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

Digital Research Community Newsletter
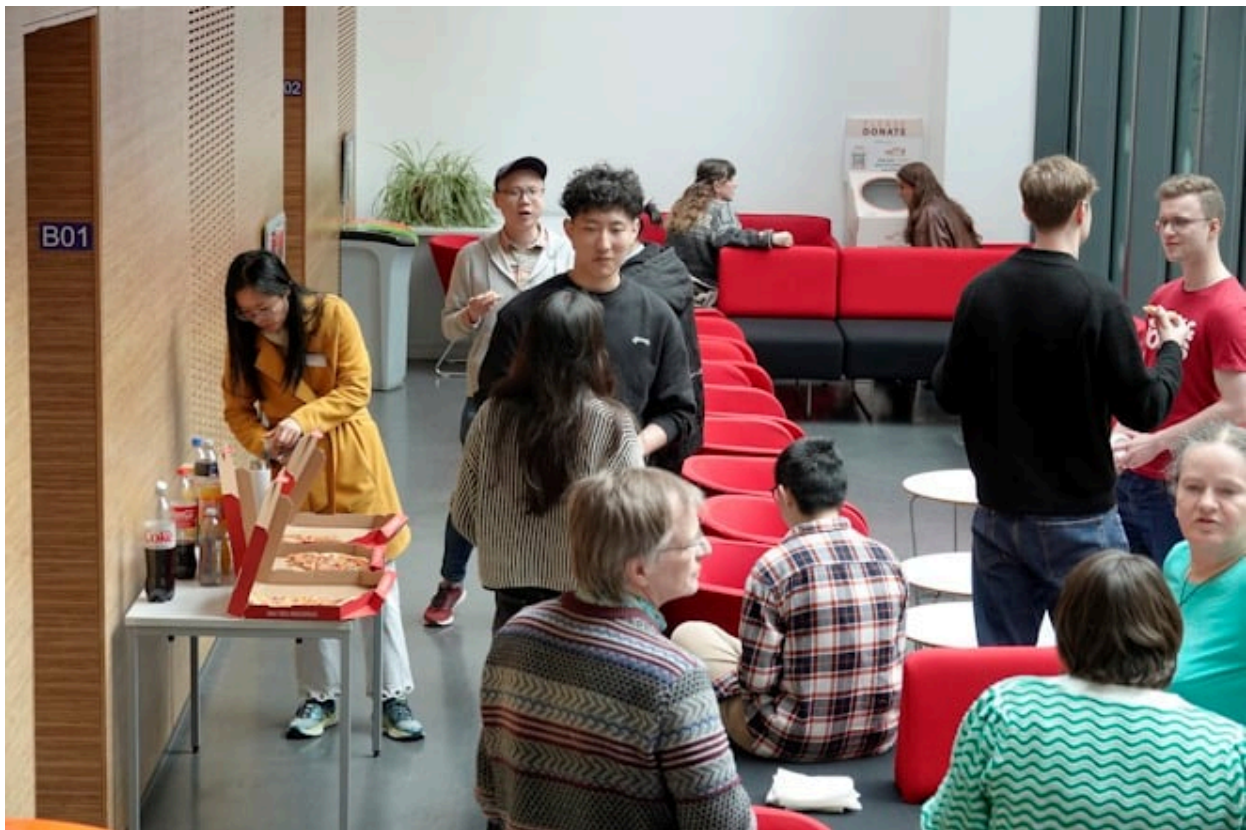
Issue 8

Dear Colleagues,

Welcome to the eighth 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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ARC Student Cluster Club

The ARC Cluster Club is an opportunity for students at all levels to develop their

programming and high performance computing skills. The club is open to all UCL

students regardless of their existing knowledge and skills; the next session will feature

a mini-challenge and is on **Wednesday July 31st 2024 at 2:30pm,** so please do sign

up if you haven't already - new participants are always welcome.

We are looking for students to form a UCL team for the [Computing Insight UK (CIUK) 2024 Cluster Challenge](#)! We need to have the team in place in early September, so if you are interested (or have students in your research group/department who might be) please come along to the July Cluster Club to find out more, or [drop us an email](#).

INFO & REGISTRATION

Community Updates

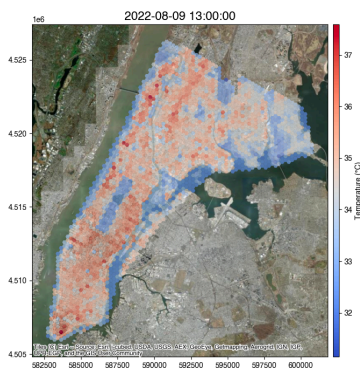## We are going to SuperComputing 24!

Atlanta, 17-22 November 2024

ARC will once again be coordinating a UCL booth at SC24, promoting engagement and interaction around digital research and innovation on a wide range of topics.

There are a limited number of funded places available for those supporting digital research, as well as early career researchers. If you are interested in attending, further information and an expression of interest form is available:

More info and apply

Deadline: Noon on 31st July 2024
(applications will be assessed and successful applicants contacted shortly after this deadline).

Case Study: Aiding the Development of Sustainable Urban Environments: Improving the Sustainability of SuPy

This open source software sustainability project, funded by last year's ARC call, focused on improving the sustainable development of SuPy, an open-source urban climate model. SuPy plays a crucial role in understanding and predicting urban climate patterns, aiding in the development of sustainable urban environments. See how this was achieved by Dr Ting Sun (UCL Institute for Risk and Disaster Reduction) working with Dr David Stansby, one of the ARC Research Software Engineers, in our latest case study.

UCL Education Awards 2024

We are proud that multiple members of ARC staff (David Pérez-Suárez, Milan Malfait, Ed Lowther, Sofia Miñano, Zakaria Senousy, Nik Aznan, Sanaz Jabbari and Miguel Xochicale) supported the work of the Learn to Discover Team from the Faculty of Life Sciences, who have won the new "Innovating" category of the UCL Education Awards.

The winning project created a set of online courses in

python on data science and machine learning, tailored for health, disease and biosciences. The ARC team helped with various aspects - from creating training material to developing the infrastructure they used for the courses and lessons, and also helping to adapt research case studies (large working examples) to their specific needs. In doing this, they also contributed upstream to the Carpentries lesson infrastructure.

UCL AI tool wins prestigious award

Congratulations to ARC's Healthcare team for their work on EMAP which underpins this award-winning AI tool. The software won the Healthcare Partnership of the Year category at the London Higher Awards 2024.

The tool estimates how many hospital beds will be needed in eight hours' time, incorporating live data of patients who have arrived at the hospital's emergency department. It has been used by University College London Hospital for the last year on a daily basis and research has found it to be significantly more accurate than the traditional way of trying to predict patient flow.

Read the case study explaining more about the work in ARC's research showcase.

Monthly Tech Socials

We are taking a break for July, but on **Wednesday 14th August from 4-6pm** the next ARC TechSocial (in association with KQCodes) features Jasmin Jahić with: 'Software architecture: between rigid process and "somehow I manage" approach'.

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 (opening soon!)

For future events, keep an eye on the ARC website.

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:
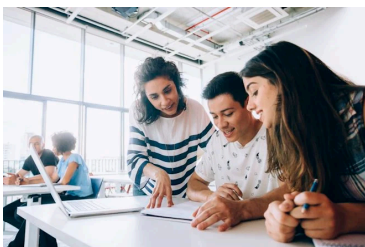
- choosing the right software, hardware and services,
- research programming,
- task automation and scripting,
- high performance computing,
- storing large datasets,
- Research Data Storage (RDS) service induction,
- handling sensitive data,
- research data management (including writing data management 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 at least 2 days before the session, so we can try to make sure a member of staff with appropriate expertise is available.

The next drop-in session is on **Tuesday 16th July 2024 from 11am - 12pm**, at Charles Bell House, G03 (Seminar Room 1).

Further details of the drop-in sessions and other support available.

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 which also runs termly as a synchronous online workshop.

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.

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 Thesis Writing Clinics

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.

During July and August, they are running dissertation and thesis writing clinics for students in conjunction with Library Skills on the following dates, online or in-person:

- **Tuesday 16th July - 10:00-12:00**
- **Wednesday 24th July - 14:00-16:00**
- **Tuesday 30th July - 10:00-12:00**
- **Wednesday 7th August - 14:00-16:00**
- **Tuesday 13th August - 10:00-12:00**
- **Wednesday 21st August - 14:00 - 16:00**

Staff at the clinics can help with formatting your dissertation, using statistical software and bibliographic referencing using Word, LaTeX, SPSS, R, NatBib, Endnote, Mendeley and Zotero.

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

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](#)

[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 - coming up in July and August:

- [Enhancing longitudinal data sharing: Data management strategies and best practices,](#) **2 and 4 July, 2 and 5 August, 10:00am - 2:30pm (two-day workshop)**

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

Prof. James Cole (UCL CMIC) - inaugural lecture 'The Four (brain) Ages of Man'
Fri 5 July 2024, 5:30-8pm, UCL Roberts Building

Professor Cole will talk about his research career to

date, with a particular focus on neuroimaging as a tool to address clinical needs for neurological and psychiatric disease. He will expound upon four career stages, from undergraduate Psychology to a PhD in psychiatric neuroimaging genetics, to his work on the brain-age paradigm, and finally his current role at UCL. He will propound his perspective on the power of statistical modelling, machine learning and artificial intelligence to harness neuroimaging and related healthcare data to better understand and promote brain health throughout life.
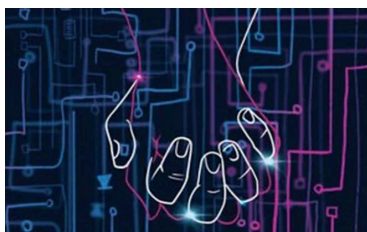
[Further information and booking](#)

Generational health drift: perspectives, evidence, and consequences from the British birth cohorts
Wed 10 July 2024, 1pm - 4:45pm (followed by a networking reception)

Less than a week after the general election the UCL Centre for Longitudinal Studies will be hosting an event presenting the evidence on generational health drift. We will focus on data from the CLS cohorts, which provide a powerful tool to understand generational changes in health as well as inequalities in health.

This event is free to attend but registration is essential.

[Further information and booking](#)

UCL Knowledge Lab - Digital Touch book launch
Wed 10 July 2024, 4:30 - 5:30 pm, Large Seminar Room (G02), UCL Knowledge Lab (hybrid event)

Digital touch is embedded in many technologies, from wearable devices and gaming hardware to tactile robots and future technologies. What would it be like if we could hug or touch digitally across distance? How might this shape our sense of connection? How might we establish trust or protect our privacy and safety?

Offering a rich account of digital touch, the book introduces the key issues and debates, as well as the

design and ethical challenges raised by digital touch. It shows how touch — how we touch, as well as what, whom and when we touch — is being profoundly reshaped by our use of technologies.

[Further information and booking](#)

More or less technology in the classroom – the value and purposes of technology use in school
Tue 16 July 2024, 5:30 - 7pm, online

This panel discussion will bring together researchers, policymakers, practitioners and campaigners to debate where priorities should lie as education comes to grips with rapid technological change. Before we rush too fast into innovating in counter-productive ways, what kinds of questions most urgently need answering?

Join the debate and put your questions to our speakers. Book your place now

[Further information and booking](#)

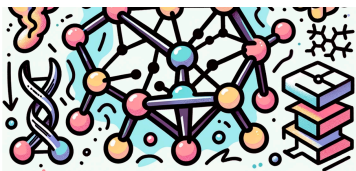### UCL Festival of Engineering Fringe: Computer Science Responsible AI Event.
Wed 17 July 2024, 3-7pm, UCL (90 High Holborn)

Artificial Intelligence and the emergence of tools such as chat GPT and LAMA have highly influenced our modern day lives. We ask them factual questions such as directions, timetables, and prices. We ask their advice and opinion about important matters such as relationships, who to vote for, and what is best to do in a situation. More and more the codes generated by these tools are run on our computers and used to analyse our data; the corrections they suggest on our writings are chosen above our own ways of writing. In order to raise awareness, share difficulties, and improve the EDI of our digitised data-driven community, we ask our experts what a responsible AI means to them and can it be achieved.

[Further information and booking](#)

Thomas Young Centre July Seminar

Thu 18 July @ 4:00 pm - 5:30 pm, Ramsay LT, Christopher Ingold Building) refreshments in the Nyholm Room)

Modelling of organic optoelectronics – David Casanova, Donostia International Physics Center

External Events

London Data Week - Empowering People In Data: Exploring Skills And Building Community (Alan Turing Institute)
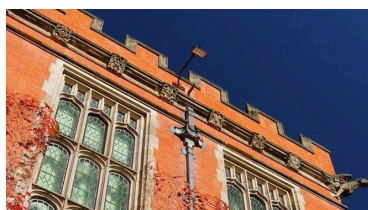
5 July 2024, 9:30am - 5:00pm, Impact Hub London, 1 Triton Square, London, NW1 3DX (hybrid event)

The morning workshop will focus on sharing/mapping approaches from across London to developing data and AI skills. We will start with some lightning presentations before participants discuss and share in small groups on possible opportunities, challenges and goals for the future. The afternoon workshop will focus on the data professionals workforce and the People in Data project. We will start with a diverse panel of speakers who will talk about their experience of working in data and the need for capacity building in this community and highlight some of the current challenges. We will then have small group discussions about: Who are the People in Data?, What skills and competency work, or training development have you done in this area or know of?, What are the main challenges of working in a data focused role?

The event is free to attend and is suitable for data professionals, those who manage data professionals and anyone interested in a career working in data.

[Further info and registration](#)

[See other London Data Week events](#)

Changing Research Culture

9 July 2024, 10am - 3pm, University of Sheffield (with online attendance available for keynote talks)

In anticipation of REF2029's heightened emphasis on

People, Culture and Environment, 'research culture' is increasingly coming into scope as a focus of attention for UK institutions. But critical and reflective work is needed to avoid the term becoming, like 'excellence' itself, a floating signifier that obscures the genuine conditions, processes and limitations of academic practice.

This one-day workshop will address this task with a particular focus on practices around openness and transparency. With reference to UKRIO's component principles of research integrity, we will examine the degree to which open practices present a necessary condition of a culture of research integrity and inclusion and explore the extent to which embedding and facilitating open practices offers a significant mechanism of culture change.

Further info and registration

Family Finance Surveys User Conference 2024

10 July 2024, 9:45am - 4:00pm, online

The user conference brings data producers and data users together to share updates on the development of the surveys and to showcase research that is being carried out using the data. Surveys include the Family Resources Survey, Living costs and food survey and Wealth and Assets Survey.

We are very pleased to announce that the keynote speaker for this year's conference is Daniel Edmiston, from London School of Economics and the Autonomous University of Barcelona, who will discuss his paper Understanding the prevalence and effects of deep poverty through existing data infrastructure.

Further info and registration

RSLondonSouthEast 2024

Tuesday 16th July 2024, 9.30am – 5pm, South Kensington Campus, Imperial College London

The RSLondonSouthEast workshop is back for 2024! This year, our 5th workshop in the series will begin the process of growing our regional community to support a wider group of "digital Research Technical Professionals"

(dRTPs). Whether you're already an experienced technical professional or researcher developing software, working with research data, or managing specialist computing infrastructure, or whether you're new to the space and are keen to develop your skills and meet others working in the field, the workshop will provide an excellent opportunity to engage with the community and develop your research technology skills.

Workshop Schedule

Registration

The MD Analysis UGM (User Group Meeting) in partnership with the Thomas Young Centre

21-23 August 2024, King's College London

The UGM will bring together users of the MDAnalysis package from different communities. Our goal is to foster an opportunity to connect for interdisciplinary researchers and developers across biomolecular simulations, soft matter, materials science and more.

Whether you are a new MDAnalysis contributor, an MDAnalysis core developer, or a researcher using (or interested in using) MDAnalysis for your work in academia or industry, this UGM is for you. You can expect:

Keynote talks from experts in the molecular dynamics simulations space (see Keynote Speakers below)
Talks related to developing and using MDAnalysis for diverse scientific applications
Tutorials diving into new features
Direct access to the MDAnalysis core developer team to help shape future development of MDAnalysis
Networking opportunities to foster new collaborations
Hackathon and other social outings.

Further info and registration

NERC Digital Gathering 2024
11-12 September, University of Manchester

The NERC Digital Gathering will bring together our research community to highlight the increasing role of

research community to highlight the increasing role of digital technologies in environmental research, including spotlighting the outcomes from NERC funded research, the on-going work of the Environmental Data Service and NERC's Data Centres. We will also hear from experts in other digital fields and industry leaders including IBM and Microsoft. The event is free to attend for all registered participants.

Link for more information and to register: NERC Digital Gathering 2024.

Abstract submissions deadline: Monday 22nd July 2024

Registration deadline: Friday 9th August 2024

MethodsCon: Futures
12-13 September 2024, Manchester

MethodsCon: Futures is a free, in-person event that will take place over two days in Manchester, UK on 12-13 September 2024. It will provide a unique opportunity for attendees to engage with, explore and develop futures, with a particular focus on themes that are likely to have significant impact on humanity's development over the next decades.

The event will be part conference, part learning opportunity and part innovation forum, with more than 30 sessions spread over two days. It has been designed to connect and energise people with a focus on futures and follows on from the success of the first MethodsCon in 2022.

Further information and applications (deadline to apply: **Wed 31 July 2024**).

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 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**. This bespoke event will showcase and celebrate the work of ECRs and provide a range of practical training workshops.

[Find out more](#).

Dates for your Diaries!

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.

Early Bird registration deadline: 18th August 2024
Standard registration deadline: 15th September 2024
Abstract submission deadline: 1st September 2024

[Further information and booking](#)

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 it's 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

Regards,
UCL Centre for Advanced Research Computing