

DACOMSIN 2023

The workshop on Data and Computation for Materials Science and Innovation

October 24, 2023, HSE University, Moscow, Russia

Rationale

Materials data collection and systematization that initially used traditional means of data publication then acquired a status of a discipline of its own and much accelerated with the advent of computers. The proliferation of Big Data in materials characterization added up to the requirement of having scalable and interoperable data infrastructures for materials research and innovation.

Extensive bibliographic and material properties databases laid a foundation for machine-assisted data harvesting, data analysis and data repurposing. Design of new materials with the predefined functional properties, and matching in silico models with experimental data have become a reality across the globe and inspired a few national initiatives in materials genome.

The progress of information technology has made it possible to not only use computers for data management and data analysis, but also made computers a viable tool for experimentation on par with physical and chemical experiments. Powerful software platforms and high quality simulated data are now prime citizens in many research and innovation settings.

The domains of materials data infrastructures, materials data analysis and materials in silico experiments have accumulated thriving communities that enjoy regular gatherings and have dedicated professional bodies for ongoing discussions. There is a lack of a common forum though with the prime purpose of multilateral and mutually beneficial discussions across all three communities.

The DACOMSIN workshop is going to address this communication gap and bring together professionals from across research and innovation to share their experience and perspectives of using information technology and computer science for materials data management, analysis and simulation.

Information technology and computer science that intrinsically underpin each of the three pillars of the workshop should be able to become a universal glue, too, that can get these areas closer to each other and can support seamless transition from materials research to pilot innovative applications and eventually to scalable industrial deployments.

Scope

The workshop main topics are:

- Databases and data repositories on experimental and simulated properties of substances and materials
- National and international data infrastructures and data services in support of materials science
- IT applications and IT platforms for materials design and simulation: quantum-mechanical, thermodynamical and other computation
- Software tools for materials data management, data analysis and data visualization
- High-performance computing as an infrastructure for materials advanced characterization and modelling
- Text and data mining, knowledge discovery and machine learning in materials research
- Data formats, metadata and ontologies in support of materials research, innovation and manufacturing
- Extended articles, research objects, executable workflows and other novel means of knowledge representation and professional communication in materials research community (beyond plain publications and data repositories)

The workshop welcomes contributions focussed on other topics, too, as long as they clearly relate to the needs of materials research and development community and as long as they are underpinned by novel applications of information technology or computer science.

Contributions from industry and small business are welcome, along with those from research organizations and academia that are expected to be the workshop mainstream.

Forms of contribution

Workshop contributions may come in the form of keynote talks with the invited speakers list currently under development, also in the forms of conference papers and posters that will be presented in the workshop. Paper and poster submissions will be peer-reviewed.

Papers are advised to be between 5 and 15 pages long. The authors of shorter papers are likely to be offered less time for presenting them in the workshop. Poster abstracts are advised to be one or two pages long.

There will be a smaller opportunity to demonstrate particular IT solutions and disseminate information about them (flyers). If you feel that your main or your only contribution may come in this form, please contact the Programming Committee as early as you can, to ensure that the workshop logistics can actually meet your demonstration requirements. The demo abstract should be submitted anyway and is advised to be one or two pages long.

The working language of the workshop is English. A few oral presentations may be delivered in Russian, with the corresponding slides and papers required to be in English.

Formatting requirements for your workshop submissions are common with the DAMDID conference and are published on the conference website <https://damdid2023.hse.ru/>.

Sponsors

The workshop will be delighted to discuss information dissemination and publicity needs of potential sponsors.

Organization

The workshop will share logistics with DAMDID (Data Analytics and Management in Data Intensive Domains) conference and will benefit from DAMDID participants attending the DACOMSIN and contributing their feedback to materials research and innovation community. In turn, the DAMDID conference will benefit from talking to the materials research and innovation community that can express their needs and intentions in respect to IT infrastructure, algorithms and computer simulation required for the progress with new materials and their applications.

The workshop is organised as a hybrid event with online attendance or live attendance in the Moscow Higher School of Economics, dependent on the participant preferences.

Moscow is a global city that made significant investments in infrastructure and public spaces. According to the United Nations global cities ranking for 2022, Moscow is awarded the top spot among large cities for quality of life and infrastructure, commending the metropolis for its transportation and its citizens' well-being. For those attending in person, travel advice and visa support will be provided.

Moscow is great city that has made significant investments in its infrastructure and public spaces, with certain attention to the needs of business visitors and tourists. Travel advice and visa support will be provided.

Dissemination of outcomes

Full-text papers and abstracts of posters, demos and keynote talks from the DACOMSIN workshop and the DAMDID conference will be published electronically on the Web.

Categories of contributions to be submitted for publication and presentation:

- regular papers reflecting original scientific results (from 10 to 15 pages);
- short papers (work in progress) (from 5 to 9 pages);
- posters (up to 2 pages abstract);
- demonstrations (up to 2 pages abstract).

The longer contributions (5+ pages) will be also published electronically in CEUR Workshop Proceedings series.

Soon after the conference two post-proceedings volumes will be submitted as special issues to the Lobachevskii Journal of Mathematics (<https://www.springer.com/journal/12202>) and to the Pattern Recognition and Image Analysis (<https://www.springer.com/journal/11493>) for the sake of better visibility of the conference publications by the international scientific community, as well as for indexing papers in Scopus and Web of Science.

<u>Programming Committee</u>	<u>Organizational Committee</u>
Nadezhda Kiselyova (IMET.AC.RU), co-chair Victor Dudarev (RUHR-UNI-BOCHUM.DE), co-chair Alexandra Khvan (MSU.RU), co-chair Galina Kuzmicheva (MIREA.RU) Igor Morozov (IHED.RAS.RU) Irina Uspenskaya (MSU.RU) Karine Abgaryan (CCAS.RU) Martin Horsch (NMBU.NO) Toshihiro Ashino (TOYO.AC.JP) Vasily Bunakov (STFC.AC.UK), Vladislav Blatov (SAMGTU.RU) Yibin Xu (NIMS.JP)	Alexandra Khvan (MSU.RU), co-chair Sergey Stupnikov (IPIRAN.RU), co-chair Natalya Polkovnikova (RUSNANO.RU), co-chair