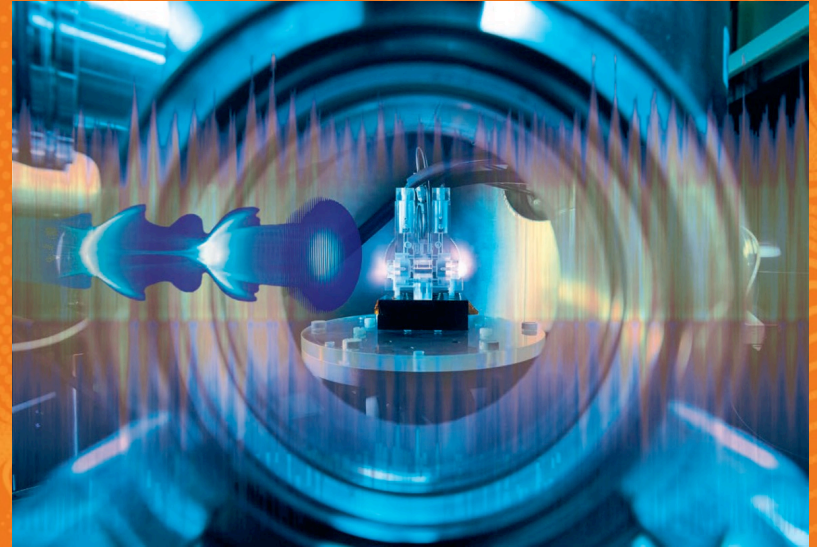
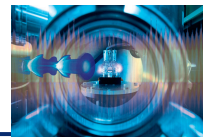


MT-DMA-ST 2 Highlights

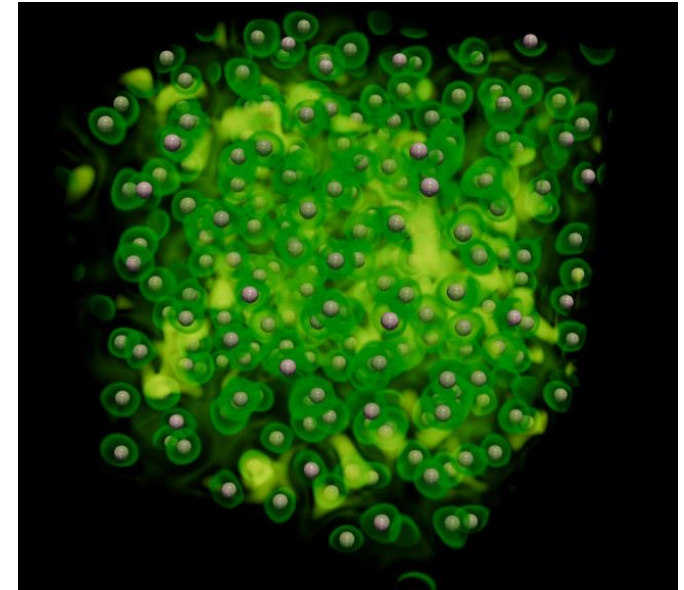
Guido Juckeland, Mohammad Al-Turany



DMA ST 2: Looking back at 2021

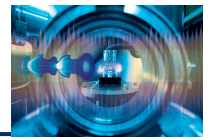


- Ongoing collaboration with ESCAPE-OSSR on curated software publication repository -> R3BRoot now onboarded
- SIMD vectorization (Vc) now available with GCC ≥ 11.1 for x86, ARM NEON + POWER CPUs
- Accelerator/Threading abstraction library Alpaka now also in use by CERN CMS
- Successful work on various quantum algorithms (simulations and ML, but also hardware optimizations)



Simulated density function of electrons (green) in a material (nuclei in grey)

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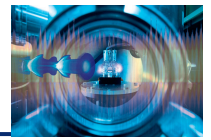
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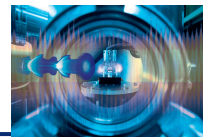


 <p>Dr. Michael Bussmann Founding Manager Center for Advanced Systems Understanding, Helmholtz-Zentrum Dresden - Rossendorf</p>	 <p>Prof. Dr. Michelangelo Canzoneri Global Head of Digital Data Healthcare business of Merck</p>	 <p>Dr. Gabriele De Canio Transformation Officer European Space Operations Centre</p>	 <p>Prof. Dr. h.c. Andreas Dengel Executive Director Deutsches Forschungszentrum für Künstliche Intelligenz (DFKI)</p>
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<h2>Co-chairs</h2>		
 <p>Dr. Gabriele De Canio Transformation Officer, European Space Operations Centre</p>	 <p>Dr. Mohammad Al-Turany Head of the Software Development for Experiments group, GSI Helmholtz Centre for Heavy Ion Research</p>	 <p>Dr. Jean-Enno Charton Director Bioethics & Digital Ethics, Merck</p>

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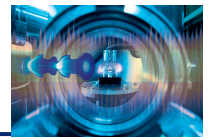


DMA was in the organization and Speakers

 Dr. Michael Bussmann Founding Manager Center for Advanced Systems Understanding, Helmholtz-Zentrum Dresden - Rossendorf	 Prof. Dr. Michelangelo Canzoneri Global Head of Digital Data Healthcare business of Merck	 Dr. Gabriele De Canio Transformation Officer European Space Operations Centre	 Prof. Dr. José Manuel Gómez-Pérez Director, Language Technology Research Expert.ai			
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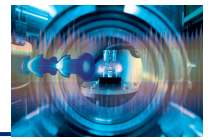
DMA ST 2 – Towards Milestone DMA-7 (2023)



- Provision of a directory of interconnectable software packages including examples to cover the whole simulation and experiment life cycle
 - ESCAPE-OSSR: provides a very good curation workflow, actual directory is a repository
(<https://zenodo.org/communities/escape2020/search?q=&type=software>)
 - HIFIS Research Software Directory: highly flexible software directory, but (currently) no curation
(<https://helmholtz.software>)
 - Idea: Combine workflows from both
 - MT Software list: To be built later today



DMA ST 2: What is next today?



- Kerstin Borrás: Quantum Machine Learning lies at the intersection of Quantum Computing and Machine Learning
- Anna Willmann: Towards a Data-driven Digital Twin of a Free Electron Laser
- Christian Tacke: Onboarding DMA Software to ESCAPE-OSSR Catalogue
- All: collecting list of software for milestone DMA-7

More in the next DMA session