Session Program

October 23, 2023

9th bwHPC Symposium

Talks

University of Mannheim, Aula
Schloss Bismarckstr. 40 68161 Mannheim

Mon, October 23

11:30 AM

Talks: Applied Mathematics and Engineering

Session | **Location:** University of Mannheim, Aula, Schloss Bismarckstr. 40 68161 Mannheim | **Convener:** (Chair) Jordan Asenov Denev

11:30 – 11:45

A Fully Parallelized and Budgeted Multi-Level Monte Carlo Method and the Application to Acoustic Waves

Speaker

Niklas Baumgarten

11:45 – 12:00 **Simulation of pyrolysis process of waste plastics**

Speaker

Dr Feichi Zhang

12:00 PM

1:00 PM

Talks: Advanced Workflows and Data Management Methods in Materials Science and High Energy Physics

Session | **Location:** University of Mannheim, Aula, Schloss Bismarckstr. 40 68161 Mannheim | **Convener:** (Chair) Bernd Wiebelt

13:00 – 13:15

Concurrent multi-scale simulation of lubrication, enabled by machine learning

Speaker

Prof. Lars Pastewka

13:15 – 13:30 **Exploring the limits of new physics at the LHC**

Speaker

Nikita Schmal

13:30 – 13:45 **End-user data analysis at the LHC**

Speaker

Nils Faltermann

13:45 – 14:00 **Fair sharing of resources between clusters with AUDITOR**

Speaker

Dr Benjamin Rottler

2:00 PM

2:15 PM

Talks: Computational Chemistry and Materials Science

Session | **Location:** University of Mannheim, Aula, Schloss Bismarckstr. 40 68161 Mannheim | **Convener:** (Chair) Christian Mosch

14:15 – 14:30

Propane/Propylene Separation via Molecular Dynamics Simulations in Metal-Organic Frameworks.

Speaker

Dr Mikhail Suyetin

14:30 – 14:45

Computational Microstructure Exploration for Batteries: Leveraging High Performance Computing

Speaker

Mr Julius Weinmiller

14:45 – 15:00   **Advanced Training-Data Generation for Machine-Learned Potentials**

Speaker

Moritz René Schäfer

3:00 PM

3:30 PM

Talks: Bioinformatics, Geosciences and Global Systems Science

Session | **Location:** University of Mannheim, Aula, Schloss Bismarckstr. 40 68161 Mannheim | **Convener:** (Chair) Jens Krüger

15:30 – 15:45

Introducing Galaxy: A new cloud and HPC gateway for data-driven computational research

Speaker

Mr Sanjay Kumar Srikakulam

15:45 – 16:00

The agroecosystem multi-model library, Expert-N on high-performance computers (HPC)

Speaker

Fasil Mequanint Rettie

16:00 – 16:15

High-resolution global weather simulations with the Model for Prediction Across Scales (MPAS) on the Hawk HPC system

Speaker

Thomas Schwitalla

4:15 PM