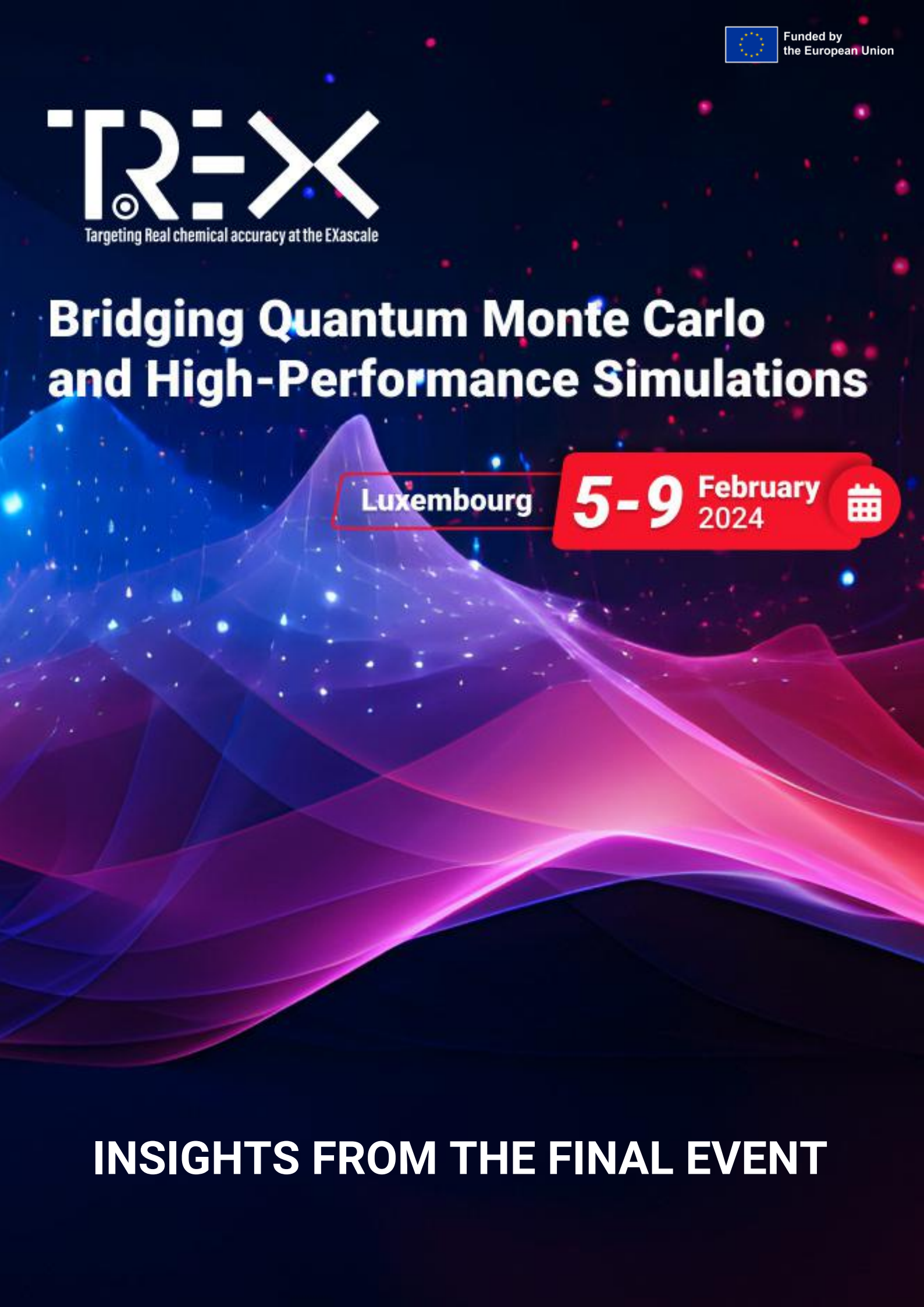
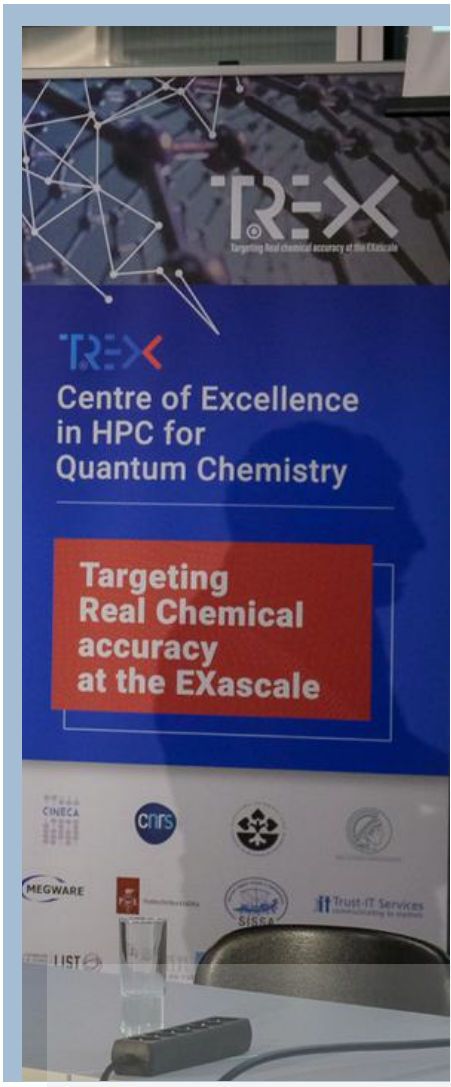

Funded by
the European Union
TREX
Targeting Real chemical accuracy at the EXascale
Bridging Quantum Monte Carlo
and High-Performance Simulations
Luxembourg
5-9 February
2024
INSIGHTS FROM THE FINAL EVENT

In the realm of HPC, quantum chemistry and materials science, the TREX Centre of Excellence stands as a beacon of innovation.

At its core, TREX has not just been about pushing the boundaries of computational capabilities but also fostering a synergistic ecosystem where researchers, developers, and other experts converge to redefine what's possible with Quantum Monte Carlo (QMC) technologies. The project's final event reflected a collective ambition to bridge the gap between theoretical potential and practical application, ensuring that the tools developed are not only powerful but accessible to a broader scientific community.

TREX: DRIVING THE QUANTUM MONTE CARLO INNOVATION

From 5 to 9 February 2024 the TREX Symposium showcased significant progress in the world of Quantum Monte Carlo (QMC) technology. Experts from across Europe and oversea converged to celebrate the project's achievements, discuss ongoing challenges and latest developments in QMC methods, also in relation to high-performance computing (HPC).

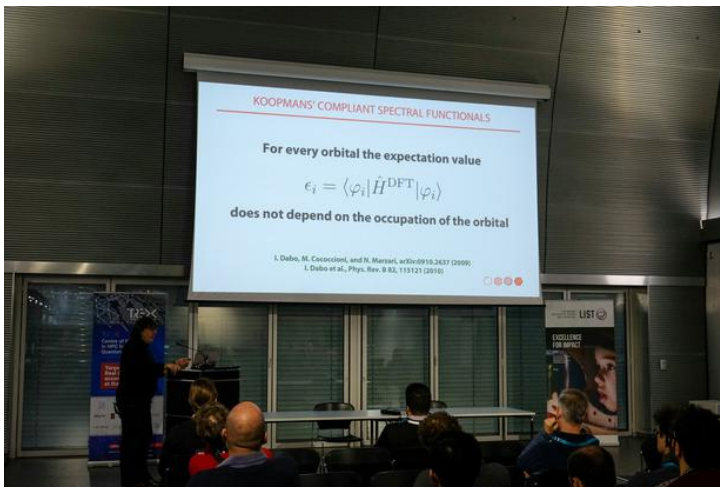


The conference brought together a diverse group of participants, from seasoned researchers to promising PhD students, representing the forefront of Quantum Monte Carlo technology. Each participant, whether presenting or participating in discussions, engaged and contributed to the rich pool of ideas and innovations that define the cutting edge of QMC research and its applications.

THE POWER OF QUANTUM MONTE CARLO (QMC)

Quantum Monte Carlo methods offer exceptional accuracy in simulations, making them invaluable for studying complex materials and simulations at the nanoscale. As exascale computing becomes a reality, QMC's potential to unlock unprecedented insights into the fundamental properties of matter grows exponentially.

Significant steps have been made in adapting QMC methods for the exascale computing era, with experts highlighting the collaborative effort required to scale these algorithms. This includes not only enhancing computational efficiency but also ensuring that software advancements keep pace with hardware innovations. The spirit of TREX underscores a commitment to open innovation and the democratisation of high-performance computing resources.



KEY TAKEAWAYS FROM THE TREX SYMPOSIUM: SCALING QMC, ALGORITHM DESIGN, HPC, AND FUTURE FRONTIERS

The TREX Symposium highlighted the immense potential, along with the significant challenges, of scaling Quantum Monte Carlo methods to the power of exascale computing.
Dr. David Ceperley (University of Illinois Urbana-Champaign) emphasised the need to fundamentally reimagine algorithms for effective calculation distribution across massive numbers of nodes, making full use of exascale power.

This focus on tailored design for unique exascale architectures is echoed by Prof. Anouar Benali (Argonne National Laboratory). He gave great importance to the shared challenges in GPU programming faced by researchers in both the US and Europe, stressing the need for mutual learning and collaboration to overcome these obstacles.

Despite the challenges, the event showcased the value of international collaborations. Anthony Scemama (CNRS/Toulouse), discussing the QMCKL library developed within TREX, noted the benefits of such partnerships. Even a bit of friendly competition can accelerate progress, as researchers on both sides of the Atlantic grapple with similar problems and learn from each other's experiences.

However, the TREX project's long-term legacy sparks a question. Dr. Ceperley expressed a concern that successful software and training resources developed within the initiative require continued support and maintenance to ensure their lasting impact. Without ongoing investment, the project's legacy remains uncertain.

AS WE EXPLORE THE LEGACY AND FUTURE DIRECTIONS OF TREX, IT'S CLEAR THAT THE PROJECT'S IMPACT EXTENDS FAR BEYOND THE IMMEDIATE SCIENTIFIC ADVANCEMENTS.

The search for the optimal way to execute QMC calculations continues across the diverse landscape of researchers. While hardware capabilities expand the limits of what's possible, a keen focus on algorithm efficiency remains vital to maximising performance gains. Mladen Skelin (EuroHPC JU) said that software development should evolve in tandem with hardware innovation through a co-design approach. Researchers, he observed, are adopting system-level perspectives to ensure their creations take full advantage of exascale machines.

This focus on tailored design is also promoted by Shiwei Zhang (Flatiron Institute). While not directly part of the TREX project, he underscored the value of the US-European collaboration fostered by TREX in advancing QMC methodology.

Nicola Marzari (EPFL and Paul Scherrer Institut) delved into the core issue of accuracy. He did acknowledge the TREX project's aim for ultimate precision, while also proposing more flexible methods that might trade a degree of precision for the ability to explore broader properties.

The TREX Project Final Event underscored the deep connection between QMC progress and access to powerful computing resources.
For researchers like Zoran Sukurma (University of Vienna), the importance of continued support for QMC development is clear. Despite the conclusion of the TREX project, the demand for advancements in this computationally-hungry field will only grow.

Emiel Slootman (University of Twente) exemplified the real-world benefits of the collaborative spirit embodied by TREX.
He highlighted the project's role in creating shared, interoperable tools essential for accelerating research in QMC and the necessity for ongoing efforts in developing these integrative tools to avoid the fragmentation of research into isolated islands.

Michele Casula (CNRS Paris), a key contributor to TREX, emphasised the inseparable nature of software advances and scientific discoveries. His breakthrough work on the hydrogen phase diagram and proton transfer mechanisms was directly enabled by code optimization and the efficient GPU porting of the TurboRVB. This is an example of how QMC researchers and HPC experts must work in tandem to unlock the full potential of both hardware and algorithms.

The TREX Project Final Event also gave reflections on how QMC is rapidly evolving, with researchers exploring how it can be combined with powerful techniques like machine learning and artificial intelligence. Kosuke Nakano (National Institute for Materials Science) talked about recent algorithmic advancements in QMC, demonstrating that the project isn't just about code development, but also about fundamental scientific progress in tackling long-standing QMC challenges.

Giuseppe Carleo (EPFL), emphasised the value of interactions fostered by such projects. He also underscored the need for future initiatives that support code development, open-source practices, and collaborations between scientists and software engineers to advance computational science and make sophisticated tools widely accessible.

Matthias Rupp (Luxembourg Institute of Science & Technology) delved into the potential of machine learning for accelerating QMC simulations. He discussed how AI techniques can identify correlations and streamline calculations, but also acknowledged the need to understand these complex models to ensure a better understanding of how the models work.

IT'S ABOUT CULTIVATING A COMMUNITY POISED TO TACKLE THE GRAND CHALLENGES OF OUR TIME, WITH QMC INNOVATION AT THE HEART OF THIS QUEST FOR KNOWLEDGE.

A Success Story: Meet Liam Bernheimer, Winner of the TREX School QMC TurboRVB 2023 Poster Competition

Liam Bernheimer, a dedicated PhD student from Tel Aviv University, emerged as the winner of the poster competition organised during the TREX School QMC TurboRVB in summer 2023. His journey into the realm of Quantum Monte Carlo (QMC) technologies is a great example of the innovative spirit driving the next generation of quantum researchers. Bernheimer's work focuses on the development of groundbreaking Monte Carlo algorithms and methods for quantum systems, reflecting a deep engagement with the foundational aspects of QMC methodologies.

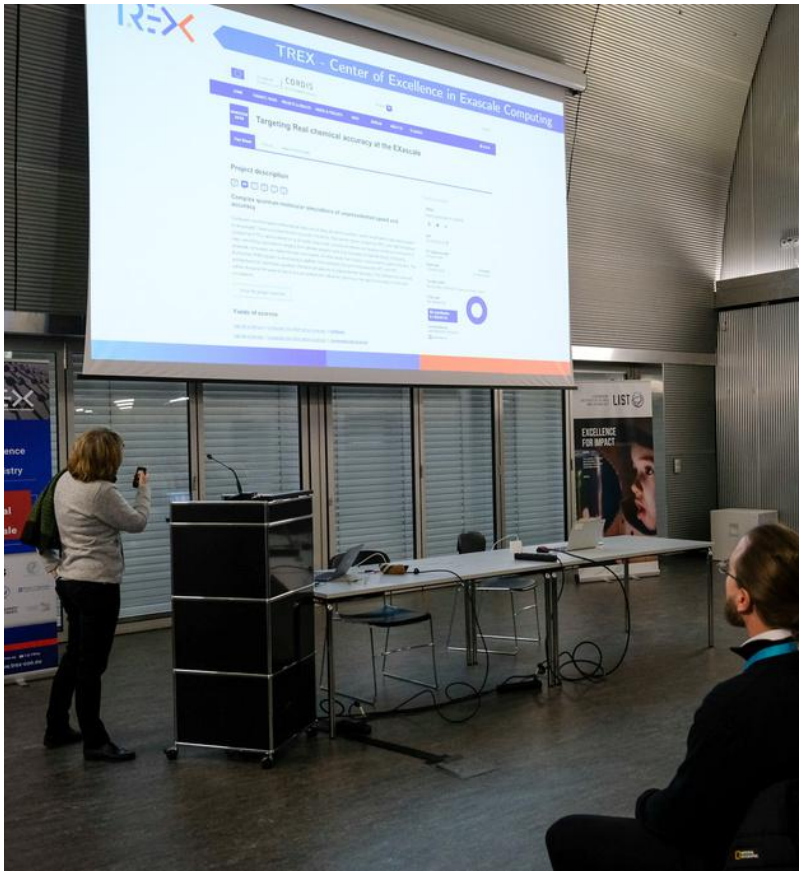
Liam Bernheimer's story is a legacy to the impact initiatives like the TREX project have on developing emerging talent. The TREX School, with its poster competition, offered both recognition for exceptional early-career researchers and a platform for them to connect with leaders in their field. Programs like this are instrumental in propelling QMC research forward, not just by advancing the tools and methods, but also by training and empowering the next generation of innovators.

" ...there are a lot of people who really pioneered the quantum Monte Carlo.."

...it's interesting to see this point of view that I'm not usually seeing..."

With these words Liam highlighted the opportunity to interact with pioneers in QMC, gaining mentorship and insights that shape his own research. Attending TREX events has also exposed Bernheimer to the real-world uses of QMC tools.

Prof. Claudia Filippi
TREX Project Coordinator



Our vision? Real chemical accuracy at the exascale.
We envisioned simulating complex molecular interactions with unprecedented precision and speed.
TREX aimed to make these visions tangible.

TREX has developed novel algorithms and software solutions, and fostered interdisciplinary dialogues.

Learn more about

Targeting Real chemical accuracy at the EXascale

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