

Perspectives and challenges of future high-performance computing for atomistic and molecular simulations

CECAM Flagship Workshop, Berlin, 19 to 21 February 2024

Highlights in classical molecular simulations

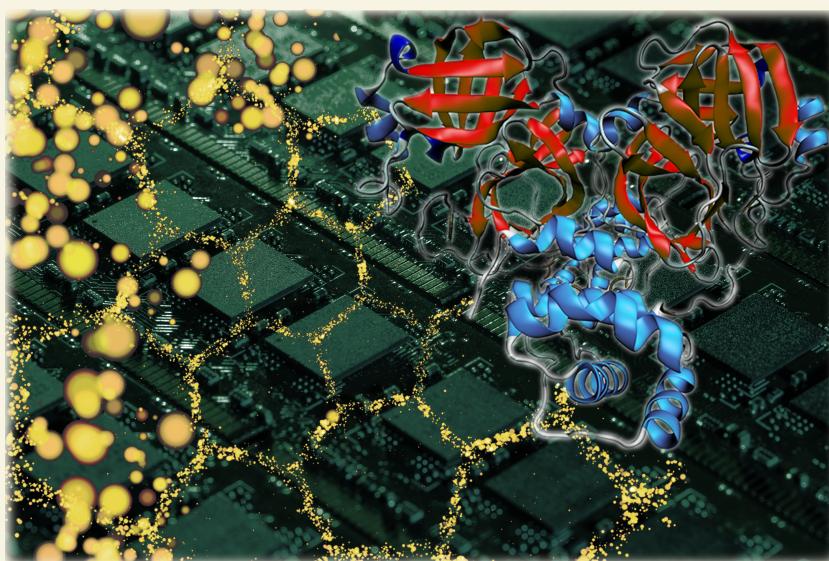
Advances in quantum mechanical modelling

Hybrid QM/MM methods and their applications

Algorithms and co-design for novel hardware

Parallel programming models

Technological trends & new computing paradigms



An interdisciplinary platform for researchers, software engineers, and hardware specialists

Invited speakers

Rommie Amaro (UC San Diego)

Christian Carbogno (FHI Berlin)

Tom Deakin (Univ. Bristol)

Michael Hennecke (Intel Germany)

Martin Herbordt (Boston Univ.)

Hans-Christian Hoppe (FZ Jülich)

Michael Klemm (AMD/OpenMP ARB)

Hector Martinez-Seara (IOCB CAS Prague)

Dmitry Morozov (Univ. Jyväskylä)

Giulia Palermo (UC Riverside)

James C. Phillips (Univ. Illinois)

Sereina Riniker (ETH Zürich)

Michèle Weiland (EPCC Edinburgh)

and 2–3 ASC Lectures (by application)

Organisers F. Höfling (FU Berlin) P. Imhof (FAU Erlangen–Nürnberg) T. D. Kühne (HZDR Dresden/Görlitz)

Venue Zuse Institute Berlin, Germany

Sponsors Atomistic Simulation Center (ASC) of the NHR Alliance, Freie Universität Berlin

Important dates Abstract submission: 10 Jan 2024, notification of acceptance: 15 Jan 2024

Registration <http://bit.ly/HPC-atomistic-CECAM2024>