
ASHPC21 - Austrian-Slovenian HPC Meeting (May 31 - June 2, 2021, <https://ashpc21.si>)

Monday May 31, 2021

08:30		JOIN IN	
09:00	OC & PC	WELCOME	Welcome talks to ASHPC21 online (by chairs: Zoran Ren, Davor Bračko, Claudia Blaas-Schenner)
09:15	Chair: Christoph Dellago	Topic	Materials science / materials discovery
09:15	Nicola Marzari	KEYNOTE	Materials discovery at the intersection between high-performance and high-throughput...
10:00	Santanu Saha		Exploring B-C phase diagram using Crystal Structure and High-Throughput Screening...
10:20	Soner Steiner		DFT simulation of the physical properties of the newly discovered borides Mn _{3-x} {Rh,Ir}5B ₂ ...
10:40		BREAK	
11:00	Chair: Siegfried Höfner	Topic	Running and using HPC clusters efficiently
11:00	Jan Eitzinger		ClusterCockpit — A web application for job-specific performance monitoring
11:20	Alois Schlögl		Managing Software on a heterogenous HPC cluster
11:40	Vladislav Kashansky		Automated Workflows Scheduling via Two-Phase Event-based MILP Heuristics for MRCSP...
12:00		LUNCH	
13:00		POSTERS	Poster Session
P 1.	Hermann Schwärzler	Poster	Embarrassingly Parallel: mothur's pairwise.seqs is a Case in Point
P 2.	Blaž Stres	Poster	Metagenomics data analysis software: trouble in HPC paradise
P 3.	Thomas Klammsteiner	Poster	How high-performance computing brings our understanding of insect-based gut microbiomes ...
P 4.	Leon Deutsch	Poster	HPC in biomed: from bacterial taxonomy to functional gene microbiology and machine learning
P 5.	Soner Steiner	Poster	The effect of magnetism to the elastic constants in the the high entropy alloy CoCrFeMnNi
P 6.	Lorenz Romaner	Poster	Hybrid approaches for DFT simulations of crystallographic defects for physical metallurgy applications
13:30	Chair: Andrej Filipčič	Topic	Climate and EuroHPC & EuroCC
13:30	Emily Collier		Exploiting kilometer-scale grid spacing for climate simulations over the Himalayas and...
13:50	Bastian Koller	KEYNOTE	Strengthening the European HPC ecosystem - strategy, technology, synergies
14:25	Damjan Harisch		Slovenian National Competence Centre HPC
14:40	Markus Stöhr		Introducing EuroCC Austria
14:55		short break	
15:00	Chair: Andrej Filipčič	Q & A	EuroHPC & EuroCC with: Bastian Koller, Damjan Harisch, Jan Jona Javoršek, Markus Stöhr, Christoph Dellago, Andrej Filipčič
16:00		end	

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Tuesday June 1, 2021

<i>08:30</i>		<i>JOIN IN</i>	
<i>09:00</i>	<i>Chair: Janez Povh</i>	<i>Topic</i>	<i>Molecular simulation</i>
09:00	Matej Praprotnik	KEYNOTE	Multiscale simulations of open molecular systems
<i>09:45</i>	<i>Jernej Stare</i>		<i>Scientific computing at National Institute of Chemistry: Elucidation of the driving force ...</i>
<i>10:05</i>	<i>Thomas Stockner</i>		<i>Using MD simulations to study the occlusion of the neurotransmitter serotonin by SERT ...</i>
<i>10:25</i>	<i>Blaž Kamenik</i>		<i>Multilevel computational modeling of freeze-drying</i>
<i>10:45</i>		<i>BREAK</i>	
<i>11:00</i>	<i>Chair: Siegfried Höfner</i>	<i>Topic</i>	<i>Facilitating HPC access for our users</i>
<i>11:00</i>	<i>Miran Ulbin</i>		<i>Web-based user interface to SLURM</i>
<i>11:20</i>	<i>Florian Goldenberg</i>		<i>A jupyterhub at the Vienna Scientific Cluster</i>
<i>11:40</i>	<i>Soner Steiner</i>		<i>Presenting the jupyterhub at Vienna Scientific Cluster ...</i>
<i>12:00</i>		<i>LUNCH</i>	
<i>13:00</i>	<i>Chair: Christoph Dellago</i>	<i>Topic</i>	<i>HPC Training & Education</i>
<i>13:00</i>	<i>Pavel Tomšič</i>		<i>Erasmus+ project: SCtrain</i>
13:15	<i>Chair: Christoph Dellago</i>	Q & A	HPC Training & Education with: Pavel Tomšič, Claudia Blaas-Schenner, Christoph Dellago, et al.
<i>13:30</i>	<i>Chair: Zoran Ren</i>	<i>Topic</i>	<i>EuroHPC systems available (soon)</i>
13:30	Mirko Cestari	KEYNOTE	Leonardo precursor of exascale system hosted in Italian Big Data Technopole
14:15	Dejan Valh	KEYNOTE	HPC Vega
<i>15:00</i>		<i>BREAK</i>	
<i>15:15</i>	<i>Chair: Ernst Haunschmid</i>	<i>Topic</i>	<i>Vienna Scientific Cluster (VSC)</i>
<i>15:15</i>	<i>Jan Zabloudil</i>		<i>The Immersion Cooled VSC-3 – an Obituary</i>
<i>15:30</i>	<i>Herbert Störi</i>		<i>VSC-5 and Beyond — a Peek Preview</i>
<i>15:45</i>	<i>Chair: Ernst Haunschmid</i>	Q & A	VSC with: Herbert Störi, Christoph Dellago, Alexander Ostermann, Jan Zabloudil, Markus Stöhr, Dieter Kvasnicka, Ernst Haunschmid
<i>16:00</i>		<i>end</i>	

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Wednesday June 2, 2021

08:30		<i>JOIN IN</i>	
09:00	<i>Chair: Zoran Ren</i>	<i>Topic</i>	<i>HPC & Industry</i>
09:00	Tomi Ilijaš	KEYNOTE	Is your company ready to benefit from HPC services and lift to Industry 4.0?
09:45	Maruška Čuš		Digital Innovation Hub facilitating the supporting environment for HPC services
10:05		<i>BREAK</i>	
10:20	<i>Chair: Janez Povh</i>	<i>Topic</i>	<i>HPC fundamentals</i>
10:20	Josef Weinbub		Evaluating Parallel Feature Detection Methods for Implicit Surfaces
10:40	Sascha Hunold		An In-Depth Analysis of MPI Collectives or Why MPI Introspection is Needed
11:00		<i>BREAK</i>	
11:20	<i>Chair: Eduard Reiter</i>	<i>Topic</i>	<i>HPC heart</i>
11:20	Mojgan Ghodrati		Effect of left atrial appendage occlusion on thromboembolic risk under mechanical circulatory ...
11:40	Elias Karabelas		Incorporating Heart Valves Using a Varying Permeability Approach
12:00		<i>LUNCH</i>	
13:00	<i>Chair: Alexander Ostermann</i>	<i>Topic</i>	<i>Big Data & AI</i>
13:00	Aleš Zamuda		Parallelization of Benchmarking using HPC: Text Summarization in Natural Language...
13:20	Rok Hribar		Clustering scientific bibliographic data with symmetric orthogonal matrix tri-factorization
13:40	Giovanna Roda		Big Data on the Vienna Scientific Cluster
14:00		<i>BREAK</i>	
14:20	<i>Chair: Andrej Filipčič</i>	<i>Topic</i>	<i>High-energy physics</i>
14:20	Jakob Novak		Uncovering new physics with vector boson scattering
14:40	Martin Schwinzerl		Optimising Parallel Performance In Beam-Dynamics Simulations
15:00	Ivona Vasileska		Task based parallelisation of the Particle-In-Cell codes
15:20	<i>Chair: Andrej Filipčič</i>	CLOSING	Farewell and thank you for attending ASHPC21 with: Andrej Filipčič and outlook towards 2022
16:00		<i>end</i>	