

ONETEP Coding Retreat 2018 – Report

The ONETEP Coding Retreat 2018 took place from the 10th-14th September, at the Cedar House in the village of Castor, near Peterborough. The Coding Retreat is a semi-regular event, last occurring in 2016, where the active developers of ONETEP, including the ONETEP Developers' Group (ODG), are able to meet and work together for an extended period of time. This allows both broad decisions about the code and its future direction to be made, and facilitates collaboration and co-operation on more detailed aspects of the code. The thirteen attendees at the 2018 retreat came from various locations, including London, Cambridge, Southampton, Warwick and even Barcelona.

A list of projects to work on had been written collectively in the lead-up to the retreat, which was further added to at the beginning of the event. These included projects related to specific functionalities, such as those covered by the Excitations in Complex Environments CCP9 Flagship grant, as well as updating documentation for the code and improving guidance for making future contributions. These projects were then allocated to various developers according to their interests and proficiencies.

One of the major outcomes of the retreat was in enabling the attendees to discuss and become familiar with new aspects of the development process, following ONETEP's recent move from SVN to Bitbucket. This also provided an excellent opportunity for guidelines for future contributors to be written. Documentation for several parts of the code was also updated, and a template for creating new modules was itself created. Projects pertaining to specific functionality made significant progress as well, including work on ensemble DFT and implementing new geometry optimisation methods. The three strands of the Excitations in Complex Environments project – quantum embedding, exact exchange in TDDFT, and excited state forces – also saw significant progress, aided by the ability to ensure the three strands mesh together well by having the appropriate developers in the room together.

The Coding Retreat offered a chance to direct the future of the ONETEP code, as well as focus on improving the current code, making it more accurate, user-friendly, and with a broader range of functionality, rendering it more useful to the entire scientific community. In this respect, the retreat has certainly already had an impact, thanks to the significant progress made in Castor. It also provided an opportunity to introduce new developers to the code in a supportive and expert environment, making sure that they get off to the best possible start. In conclusion, the ONETEP Coding Retreat 2018 was an extremely productive and useful event, ensuring that one of CCP9's flagship codes is as scientifically valuable as possible, and is well-positioned to progress into the future.



The attendees hard at work coding



The group dinner