Jim Gatheral Travel Scholarship Report

About me

My name is Clément Civrais, and I am currently a third-year postgraduate researcher at the School of Engineering, University of Glasgow. My work is in the fields of hypersonic flow, quantum mechanics, mathematical modelling, and numerical simulation, with the aim of introducing new models to be used in the simulation of the vibrational and electronic modes of molecules. In my third year of studies, I was awarded the Jim Gatheral Travel Scholarship (£4,000). This generous scholarship facilitated my academic stay at the Institut für Raumfahrtsysteme, University of Stuttgart.

Figure 1. Institut für Raumfahrtsysteme, the University of Stuttgart.


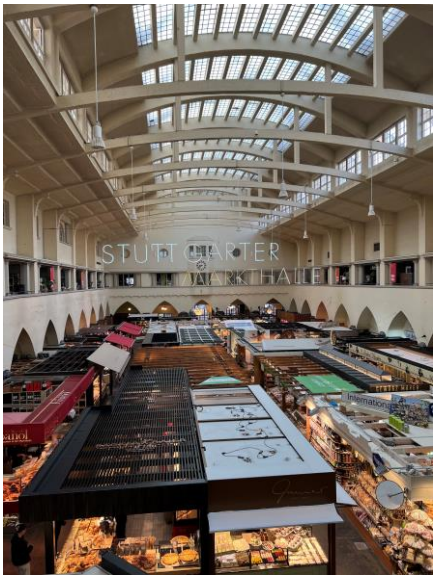
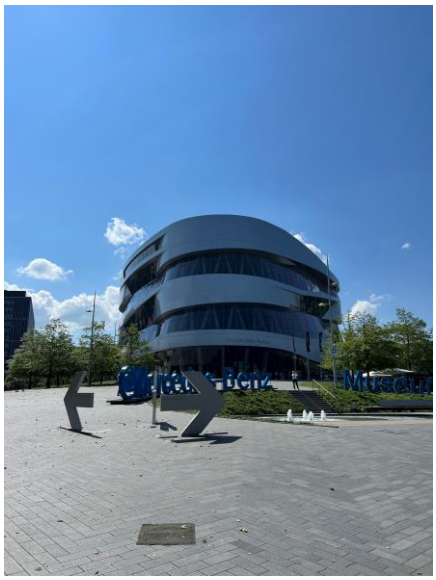


Figure 2. From top left to bottom right. Marktplatz and Stiftskirche, Stuttgart Markthalle, Mercedes-Benz Museum, Unterturkheim vineyards.

Why did you apply for the Travel Scholarship?

My work is in the fields of hypersonic flow, quantum mechanics, mathematical modelling, and numerical simulation, with the aim of introducing new models to be used in the simulation of the vibrational and electronic modes of molecules. The work so far on vibrational energy has resulted in three journal articles (one published, one under-review and one forthcoming) and two conference articles. This series of papers illustrates the development of the novel model and validates it against well-established test cases and high-accuracy numerical and experimental data, before applying it to different problems. It is shown that the new vibrational model significantly improves the predictions of critical flow properties such as the specific heat capacity.

As with many articles dealing with the electronic mode, my work until now considered only the ground state as vibrationally active. To further explore the importance of this contribution, I have conducted some preliminary studies. In these studies, four

mathematical models have been derived in which the internal modes of a molecular system are coupled to one another with varying degrees of physical accuracy. The study has revealed that considering all the electronic excited states of a molecular system to be individually vibrationally active, i.e., coupling the vibrational and electronic modes, substantially improves the accuracy of the flow properties compared to experimental data, e.g., specific heat capacity. Such a finding has, therefore, motivated the development of a novel technique to couple the vibrational and electronic excitation of all the electronic excited states.

The Space and System Institute at the University of Stuttgart is a world-recognised research institute in electric propulsion, which is an area where my current research can have a significant impact. As a result, it has naturally brought me and my supervisors to initiate a collaboration with the Space and System Institute.

I applied to the Jim Gatheral Travel Grant to facilitate the collaboration between two research institute by supporting the travel expenses incurred by the visit of the Space and System Institute at the University of Stuttgart. Beyond the collaborative aspect, I also saw this opportunity as an instance for personal and professional growth. I aimed to acquire new skills, enrich my understanding of hypersonic research and broaden my professional network, connecting with experts, researchers, and fellow enthusiasts in the field.

Details of your visit

The placement was hosted at the University of Stuttgart in the Space and System Institute (ISS). It lasted for 12 weeks, starting at the beginning of April and ending early July. It was supervised by Dr Marcel Pfeiffer, a knowledgeable researcher in DSMC-related research and kinetic theory. I was integrated within Marcel Pfeiffer's research division composed of 7 PhD researchers.

The primary objective of this academic stay was to derive, implement and validate a novel model for the electronic excited states in high thermal conditions. The idea behind traveling to University of Stuttgart and collaborating with Dr Marcel Pfeiffer was to leverage his expertise to enhance the capabilities of our model and expand its range of applicability.

The placement was divided into three steps:

a) The first two to three weeks were allocated to a literature survey of the available mathematical models to provide a solid background for the development of a novel methodology,

b) The following five to six weeks were dedicated to the implementation of the numerical technique,

c) The remaining time was devoted to benchmarking and validation of the model.

The coupled approach represents a significant achievement, having been both successfully derived and implemented within an in-house DSMC solver developed at the University of Glasgow. To ensure its accuracy and effectiveness, the model has been subjected to benchmarking under typical hypersonic flow conditions. The outcomes of these meticulous tests have shown promising results.

Additionally, in May 2023, I had the opportunity to deliver a talk at the Rarefied Gas Dynamics NextGen Meeting. Subsequently, I received an invitation to present an extended seminar at the DLR Göttingen in June 2023.

Impact of the Travel Scholarship

The project aims to deliver a joint journal paper and a presentation of the work-in-progress at the International Symposium of Rarefied Gas Dynamics, held in Göttingen, Germany, in 2024. The journal article is currently in preparation and focuses on the implementation and validation of a novel methodology for the modelling of excited electronic states.

This collaboration is part of a long-term project in which both research institutes aim to improve the understanding of the electronic modelling of molecular systems. It will enable mutualising resources and sharing of knowledge which will consequently improve the quality and the validity of the research.

This academic stay was an opportunity for me to develop as a researcher. Actively working with Dr Marcel Pfeiffer was highly beneficial that allowed me to expand my understanding of gas kinetic modelling in high thermal conditions. Such an exposition diversified my research profile and broaden my professional network. Such a placement allowed me to practice my linguistic skills as well as be exposed to a new culture. This experience was therefore a valuable asset for my career.

Acknowledgements

First, I would like to thank the University of Glasgow and the Jim Gatheral Travel Scholarship for making this research trip possible. I would also like to thank Dr Marcel Pfeiffer for welcoming me to his research group and for the guidance during my stay. Moreover, I would like to thank my supervisors, Dr Craig White and Dr Rene Steijl, for their support throughout the process. Finally, a special thanks to the extended numeric research group for the coffee breaks, foosball and football matches and the stammtisches making it a vibrant environment.