped bandwidth data transfer problem is only really an issue for the very large infrastructures in SCD. The rest of the very extensive RAL /Harwell campus backbone network is designed to cope with the thousands of desktop computers and their enterprise functions (email, internet etc), so solving this problem at the campus level isn't economically justified.

In late 2016 the JASMIN infrastructure was starting to plan an upgrade to its internal network to, as it turned out, more than double the computing and storage capacity and capability. This would take the internal bandwidth of the project to 20Terabits/sec compared to the 80 Gigabit/sec of the uplink it was connected to. The existing JASMIN network used a 2 tier routed "CLOS Tree" network of 12 spine routers and 23 leaf routers as in Figure 2, in a "non-blocking" arrangement where all the servers can exchange data with all the other servers at the same time at full rate, without saturating any uplinks.

This JASMIN network had about reached the extent of expansion (1,500 ports at 10Gigabit/s), so to double its capacity we would need to start a new CLOS network and somehow connect it to the existing one, ideally also in a non-blocking configuration. Through extensive research with industry advisors and, eventually, an open public sector tender procurement, we selected a 5 tier CLOS network architecture as in Figure 3.

This "Data Centre Network" 5 Tier CLOS is similar to that used by the extreme scale internet companies such as in Facebook's data centres (Ref 1). In these data centres the racks are divided into "Pods" where each Pod looks similar to our 2 Tier CLOS networks in JASMIN2 and now in our JASMIN Phase 4 upgrade (JASMIN4) and provided a route to add more Pods as JASMIN expands. This prompted me to realise that perhaps the other infrastructures in SCD could also be connected to the "Super Spine" middle tier of the 5 Tier CLOS. This would then allow them to exchange data at very high rates without needing to go via the RAL backbone network. Hence the concept of the "SCD Bridge Network" was conceived, where each SCD service could be considered as one or several "Pods" and connected together via a common superspine.

The SCD Bridge Network as shown in Fig 4 architecturally looks like a scaled out version of the 5 Tier CLOS shown in Fig 3 with a larger middle Tier, to accommodate not just the JASMIN expansion but also all other SCD services as Pods. However beneath the symmetry of the connection diagrams lies a wealth of complexity. For example we needed each service or Pod to be able to control which parts/subnets it wanted to expose onto the Bridge and which other services or Pods it would accept traffic from. This is implemented in a fairly complex static table of BGP (Broader Gateway Protocol) routing rules in the top of each SCD service or Pod.

Unusually for such data centre networks we also need the Bridge to be a high speed alternative to the path via the RAL backbone as described above. This is so that each infrastructure can operate on its own if there is a problem with the Bridge. To enable this, each Pod must maintain a routing "default route" of its own to the backbone. This has to be carefully controlled when connecting to the Bridge, as BGP is a dynamic routing protocol and if all the Pods broadcast that they are the default route, network traffic does not have a clear path to the internet, for example, and chaos reigns.

JASMIN itself is reliant on the Bridge to connect the JASMIN phases 1,2 & 3 CLOS network to JASMIN4, so over time, with further operational confidence from JASMIN, we may choose to provide one resilient gateway from the Bridge for all SCD Pods to use, to avoid the default routing problem.

The Bridge also solves a long standing issue of connecting our R89 and Atlas data centres, which are both located on the Harwell site, together without using the RAL backbone. Part of the SCD Bridge project is funding 64 100Gigiabit/sec fibre links from the Bridge superspine in the R89 data centre to new Pods in the Atlas data centre – starting at 6Terabits/sec with expansion to 128 fibres and 200Gbit optics in future rising to 24 Terabits/sec capacity. This bandwidth will allow us to site Pods in Atlas as if they were in R89, providing much needed data centre floor space and maximising the STFC investments in the Atlas data centre refurbishment.

The R89 and Atlas data centres are 0.5-1km apart and it's interesting to note that these very 21st Century network connections are routed through a thoroughly 20th Century "stream pipe" that was left over from a combined heat and power scheme from when the site housed the Atomic Energy Authority in the 1950s, ducting waste heat from nuclear reactors on the Harwell site to heat office spaces in the Rutherford Appleton Labs.

At the time of writing the SCD Bridge comprised of 16 Mellanox SN2700 32 port 100Gb routers which are installed and operating between the two JASMIN Pods, with high bandwidth links to the other SCD services already run in but not configured. We have seen sustained data rates of 220Gbytes per sec to the new JASMIN4 42PetaByte storage (1.7 TeraBits/sec) alone in testing (placing in the top 5-10 in the world for IO (input/output) performance) to add to the (at least) 240Gbytes per sec of the existing JASMIN storage, let alone our Tier1 storage infrastructure and the ~40,000 cores of computing SCD operates, fully justifying the needs for the apparently extreme scale networking of the Bridge network.

Once the JASMIN4 is in production and we have a few months of operational experience we will enable the links to the other services, so that sometime in 2019 all of the SCD services will be able to exchange the PetaBytes of data (1 PetaByte = 1,000,000 Gbytes) needed by today's big data driven science projects and resolve the "trapped bandwidth" problem.

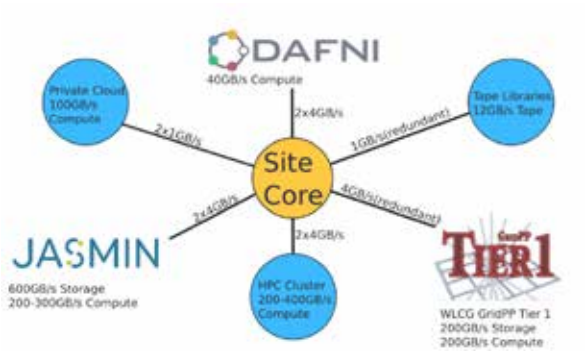

Figure 1: "Trapped bandwidth" : The SCD services have significantly more internal bandwidth than the uplinks to the RAL site core/backbone network

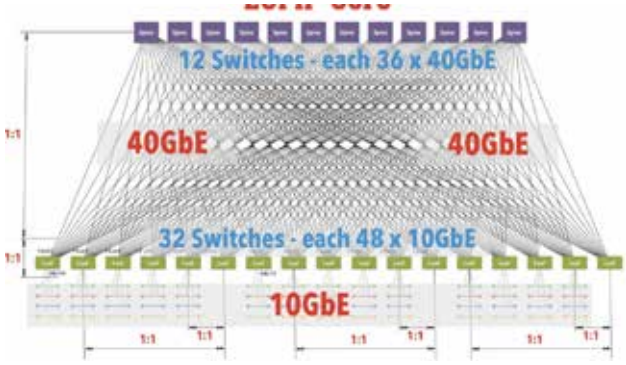

Figure 2: JASMIN 2 tier CLOS Network: This network connects up to 1,500 servers each at 10Gb from the "Leaf" switches. It hosts all the servers and storage for JASMIN phase 1,2,3

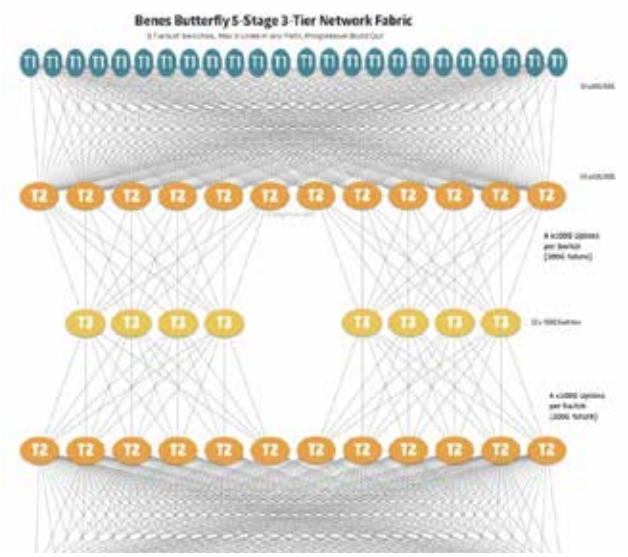

Figure 3: A 5 Tier CLOS: The upper and lower T1 and T2 switches are equivalent to the JASMIN2 and JASMIN4 networks Pods as in Fig2 . They are connected using the T3 switches which are equivalent to the SCD "Bridge" network

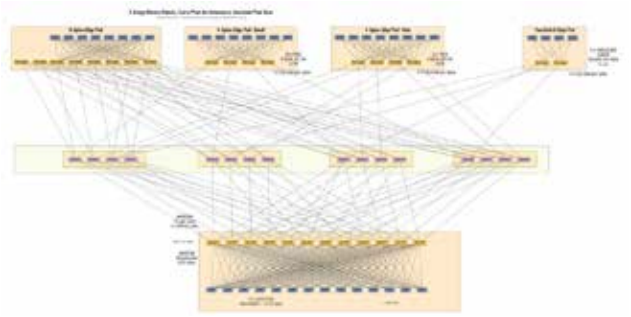

Figure 4: SCD Bridge Network : This diagram shows how different sizes of networks can be connected to the Bridge network. The bottom "Pod" is an example of a JASMIN2 style network. The top "Pods" are examples of other networks like DAFNI (top right) or a Tier1 (top middle)

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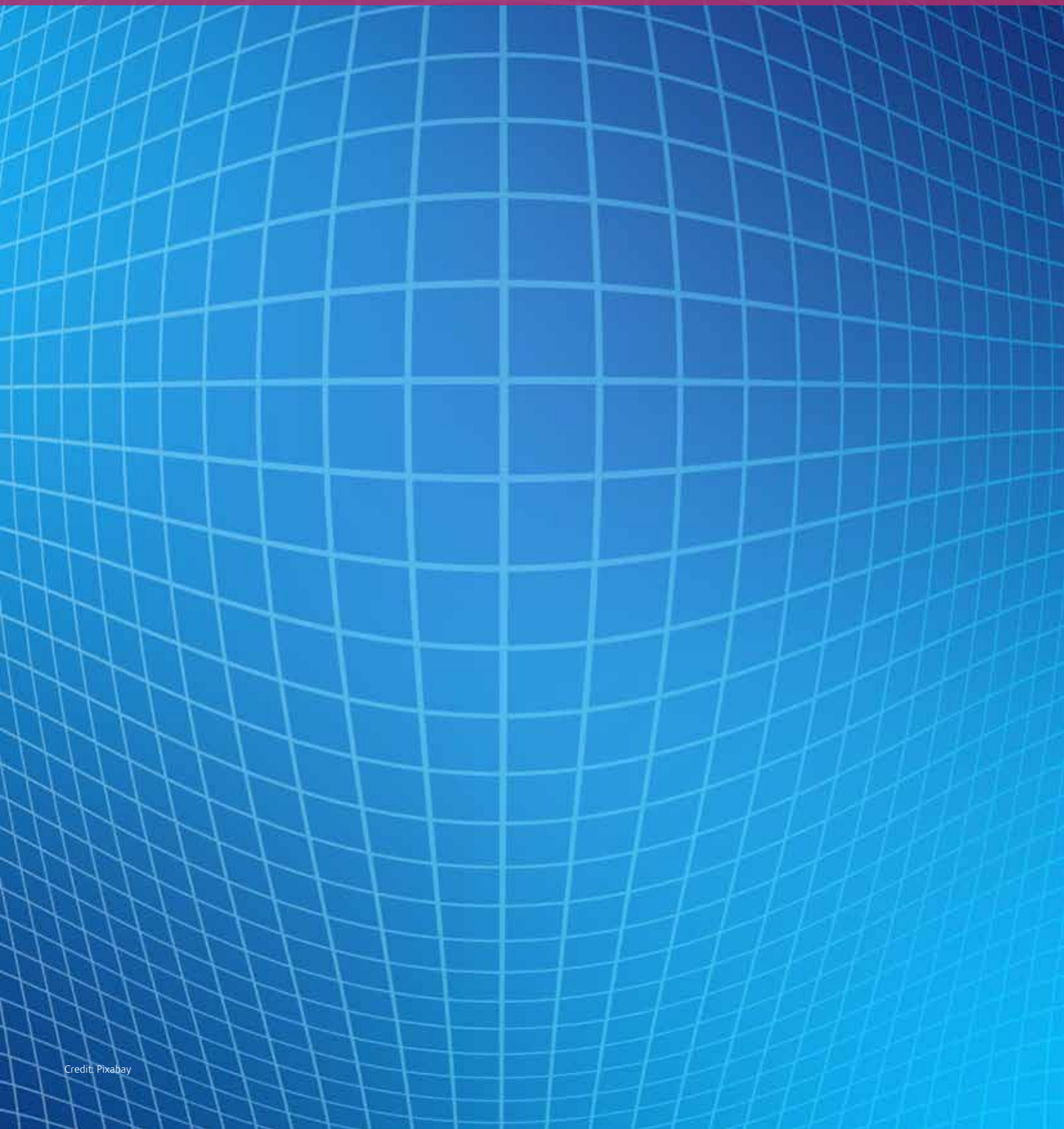
https://code.facebook.com/posts/360346274145943/introducing-data-center-fabric-the-next-generation-facebook-data-center-network/

Strategic Theme 1

SCD will build and strengthen our existing capability of providing enabling computational expertise and e-infrastructure to support STFC in fulfilling its strategic goals: "world class research, world class innovation, and world class skills."

Dealing with catastrophic fill in sparse least-squares problems



Credit: Pixabay

The method of least squares (LS) is a commonly-used approach to computing an approximate solution (or a 'best fit') when you have more equations than unknowns. "Least squares" means that the solution minimizes the sum of the squares of the residuals made in each equation. LS solvers are used across a wide range of disciplines, for everything from simple curve fitting, through the estimation of satellite image sensor characteristics, data assimilation for weather forecasting and climate modelling, to powering internet mapping services, exploration seismology, NMR spectroscopy, piezoelectric crystal identification (used in ultrasound for medical imaging), aerospace systems, and neural networks.

Since its development in the 18th century, the solution of LS problems has been and continues to be a fundamental method in scientific data fitting. Solving these problems can present a number of challenges. Our scientists have been exploring a method of 'matrix-stretching' that has the potential to solve some large-scale problems that were previously intractable.

An important special case is the linear LS problem

$$\min_x \|Ax - b\|_2, \tag{1}$$

where the system matrix $A \in \Re^{m \times n}$ $(m \geq n)$ and the right-hand side vector $b \in \Re^m$ are given. Necessary and sufficient conditions for (1) are that

$$A^T r = 0, \quad \text{where } r \text{ is the residual } \; r := b - Ax.$$

Thus a solution x satisfies the normal equations

$$Cx = A^T b, \qquad C = A^T A. \tag{2}$$

If A is of full rank, then this n x n system is symmetric and positive definite. For small problems, the solution x may be found from a singular-value decomposition of A or from a rank-revealing QR factorization. But in many practical applications, A is large and sparse (that is, the vast majority of its entries are zero), and because of the paramount need to preserve sparsity in the solution process for such problems to be tractable, algorithms developed for dense linear LS problems are unsuitable. The direct solution through a sparse Cholesky factorization of the normal matrix C may be possible or, for really large problems, iterative solvers are needed.

In practice, although most rows of the matrix A are sparse, it can often contain a small number of much denser rows. **A single dense row leads to catastrophic fill in** C. Even rows that are not fully dense can lead to such large amounts of fill in the normal matrix that for large problems forming the normal matrix explicitly and attempting to directly solve (2) is impossible. To try and overcome this issue, we have recently been exploring the use of matrix stretching. The idea here is to "stretch" the dense rows in the matrix A to give a new larger matrix $\hat{A}$ in which none of the rows leads to catastrophic fill in the corresponding stretched

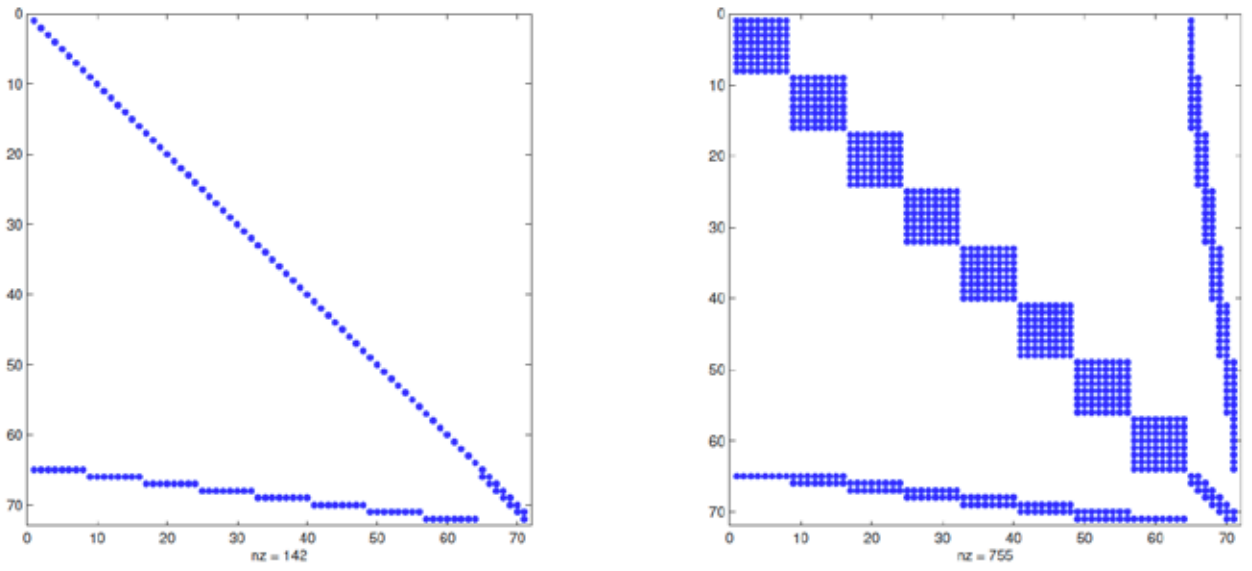


Figure 1: Structure of $\hat{A}$ (left) and $\hat{C}$ (right) for the matrix A with a single dense row and A_s diagonal with n = 64 and the dense row stretched into 8 parts.

normal matrix $\hat{C} = \hat{A}^T\hat{A}$; the solution of the original problem (1) can be recovered from that of the stretched problem. To illustrate this with the simplest possible example, consider the case where A is diagonal except for the final row which is dense. The sparsity pattern of the stretched matrix $\hat{A}$ and the stretched normal matrix $\hat{C}$ is illustrated in Figure 1. Here, $n = 64$ and the dense row is stretched into 8 equal parts; for the resulting stretched matrix $\hat{n} = 72$. We see that $\hat{C}$ is sparse.

The same technique can be applied to more general matrices with one or more dense rows. However, we have observed that for problems arising from practical applications, standard stretching based on the simple splitting of dense rows into a number of equally-sized contiguous segments can result in significant fill in the stretched normal matrix and, in particular, in its Cholesky factor. Furthermore, for any given example, it is unclear how to choose how many parts to split the dense rows into. Simply increasing the number of parts into which the dense rows are split does not necessarily alleviate the problem and can lead to a poorly conditioned system. This led us to develop a new sparse stretching strategy that aims to limit the fill in $\hat{C}$ and its factors and, in doing so, determines how many parts each dense row should be split into: the number will be different for each dense row within A and the parts will not be of equal size. Let us write A in the form

$$A = \begin{pmatrix} A_s \\ A_d \end{pmatrix},$$

where the rows of A_s are sparse and the rows of $A_d = (f_1,...,f_p)^T$ are dense. If each dense row f_i^T is stretched into a matrix F_i^T then the stretched matrix and corresponding stretched normal matrix have the form

$$\hat{A} = \begin{pmatrix} A_s \\ F^T \quad S \end{pmatrix} \quad \text{and} \quad \hat{C} = \begin{pmatrix} A_s^T A_s + FF^T & FS \\ S^T F^T & S^T S \end{pmatrix} \tag{3}$$

where $F = (F_1,...,F_p)$ and S is a block diagonal matrix with entries +1 and -1. It can be shown that $S^T S$ is tridiagonal and so the number of entries in the (2,2) block of $\hat{C}$ depends only on the order of S (that is, on the number of parts the dense rows are split into). Moreover, the fill in $A_s^T A_s + FF^T$ resulting from the dense rows is a minimum if the sparsity pattern of FF^T is contained within that of $A_s^T A_s$. Thus the idea behind sparse stretching is to choose the splitting of each dense row so that the structure of FF^T is embedded within that of $A_s^T A_s$. Our approach is illustrated in Figures 2 and 3.

So far, we have been able to show that sparse stretching is able to overcome the limitations of standard stretching for LS problems [2]. However, some issues remain. In particular, when the matrix A is stretched to $\hat{A}$ the increase in the size of the matrix can be significant, adding to the cost of the factorization of the stretched normal matrix. Thus we are currently exploring the idea of limited sparse stretching which will combine updating techniques with sparse stretching. Updating techniques [1] aim to use a factorization of the sparse reduced normal matrix $C_s = A_s^T A_s$ combined with the factorization of a dense subproblem involving A_d. However, even if A is of full column rank, removing the dense block A_d can result in the sparse part A_s being rank-deficient. In particular, A_s may contain one or more null columns and the Cholesky factorization of C_s then breaks down. A possible option is to select some of the rows of A_d, stretch them and then add the sparse parts to A_s to recover full rank. Again, the original problem will be replaced by a larger one but the hope is that the increase will be modest and will allow us to exploit the advantages of both updating and stretching in a single approach.

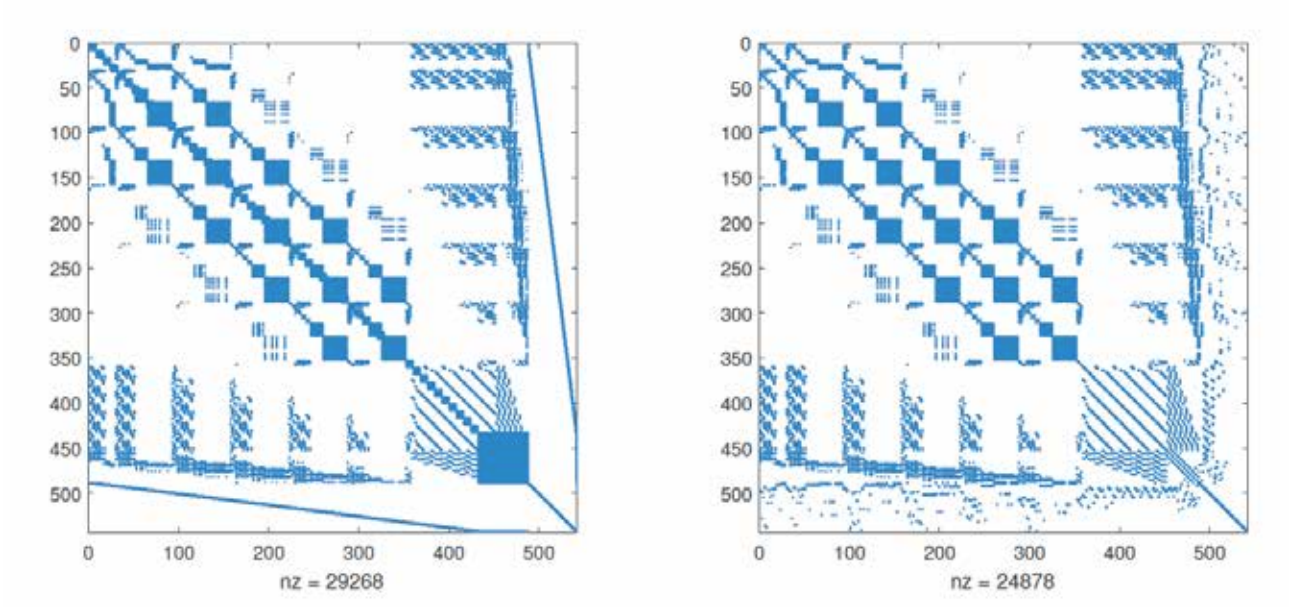


Figure 2: Problem with single dense row. The sparsity pattern of the stretched normal matrix for standard stretching (left) and sparse stretching (right)

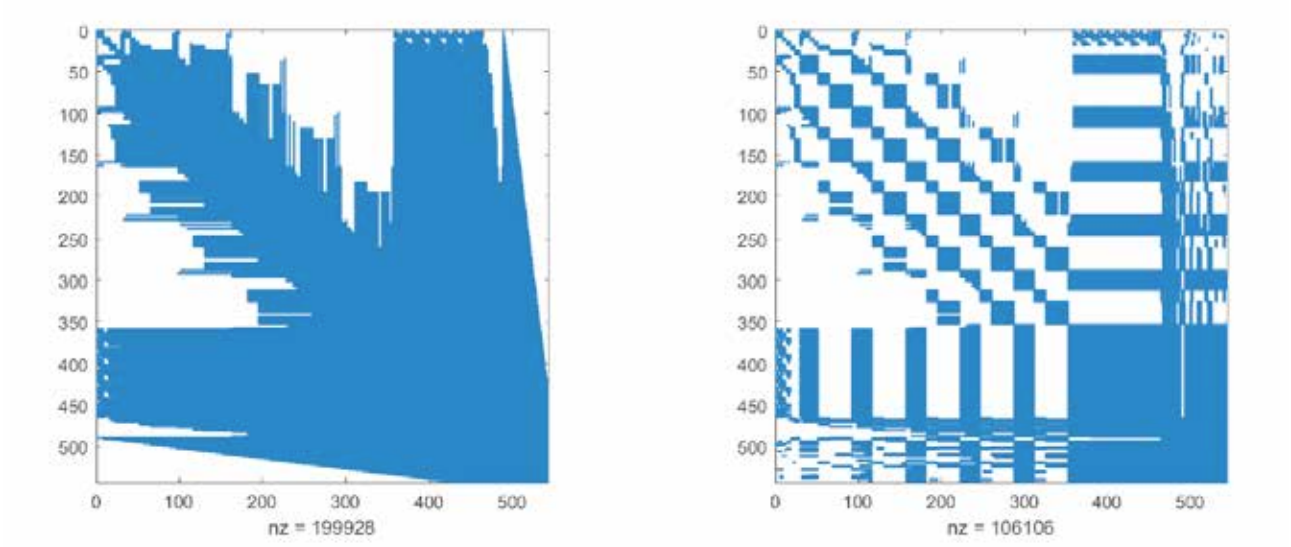


Figure 3: The sparsity pattern of the Cholesky factor of the stretched normal matrix for standard stretching (left) and sparse stretching (right)

Authors
J. Scott – STFC Rutherford Appleton Laboratory and the University of Reading, M. Tuma – Charleš University, Czech Republic.

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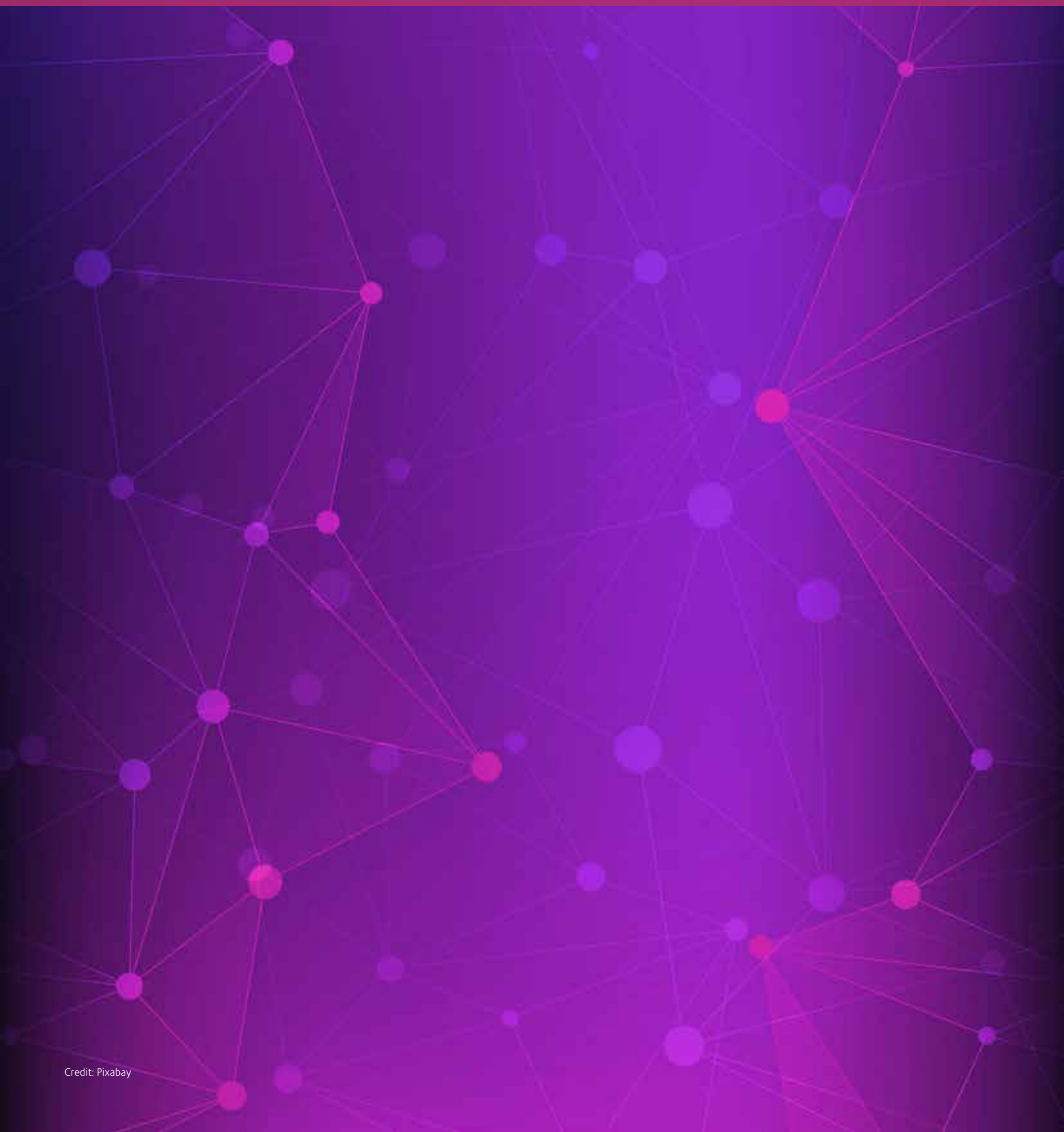
Strategic Theme 1

SCD will build and strengthen our existing capability of providing enabling computational expertise and e-infrastructure to support STFC in fulfilling its strategic goals: "world class research, world class innovation, and world class skills."

Longbow – lowering technological barriers in advanced computing



Credit: Pixabay

Scientists and academics need to run computer simulations designed to imitate a real-life situation – such as exploring how a new drug will attack a cancer cell – using the advanced capability and power of supercomputers. This can be a daunting task as these very high-speed, high-tech computers are expensive to run and can be both difficult and very time consuming to use. Each machine is likely to have a different interface – so the user would have to spend time learning about each system and then write separate configuration files for each one before they could run a simulation.

Additionally, users will need to write a submission file for each simulation, so if an experienced user is running 1,000 simulations they will usually need 1,000 submission files. This manual preparation not only takes a lot of time but also increases the risk of errors being made.

Enter Longbow…

Longbow is a tool that runs simulations on supercomputers whilst giving the impression that they are running on your own desktop or laptop computer. Developed by the High End Computing consortia for Biosimulation (HEC-Biosim*), Longbow will:

- Automatically create the configuration files required to run high-end simulations, lowering technological barriers to make complicated computing infrastructure simple. Users no longer need to spend time reading documentation before sending a simulation; they can just submit it and forget it. Longbow is pre-programmed with defaults for different systems, so it will learn the new system and adapt to the individual computer's configuration.
- Write the submission files for each simulation, so what might have taken several weeks to prepare manually now takes less than a second. Longbow will create the files and perform checks – and it doesn't make mistakes.
- Mimic the software the user is familiar with; so there is a very low learning curve from what they are already doing to having the power of a supercomputer at their fingertips.
- Provide seamless file transfers to bring data back to the user – so although the simulation could be running on millions of processors a thousand miles away, it appears to be running on their own laptop or desktop.
- Save vast amounts of time and money, which in turn enhances the value of the research grant or other funding stream.

Who is it for?

Longbow was originally designed for use by researchers and academics working in the field of bio-simulation. Due to its popularity, however, Longbow has been developed into a more generic tool so it is now available for other subject areas and is used in related industries. Users are encouraged to share the knowledge gained from using it with their own communities so that others can benefit.

There are two broad user categories:

- The novice – people new to simulation work, or they come from a non-computing background. Longbow makes it easy for them to use complex machines.
- The experienced experimentalist – highly knowledgeable users with many years' experience and who are likely to run thousands of simulations. Longbow allows them to spend more time doing science rather than unproductive computing set-up tasks.

An added bonus is that researchers working in the field of bio-simulation can also apply to HEC-Biosim for time on ARCHER, the UK's national supercomputing service.

How can you get Longbow?

Longbow is available via public repositories so you can download it from:

- github https://github.com/HECBioSim/Longbow
- pypi https://pypi.python.org/pypi/Longbow/

Or if you don't have access to those you can download the Longbow tool and get support from the HEC-Biosim website: http://www.hecbiosim.ac.uk/

Longbow is already being used to help experiments dealing with:

- New drug discovery and design
- DNA superstructures – understanding the mechanisms of how DNA forms supercoils and ultimately how it creates chromosomes
- Protein folding (where a protein structure assumes its functional shapes) – important for understanding some diseases
- Developing more environmentally-friendly engines

Authors

J. Gebbie, STFC Daresbury Laboratory. M. O'Sullivan, STFC Rutherford Appleton Laboratory

*HEC-Biosim supports the bio-molecular research community. It is helping to bring high-end computing to non-traditional users and experimental bio-scientists, as well as engaging physical and computer scientists in biological applications. It is supported by the Science and Technology Facilities Council and the Engineering and Physical Sciences Research Council through CoSeC (the Computational Science Centre for Research Communities).

Strategic Theme 2

SCD is committed to deliver and further develop its expertise in scientific analysis, data science, modelling and simulation, to support STFC's commitment to: Establish the Ada Lovelace Centre, an integrated, cross disciplinary, data-intensive science centre, to transform the use of real time data processing, computer simulation and data analytics to deliver more effective research at our national facilities.

CCP-EM: determining biomolecular structures by electron cryo-microscopy

Credit: Pixabay

Electron cryo-microscopy (cryoEM) uses beams of electrons rather than light to image very small objects. Recent improvements in the technology have meant that individual biological molecules, such as proteins or viruses, can now be seen with an electron microscope. The resolution is so good that pharmaceutical companies are beginning to adopt the technique in their drug development pipelines. The Scientific Computing Department set up and leads a Collaborative Computational Project for cryoEM (CCP-EM) which provides computational support for the community of scientists in cryoEM. CCP-EM has released a software suite which currently focuses on the interpretation of 3D molecular shapes obtained from images taken on the microscope in terms of thousands of individual atoms. This step allows chemists to understand the role of these molecules in vivo, and a correct interpretation is vital for all downstream use of the data. CCP-EM also organises training and collaboration events, the highlight of which is the annual Spring Symposium. While CCP-EM supports all scientists in the UK and overseas, it has a particularly close relationship with the eBIC national cryoEM facility at the Diamond Light Source, and together these projects form a significant part of the UK infrastructure in cryoEM. The CCP-EM community is also supported through CoSeC (the Computational Science Centre for Research Communities).

Your genome, and those of all living things, code for a set of protein and nucleic acid molecules that combine to create the complex organisms we see. Structural biology is the science of understanding the three dimensional nature of these molecules, and how they interact with each other, with applications in fundamental biology through to drug design. Until recently, structural biology was dominated by macromolecular crystallography, but there is a new kid on the block – or rather, a kid that has grown up enough to get a well-paid job. Improvements in instrumentation and in computation means that electron cryo-microscopy (cryoEM) can now provide sufficient structural detail to rival crystallography. This has led to a substantial investment in the technology, and the award of the Nobel Prize for Chemistry in 2017 to three pioneers of the field.

In fact, cryoEM has been around for several decades, but it is the progress overcoming two serious limitations that has generated the enthusiasm. Firstly, as shown in Figure 1, there has been a dramatic improvement in the typical resolution attained since around 2014. The 2Å barrier was broken in 2016 by the structure of glutamate dehydrogenase at 1.8Å resolution, while this year has seen two structures of apoferritin at 1.62 Å and 1.65 Å (see Figure 2). More importantly, to-date in 2018 around 30% of deposited structures have a resolution better than 4Å, beyond which atomic detail can begin to be discerned. Secondly, single particle reconstruction requires a sufficiently large molecule or complex to accurately determine the orientations of particles on the cryoEM grid. Smaller molecules are now being imaged, approaching a suggested theoretical limit of ~40 kDa. For example, a cryoEM structure of the 64 kDa haemoglobin at 3.4 Å was solved in 2017, with the help of a Volta phase plate. These improvements in resolution and minimum size raise the possibility of imaging the binding of drug candidates, so that pharmaceutical companies are now investing in cryoEM.

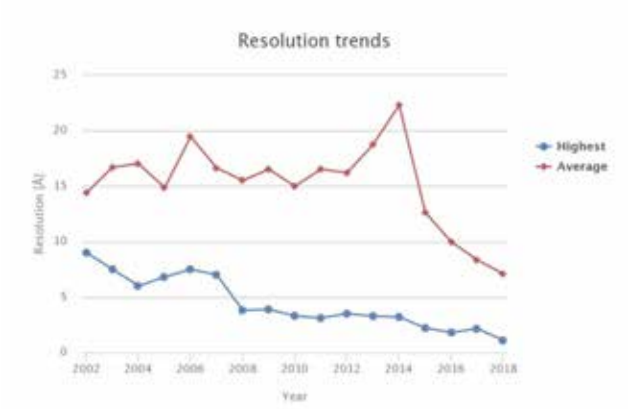
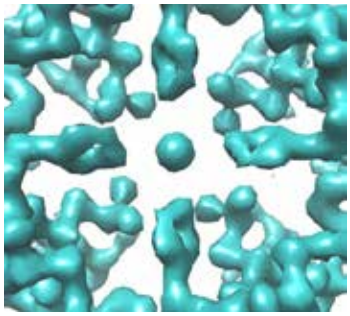


Figure 1: Average and highest resolutions achieved by single particle reconstruction. The graph was taken from the Protein Data Bank in Europe on 22/8/2018 (see http://www.ebi.ac.uk/pdbe/emdb/statistics_sp_res.html/)

A



B

Figure 2: Murine apo-ferritin at 1.62Å (A) and a zoomed in region (B) showing the high resolution detail around the iron binding site

The Collaborative Computational Projects (CCPs) provide national support in certain scientific domains. The CCP for Electron cryo-Microscopy (CCP-EM) was set up in 2012 as interest was growing in the technique, but before the "resolution revolution" had taken off. It is funded by the Medical Research Council (MRC) and coordinated by a core team in the STFC Scientific Computing Department. CCP-EM is a member of the Computational Science Centre for Research Communities (CoSeC) which facilitates the interchange of ideas on software best practice as well as specific algorithms in areas such as imaging and machine learning.

CCP-EM provides a software suite, with version 1.1 released in July 2018 [1]. This provides the basic framework of the suite and initial functionality around model building and refinement. Binaries are built with the help of the SESC build service (Anvil, based on Jenkins). A large part of the current suite is concerned with interpreting cryoEM volumes in terms of atomic coordinates. Depending on the resolution achieved, atomic models of components determined e.g. by crystallography can be fitted (rigidly or flexibly) into the map, or the coordinates can be built de novo.

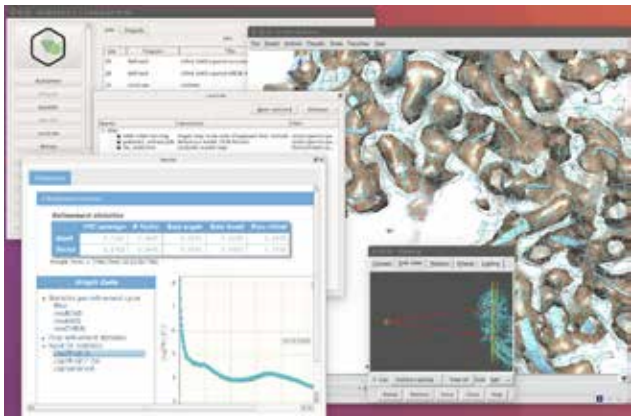


Figure 3: The CCP-EM software suite, showing an example of the application of LocScale applied to human γ-secretase complex, and the built-in link with UCSF Chimera for molecular graphics

Figure 3 shows an example of building and refining an atomic model for human gamma-secretase complex at 3.4Å using CCP-EM. Identifying atomic positions in cryoEM maps can sometimes be helped by sharpening the map, e.g. by increasing the weight on higher frequency Fourier components. However, it is a well-known feature of cryoEM maps that the resolution varies across the structure, and hence the optimum sharpening for interpretation can vary. The CCP-EM software suite includes the application LocScale from Arjen Jakobi at TU Delft which provides optimum local sharpening based on a reference atomic model, with the aim of facilitating additional model building and refinement [2].

While much of the current excitement is focused on single particle reconstruction with cryoEM, there are other experimental modalities of electron microscopy. Electron diffraction can be used for crystallography in much the same way that X-rays have for many years. The stronger scattering of electrons means that smaller crystals can (and must) be used, which can be useful for poorly crystallising molecules. Electron tomography, where a single sample is rotated in the microscope, is useful where particles cannot be isolated, are pleiomorphic (vary significantly in size and shape, e.g. enveloped viruses), or where larger cellular structures are of interest. In subtomogram averaging, particles are identified in tomograms and averaged, yielding information similar to single particle reconstruction, albeit at lower resolution. CCP-EM intends to provide software for these other modalities, and work is underway on the inclusion of a pipeline for subtomogram averaging and an application for segmenting tomograms.

The flagship event for CCP-EM is the annual Spring Symposium, the 4th edition of which was held at Keele University in April 2018. The talks are available on YouTube, and the proceedings are published by Acta Crystallographica D. CCP-EM organise training courses for 3rd party software (e.g. Dynamo for subtomogram averaging) as well as for their own software (e.g. the Icknield workshops on building and refinement of atomic models), and contribute cryoEM sessions in various international workshops (e.g. the CeBEM/CCP4 macromolecular crystallography school in Uruguay).

The CCP-EM team work closely with staff and users of the eBIC cryoEM facility at Diamond. They maintain the set of analysis programs available to on-site users, benchmark and optimise new software, and develop bespoke automated pipelines to provide rapid feedback on data collection. The experience gained at eBIC is fed into the CCP-EM suite, and disseminated to other cryoEM facilities around the UK.

Authors
M. Winn, T. Burnley, C. Palmer, A.P. Joseph, STFC Rutherford Appleton Laboratory

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Strategic Theme 2

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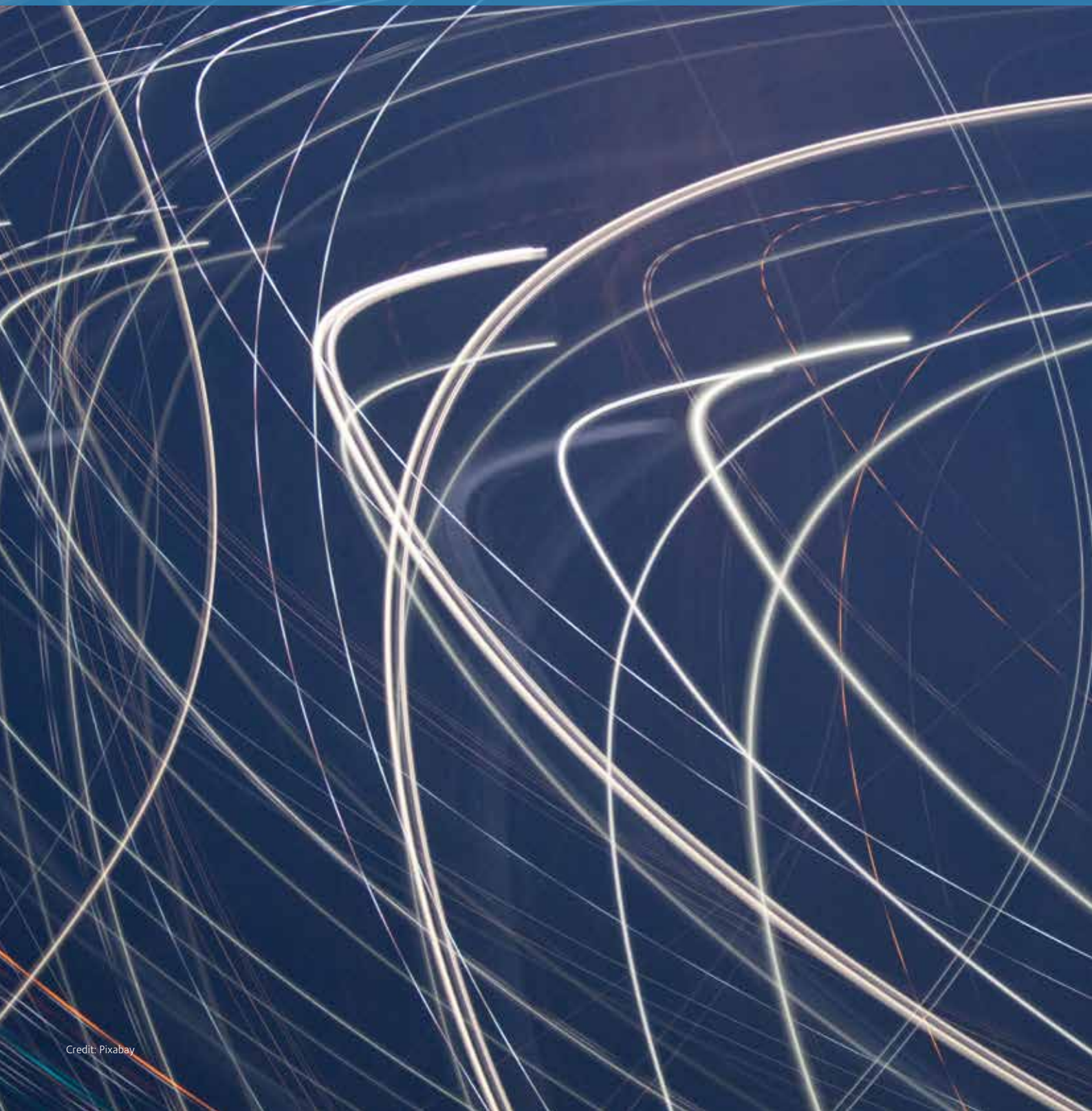
Dynamic Federations (DynaFed) system



Credit: Pixabay

Scientific experiments frequently require large-scale data storage, which may be achieved by distributing data across many sites. The Dynamic Federations (DynaFed) system from CERN can combine data stored at multiple sites into a single federation. Louise Davies, a graduate in the Scientific Computing Department's Data Services Group, has made DynaFed more widely usable by allowing access with either an existing username and password or a Grid certificate.

CERN created the DynaFed project to federate access to the various storage technologies used within the Worldwide Large Hadron Collider Computing Grid [WLCG]. The Scientific Computing Department (SCD) operates the ECHO [ECHO] cluster to provide storage for various experiments, such as the Large Hadron Collider (LHC), the Laser Interferometer Gravitational-Wave Observatory (LIGO), and Collaborative Computational Project 4 (CCP4). ECHO participates in a DynaFed federation, where the main goal is to enable access to data stored in various locations without users needing to know where the data resides.

DynaFed allows users to access data via standard clients such as web browsers, and supports traditional Grid storage resources such as dCache and DPM via the HTTP and Web Distributed Authoring and Versioning (WebDAV) protocols. DynaFed also allows users to access data via the Amazon Web Services Simple Storage Service protocol for accessing object storage [S3], which has become a de facto industry standard. This is of particular interest because the Ceph [Ceph] object store underlying ECHO also has an S3 interface, allowing us to use DynaFed to access data stored in ECHO.

SCD uses DynaFed to provide a hierarchical view of data stored in ECHO S3, and to authenticate and authorize access to the data. Previously, SCD's configuration of authentication for DynaFed assumed that access was from automated data production processes or privileged users providing an X.509 Grid certificate [X.509]. However, with more interest in interactive access from new projects - such as LIGO - and new users, the need for a more convenient form of authentication became obvious. As DynaFed runs under the control of the Apache web server, there are many authentication modules available, and these can coexist to allow multiple methods for user authentication to the same data storage. Figure 1 shows the default architecture of a DynaFed installation.

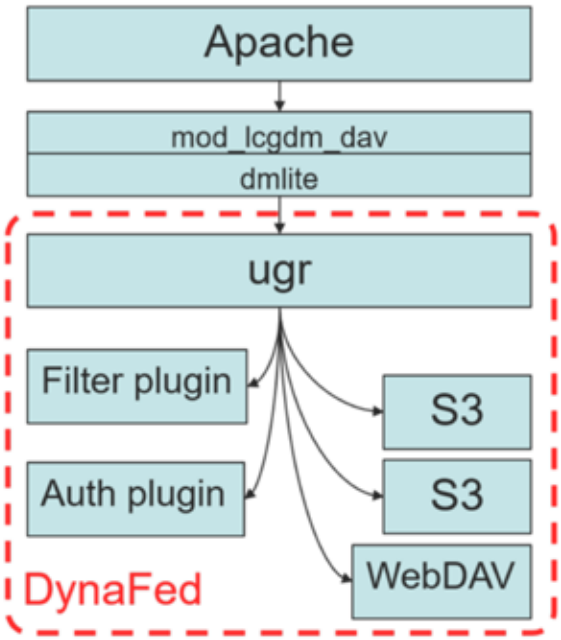


Figure 1: DynaFed Architecture

Structure and Operation of DynaFed

DynaFed is a collection of several plugins that a front-end server can load to provide the federation functionality. The front-end must provide HTTP access and optionally WebDAV.

An Apache web server acts as the frontend, communicating with the client via WebDAV. The figure shows two endpoints configured for accessing storage through S3, and one for WebDAV. The **mod_lcgdm_dav** plugin and **dmlite** communicate between Apache and the Universal Generic Redirector (UGR), the core of DynaFed. UGR transforms a client HTTP request for a desired resource into an HTTP Redirect response specifying the resource at one of the configured storage locations. UGR can use default rules (such as preferring the storage location 'closer' to the client) or logic in a Filter plugin to determine the best storage location for the client to access the resource.

Figure 2 shows how DynaFed can redirect a user request to the best location for the desired resource. The user requests **/dir/file2**, which is stored in two locations (**Site 1** and **Site 2**). DynaFed determines that the user is closest to **Site 2**, and redirects the user request to **Site 2**.

Authentication Options for DynaFed

To allow more convenient user authentication in addition to the established X.509 method, we considered two options.

Authentication with LDAP

The Lightweight Directory Access Protocol [LDAP] is an industry-standard lookup protocol currently in use within STFC. Apache provides **the mod_ldap** and **mod_ldap_authnz** modules that together can be used to provide Apache the ability to communicate with an external LDAP server to verify user credentials.

The options available in web browsers to prompt the user for their credentials include HTTP Basic Authentication [RFC7617] and HTTP Form-based Authentication [RFC8053]. Basic Authentication can also be used from a command-line tool, but doesn't provide an option to logout the user. The solution was to use Form-based Authentication as it allows the user to logout.

Authentication with Shibboleth

Shibboleth [Shibboleth] is a Single Sign-On system that enables users to authenticate with federations of many different organisations.

Shibboleth is already widely established in the academic community and can be used to gain access to identity federations such as the UK Access Management Federation for Education and Research UKFed [UKFed] and eduGAIN [eduGAIN]. Integration of Shibboleth authentication with DynaFed would significantly increase the number of potential users. To be able to gain access to the large user base provided by the identity federations, an administrator must first apply to be a service provider for those federations. The application process generally requires the organisation be registered as part of the federation to establish trust in the new service, and involves a certain amount of administrative work, ensuring both the security of the service and that processes are in place to maintain and provide support for the service.

Shibboleth authentication in Apache uses the **mod_shib** module. There was a little difficulty in passing Shibboleth attributes to the DynaFed authorization plugin in a secure manner; currently, DynaFed only receives HTTP headers and query strings to pass on to the Python authorization function. Concerns over client spoofing make the use of HTTP headers to store Shibboleth attributes unattractive. Shibboleth would prefer to use server environment variable as these are secure from the client, so a modification was made at STFC to the **mod_lcgm_dav** module to allow passing environment variables onwards.

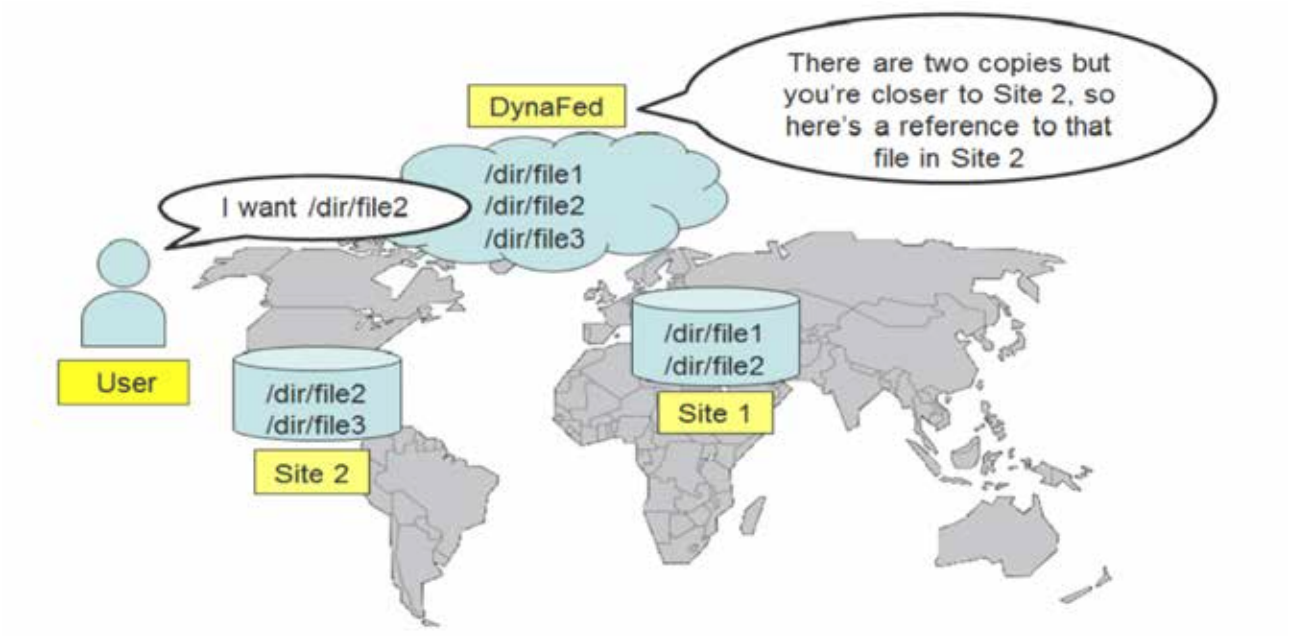


Figure 2: DynaFed Redirection

Writing a DynaFed Authorization Plugin

As the integration of Shibboleth with DynaFed mentioned above is not currently suitable for production, we decided to authenticate with LDAP to verify the credentials that a user supplies. This requires a matching authorization module that can use the LDAP user attributes to determine whether the request is permitted.

DynaFed has a plugin based approach to authorization and any number of authorization plugins can be activated within the same DynaFed installation. DynaFed will check each plugin to see if it grants access to the request and if any plugin accepts the request then access is granted, otherwise if no plugin authorizes the user then permission is denied. Since multiple authorization plugins are allowed simultaneously, this makes supporting separate authentication schemes much simpler. Providing a separate authorization plugin corresponding to each authentication method means that it is simpler to add or remove authentication methods.

DynaFed will invoke a function in a Python authorization module that returns a value indicating whether the request is allowed or not, based on attributes of the incoming request passed to the function. These parameters include the client username, the path of the resource being accessed and the access mode of the request (list/read/write/delete). This function is called every time a request is made; therefore only code that needs to be run per request should be placed in this function, whilst other items should be initialised in other places in the module. This is relevant since most authorization plugins will need to query some type of configuration file that contains the user access permissions and this should be processed outside the main access granting function. Additionally, there is a timing constraint in that DynaFed logs a warning for any authorization plugin that takes longer than 5 milliseconds to execute, in the interest of maintaining good performance of the service.

To complement the LDAP authentication applied by Apache, an authorization plugin that could use LDAP attributes to authorize users was created. The LDAP plugin uses a JavaScript Object Notation (JSON) file to manage path permissions based on LDAP attributes. JSON was chosen because Python has good interaction with JSON files, with the json module being part of the Python Standard Library, and because JSON is a human-readable file format, so the file could be administrated both manually and programmatically. The JSON file is used to verify that the user has the correct permissions to perform the relevant action on the path they are requesting.

Administration scripts provide a convenient means of creating and modifying the authorization files.

Current Status

This work has successfully combined X.509 and LDAP authentication to enable existing Grid access to DynaFed resources and also provide a more user-friendly interface through LDAP. The new LDAP authentication method has been added to the production DynaFed instance at STFC and is ready for trials to start with Facilities users . The code change to allow passing environment variable from **mod_lcgdm_dav** is currently under consideration by the DynaFed developers.

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L. Davies, A. Dewhurst, I. Johnson, STFC Rutherford Appleton Laboratory

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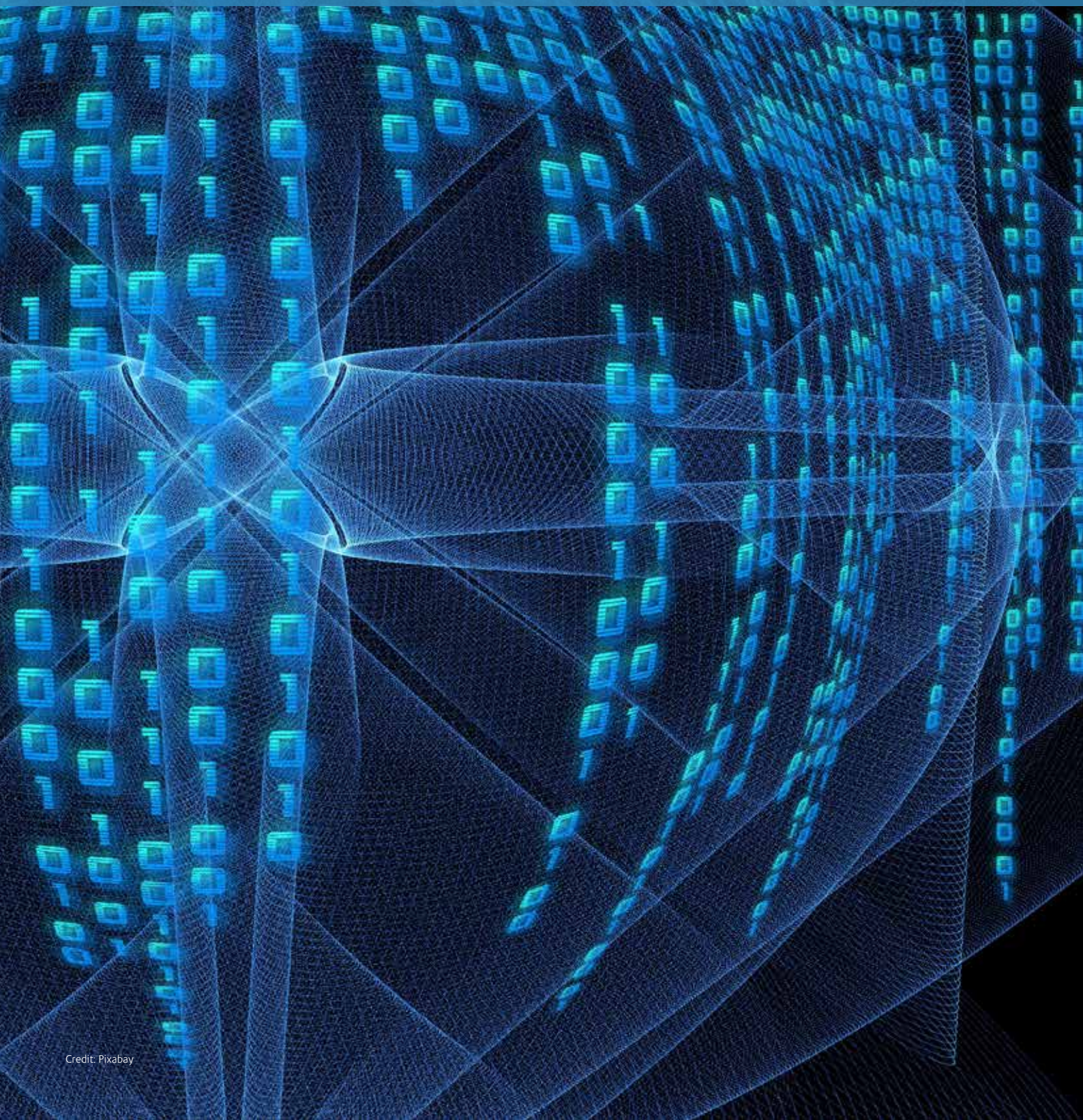
Software Collaboration and Cooperation



Credit: Pixabay

Creating software can be a very collaborative experience and this year the Software Engineering Group (SEG) has been working with peers in the UK, Europe and beyond. Our activities have spanned efforts to change the culture of delivering software. SEG provides the ICat data management cataloguing and discovery tools to STFC Facilities, data and publication repositories to STFC and software development tools to communities in the wider Collaborative Computational Projects (CCPs). To be able to do that effectively we need to be part of our own peer groups.

ICat development community encompasses STFC and European neutron and photon sources, with the ICat project manager, Stuart Pullinger, based in SEG. The community virtually meets every month to discuss development progress; this is usually focused on code. However good code is not the only thing needed for effective software development. Following a review of ICat using the Software Sustainability Institute's software audit tool, Stuart identified improvements were needed to the website and documentation and he hosted a document hackathon at the annual ICat face-to-face meeting. There was also ICat team representation at the Scientific Data Management for Photon and Neutron Facilities meeting, where the latest ICat roadmap was discussed.

The Research Software Engineers (RSE) community [1] is a growing one which brings together those involved in software development in research. Catherine Jones, who leads SEG, is a member of the RSE Leaders network which gives an opportunity to share expertise and best practice. In particular she spoke about her career at a Birds of a Feather session during the Supercomputing conference (SC17)in Denver.

Catherine, who was on the organising committee for the RSE18 conference as Workshop co-chair, also attended this International meeting, held in London in January 2018. Participants were world-wide, with colleagues from UK, Europe, USA, Canada, Brazil, Africa, New Zealand and Australia. The colleagues discussed topics including RSE career paths, software engineering tools, the importance of RSEs as an identifiable group and how the emerging national groups can work together in an international context. A flavour of the day was given by the tweets under the hashtag #intrse.

Software as a research output in its own right is an area which is gaining momentum. To be able to ensure that software is treated in the same way as publications and data then aspects such as citation, description and preservation need to be discussed and decided. SEG is involved in initiatives in this area such as the Force 11 Software Citation Implementation Working Group [2] and contributed to the Jisc/Software Sustainability Institute workshops on software preservation.

Understanding the role of software in research, finding specific software cited in specific research, and software as a research output in its own right are important areas for continued discussion and debate, and SEG will continue to contribute to this with the community.

Catherine speaking at the International RSE18 conference

Catherine with colleagues Alys Brett from Culham Centre for Fusion Energy, Ian Cosden from Princeton University & David Bernholdt from OakRidge National Laboratory in the STFC machine room.

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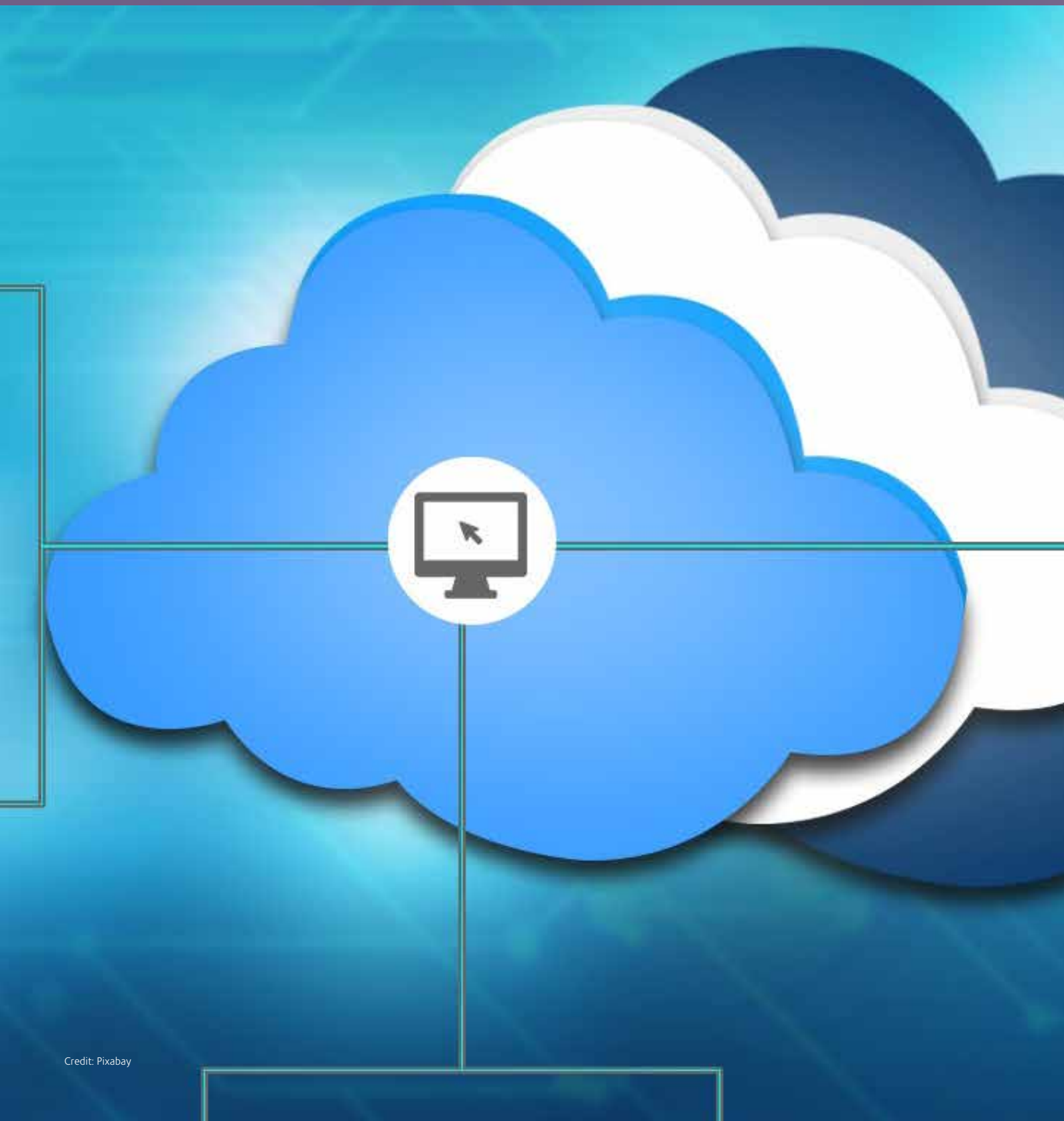
1.www.rse.ac.uk

2. https://www.force11.org/group/software-citation-implementation-working-group

Strategic Theme 3

SCD delivers a comprehensive programme of computational and data science services, research and development to underpin STFC's Data Intensive Science ambition: to develop and deliver cutting edge solutions for academia and industry to advance data intensive science and innovation.

SCD Cloud and IRIS National e-Infrastructure



Credit: Pixabay

The requirements for scientific computing continue to grow in scale and complexity. More flexible provisioning, both in terms of capability and scale are becoming more vital. The Scientific Computing Department (SCD) has been at the forefront of providing high performance and high throughput computing (HPC and HTC) to STFC communities for decades. STFC has also been at heart of international petascale grid computing development for over a decade – running the UK Tier 1 as part of the global effort to support the Large Hadron Collider (LHC) computing grid.

The SCD Cloud has been developed over the last three years. A new OpenStack platform was launched this summer and is ready to take its place alongside the Tier 1, SCARF and JASMIN.

We are now positioned for a new era of more flexible large scale distributed scientific computing integrated into IRIS, a UK wide distributed e-Infrastructure, for the range of STFC science such as LHC, Square Kilometre Array and STFC facilities.

The SCD Infrastructure-as-a-Service Cloud

The STFC Cloud is an Infrastructure-as-a-Service platform which is designed to enable users from STFC funded projects to perform research. It is based on the OpenStack cloud management framework and makes use of other open source technologies such as QEMU, KVM, Ceph and MariaDB. Currently it delivers around 5000 cores of compute and around 16TB of memory to around 50 projects. The STFC Cloud also delivers 60 GPUs of various types to the Ada Lovelace Centre and IRIS.

The STFC Cloud is designed to meet STFC's requirements for a secure, reliable and performant elastic compute resource. Security is achieved by making use of the OpenStack platforms capability to create private networks for projects and by making use of OpenStack Security Groups as a layer of firewalling in addition to the site firewalls. These features allow research groups to be separated from each other and the STFC internal network. It also allows users to run their own virtual machines without time consuming configuration on our part. Reliability is achieved through many levels of redundancy, multiple instances of every OpenStack service, highly available databases using MariaDB and Galera, highly available load balancers using haproxy and keepalived and a highly available messaging service using RabbitMQ. It uses the SIRIUS Ceph cluster to make virtual machine images and volumes highly available. To ensure that Virtual Machines perform as required the hypervisors are aware of the layout of the hardware, allowing for efficient scheduling of Virtual Machines. Virtual Machines can also be configured with either over-committed or dedicated CPU cores depending on the requirements of the user. To minimise the overheads of using the isolated project networks we carefully tune the high performance networking hardware.

The network architecture for the Cloud is also interesting. The network is architected as a Leaf-Spine network with the ability to scale out to many racks of hardware while also having the ability to scale the bandwidth between racks of hardware (currently 200Gbps with 2 spine routers, about 4000 times faster than the average home broadband speed in the UK of 46.2Mbps as of May 2018). Hypervisors and storage nodes are each connected to a leaf at 25Gbps (10Gbps for some of the older hardware). This enables complex work flows involving large datasets to be completed quickly.

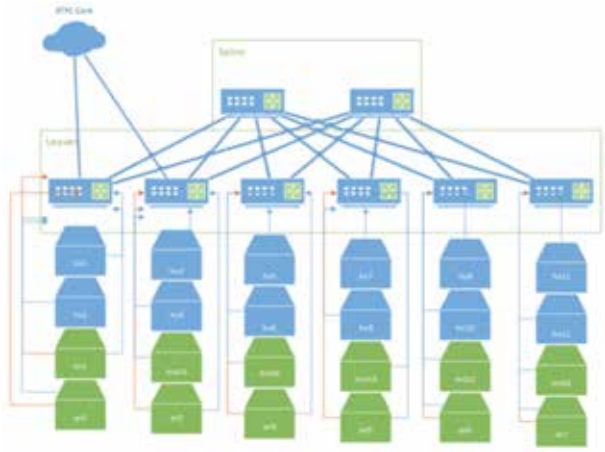


Figure 1: The layout of the cloud network

There are many use cases currently using the STFC Cloud, a few examples are:

- The Software Engineering Support Centre (SESC) Build Service, a service run by SCD for the Engineering and Physical Sciences Research Council (EPSRC) – which creates Virtual Machines as they are needed for builds and destroys them when they are done. This allows users of the Build Service within STFC and EPSRC to perform robust building and testing of software on multiple operating systems.
- Cloud Bursting the Worldwide LHC Computing Grid (WLCG) Tier 1 Batch Farm – The STFC Cloud provides additional compute capacity to the Tier 1 to enable it to support more use cases from outside of the WLCG.

- SeaDataCloud is a Horizon 2020 project to support Ocean science. The STFC Cloud enables STFC to participate in and provide resource to the project. They will use Rancher on top of OpenStack VMs to operate the containerised services they require.
- Data-Analysis-as-a-Service – The STFC Cloud will create bespoke Virtual Machines with tailored research environments for the ISIS Neutron and Muon Source, Diamond Light Source and Central Laser Facility users as they require them for analysing the data from their visits.

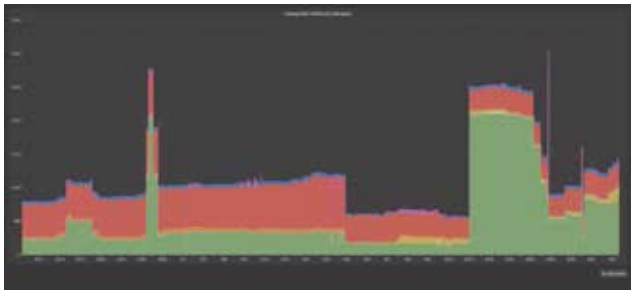


Figure 2: cloud usage increasing due to cloud bursting

IRIS – UK National e-Infrastructure to enable STFC Science

The UKT0 (UK Tier Zero) activity over the last few years has aimed to link diverse resources into a coherent whole – providing a national e-Infrastructure of both high performance (HPC) and high throughput (HTC) computing resources to support STFC science.

This has evolved into IRIS (e-Infrastructure to enable STFC Science), and is supported by communities including:

- Particle Physics: LHC+and other Particle Physics experiments (GridPP)
- DiRAC (UK HPC for theoretical physics)
- National Facilities such as Diamond Light Source and ISIS Neutron and Muon Source
- Astro: LOFAR, LSST, EUCLID, SKA, ...
- Astro-particle: LZ, Advanced-LIGO
- STFC Scientific Computing Dept (SCD)
- Culham Centre for Fusion Energy

These efforts have resulted in a £16M capital investment from the Department for Business, Energy and Industrial Strategy (BEIS) for the next four years. This will mostly provide compute and storage resources going some way to restore the erosion over the last several years of flat cash, and provide some support for emerging science but will also fund some cross cutting activities such as linking resources (federated identity management and SSO, resource accounting & management tools) across the UK.

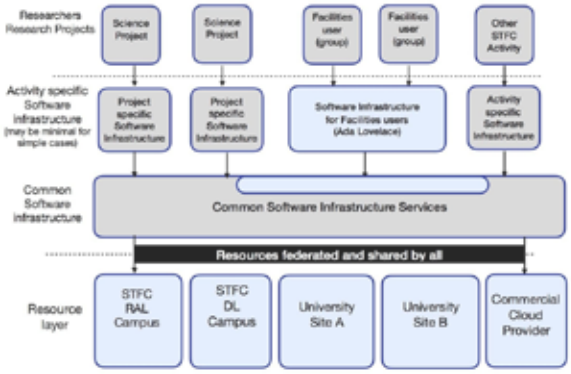


Figure 3: How IRIS will provide software and infrastructure to enable science

While UKT0 and now IRIS have been led by the communities it will serve, SCD has played an important coordinating role, and central to our ability to do that has been both our track record in delivering computing at scale to the national and international communities, but more recently the development of cloud capabilities that will sit at the centre of IRIS.

Emerging use cases with workflows that may move from one facility to another – some HPC, some HTC, some dedicated GPU etc., will require identity, authentication and authorisation that is unified across the different resources and some overview of whole infrastructure.

The cloud platform designed and deployed by SCD, leveraging the experience and tools used to deliver the Tier 1 to the Worldwide LHC Computing Grid, is an essential component along with the Echo large scale datastore. The coupling of the SCD cloud platform to the Tier 1 batch farm, and the development of other SCD activities, most notable the Data Analysis as a Service project (DAaaS) has ensured it is rooted in delivering flexible computing at the scale and with the performance, robustness and security required by modern scientific computing use cases.

In addition SCD's experience developing tools for resource accounting, and at the heart of projects like AARC (Authentication and Authorisation for Research and Collaboration) – developing standards and blueprints for distributed AAI will prove invaluable as IRIS evolves.

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Strategic Theme 3

SCD delivers a comprehensive programme of computational and data science services, research and development to underpin STFC's Data Intensive Science ambition: to develop and deliver cutting edge solutions for academia and industry to advance data intensive science and innovation.

Data and Analytics Facility for National Infrastructure (DAFNI)

Credit: Pixabay

National infrastructure systems (energy, transport, digital communications, water etc.) are undergoing a rapid change which is based upon the availability of digital data, communications, and computer power. There are opportunities to improve the efficiency, reliability and sustainability of infrastructure through better sharing and use of data, exploitation of simulation and optimisation techniques, and engagement with stakeholders through visualisation. The Data and Analytics Facility for National Infrastructure (DAFNI) represents an £8 million investment from the UK Collaboratorium for Research on Infrastructure and Cities (UKCRIC) to provide world leading infrastructure systems research capabilities and enhance the quality of outputs. In this report we describe capabilities of the DAFNI platform: (1) a secure yet accessible National Infrastructure Database; (2) a new software platform to enable analysis, modelling and simulation of national infrastructure systems; and (3) new remote and local visualisation facilities to enable access to and interpretation of the results by researchers, practitioners and decision makers.

Background

The Organisation for Economic Co-operation and Development (OECD) estimates that globally US$53 trillion of infrastructure investment will be needed by 2030 [1]. In line with this, the UK's National Infrastructure Plan has set aside over £460 billion of investment for the next decade. However, it is not yet known what effect the investment will have on the quality and reliability of national infrastructure services, economic productivity, the resilience of society or its impacts upon the environment. This uncertainty exists as a result of the inherent complexity of infrastructure networks and their interactions with people and the environment.

At a fundamental level the effectiveness of these investments is underpinned by the quality of the analytics used to inform decision making. Big data analytics, simulation, modelling and visualisation are now providing the possibility to improve this situation. Addressing this step change is intrinsically complex in nature and represents a broad set of distinct challenges for DAFNI. The key challenge is oriented around supporting the multitude of areas encompassed within National Infrastructure modelling.

DAFNI

Although the problem that DAFNI is looking to address is both broad and complex, an initial requirement-gathering exercise elicited a number of core capabilities. This activity took place over a 4-month period between August and November 2017 consisting of interviews, research proposal analysis, analogous facilities review, a number of public engagement activities and commencement of a case studies programme. From these activities, a series of themes have emerged. These have enabled us to define a series of axioms upon which DAFNI's implementation will be based. Our axioms combine to illustrate the high-level capabilities DAFNI must offer and the logical structure of the components that will deliver them.

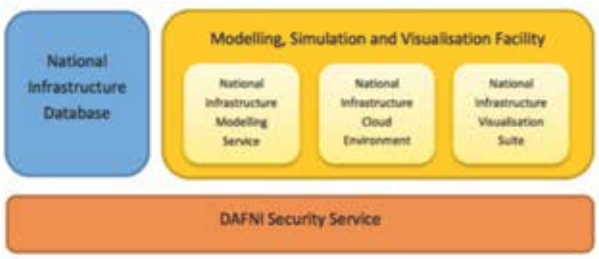

Figure 1: DAFNI Core Capabilities. The five core components are shown here encapsulated by the initial separations that were defined as Modelling Simulation and Visualisation Facility (MSVF) and National Infrastructure Database(NID)

National Infrastructure Database (NID): The NID exists at a fundamental level to provide centrally managed access to national infrastructure datasets and those required to support national infrastructure research. This however, requires a number of functional capabilities to be available on the platform to enable this data-store to be usable, efficient and reliable. The requirements for the NID identify a number of core features: a centrally managed data-store; an Extract Transform and Load (ETL) framework; a data catalogue; and a data access and publication service.

National Infrastructure Modelling Service (NIMS): The requirements for NIMS identify the need to provide the user community with the ability to improve performance of existing models, reduce the complexity of creating models and facilitate the creation of complex system-of-systems models. In order to provide this functionality, there are a number of logical components that will support this activity.
They are as follows: a workflow framework and creator; a workflow engine; a model catalogue and a data transformation library.

National Infrastructure Cloud Environment (NICE): The foundation of all of the capabilities that DAFNI will provide are based upon the existence of a high performance, flexible and scalable cloud environment. Fundamentally this will replicate the functionality available at other analogous cloud environments. The DAFNI project will, however, provide a series of adaptations to increase the suitability for the intended user community. The breakdown of this is as follows: a cloud environment; a cloud services user interface and command line interface; a number of PaaS offerings (e.g. data science notebooks and databases); and a centralised resource pool in support of PaaS and workflow manager (NIMS) activities.

National Infrastructure Visualisation Suite (NIVS): Visualisation is an often overlooked or underinvested area of a platform, but is often the primary means through which meaning from results is attained. This is the core role that visualisation will play for DAFNI. It will act as an enabler for facilitating understanding of data, models, outputs and translation of findings to decision makers. In order to achieve this means, the platform will provide the following core functions: traditional visualisation as a service (e.g. graph and tabular representations); and advanced visualisation as a service (e.g. virtual/augmented reality)

DAFNI Security Service (DSS): The DSS forms the crux of all the guarantees the platform will provide with regards to security. In order to ensure the robustness of the platform this aspect manages all security aspects internal to the platform. To achieve this it must allow users to seamlessly access and use services without being hindered by the platform whilst maintaining security. To achieve this the platform will provide the following functional components: an authentication service; an authorisation service; a monitoring service; and an accounts management service.

Impact

Ultimately, everyone can benefit from infrastructure systems that are more efficient, reliable, resilient and affordable. DAFNI's core aim is to improve and enhance all of these. The causal effect aiming to maximise the benefits of the UK investment for infrastructure directly impacting and driving these economic and societal gains. It will achieve this by enabling the research community to conduct research that is able to generate new insights at a higher level of detail and a higher level of accuracy than ever before, alongside enabling exploitation of this at a more accessible level.

This revolution created by DAFNI will be ushered in by the increased data availability and computational resource availability. Access to bigger and more granular datasets mean that it will be possible, for example, to characterise the demand for infrastructure services at a household level for every household in the UK. Enhanced computational resources mean that calculations of traffic movements or pipe flows can be computed for networks that are vastly bigger than was hitherto the case. Utility companies are rapidly advancing the systems that they use to control their networks. These rapid advances are opening up new possibilities for infrastructure owners, operators, policy makers, regulators and their engineering consultants.

The potential impact resulting from this wave of innovation in infrastructure systems analysis and decision making is a crucial part of the UK's development strategy. As part of this the breadth of potential communities that can benefit is broad too. Key communities include:

- The applied research community in the public and private sectors (recognising that academic benefits have been described elsewhere in this proposal) e.g. Catapults, BRE, JBA Trust, etc.;
- Business: utilities (energy, water, digital communications, solid waste) and transport (road, rail, ports, airports) owners and operators, and their consultants and contractors;
- Infrastructure finance, investment and insurance;
- Infrastructure security and asset management; and
- Public bodies including, government departments and agencies, the National Infrastructure Commission, regulators, devolved administrations and city/local councils.

Figure 2: Advanced visualisation example from 3DStock at UCL: the picture demonstrates the level of detail that is available with the emergence of data and technology and the scale that will be achievable with DAFNI [2]

Figure 3: Example of interactive modelling from QUANT [3]. Demonstrating the creation of a chosen simulation without requiring access to the underlying model code

Authors
S.A. Chorlton, P.M. Oliver – STFC, Rutherford Appleton Laboratory. J. Hall - Environmental Change Institute (University of Oxford)

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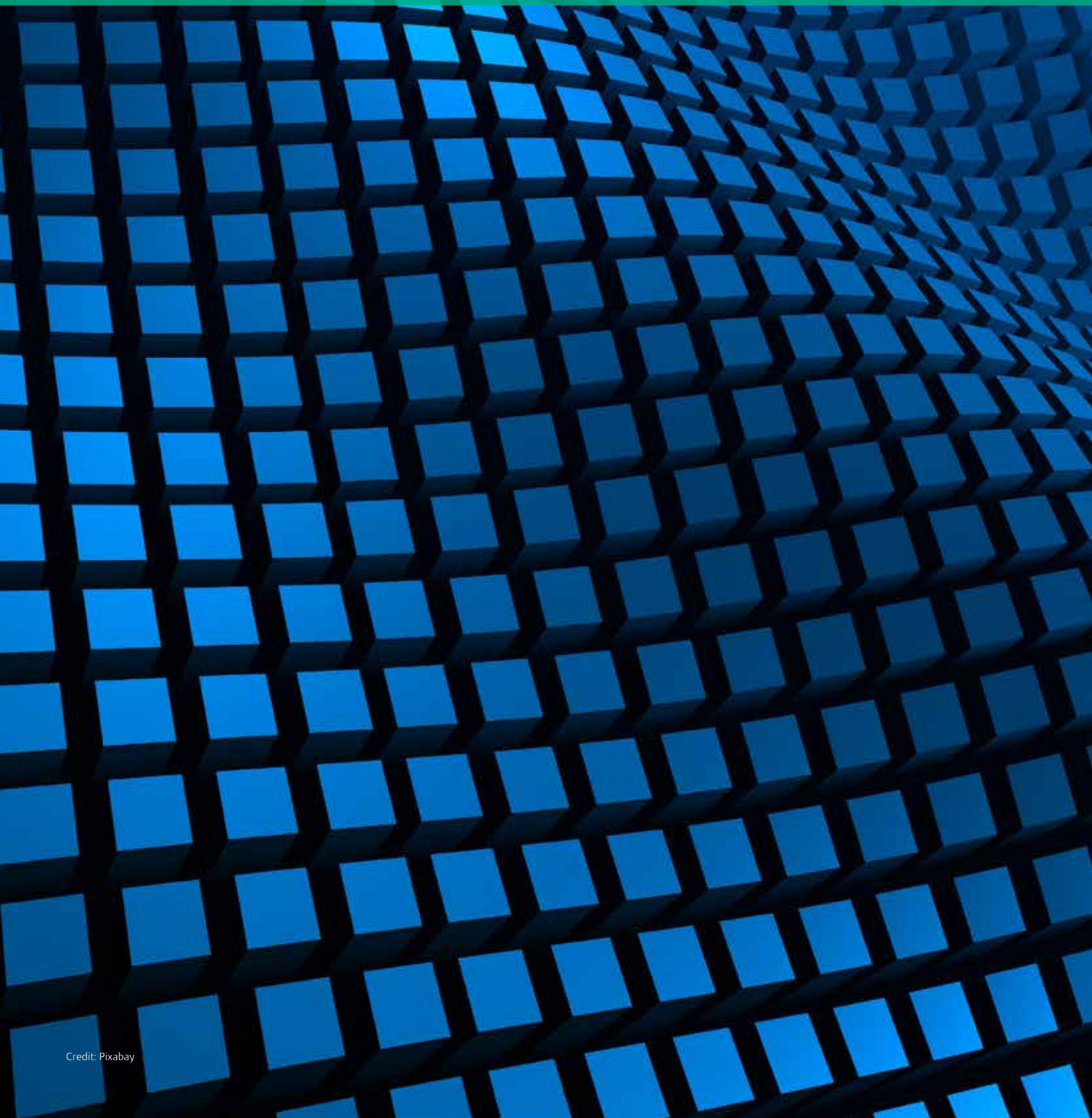
Strategic Theme 4

In order to ensure that the UK's e-infrastructure supports the country's leading international research status and delivers the data capabilities essential for academia, industry and STFC's science program, SCD will collaborate with our Research Council UK partners and stakeholders, and with Innovate UK, and JISC, as part of the emerging UK Research and Innovation (UKRI), to shape and build an efficient and effective UK e-infrastructure for UK science and industry.

Federated Identity Management Promotes Collaboration for Research



Credit: Pixabay

One of the challenges facing scientists today is how to analyse large volumes of data from large international collaborations. Whether it is the Large Hadron Collider, the Square Kilometre Array or Next Generation Sequencing, there is almost no area of research that does not find increasing volumes of data. So it makes sense to analyse the data collaboratively.

Let's say that Alice and Bob are two such scientists. Alice is based at University College London and Bob at the University of Edinburgh, but collaborate on analysing molecular crystallography held by STFC. Neither Alice nor Bob has enough resources available so they use some shared computing resources on the network to analyse their data.

The researchers now need to share access to both their data and the IRIS cloud computing resource (IRIS is described earlier in this report). Instead of registering and getting new accounts with the data centre and with each of the services, would it not be nice if they could use the user names they already have? This is the benefit of using identity federations. Using their home organisation user ID, they authenticate themselves to the data service and the computing cloud, and their home organisation makes the assertion that they are members of those organisations.

Because the IRIS infrastructure and the STFC data store both trusts UCL and Edinburgh to provide identities for their members of staff, there is no need for Alice or Bob to have separate usernames for each resource, and no need for them to reset their passwords whenever they forget.

This is a win-win situation: the registration process becomes easier because the researchers already have their identities; the use of the infrastructure becomes easier because they don't have to spend time looking up their passwords. And the infrastructure gets better quality identities, because it gets them from

organisations it trusts, not from people it does not know who register with an email address. The organisations release data because they know federations have policies that protect the data.

Federated identity management is not new; it has been best practice for authenticating researchers for well over a decade. No one should set up a service anywhere that uses username/password authentication, unless it is used only by half a dozen people. What is new, however, is the usefulness of the identity. It now has a passport and can travel: identities from UK federations are accepted across Europe, and (some) globally. And there is also a recognition that researchers have more than one identity, and more than one role. They may be in several collaborations, and they may use other cloud services to share documents, and use social media to communicate their work. Infrastructures recognise that although social media identities are not strong enough for everything, they are OK for some types of work, e.g. read-only access, or for more privileged access when linked to a stronger account. Alice and Bob can share documents in the cloud using simple identities, and once they get to the shared data they get asked to "step up" and provide stronger assurance that they are who they claim to be.

STFC is at the forefront of this work in collaboration with JISC and with our peer organisations throughout Europe, which are working together to build the European Open Science Cloud. In particular the AARC project – Authentication and Authorisation for Research Communities (https://aarc- project.eu/) – brings together research institutes, identity federations, and infrastructure providers to document best practices for use of credentials, and for establishing authorisation and shared policies. By shaping and following best practices, we help ensure that researchers can get access to the resources they need, and spend less time worrying about how they will get access to them.

Authors
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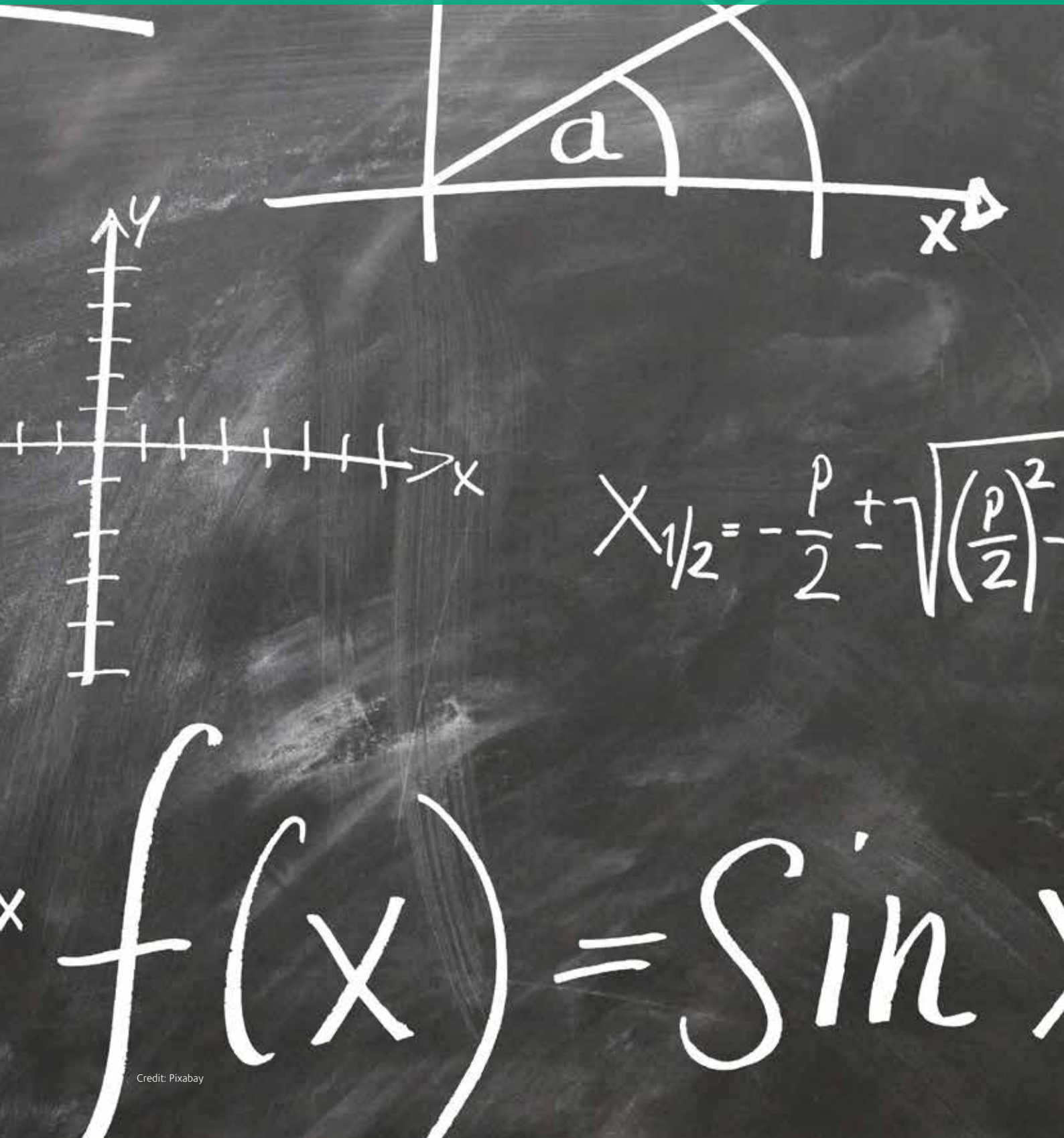
Strategic Theme 4

In order to ensure that the UK's e-infrastructure supports the country's leading international research status and delivers the data capabilities essential for academia, industry and STFC's science program, SCD will collaborate with our Research Council UK partners and stakeholders, and with Innovate UK, and JISC, as part of the emerging UK Research and Innovation (UKRI), to shape and build an efficient and effective UK e-infrastructure for UK science and industry.

SCD Public Engagement Committee



Credit: Pixabay

The Scientific Computing Department (SCD) Public Engagement Committee has continued to meet regularly over the financial year 2017-8 and has made key contributions to the National Laboratories Public Engagement Programme. In addition to the 'Girls in Tech' event with IBM, which involved 15 members of SCD and saw students and teachers visit both the Rutherford Appleton and Daresbury Laboratories (RAL and DL), we have also reached over 6000 people over the course of the year at smaller events. New resources and workshops have also been developed, and are now a core part of the public engagement programme.

• The Computational Chemistry group and the DL Public Engagement (PE) team worked together to come up with an inspirational hour long talk with demonstrations to showcase to Year 10 students how the computational chemists at DL work with supercomputers to do chemistry in novel and exciting ways - from making the perfect shampoo to materials for the next generation of space satellites! This talk formed part of the 'Chemistry at work' week hosted at the Catalyst Science Discovery Centre.

• In spring 2017, the popular KS2 Big Data workshop was updated to include a GAIA theme. The new workshop built upon the work previously done by SCD staff, which had discussed the big data implications for the SKA telescope. Adapting the session to include a space-based telescope allowed the teacher training session to be run at the UK Space conference, organised by ESA. The workshop was a celebration of the work of scientific computing, and gave an introduction to GAIA and explained the role of STFC in processing the vast amounts of data from the telescope. Activities included an updated BeeBot mission and an activity to explain parallax. This activity has also been developed by the DL PE team into Big Data themed teacher training activities aimed at primary school teachers.

• In July, RAL hosted a Robot Challenge Day in the R18 visitor centre. A culmination of three months of outreach work at four local primary schools, the event brought teams of pupils to RAL to compete in a range of different tasks, primarily focussing on a set of challenges using the LEGO Mindstorms robotics system. The After School Club sessions started at the end of April 2017, with members of SCD taking the role of mentors. Mentors ran weekly sessions teaching the children how to use the Lego Mindstorms kits, starting by teaching them the basics of good coding practice. They then moved onto teaching the children how to code using the Mindstorms, using the switch and loop functions required to make the robot complete the tasks they had been set. Teams also produced a poster showcasing their work, took part in a group exercise and gave a presentation about some of the work undertaken at STFC with a small code project to accompany it – typically using the Scratch programming language for most groups.

• RAL once again hosted a successful Summer Coding week, supported by mentors from SCD. This saw 22 children, aged 7-17, choose a challenge related to data and solve it using the technology of their choice. Among the projects were: A Python 'ChatBot' that would use Wikipedia to learn about new topics, a Scratch-based animal guessing game and a material simulation project using data from an on-site experiment. The feedback from the participants, parents and SCD mentors was excellent.

At the end of the week, the Summer Coding participants presented their work to the other teams, as well as family, mentors and staff

The Summer Coding week participants with their certificates

The winners of the 'Girls in Tech' Innovation challenge at DL

• In October, both RAL and DL hosted joint 'Girls in Tech' events with IBM to celebrate Ada Lovelace day. This event was the first joint computing outreach event between RAL and DL, as well as the first IBM outreach event hosted at RAL. The day was a mix of hands-on practical activities, Q&A sessions and innovation challenges. For the coding challenge, the girls had to code and wire up an Arduino-based temperature sensor. The Q&A sessions proved to be the most popular session of the day and offered the girls the chance to understand how to get into a technology career with all the different avenues available to them, from work experience, apprenticeships, graduate schemes and professional career development. The innovation challenge was to come up with an innovative idea, outline a prototype and do a one-minute pitch at the end of the day. The winning team at Daresbury invented 'Reflect and Select', a smart mirror in which you can try on online shopping items virtually in the mirror and purchase one. The winning team at RAL introduced a hovering wheelchair to allow disabled people a new found freedom in movement, a wonderful example of 'out-of-the-box' thinking!

A Q&A Session at the 'Girls in Tech' DL event

• In November, RAL hosted a computing themed event for ten teams of children in Years 8 and 9. Their task was to repair the first ship to Mars carrying a crew, after mission critical hardware and software systems were damaged. Each team was assigned one of the damaged systems to design and implement hardware and software replacements: the solar panel system, the communications system and the magnetic airlock system. The teams successfully repaired the damaged areas using Arduino microcontrollers and Ardublock (graphical coding), having only been introduced to these in the morning. All teams quickly got to grips with the use of graphical Arduino programming, with little previous experience. Each group also received a tour of the RAL data centre, and each school received an Arduino starter kit to take away along with a resources pack so they could replicate the day at their own schools – several teachers were already planning lessons around Arduinos as they left!

• In January, SCD and the Diamond Light Source hosted a Computing Your Future event. The day involved learning how scientific computing underpins modern science, practical activities and a networking lunch. The activities included an Arduino workshop, a LEGO Mindstorm workshop and a demonstration of SCD's Visualisation Suite. The Visualisation Suite demonstration introduced students to some of the techniques that SCD's Visual Analytics and Imaging Systems group specialise in, such as building 3D models from stacks of 2D images (tomography) and visualising 3D models, as well as explaining what these techniques can be used for. As the students explored the demos, the work behind what they were seeing was explained, with emphasis on the importance of visualisation of data and objects in the modern world. The students had a lot of fun interacting with the novel technology the facilities within SCD have to offer and asked a lot of questions, both about the things that they were seeing and also the technology and algorithms behind it all.

• On 22 March 2018 DL hosted the Northwest Science Network Event, headed up by Professor Peter D Nellist. The network is a joint venture between Corpus Christi College and Pembroke College (both University of Oxford), South Cheshire College (Crewe), and Xaverian College (Manchester). The network aims to engage students from the Northwest with research-level science, designed to equip them for application and entry into higher education. Events take place across the year both in the Northwest and in Oxford. Research and Teaching Fellows from the University of Oxford and other research-intensive universities deliver a series of lectures across the scientific disciplines, whilst the network also provides students from the Northwest with the opportunity to visit regional laboratories – such as SuperSTEM at DL. As part of the SuperSTEM Event, staff in the Computational Chemistry Group delivered a solar cell computational workshop to 25 KS5 students in conjunction with project colleagues from Swansea University. This workshop was incorporated into the programme to give the students more exposure to other types of research and development work going on at DL, broadening their experience on the day.

• A 'Saturday Coding' club has continued to run at RAL over the 2017-18 year. Once a month, a four hour session is held on site where participants work on projects of their own choosing with help and support from SCD mentors and the RAL PE team. The focus of these events is on peer learning, rather than working from a lesson plan. This gives the participants a chance to explore computing for themselves, using the Arduino, Mindstorms and other resources, and builds their confidence. At the end of each club a peer presentation session is run, to which parents and family are invited, giving the participants a chance to show what they have achieved. This also demonstrates the 'soft skills' side of working in the sciences, improving the participants' communication and presentation skills. The club has become steadily more popular, and there is now a waiting list, despite the fact that no direct marketing has taken place. The long-term format of the club also allows SCD mentors to build relationships with the participants and several of them have gone on to do work experience at the lab as a direct result of attending the club. These events take place once a month and reach approximately 20 people per event.

• SCD once again played an important role in the popular work experience programmes at RAL and DL. This year the SCD Public Engagement committee organised workshops for both supervisors and students. The supervisor workshop (held at both sites) served to share best practice and help new supervisors develop suitable projects. The student workshop was a three-day computing workshop at RAL to give them an introduction to coding. SCD also supervised 16 placements for work experience at RAL and 2 at DL.

In addition to the above activities, previously established events and workshops continued to be an integral part of the public engagement programme. Throughout the year, there were also regular tours of the data centres and visualisation suites, teacher training sessions, and Arduino and Bee-Bot activities at school and public events.

The department will be building on the success of its Public Engagement work in the coming year by developing new Lego Mindstorms activities, improving the evaluation of activities, and by running a Computer Celebration Access Day at RAL and DL. There is also a Talking Science Public Lecture to be given in May by staff in the Computational Chemistry Group at DL, and a week of work experience is planned for thirteen Year 12 students in July that will be presented as a mixed work experience/summer school. This week will optimise the time that staff have available to spend on PE and mentoring activities, while ensuring the students are offered a wide and varied work-like experience.

Participants at the Arduino Challenge Day (above and right)

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Strategic Theme 4

In order to ensure that the UK's e-infrastructure supports the country's leading international research status and delivers the data capabilities essential for academia, industry and STFC's science program, SCD will collaborate with our Research Council UK partners and stakeholders, and with Innovate UK, and JISC, as part of the emerging UK Research and Innovation (UKRI), to shape and build an efficient and effective UK e-infrastructure for UK science and industry.

International Presence

Credit: Pixabay

The Scientific Computing Department (SCD) continues to form new partnerships and strengthen existing collaborations with institutes in the UK and around the world. During 2017-18 SCD presented, demonstrated and discussed its research and services in over 32 countries across the globe. Here we highlight just a few of the conferences and events that we have participated in.

Supercomputing Conferences in the USA and Germany

Once again the Scientific Computing Department (SCD) and its close relation, the STFC Hartree Centre, had a strong presence at the world's largest supercomputing conference, SC17, where we showcased some of STFC's excellent data-intensive science. In 2017 it was held at the Colorado Convention Centre in Denver, easily recognisable because of the gigantic blue bear peering in through the glass wall! The SCD and Hartree Centre staff were involved in a number of talks, workshops and knowledge exchange sessions within the SC17 technical programme, and we had a large display booth in the exhibition hall. One of our first visitors was Erin Kuhn from the British Consul in Denver. She came along to view the displays and hear a talk by Professor Tony Hey, our Chief Data Scientist. Erin was impressed with the range of computational science that we carry out, and keen to set up visits to some of the US National Laboratories.

The SCD and Hartree teams also took a display to ISC2018, which was held in Frankfurt, Germany, and participated in the many technical sessions being presented. Our staff were on hand to explain what we do and discuss the latest developments to a steady stream of delegates at what proved to be our busiest year so far. We were delighted to see people that we knew and have worked with for many years amongst the visitors to our booth, as well as some new collaborators who dropped by just to say hello.

Blue bear, credit Pixabay

A prestigious STFC event in the UK

Developed, organised and managed by SCD, Computing Insight UK (CIUK) is one of the UK's premier conferences for advanced computing and data-intensive science. It was held in December 2017 at Manchester Central with the theme of 'Joining up the UK e-Infrastructure.' Speakers gave passionate presentations about their chosen topic and the event was buzzing with the energy and enthusiasm of people excited about the science, the products and the ideas being showcased.

This annual conference, which is growing in popularity with speakers, delegates and exhibitors, included two full days of presentations, talks and panel sessions running alongside an exhibition of the latest technologies from the leading hardware and software developers and resellers, an exhibitor forum and a series of breakout sessions.

A Forum in Belgium

Over 300 people gathered in Brussels for the first European Open Science Cloud (EOSC) Stakeholder Forum. The opening address was delivered by SCD's Dr Juan Bicarregui, coordinator of the EOSCpilot project that is supporting the first phase of its development. The European Open Science Cloud will offer 1.7 million European researchers and 70 million science and technology professionals a virtual environment with open and seamless services for storage, management, analysis and re-use of research data that are today blocked by geographic borders and scientific disciplines. This Stakeholder Forum provided an ideal opportunity to discuss the scientific challenges and to identify the first steps and building blocks to make European Open Science a user-friendly reality.

Team SC17

Juan Bicarregui speaking at the EOSC Forum in Brussels

A busy time for exhibitors at CIUK

Debates in Sweden and Bulgaria

Brian Matthews, SCD's Data Science and Technology group leader, joined an expert panel together with colleagues from the European Spallation Source and MAX-IV facilities, the Worldwide LHC Computing Grid, and the Swedish research funding body, for a lively debate on the opportunities and challenges of research data. It was held at Pufendorf Institute for Advanced Studies at the University of Lund in Sweden, on the theme " Data management and infrastructure - from policy to practice". This was part of a 'Big Science & Society' project, exploring the changes resulting from data driven science and how a major research institute such as Lund should respond to it.

Our Computational Chemistry Group leader, Ilian Todorov, participated in a panel debate in Sofia, Bulgaria, on 'Shaping Europe's Digital Future'. He was invited to speak by the Bulgarian Presidency of the Council of the European Union and the European Commission.

Keynotes in Germany, Spain and the USA

Our Chief Data Scientist, Tony Hey, spoke at the Big Data Science in Astroparticle Research - HAP Workshop, at Aachen University in Berlin. Topics covered at this event included machine learning, open data-software-analysis and developments in national and international strategies, as well as hands-on tutorials in deep learning network architectures. He also gave keynote speeches at two other events: a workshop for High-Performance Systems and Analytics for Big Data (HPSA) in the USA; and High Per, the International Spring School on High Performance Computing in Spain.

Symposia in Japan

Iain Duff and Florent Lopez, who are both members of our Computational Mathematics Group, attended the SIAM Conference on Parallel Processing for Computational Science meeting in Tokyo in March 2018. As well as attending the conference, they co-organized two mini-symposia describing work in the H2020 FET-HPC Project NLAFET (Parallel Numerical Linear Algebra forFuture Extreme Scale Systems).

Mt. Fuji - one of the views from the SIAM conference in Japan

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