ONETEP Masterclass 2019 – Report

The ONETEP Masterclass 2019 took place from the 27th-30th August, at the Arden Conference Centre in the University of Warwick, generously sponsored by CCP9. The ONETEP Masterclass is a biennial event, last occurring in 2017, and this year the organising committee consisted of James Womack, Joly Aarons, Joseph Prentice, and Nicholas Hine. The event provided a forum for researchers, from both industry and academia, to learn about the capabilities and best usage of ONETEP from the current developers of the code, including the ONETEP Developers' Group (ODG). The aim is to help people make use of ONETEP in their research, by giving an overview of the code's functionality so they can determine what features they need, and by providing one-to-one tuition on the application of ONETEP to the attendees' research problems. In the 2019 event, there were 26 attendees from institutes across the globe, including from China, South Africa, Mexico, Spain, Poland, and Ireland, in addition to those from academia and industry in the UK. There were also 9 active ONETEP developers present to act as tutors. The Masterclass was also used as an opportunity to award the first Karl Wilkinson Memorial Prize, for 'research contributing most strongly to the advancement of electronic structure theory and its applications with the ONETEP linear-scaling DFT code'.

Prior to the event, attendees were asked to list what their interests were, and were each assigned a tutor whose expertise aligned with their interests. This meant that the attendees were able to obtain expert help directly from those who had written the code, and therefore make use of the code more effectively. Attendees were also asked to vote on which functionalities they would like to hear short introductory talks on, so that the information provided by the tutors was tailored to the attendees' interests.

The Masterclass was very successful, and achieved its main goal of providing a place for both first-time and experienced users of ONETEP to interact and receive help from the developers of the code. Feedback from all the attendees was very positive, and many have used the knowledge gained at the Masterclass to continue using ONETEP in their research after its completion. The developers themselves also had their attention drawn to any shortcomings in documentation, and enjoyed spending a week helping many different research projects move towards their goals. All participants, developers and attendees, were able to spend a week working alongside both familiar and new researchers, enabling co-operation and collaboration. In conclusion, as with previous Masterclasses, the 2019 iteration was an extremely interesting and useful event to be a part of, providing both experienced and novice users one-to-one tuition on how to use ONETEP best for their precise purposes, and fostering an interactive and friendly community around the code. It has helped ensure that one of CCP9's flagship codes is as scientifically valuable as possible, and is well-positioned to expand its use into many different strands of research across the globe.