

MONDAY

Room o.119, Erwin-Schrödinger-Zentrum

14 ⁴⁵ Welcome	Matthias Scheffler FHI @ IRIS/HU, Germany
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Session 1: Architectures of exascale computers and necessary coding concepts

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15 ¹⁵ Moderation & Introduction	Erwin Laure MPCDF, Germany
15 ³⁰ The supercomputer Fugaku - AI and Big Data	Kento Sato RIKEN, Japan
16 ¹⁰ Coffee break	
16 ³⁰ El Capitan: The LLNL Exascale System	Bronis de Supinski LLNL, USA
17 ¹⁰ Material modelling in Aerospace Applications using HPC and Cloud computing	Carlo Cavazzoni Leonardo Lab, Italy
17 ⁵⁰ Title to be announced	Jesus Labarta Mancho BSC-CNS, Spain
18 ⁴⁰ Dinner with Poster Session Foyer, IRIS Adlershof	

Wifi: _FREE_WIFI_BERLIN

Emergency numbers:

Police	110
Ambulance	112
Fire brigade	112
US embassy	+49 30 83050
Nora Butter	+49 179 2965817

TUESDAY

Session 2:

Multi-scale modeling at the exascale

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9 ⁰⁰ Moderation & Introduction	Sara Bonella CECAM/EPFL, Switzerland
9 ¹⁵ Exascale challenge for workflows and multi-scale modeling	Modesto Orozco IRB Barcelona, Spain
9 ⁵⁵ Exascale workflows	Geoffroy Hautier Dartmouth College, USA
10 ³⁵ Coffee break	
10 ⁵⁵ Mesoscale algorithms and codes in exascale architectures	Massimo Bernaschi CNR, Italy
12 ¹⁵ Lunch break at Restaurant I Due Amici	
13 ⁴⁵ Kinetic Monte Carlo	Qian Yang U Connecticut, USA
14 ²⁵ Multiscale modeling in soft and biological matter	Matej Praprotnik Kemijski Inštitut, Slovenia
15 ⁰⁵ Coffee break	

Session 3:

AI for molecular modelling

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15 ²⁵ Moderation & Introduction	Kurt Kremer MPIP, Germany
15 ⁴⁰ Extracting Design Principles from Physics-Inspired Machine Learning	Rose K. Cernovsky U Wisconsin, USA
16 ²⁰ Machine Learning Dielectric Screening for the Simulation of Excited State Properties of Molecules and Materials	Giulia Galli PSME, USA
17 ⁰⁰ Compound discovery by multiscale modeling and machine learning	Tristan Bereau U Amsterdam, Netherlands
17 ⁴⁰ Big data science in porous materials	Berend Smit EPFL, Switzerland
19 ⁰⁰ Dinner with Poster Session Foyer, IRIS Adlershof	

WEDNESDAY

Session 4:

Artificial intelligence concepts

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9 ⁰⁰ Moderation & Introduction	Claudia Draxl IRIS/HU @ FHI, Germany
9 ¹⁵ Finding structure in data, identifying maps of materials properties, and detecting the „materials genes“	Matthias Scheffler FHI @ IRIS/HU, Germany
9 ⁵⁵ Molecular Dynamics with the Deep Potential Method	Roberto Car Princeton U, USA
10 ³⁵ Coffee break	
10 ⁵⁵ Machine learned potential-energy surfaces	Cecilia Clementi FU Berlin, Germany
11 ³⁵ Data-driven discovery of rare phenomena	Mario Boley Monash U, Australia
12 ¹⁵ Lunch break at I Due Amici	

Session 5:

Challenges in atomistic modelling

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13 ⁴⁵ Moderation & Introduction	Ignacio Pagonabarraga CECAM/EPFL, Switzerland
14 ⁰⁰ Exhilarating exascale explorations in materials space	Nicola Marzari EPFL, Switzerland
14 ⁰⁰ Design of macromolecular products and processes from scratch	Juan de Pablo PSME, USA
15 ²⁰ Grand canonical replica exchange MD from first principles	Luca Ghiringhelli IRIS/HU @ FHI, Germany
16 ³⁰ Departure from Dorint Hotel to the conference outing: Graffiti tour at the former US listening station Conference dinner in the Grunewald	

THURSDAY

Hands-on tutorial: Day 1

Room 1.427, Lise Meitner-Haus

9 ⁰⁰ Introduction to ab initio molecular dynamics and DFT Giulia Galli, PSME Francois Gygi, UC Davis, USA
11 ⁰⁰ Coffee break at IRIS Adlershof
11 ¹⁵ Introduction to advanced sampling methods Juan de Pablo, PSME Ludwig Schneider, PSME
13 ¹⁵ Lunch at IRIS Adlershof
14 ³⁰ Hands-on: Introduction to QBox Francois Gygi, UC Davis, USA Arpan Kundu, PSME
15 ³⁰ Hands-on: Introduction to SSAGES Pablo Zubieta, PSME Ludwig Schneider, PSME
16 ³⁰ Coffee break at IRIS Adlershof
16 ⁴⁵ Hands-on: Coupling of ab initio and advanced sampling techniques Elizabeth M. Y. Lee, PSME Gustavo Perez, PSME
18 ⁰⁰ BBQ @ Gerdans Erwin-Schrödinger-Zentrum

FRIDAY

Hands-on tutorial: Day 2

Room 1.427, Lise Meitner-Haus

9 ⁰⁰ Hands-on Problem # 1 Arpan Kundu, PSME Elizabeth M. Y. Lee, PSME
11 ⁰⁰ Coffee break at IRIS Adlershof
11 ¹⁵ Hands-on Problem # 1 Gustavo Perez, PSME Pablo Zubieta, PSME Ludwig Schneider, PSME
13 ¹⁵ Lunch at IRIS Adlershof
14 ³⁰ Parallel Sessions: - Session 1: Hands-on Problem # 3 - Session 2: Exploratory/discovery session with experts Giulia Galli, Francois Gygi, Juan de Pablo, and all PD and students of previous sessions