D5.1 - UEDIN-EPCC and ICHEC Transnational Access success story

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Author, Institution: E-Mail:	Catherine Inglis, UEDIN-EPCC – c.inglis@epcc.ed.ac.uk
Other contributors	Mats Simmermacher, Technical University of Denmark

ABSTRACT:
This document describes the HPC-Europa3 visit of Dr. Mats Simmermacher, Technical University of Denmark, to Dr. Adam Kirrander, University of Edinburgh, and their subsequent ongoing collaboration. This extremely successful visit led to several publications in some of the most prestigious journals in the field, and helped Dr. Simmermacher to secure a one-year lectureship in the department which hosted his HPC-Europa3 visit. The strength of the collaboration has also led to Dr. Simmermacher submitting another successful HPC-Europa3 application to return to Edinburgh to work with Dr. Kirrander.

KEYWORD LIST:
HPC-Europa3, Transnational Access, research, collaboration, EPCC, HPC, chemistry, photochemical reactions, quantum simulations, ultrafast x-ray scattering, XFEL

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TABLE OF CONTENTS

Executive summary

Dr. Mats Simmermacher, Technical University of Denmark, carried out an extremely successful HPC-Europa3 visit to Dr. Adam Kirrander, University of Edinburgh, from January to April 2018. This visit led to several publications in some of the most prestigious journals in the field (Physical Review Letters and the Journal of Chemical Physics). The visit was also instrumental in helping Dr. Simmermacher to secure a one-year lectureship post in the School of Chemistry at the University of Edinburgh, which was the host department for his visit. The strength of the collaboration led to Dr. Simmermacher submitting another successful HPC-Europa3 application to return to Edinburgh to continue his collaboration with Dr. Kirrander on a new project. This second application was approved in September 2020, but, at the time of writing, the visit has been postponed due to the Covid-19 pandemic.

1 Introduction

Mats Simmermacher was a postgraduate student in the Department of Chemistry at the Technical University of Denmark when he submitted a successful application to the first HPC-Europa3 call, in September 2017. His 3-month visit was hosted by Dr. Adam Kirrander, from the School of Chemistry at the University of Edinburgh, who collaborated with him on his project, "Quantum simulations of ultrafast scattering experiments at X-Ray Free-Electron Lasers". This project was carried out using the High Performance Computing (HPC) resources at EPCC. Visiting between January and April 2018, Mats was one of the first EPCC visitors under HPC-Europa3.

It was Dr. Kirrander himself who had informed Mats about HPC-Europa3 and encouraged him to apply for a visit to work with him. The two had met for the first time during the Faraday Discussions in Edinburgh in 2016, and Mats had subsequently made two brief visits to Dr. Kirrander to find common objectives for their collaboration, to discuss the theory and code they planned to apply, and to choose a suitable molecule to simulate. HPC-Europa3 provided the perfect opportunity for Mats to carry out a longer visit to the group in Edinburgh in order to pursue these objectives.

Mats is now a post-doctoral researcher in the Department of Chemistry at the Technical University of Denmark, where he completed his Ph.D., and continues to work in close collaboration with Dr. Kirrander.

2 First project: Quantum simulations of ultrafast scattering experiments at X-Ray Fee-Electron Lasers

Mats' first visit took place between January and April 2018.

2.1 Project overview

Many natural processes such as photosynthesis, vision in living organisms, and the formation of vitamin D in our bodies, as well as industrial or medical applications such as photocatalysis, solar energy harvesting, and photodynamical cancer therapy, are based on photochemical reactions. Despite their importance for technology and for life itself, photochemical reactions are poorly understood. In order to develop innovative new technologies that may offer solutions for efficient and sustainable synthesis, renewable and carbon-free energy, or medical treatments, it is crucial that we significantly improve our understanding of photochemical reactions.

Generally, a photochemical reaction is initiated by light. Absorption of light stimulates motion of a molecule's constituent particles, its electrons and nuclei, leading to the molecule changing shape and chemical bonds breaking or forming. As this motion happens on very fast timescales, its direct observation was long considered impossible. This changed with the advent of ultrafast optical lasers that paved the way for the pioneering work of Ahmed Zewail, for which he was awarded the Nobel Prize in Chemistry in 1999.

This HPC-Europa3 project capitalised on recently emerging scientific facilities, the X-Ray Free-Electron Lasers (XFELs), which open the potential for even more transformative ultrafast x-ray scattering experiments, and enable chemists and physicists to obtain unprecedented insights into the dynamical behaviour of matter. The ultrashort, intense, and coherent x-ray pulses that XFELs generate allow for real-time observation of photochemical reactions via ultrafast x-ray scattering: a photochemically reacting molecule scatters short bursts of x-rays onto a detector and thereby reveals how it changes with time. The properties of the XFEL radiation furthermore allow for the observation of new and exciting physics such as the theoretically proposed Coherent Mixed Scattering (CMS, see Figure 1), which could provide particularly useful and otherwise inaccessible information about how photochemical reactions proceed.

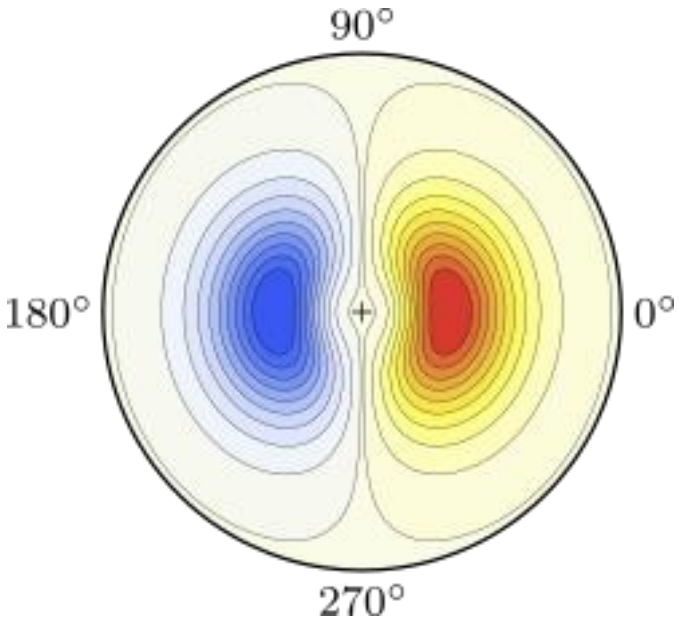

Figure 1: Simulated detector image of Coherent Mixed Scattering by a photoexcited hydrogen molecule (H_2) in two coherently populated electronic singlet states

XFELs are large-scale scientific infrastructures which require billions of euros of investment. There is currently one such infrastructure in the EU – the European XFEL in Hamburg/Schleswig-Holstein – and the construction of one in the UK is under consideration, at an estimated cost in the region of half a billion euros. A single beamtime, i.e. a week of experiments performed by one team at a single hub of such a machine, costs something in the order of a million euros. To make the most out of these massive investments, to really exploit the vast potential of the XFELs, it is extremely important to carry out theoretical and computational work. Accurate simulations are needed to plan experiments in advance, to maximise the chance of success. Simulations are also required to assist the interpretation of the results.

These extensive in silico simulations are based on quantum electrodynamics and require new computer codes that allow the evaluation of the necessary scattering matrix elements from accurate ab initio wave functions. The objectives of this HPC-Europa3 project were to develop, parallelise, and test such a code and apply it to a molecule to perform a simulation of ultrafast non-resonant x-ray scattering in a fully quantised framework.

2.2 The HPC-Europa3 visit and impact of the work

During the 3-month visit, Mats and his host successfully developed, parallelised, and tested a code that evaluates one-electron scattering matrix elements from multiconfigurational wave functions (see Figure 2). They applied this code to the hydrogen molecule and performed a simulation of ultrafast non-resonant x-ray scattering in a fully quantised framework, thereby revealing a novel physical effect which had not previously been observed, but which may potentially be measured in experiments at XFELs. This may then be able to provide researchers with unprecedented information about how chemical reactions initiated by light proceed.

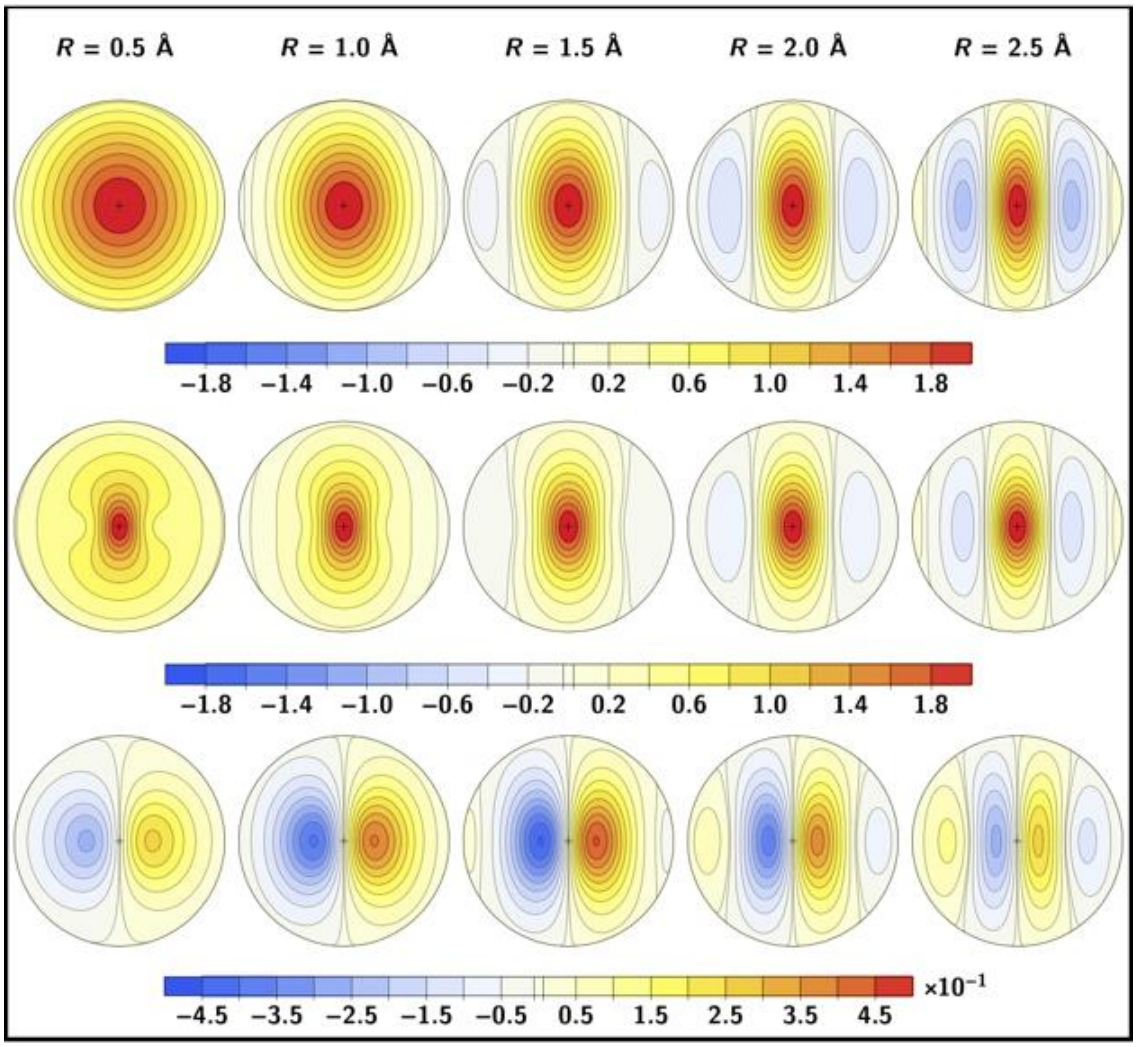

Figure 2: Simulated two-dimensional detector images of three different scattering matrix elements of the hydrogen molecule at five different bond lengths

The results obtained during the visit formed an important part of Mats' PhD thesis [1].

The results were also published in two renowned physics journals [2, 3]. Physical Review Letters is the world's premier physics letter journal and the American Physical Society's flagship publication. It has a 2019 Impact Factor of 8.385 (Journal Citation Reports, Clarivate Analytics, 2020). The Journal of Chemical Physics is an international journal that publishes cutting edge research in all areas of

modern chemical physics and physical chemistry. It has a 2019 Impact Factor of 2.991. Mats is the first author for both papers, with his host and other members of both research groups being co-authors. The support of the HPC-Europa3 programme is mentioned in the Acknowledgements section of both papers.

Following his visit, Mats obtained a 1-year post as a lecturer in the School of Chemistry at the University of Edinburgh, his former host department, from August 2018 until July 2019. Mats believes that his HPC-Europa3 visit "definitely helped" him to secure this position.

Collaboration between Mats and his host continued even once Mats had returned to the Technical University of Denmark to take up a post-doctoral research position, resulting in more jointly authored journal publications [4, 5, 6].

Mats comments: "We have developed theory and code that allows the accurate simulation of these new effects and experiments, and we can run them on HPC now. Previously, people used cheaper, more approximate methods that may fail to catch the new physics involved. Before our project, we were simply not able to perform these computationally more demanding calculations. It was novelty both for us and in our field. The simulations we published in our Physical Review Letters article [2] were the first of their kind. Now, we can apply the same methods to different systems and have actually used them in other research projects since. To mention one concrete example: together with our experimental collaborators, we published a paper in Nature Communications last year that involved simulations that were performed with codes very similar to those used in our HPC-Europa3 project [5]. The HPC-Europa3 project was extremely helpful in the development of our computational tools and without it, we most likely wouldn't be where we are today."

As mentioned above, a deeper understanding of photochemical reactions could have a huge impact on our understanding of many natural processes such as photosynthesis and the formation of vitamin D in our bodies, and could lead to new developments in industrial or medical applications such as solar energy harvesting and photodynamical cancer therapy. The resulting new knowledge will transform fundamental science and boost scientists' ability to design new and better materials at the molecular level. Although the research undertaken in the context of this HPC-Europa3 visit was fundamental research and not directly related to any of these processes, it may lay the theoretical foundation that aids such developments in the future, and the resulting socio-economic benefits are clear.

3 Second project: Signatures of Intersystem Crossing in Ultrafast X-Ray Scattering

In September 2020, Mats submitted a second successful HPC-Europa3 application for a new project which will bring together his own theoretical and computational skills and Dr. Kirrander's extensive experience in both ultrafast x-ray scattering and nuclear dynamics – and in particular the dynamics of carbon disulfide. The project will build on codes that have been developed within the host research group. This second visit is currently postponed due to the Covid-19 pandemic.

3.1 Scientific background

A major breakthrough in understanding how photochemical reactions proceed is necessary to fulfil their promise as a basis for new light-based technologies, which will provide efficient and sustainable synthesis, renewable and carbon-free energy, and new and innovative medical treatments.

Generally, photochemical reactions are initiated by light. Absorption of light stimulates motion of a molecule's constituent particles, the electrons and nuclei, leading to the molecule changing shape and chemical bonds breaking or forming. These dynamics, and the associated flow of energy through the molecule, are controlled by processes known as internal conversion and intersystem crossing (see Figure 3 and Figure 4). These processes redistribute the absorbed energy and are characterised by radiationless transitions from one electronic quantum state to another. These transitions have a decisive impact on the evolution and outcome of photochemical reactions. Unfortunately, no experimental technique exists yet that can probe these transitions directly.

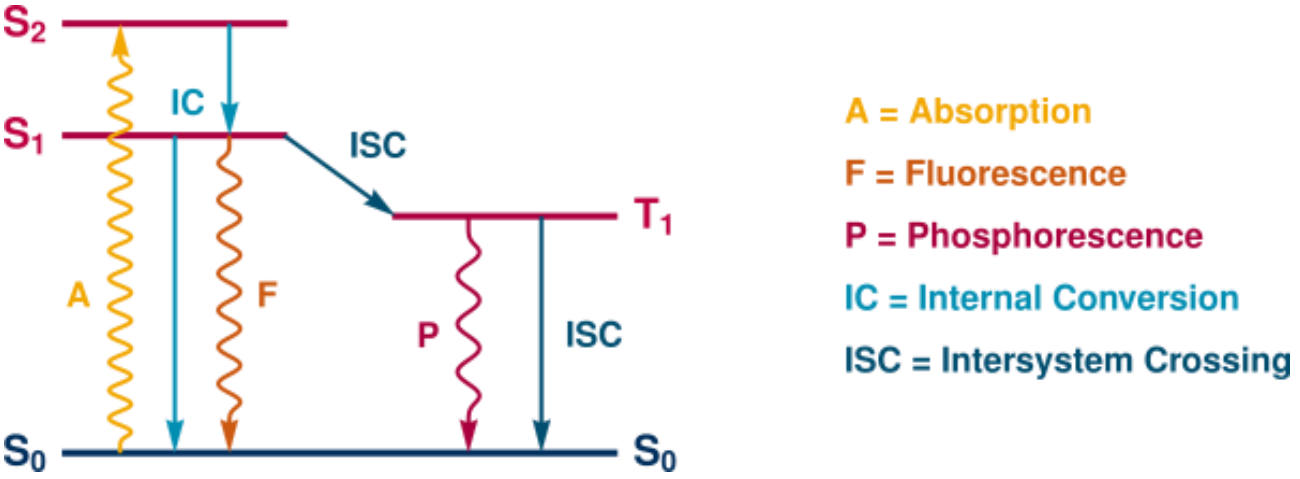

Figure 3: Illustration of different processes during a photochemical reaction. S_0, S_1, and S_2 represent electronic states with singlet spin multiplicity, T_1 and T_2 represent electronic states with triplet spin multiplicity. Processes that involve the absorption or emission of light are depicted by curly arrows. Processes that imply radiationless transitions between electronic states are depicted by straight arrows.

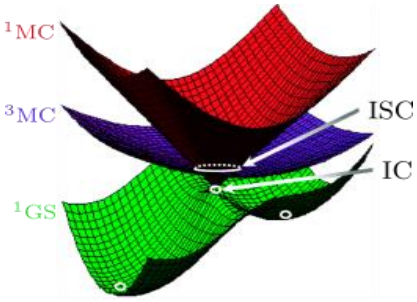

Figure 4: Example of schematic potential energy surfaces with regions where intersystem crossing (ISC) and internal conversion (IC) can occur – *Greenough et al., Phys. Chem. Chem. Phys. 16, 19141 (2014)*

New sources of x-rays, the X-Ray Free-Electron Lasers (XFELs), may offer the opportunity to close this gap. The unrivalled properties of the XFEL radiation may allow for the detection of a proposed new effect referred to as Coherent Mixed Scattering (CMS). This effect probes short-lived electronic coherences, which emerge whenever a molecule undergoes internal conversion or intersystem crossing. Hence, CMS potentially provides as yet inaccessible information about the course of photochemical reactions.

3.2 Project overview

This project will investigate how ultrafast x-ray scattering at XFELs could measure signatures of intersystem crossing. Intersystem crossing is a process which is particularly important in quantum computing, molecular memory devices, photocatalysis, photovoltaics, and light-emitting diodes, since the implied transition between electronic states is accompanied by a change in the molecule's spin multiplicity. Spin is a quantum mechanical property without a classical analogue but can be roughly understood as the intrinsic angular momentum of an electron. Spin multiplicity defines how the spins of all electrons in a molecule combine. While a molecule undergoes a photochemical reaction, the coupling between the electrons' spin and orbital angular momentum can lead to intersystem crossing and thereby opens a reaction path across states with different spin multiplicities. Without this process, many photochemical reactions would be impossible.

Since the scattered x-rays do not interact with the electrons' spin and different spin manifolds often have different topologies as well as different electronic characters, it is likely that the scattering signal will change in a specific manner when a molecule undergoes intersystem crossing. Using highly accurate quantum dynamics simulations, this project will explore and demonstrate this effect in the benchmark molecules iodine bromide (IBr) and carbon disulfide (CS_2). These are molecules where competition between internal conversion and intersystem crossing is known to be important and they constitute likely targets for initial proof-of-principle experiments. The researchers involved in the project will compute all components of the scattering signal, elastic, inelastic, and coherent mixed, (see Figure 5) to reveal how they are all affected by a change in spin multiplicity. The work will also set new and much needed benchmarks for the quantum dynamics community, allowing for methodological advances in simulation techniques.

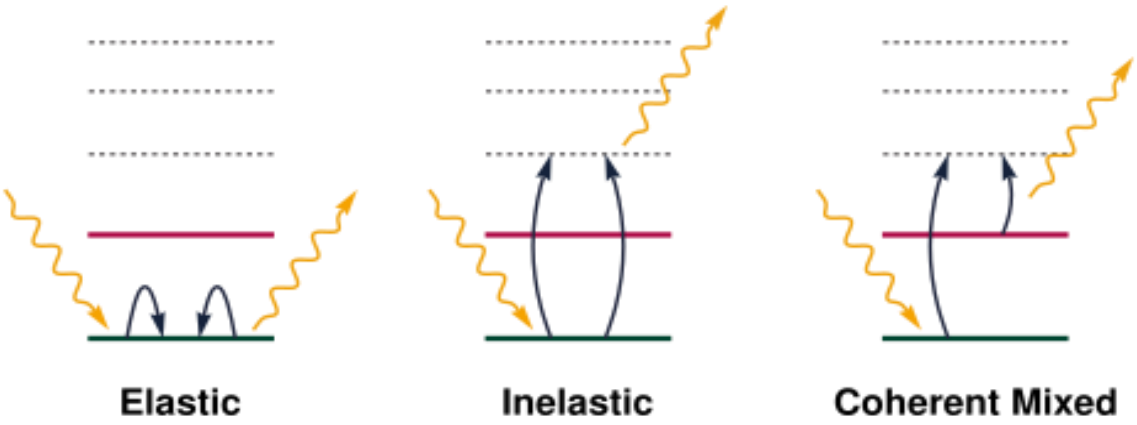

Figure 5: Illustration of the three components of ultrafast x-ray scattering. The vertical lines represent electronic states, the curly arrows depict the incident and scattered x-ray photons, and the blue arrows stand for scattering amplitudes and the electronic transitions they induce. While elastic and inelastic scattering occur from a single electronic state, coherent mixed scattering requires an electronic coherence between two electronic states.

3.3 Expected outcomes of the second project

Even though ultrafast x-ray scattering has already been explored extensively both by theory and experiment, the scientific community has just begun to understand the novel physics it offers. How intersystem crossing affects the scattering signal still remains an open question. If successful, this project will therefore provide significant new insights that will enable researchers in chemistry, molecular physics, materials science, and medicine to further exploit the vast potential of XFEL facilities and to advance our understanding of photochemical reactions.

The successful outcome of the project would also demonstrate the invaluable benefits of using high-performance computing. The advanced experimental techniques chemists, physicists, and materials scientists are using today usually lead to vast amounts of data that can rarely be analysed and interpreted without computational support. Simpler, more approximate codes which do not necessarily require high-performance computing can be used; however. such codes cannot possibly account for new physics, nor realistically explore the richness of information hidden in the experimental data. Should this project succeed in demonstrating how ultrafast x-ray scattering can be used to obtain otherwise inaccessible information about processes like intersystem crossing, it will also make a strong case for the extended use of high-performance computing in this field.

The previous project resulted in a major scientific breakthrough which was published in the prominent physics journal Physical Review Letters. This new project is expected to have a similar or even greater scientific impact by setting new and much-needed benchmarks for quantum dynamics simulations and light-matter interactions, as well as by demonstrating a new direction for ultrafast x-ray scattering experiments. This exciting new science cannot be achieved without access to high-performance computing resources.

The impact of this second visit on Mats' research career should also not be understated. Without the support of HPC-Europa3, it would be impossible for him to continue to pursue his research at the forefront of Theoretical Chemical Physics, due to a lack of available computational resources. Further, this visit will allow him to strengthen the international network which he established during his first visit.

4 Role of HPC-Europa3

The collaboration between Dr. Mats Simmermacher and Dr. Adam Kirrander is an excellent example of how HPC-Europa3 can support and strengthen international collaboration and lead to world-class scientific results.

The programme helped a junior researcher (a Ph.D. student at the time of the first visit) to consolidate a fledgling collaboration with an expert in his field in another country. By combining their expertise, their research led to the publication of several papers in some of the most prestigious journals of the field (including Physical Review Letters and The Journal of Chemical Physics). These papers were largely based on the codes written and the data produced during the first HPC-Europa3 visit.

The use of HPC was critical for the successful outcome of the project already undertaken. The research allows accurate simulation of experiments at emerging scientific facilities, the X-Ray Free-Electron Lasers (XFELs). Only a small number of these facilities currently exist, and experimental time at them is very expensive. Therefore, to maximise the chance of success, theoretical and computational simulation work of the type carried out in the project is vital in order to plan the experiments in advance. Extensive in silico simulations are also needed to interpret the experimental results afterwards. The HPC-Europa3 project developed truly novel theory and code, and as these first-of-their-kind simulations can run on HPC systems, they give faster and more accurate results than had previously been obtained using cheaper methods.

It should also be noted that this work brings together theoretical physicists and experimental collaborators, benefitting both groups.

Although this work is fundamental science, the unprecedented insights into photochemical reactions which have resulted from the work could lead to industrial or medical applications which provide significant benefits to society, such as improved knowledge of how vitamin D is formed, more efficient solar energy harvesting, or advances in photodynamical cancer therapy.

The foundations of this collaboration had already been laid before the HPC-Europa3 visit took place; however, without the support of the programme, it is extremely unlikely that Mats would have been able to spend a significant amount of time at the University of Edinburgh, and the collaboration would not have taken shape so quickly and effectively. Mats comments, “The HPC-Europa3 project was extremely helpful in the development of our computational tools and without it, we most likely wouldn't be where we are today.”

Further, the visit played a crucial role in Mats obtaining a one-year lectureship position at the University of Edinburgh, something which would otherwise have been difficult to achieve for a junior researcher from another country who had only just completed his Ph.D. Both the collaboration itself and the international experience gained will no doubt benefit Mats enormously in his developing research career.

Three years after the visit took place, the collaboration continues to be strong, with further joint papers published, and a second HPC-Europa3 visit due to take place when the current pandemic travel restrictions are relaxed.

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6 Appendix: Project report from first visit (application HPC173JPJ5)

EVALUATION OF ONE-ELECTRON SCATTERING MATRIX ELEMENTS OF MOLECULES

Mats Simmermacher,[a] *Andrés Moreno Carrascosa*,[b] *and Adam Kirrander*[b]

[a] Department of Chemistry, Technical University of Denmark, 2800 Lyngby, Denmark
[b] EaStCHEM, School of Chemistry, University of Edinburgh, EH9 3FJ Edinburgh, United Kingdom

Introduction

The advent of x-ray free-electron laser facilities (XFELs) that provide ultrashort, highly intense, and coherent pulses of x-rays permit the experimental investigation of chemical reactions or photophysical relaxation processes in real-time. They enable chemists and physicists to obtain unprecedented insights into the dynamical behaviour of matter. One of the experimental techniques that becomes possible at XFELs is ultrafast non-resonant x-ray scattering. Here, a target molecule is first excited by a laser pulse and subsequently probed by an x-ray pulse that is scattered onto a detector. By variation of the time delay between the two pulses and by analysis of the recorded scattering patterns, detailed information about the time evolution of the excited molecule is gathered.
In order to exploit the vast potential of this new technique and to interpret existing or future experiments, extensive *in silico* simulations based on quantum electrodynamics are required. These simulations necessitate new computer codes that allow the evaluation of scattering matrix elements (SMEs) from highly accurate *ab initio* electronic wave functions calculated with available quantum chemical software. SMEs describe the amplitude and probability of scattering an x-ray photon by an atom or a molecule into a certain direction in space. Many of such matrix elements for various molecular geometries and several electronic states are involved in a reliable simulation and each element is evaluated on a two-dimensional grid that covers the detector. Such a task is computationally very demanding but can be carried out in parallel. It is thus a case for the use of high-performance computing (HPC).
We report the development, parallelization, and extensive testing of a code that evaluates one-electron SMEs from multiconfigurational wave functions on ARCHER. SMEs of the hydrogen molecule H_2 in its nine energetically lowest-lying electronic singlet states for different H–H bond lengths are computed. The results serve as a basis for the first complete simulation of the two-dimensional ultrafast scattering signal of an excited molecule within a fully quantised framework.[1,2]

Methods

A one-electron SMEs can be expressed as a Fourier transform of the electron density. The electron density, in turn, is given by the absolute square of the electronic wave function where all coordinates apart from one are integrated out. Considering that most quantum chemical programmes optimise the *ab initio* wave function in terms of Gaussian functions, known as Gaussian-type orbitals (GTOs), one can construct an algorithm that computes SMEs efficiently from *ab initio* data. For that we made use of the Gaussian product theorem as well as of the fact that the Fourier transform of any Gaussian function has an analytical solution.[3,4] We have furthermore parallelised our code to make use of HPC facilities such as ARCHER. Since the evaluation of an SME on a given grid point of the detector is independent of all other grid points, the computation on the entire grid is embarrassingly parallel. Moreover, we have split the operations performed on the GTOs evenly across the available nodes by means of an MPI reduction.
We have tested the code extensively with *ab initio* data for the nine energetically lowest-lying singlet states of the hydrogen molecule H_2. The wave functions were optimised using State-Averaged Complete Active Space Self-Consistent Field theory (SA-CASSCF) and the d-aug-cc-pVQZ basis set in the quantum chemical programme package MOLPRO. Once our code consistently provided results that visually and numerically matched our theoretical expectations, the SMEs were interpolated to a finer grid and used in a simulation of ultrafast time-resolved x-ray scattering.

Results

The results of the simulations are reported and discussed in detail in References 1 and 2.

Conclusions

We have developed, parallelised, and tested a code that efficiently evaluates accurate one-electron SMEs from *ab initio* electronic wave functions. These matrix elements are urgently required for the simulation of ultrafast time-resolved x-ray scattering experiments that become possible at XFELs. Their evaluation is computationally very demanding but can be significantly accelerated by making use of HPC. The feasibility and reliability of such calculations were demonstrated for the hydrogen molecule H_2. The results are published in renowned physics journals.

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