

Bringing together the UCL community who use computational and data sciences or digital technologies in their research.

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Digital Research Community Newsletter

Issue 10



Dear Colleagues,

Welcome to the tenth edition of the UCL Digital Research Community newsletter! As we hope you already know, you are receiving this because you previously signed up for either the ARC newsletter or the old eResearch Domain newsletter.

As always, please do forward this email to any colleagues you think may be interested. If you no longer want to hear from us, you can unsubscribe using the link at the bottom of this email, although we would be very sorry to see you go...

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## CIUK Student Cluster Challenge

**Are you a python programmer?**

**Could you represent UCL at an inter-university competition?**

**Launch event: 9th September 1:30pm - 5:30pm**



Come along and learn about this national competition and how you can get involved



Python programmer?

PhD student?

Have some experience with the command line?

Join **#teamUCL** to participate in the inter-university CIUK Student Cluster Challenge - work on some challenges in Term 1, and then join UCL's Advanced Research Computing team at the CIUK conference in Manchester in December (all expenses paid).

Want to find out more (and get a free lunch)? Come along to the launch event - sign up below:

INFO & REGISTRATION

## Community Updates



## **Become an ARC Community Ambassador**

PhD student or PostDoc?

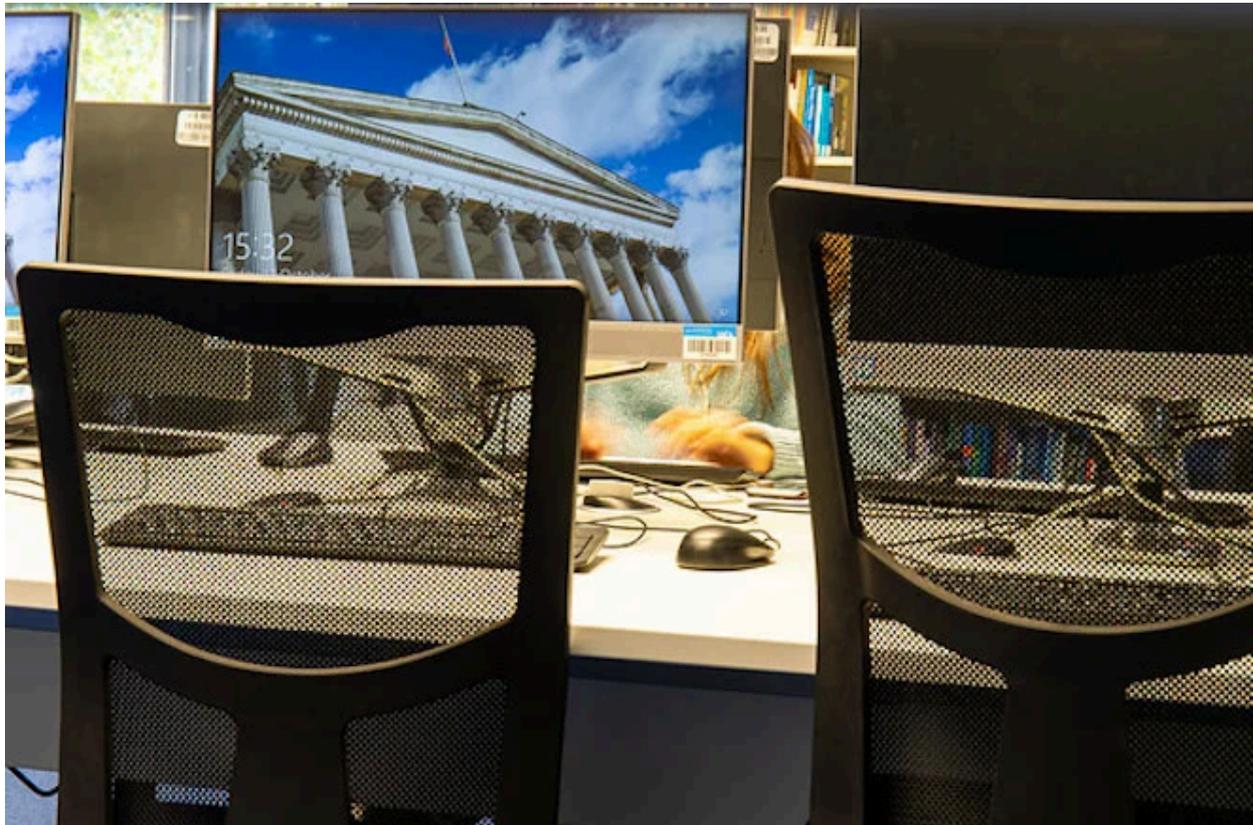
Good communication skills and event organisation experience?

Interested in helping us promote digitally-enabled research and scholarship to students and staff in your department?

From a department where ARC isn't well known?

Why not become a (paid, part-time) ARC Ambassador?

[Find out more and apply](#) (Deadline: 20th September)



## **Become an ARC Academic Fellow (20%-40% FTE secondment)**

Academic staff (Lecturer or above)?

Have an idea that will further digital research across your discipline and UCL?

Interested in creating a new line of research, co-developed with ARC, to deliver this idea?

Apply for a 20% to 40% ARC Academic Fellowship:

[Find out more and apply](#) (Deadline: 20th September)



## Festival of Digital Research & Scholarship Round-Up

A massive 'Thank You!' to everyone who engaged with our inaugural Festival. With 20 presentations, 17 posters, 5 workshops, and 302 registered to attend, the day was a huge success!

Head to the [Festival webpages](#) for a full summary, and access to the day's keynotes, presentations, posters and photo gallery.



## Community of Practice for Research Data Stewards

Do you work at UCL.....

- Writing data management plans
- Collecting and cleaning data
- Scripting data transformations
- Creating metadata
- Preparing data for sharing
- Archiving data

.....?

By supporting any part of the research data lifecycle - from writing funding applications through to data archiving - you are, by definition, a Data Steward!

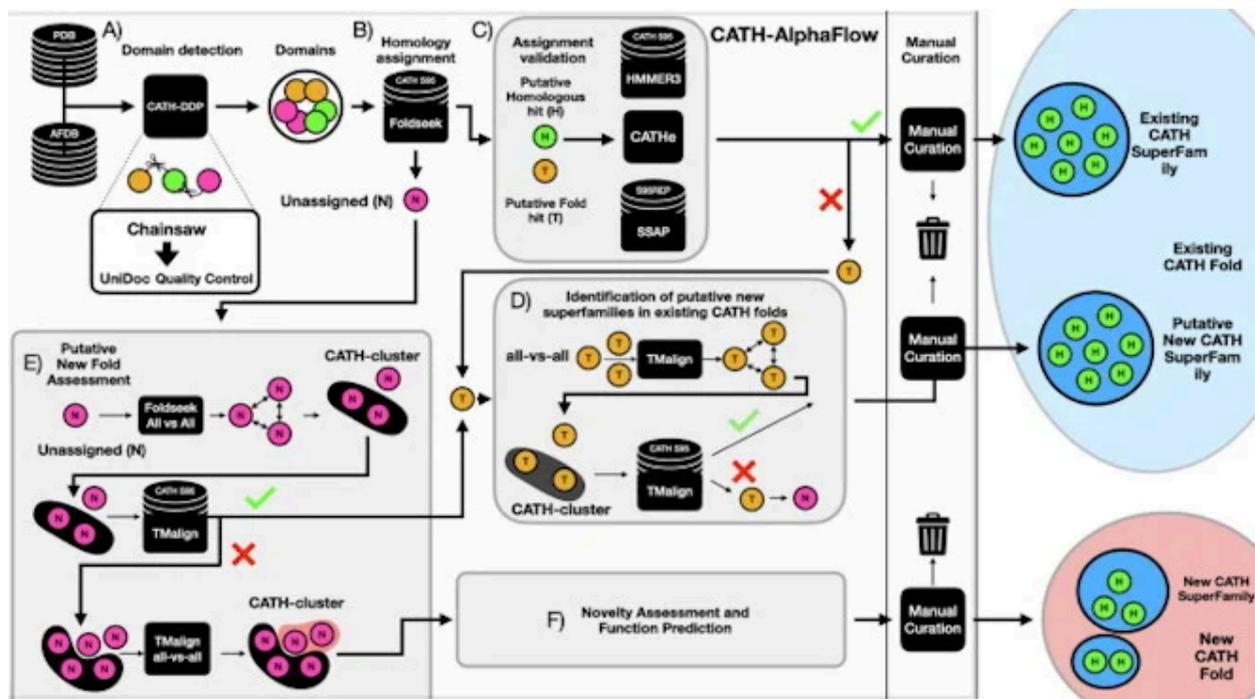
So, [come join us](#)! And be part of UCL's Research Data Stewardship Community of Practice.....



## The RDSS 2017 to RDSS 2023 project migration is complete

As a component of the overall work to replace the ageing Research Data Storage Service (RDSS 2017) with part of the new Research Data Platform (RDP), the long task of migrating all our project data is now complete! The overall work undertaken by [ARC's Research Infrastructure Developers](#) included 2321 lines of code (written mostly in BASH, with some Python) and follows on from an effort to refactor our administration portal to accommodate multiple storage end-points on a project by project basis. The migration was split into two phases, moving our 617 closed projects first which happened between 10th April and 25th May. After a short gap while dependencies were resolved in the RDP, the remaining 1181 live projects were migrated between 27 June and 7th August. The data and files were split (approximately) evenly between closed and live projects and comprised about 2.6PB and 210 million files each.

Please see [the ARC website](#) for further information about the migration and the Research Data Storage Service.



## Case Study: Repackaging legacy software for protein structural domain annotation

For this open source software sustainability project, funded by last year's call, ARC worked with the [Orengo Group](#) in the [UCL Research Department of Structural & Molecular Biology](#) to make an existing bioinformatics data pipeline more portable, scalable and ready to be applied to huge new datasets (e.g. 200 million predicted structural models from AlphaFold). Read how this was achieved by [Dr Ian Sillitoe](#) (SMB) working with Dr Robert Vickerstaff, a Senior Research Software Engineer from ARC, in [our latest case study](#).

## ARC Events



## Join us as the BBC and ARC launch the BBC 10k dataset to boost UCL Data Science Research

ARC and the BBC are collaborating to deliver a major collection of broadcast TV programmes to UCL data science researchers. The collection, known as the [BBCAVS: 10k dataset](#), comprises 10,160 programmes broadcast by the BBC in the UK between June 2007 and December 2021 and includes content originally recorded between 1962 and 2017. Subtitles and associated metadata are included with the data.

The BBCAVS 10k dataset is being made available to UCL researchers under the [BBC's Data Science Research Partnership](#).

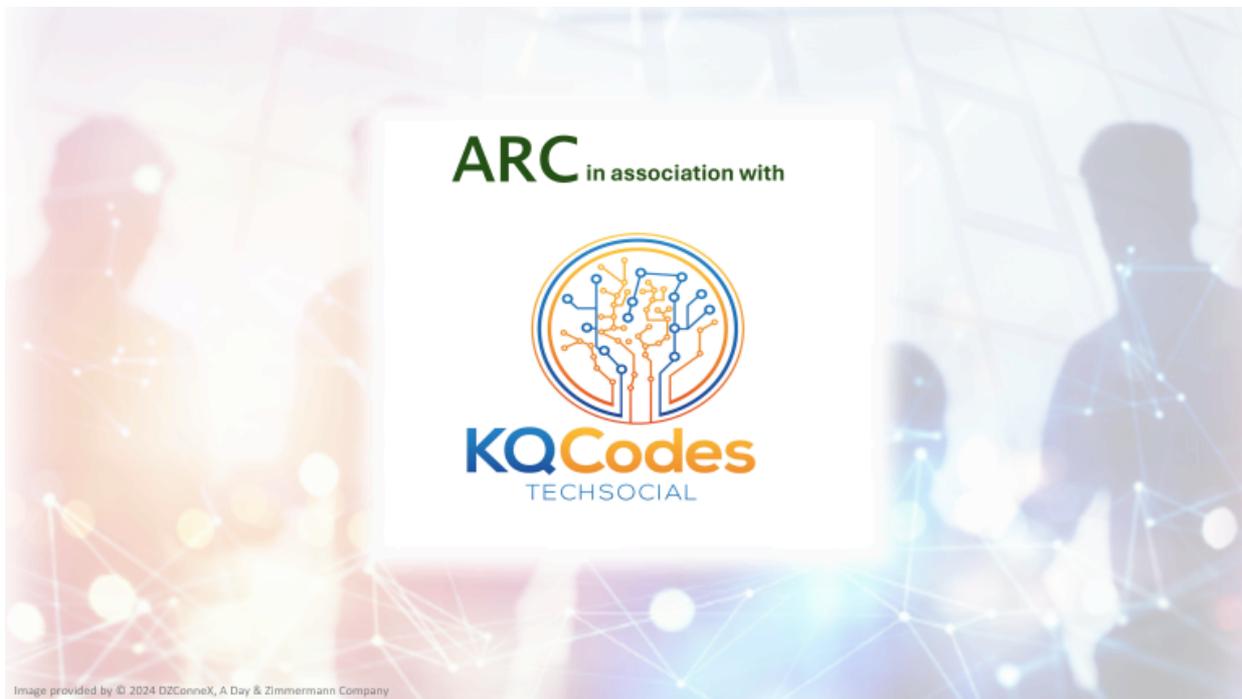
Join us at **14.00 on Tuesday 17 September on MS Teams** to hear more about the data from the BBC's Lead Data Scientist, Andy Secker.

The session will start with an introduction to Harbour, the ARC service that is facilitating access to the data.

There will be opportunities to ask questions.

Please submit a request to the Harbour team on the [MyServices portal](#) to attend the session.

If you have any questions about Harbour or would like to register interest in the BBC dataset, please reach out to the team via the [MyServices portal](#).



## Monthly Tech Socials

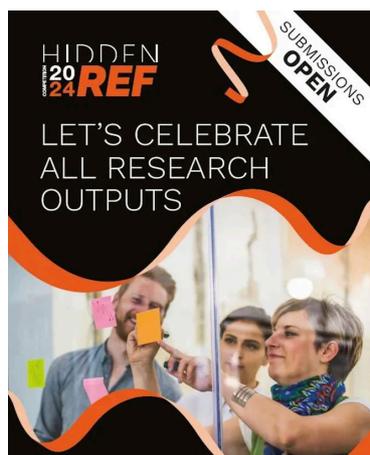
Frustrated with the lack of summer sunshine lately? Then come join ARC (in association with KQCodes) at our next TechSocial on **Wednesday 11th September from 4-6pm** as we hear from and talk with climate scientist Milan Klöwer about 'Climate modelling and low-precision floating point numbers'.

These free, informal hybrid events are for anyone with an interest in the computational methods and technology behind research, and is an opportunity to discuss and learn about useful tools and techniques which may help with your work - the **informal discussion and networking after the talks will take place over pizza and refreshments!**

[Further information and registration](#)

For future events, keep an eye on the [ARC website](#).

## Calls



### The Hidden REF: Does your work gain the recognition it deserves?

Research organisations use publications as practically the only measure of success in research, but research is fundamentally reliant on a huge range of people and many types of work that are not recognised in publications. We can't advance research if we don't recognise everyone and everything that we rely on to conduct research.

You can help us shine a spotlight on this issue by taking part in [the Hidden REF competition](#). We want to hear about your unrecognised research roles, from technicians to data stewards to research managers, and your unrecognised outputs, from software to musical compositions to anything else that is important to you. The more submissions we receive, the more evidence we have to continue our successful campaign to increase recognition for everyone who works in research.

Submissions are a maximum of 900 words. If you work in a UK organisation and take part in or support research in any way, you are welcome to take part in the Hidden REF competition.

The competition is now waiting for your submission!  
**Deadline is 11.59 on the 13th of September.**

[Further information](#)



### RAC 17 call: Computing and RSE resources on the STFC DiRAC HPC facility - now open

The DiRAC Resource Allocation Committee facility time opportunity (RAC17) is now open. The UK theory and modelling communities in astronomy and cosmology, astrophysics, solar system physics, particle astrophysics, particle physics and nuclear physics are invited to apply for computational resources on the STFC DiRAC HPC Facility.

The deadline for submission of proposals is **Thursday**

The deadline for submission of proposals is **Thursday 12th September 2024 at 16:00 UK time.**

[Further information](#)

To apply, please see <https://dirac.ac.uk/getting-access/>.



## **UKRI are calling for new members of the ARChER2 User Advisory Group**

The ARChER2 User Advisory Group, which represents the current and prospective user base of ARChER2, the UK national supercomputing service, provides recommendations and feedback to UKRI with the aim of improving the user experience of the service.

If you're an existing user of the ARChER2 national supercomputing / high performance computing services with significant experience of using ARChER2 to conduct computational research in the area of the vacancy, an appreciation of the UK's wider HPC environment and international HPC activities, experience of engaging with the ARChER2 user community and helping communication between stakeholders, a willingness to dedicate sufficient time to the role and backing or support from your organisation, please see:

<https://www.ukri.org/who-we-are/work-for-us/join-an-advisory-committee-panel-or-network/academic-research-computing-high-end-resource-archer2-user-advisory-group-vacancies/>

for further information on how to apply.

Deadline for submission of applications:  
**17 September 2024**



## **2nd GPU eCSE call**

GPU eCSE support provides funding to the UKRI research community to develop software in a sustainable manner to run on GPU-based architectures. The GPU eCSE programme is administered by EPCC through ARChER2 (<https://www.archer2.ac.uk/>) but open to all research areas across all of UKRI's remit.

The 2nd GPU eCSE call (GPU-eCSE02) opened on the 2

July 2024. Funding will enable the employment of an RSE (a Research Software Engineer, PDRA or equivalent) to work specifically on the relevant software to enable new features or improve the performance of the software to be run on GPU-based architectures. Projects may utilise the GPU component of ARCHER2 or other suitable GPU resources to complete the technical work. If the proposal plans to use the GPU component of ARCHER2, successful projects will be given access to these resources.

More details of how to apply are available by following the link to the eCSE calls page from:

<https://www.archer2.ac.uk/ecse/calls/>

**The final deadline for proposal submission is 16:00 on 17 September 2024** via the ARCHER2 SAFE.

## Training & Workshops



### ARC Training

You can find a [full list of ARC-provided training](#) on our Education pages - including self-paced courses via Moodle, for example, [our new Introduction to High Performance Computing at UCL](#).

If an in-person or online instructor-led course has no dates listed, please fill in our [expression of interest form](#) and we will contact you as soon as we have dates for the next session.



### ARC Drop-in Sessions

A reminder that we have resumed our in-person drop-in support sessions - these are for all research staff and research students, where you can get support and advice to help plan and tackle problems with your research. If you have any problems related to the following areas, we should be able to help:

- choosing the right software, hardware and services,
- research programming,
- task automation and scripting,
- high performance computing,
- storing large datasets,

- Research Data Storage (RDS) service induction,
- handling sensitive data,
- research data management (including writing data management plans).

If the problem is likely to need a lengthy discussion (half an hour or more) or requires very specific knowledge (e.g. of an unusual programming language) it would be very helpful if you could email a short summary of your problem to [arc@ucl.ac.uk](mailto:arc@ucl.ac.uk) at least 2 days before the session, so we can try to make sure a member of staff with appropriate expertise is available.

Further details of the drop-in sessions and other support available can be found [here](#) - **please note that we are taking a break in August and will resume in September! In the meantime, please email us for ad hoc advice.**



## Research Data Management Training

Learn how to write an effective data management plan for a project proposal or grant application!

Our colleagues in Library Services' Research Data Management Team run training sessions for writing data management plans, both online and in-person.

To find out more and to book a place, see their [booking calendar](#).



## Digital Skills Development Training

UCL's Digital Skills Development Team runs a variety of free training courses, many of which may be of interest to researchers - details of the programme for the autumn term will appear in due course on their [blog](#).



## ARCHER2 HPC Online Training

ARCHER2 Training is provided by EPCC (Edinburgh Parallel Computing Centre) as part of the ARCHER2 (Tier 1) national high performance computing service and is free of charge to research staff and students from academic

institutions.

Self service courses (always open):

- [Shared Memory Programming with OpenMP](#)
- [Message-Passing Programming with MPI](#)
- [QM/MM with GROMACS + CP2K](#)
- [Hands-on Introduction to HPC](#)

Upcoming online courses:

- [Introduction to LAMMPS](#), 17th October, 10:00 - 16:30 ([register now](#))

[Details of other training \(including in-person\) provided by ARCHER2](#)



## UK Data Service Training

The UK Data Service runs a comprehensive programme of free, online introductory training - they have just announced their autumn programme, including the following courses in September and October:

- [Data in the spotlight: Large scale social surveys](#), **Tuesday 24 September, 10.00 – 11.30**
- [Introduction to effective and practical research data management](#), **Monday 30 September, 10.00 – 11.30**
- [How to become a computational social scientist](#), **Tuesday 1 October, 10.00 – 11.30**
- [Dissertation projects: Introduction to secondary analysis for qualitative and quantitative data](#), **Tuesday 8 October, 10.00 – 11.30**
- [Ethical and legal guidelines in data sharing](#), **Thursday 10 October, 10.00 – 11.30**
- [Getting started with secondary analysis](#), **Tuesday 15 October, 10.00 – 11.30**
- [Role of Informed Consent in Ethical Data Collection, Sharing and Reuse](#), **Thursday 24 October, 10.00 – 11.30**
- [Introduction to copyright: Copyright and publishing](#), **Tuesday 29 October, 10.00 – 11.30**

You can also browse their [events pages](#) for a full list of

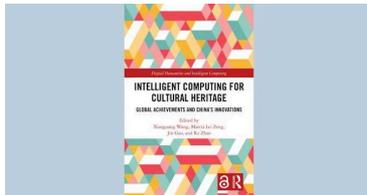
You can also browse them [events pages](#) for a full list of what is available. If you've missed a workshop, recordings of past UK Data Service events are made available on the [UKDS YouTube channel](#).



## CLOSER Learning Hub

Longitudinal studies track the same individuals and households over time. They are powerful research tools to help us understand how our early circumstances and experiences influence our later lives. The [CLOSER Learning Hub](#) has information and resources to help you explore longitudinal studies and get you started using the data.

## UCL Events



### IAS Book Launch and Symposium: Intelligent Computing for Cultural Heritage

26 September 2024, 9:00 am – 6:00 pm

IAS Common Ground, Wilkins Building

UCL's ongoing contributions to digital humanities research and teaching, specifically through its Department of Information Studies (DIS) and the UCL Centre for Digital Humanities (UCLDH), have significantly influenced our new book - Intelligent Computing for Cultural Heritage: Global Achievements and China's Innovations and the book series - Digital Humanities and Intelligent Computing. For this one-day Symposium and Book Launch, we invite chapter authors and experts in the field to give talks, and lunch and refreshments are also provided throughout the day to facilitate scholarly networking. With this event, we will not only celebrate the current achievements in the field but also mark a stepping stone towards a more connected future of digital humanities.

[Further information and registration](#)

## External Events



## MSSC – Ab initio Modelling in Solid State Chemistry

16 - 20 September, 9:00 am - 6:30 pm

AM - LT 1, Bush House, Strand Campus, King's College London

PM – Dept. of Chemistry, South Kensington Campus, London SW7 2AZ

2024 MSSC Summer School on the “ab initio modelling of crystalline and defective solids with the CRYSTAL code”. The School is addressed to PhD students, Post-Docs and researchers with interests in solid state chemistry, physics, materials science, surface science and catalysis. It provides an overview of the possibilities offered by ab initio quantum mechanical techniques adopted in CRYSTAL when applied to the characterization of crystalline materials.

[Further information and booking](#)



## CLOSER 2024 Early Career Researcher (ECR) Conference and Training Event

CLOSER is excited to announce our free, in-person ECR Conference and Training Event, **Bridging Research Policy: Unleashing the potential of longitudinal research for societal impact**, will take place in central London on **Wednesday 18 September 2024 from 09:30 - 17:00**.

This bespoke event will showcase and celebrate the work of Early Career Researchers and provide a range of practical training workshops.

[Find out more](#)

Registration deadline: **Wednesday 11 September 2024**.



## The Tech We Want: Online Summit

17 October 2024, 10:00 - 18:30

In recent years, technology has adopted a complex, wasteful, and expensive approach to serving its purpose, making it rare, even in the open movement, to find affordable, accessible, and sustainable software. There is

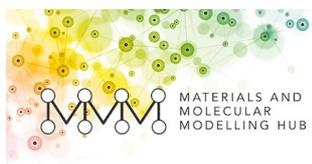
an urgent need for the technology industry to re-think how software is developed, which tools do we use and how tech solutions are currently conceived, coded, and deployed.

In this free one-day The Tech We Want Online Summit, the Open Knowledge Foundation (OKFN) is bringing together key voices working on public interest technologies to start a collective conversation about new practical ways to build software that is useful, simple, long-lasting and focused on solving people's real problems.

The Online Summit is open to everyone, especially technology workers, developers, engineers and programming language specialists who are interested in taking a critical look at current technologies.

Join us in building the tech we want and that the world needs!

[Further information and registration](#)



## **MMM Hub Conference & User Meeting 2024**

**29 - 31 October 2024**

**Venue: Battle of Britain Bunker, Uxbridge**

The conference will highlight the high-calibre scientific throughput produced across the MMM Hub's partner community and beyond, highlighting particularly the contribution of modern HPC resources (including MMM Hub's 'Young'), in enabling these advances. A selection of breakthrough materials and molecular modelling research taking place across the country will be presented, addressing challenges to society and industry through simulation at the atomic scale, alongside discussion in emerging computing trends and how this impacts materials scientists.

The meeting will provide an excellent opportunity for researchers at all levels to learn about the forefront of this important field in numerical simulation, and to showcase their most recent results.

**Standard registration deadline:** 15th September 2024

**Abstract submission deadline:** 1st September 2024

[Further information and booking](#)

## Dates for your Diaries!



### Computing Insight UK 2024 is Going Bigger and Better

**5-6 December 2024**

[Computing Insight UK will be moving to a new venue in 2024!](#)

The UK's premier conference for HPC and associated science, organised by STFC's Scientific Computing department, will still be held at the Manchester Central Convention Complex, but we are moving into the bigger Exchange Hall and Exchange Auditorium. This move marks the biggest change to the Conference since its introduction 34 years ago and is a direct result of the tremendous growth we have seen over more recent years.

Follow the [CIUK 2024 website](#) for updates.

**Subscribe to this newsletter**

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Regards,

UCL Centre for Advanced Research Computing

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