

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 9



Dear Colleagues,

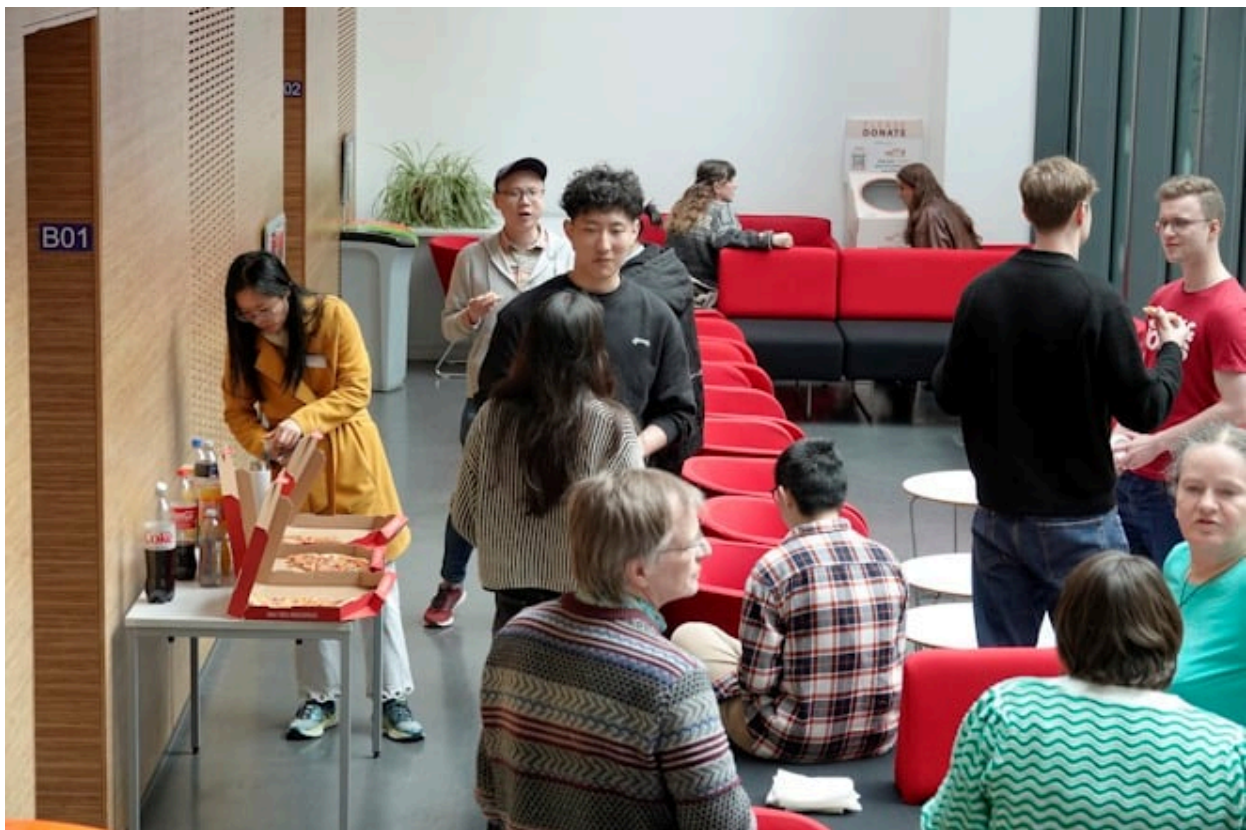
Welcome to the ninth edition of the UCL Digital Research Community newsletter! As we hope you already know, you are receiving this because you previously signed up for either the ARC newsletter or the old eResearch Domain newsletter.

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 (get your command line skills ready!) 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](#).

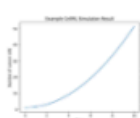
INFO & REGISTRATION

Community Updates

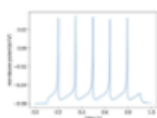
Home People Standards Events Documents [Examples](#) Contact  

COMBINE Examples

Here you will find Python Jupyter notebooks that show how to create simple models for each of the COMBINE standards



CellML



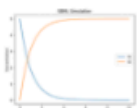
NeuroML



OMEX



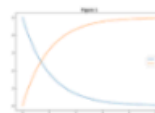
GN



SBML



SBOL



SED-ML

Case Study: Unifying API generation for COMBINE standards

For this open source software sustainability project, funded by last year's call, ARC worked with UCL Neuroscience, Physiology & Pharmacology (NPP) to unify the tools used in developing Application Programming Interface libraries for two open standards formats that facilitate modelling in computational biology. See how this was achieved by Dr Pdraig Gleeson (NPP) working with Dr Sarah Keating, one of ARC's Principal Research Software Engineers, in [our latest case study](#).



New Clinical Data Science and Technology Platform (STP) launched

ARC, in collaboration with researchers across five UCL departments have launched the [Clinical Data STP](#). The Clinical Data STP enables access to Electronic Health Records (EHR) data for UCL research through university-wide, multi-study data licenses. EHR datasets enable the study of risk factors, causation, distribution, management and prognosis of a wide range of diseases/illnesses and allow real world evaluation of the safety and effectiveness of pharmaceuticals.

Multi-study licenses offer a significant saving over single-study licenses. The costs of the multi-study licenses held by UCL under the Clinical Data STP are shared between the users. Access arrangements and policies are available on the Clinical Data STP website. The first license supported by the STP is the Clinical Practice Research Datalink (CPRD). The license is held by ARC and managed through the Clinical Data STP. To discuss your research ideas and check the fit with data held within the CPRD (and associated linked data) contact clinicaldatastp@ucl.ac.uk.



Update: Contender Novel Machines

ARC has recently completed installing several one-off computers that have novel, or esoteric, architectures. They include various kinds of GPUs and other accelerators, many useful for machine learning. There are also Arm architecture CPU hosts and even an IBM mainframe. [Check out the list of machines here](#), where there are also instructions on how to apply for access. Be amongst the first to try out the latest platforms!

IS RESEARCH DATA YOUR THING?



Do you do any of these?

- write Data Management Plans
- collect and clean data
- script data transformations
- create metadata
- prepare data for sharing
- archive data..... ?

You are a Data Steward!

Stewardship supports any part of the research data lifecycle from applying for funding, data acquisition, management and sharing, to archiving.



We want your ideas!

What do you want your community to do?

Join the new Research Data Stewardship Community!



Research Data Stewardship Community of Practice

We are setting up a Research Data Stewardship Community of Practice, and welcome anyone who is engaged in providing support for research data management within UCL, whether as formal data stewards or as part of academic or professional service roles.

Data stewardship can encompass support for any part of the data pipeline from applying for funding, data acquisition, data management, through to the onward sharing of research data and its archiving.

If that sounds like you, please use this [Microsoft form](#) to express your interest in joining, and/or suggest any ideas you have about what the Community of Practice could do!



ARC Involved in new STEP-UP Project to support research technical professionals

ARC's Head of Research Data Services, [Professor James Wilson](#), is a Co-Investigator on the recently announced STEP-UP project, which is creating a strategic technical platform for university technical professionals. The platform will link expert technical talent and career opportunities, to enable skills development to keep up with the rapid pace of developments in research computing, data and artificial intelligence (AI).

More details about this and other similar projects can be found here:

<https://www.ukri.org/news/new-funding-to-support-research-technical-professionals/>



UCL participated at the OSPOs for Good conference at the UN

ARC member [David Pérez-Suárez](#) (together with Malvika Sharan and Arielle Bennett from the Alan Turing Institute / The Turing Way and Neil Chue Hong from the Software Sustainability Institute) attended the [OSPOs for Good symposium](#) at the United Nations Headquarters representing research institutions from the UK.

Open Source Programme Offices (OSPOs) from different entities - national and local level government, institutions and private sector, together with open source communities, think tanks, and activists - joined together to discuss how Open Source can be used to help to tackle UN's Sustainable Development Goals from within the communities, companies or institutions to cross collaboration within all of them.

Read more in [David's post on the ARC blog](#).

```
("input")?"val":"html";e+="Text",r.resetText||n.data("resetText",n[i](),n[i](r[e]|this.options[e]),setTimeout(function(){e="loadingText"?n.addClass(t).attr(t,t).n.removeClass(t).removeAttr(t),0}),t.prototype.toggle=function(){var e=this.closest("[data-toggle='buttons-radio']");e&&e.find(".active").removeClass("active"),this.$element.toggleClass("active");n=e.fn.button;e.fn.button=function(n){return this.each(function(){var r=e(this),i=r.data("button"),s=typeof n=="object"?n:"button",l=new t(this,s),n="toggle"?i.toggle():n&&i.setState(n)}),e.fn.button.defaults={loadingText:"loading",button:Constructor,t,e.fn.button.noConflict=function(){return e.fn.button=n,this},e(document).on("click.button.data-api","[data-toggle='button']",function(t){var n=e(t.target);n.hasClass("btn")||(n=n.closest(".btn"),n.button("toggle"))}(w),function(e){"use strict";var t=function(t,n){this.$element=e(t),this.$indicators=this.$element.find(".carousel-indicator"),this.$options=n,this.options={pause:"hover"&&this.$element.on("mouseenter",e.proxy(this.pause,this)).on("mouseleave",e.proxy(this.cycle,this));t.prototype={cycle:function(t){return t||(this.paused=1),this.interval&&clearInterval(this.interval),this.options.interval&&!this.paused&&(this.interval=setInterval(e.proxy(this.next,this),this.options.interval),this.getActiveIndex(),return this.$active=this.$element.find(".item.active"),this.$items=this.$active.parent().children(),this.$items.index(this.$active)},to:function(t){var n=this.getActiveIndex(),r=this;if(t>this.$items.length-1||t<0)return;return this.sliding.$element.one("slid",function(){r.to(t)});n=t?this.pause().cycle():this.slide(t>"next":"prev",e(this.$items[t]))},pause(t){return t||(this.paused=0),this.$element.find(".next,.prev").length&&e.support.transition.end&&(this.$element.trigger(transition.end),this.cycle(0)),clearInterval(this.interval),this.interval=null,this,next:function(){if(this)return;return this.slide("next"),prev:function(){if(this.sliding)return;return this.slide("prev")},slide:function(t,n,r=this.$element.find(".item.active"),i=n||r[t](),s=this.interval,o=t=="next"?right:"right",u=t=="next"?first:"last",this.sliding=0,s&&this.pause(),i=i.length?i:this.$element.find(".item")[u](),f=e.Event("slide",{relatedTarget:i[0],direction:i.hasClass("active")?return this.$indicators.length&&(this.$indicators.find(".active").removeClass("active"),this.$indicators.find(f).addClass("active"));t&&t.addClass("active"))};if(e.support.transition&&this.$element.hasClass("slide")){this.$element.trigger(f);if(f.isDefaultPrevented())return;i.addClass(t),i[0].offsetWidth,i.addClass(o),this.$element.one(e.support.transition.end,function(){i.removeClass([t,o].join(" ")).addClass("active"),removeClass(["active",o].join(" ")),a.sliding=1,setTimeout(function(){a.$element.trigger("slid"),0});else{this.$element.trigger(f);if(f.isDefaultPrevented())return;r.removeClass("active"),i.addClass("active"),this.sliding=1,this.$element.trigger("slid");return s&&this.cycle(),this}};var n=e.fn.carousel,e.fn.carousel=function(n){return this.each(function(){var r=e(this).carousel(),s=e.extend({},e.fn.carousel.defaults,typeof n=="object"&&n,o=typeof n=="string"?n:s.slide;i||r.data("carousel",s),typeof n=="number"?i.to(n):o||i[0]():s.interval&&i.pause().cycle()}),e.fn.carousel.defaults={interval:5e3,pause:"hover"},e.fn.carousel.Constructor=t,e.fn.carousel.noConflict=function(){return e.fn.carousel=n,this},e(document).on("carousel.data-api","[data-slide],[data-slide-to]",function(t){var n=e(this),r,i=e(n.attr("data-target"))||(r=n.attr("data-target").replace(/.*#?(\w+)$/),""),s=e.extend({},i.data(),n.data()),o=i.carousel(s),(o=n.attr("data-slide-to"))&&i.data("carousel").to(o).cycle(),t.preventDefault()})(window.jQuery),function(e){"use strict";var t=function(t,n){this.$element.toggleClass("active"),this.$options=e.extend({},e.fn.collapse.defaults,n),this.options=this.$options.parent&&(this.$parent=e(this.options.parent)),this.options.toggle();t.prototype={constructor:t,dimension:function(){var e=this.$element.hasClass("width");return e?"width":"height"},show:function(){var t,n,r,i;if(this.transitioning||this.$element.hasClass("in"))return;t=this.dimension(),n=e.camelCase(t).join("-"),r=this.$parent&&this.$parent.find(">.accordion-group > .in");if(r&&r.length){r.data("collapse");if(!i&&this.transitioning)return;r.collapse("hide"),i||r.data("collapse",null)}this.$element[t](0),this.transition("addClass",e.Event("shown"),e.support.transition&&this.$element[t](this.$element[0][n])),hide:function(){var t;if(this.transitioning||this.hasClass("in"))return;t=this.dimension(),this.reset(this.$element[t]()),this.transition("removeClass",e.Event("hide"),this.$element[t](0)),reset:function(e){var t=this.dimension();return this.$element.removeClass("collapse")[t](e)"auto".offsetWidth,this.$element[e==null?"addClass":"removeClass"]("collapse"),this,transition:function(t,n,r){var i=this,(n.type=="show"&&i.reset(),i.transitioning=0,i.$element.trigger(r));if(n.isDefaultPrevented()}}
```

Add your research software to the Research Software Directory

Have you created a piece of research software that you'd like to announce to the world? The Research Software Directory - <https://research-software-directory.org/> - is designed to show the impact of research software on our world. Sign up and submit the software you are maintaining to the directory!

Don't have any software to publish there yet? Then, visit the directory and search through the almost 500 packages they've got registered. You may find something that does what you need already and collaborate with them!

(Please note: The research software directory is maintained by our friends at the [Netherlands eScience Center](#) and supersedes our old research dashboard).



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).



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 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 10:00 on

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

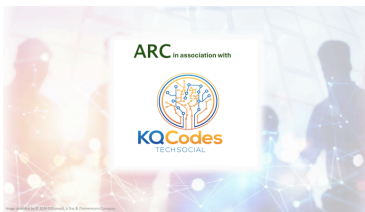


ARC achieves Silver at the 2024 Green Impact Awards!

On this Olympic Friday, we are thrilled to announce that ARC has achieved Silver in the 2024 Green Impact Awards, this recognises our commitment to a sustainable future.

A massive thanks to the ARC Green Impact Team for all their efforts getting ARC to Silver.

Now to see if we can reach Gold in 2025...



Monthly Tech Socials

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](#)

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 30th July 2024 from 11am - 12pm**, at [Charles Bell House, G03 \(Seminar Room 1\)](#).

Further details of the drop-in sessions and other support available can be found [here](#) - **please note that we will be taking a break in August and will resume in September!** (Dates to be confirmed shortly...)

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 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 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 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.

Events



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](#)



**Natural
Environment
Research Council**

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 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

NCRM NATIONAL CENTRE FOR
RESEARCH METHODS

CELEBRATING
20
YEARS

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](#)

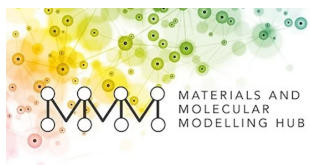


CLOSER 2024 Early Career Researcher (ECR) Conference and Training Event

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 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

Regards,
UCL Centre for Advanced Research Computing

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