Development of the Wannier90 code

Dr Arash Mostofi – 26/07/2012

Purpose of visit:

Dr Arash Mostofi is one of the principal developers of the Wannier90 code [www.wannier.org, Mostofi *et al.*, *Comput. Phys. Commun.* **178**, 685 (2008)]. Wannier90 is an open-source program that generates maximally-localized Wannier functions (MLWFs) and uses them to calculate electronic properties of materials with high accuracy and computational efficiency. Since its first release in 2008, the code has been interfaced to almost all of the major electronic structure packages that are developed in Europe, including Quantum-Espresso, AbInit, VASP, Siesta, Wein2k and Fleur. A particular advantage of Wannier90 is that once a property is implemented within the software, it is then immediately available to users of all codes that interface to it. To date, Wannier90 has been used in over 130 publications, and has almost 200 registered users on its mailing list.

The host, Prof Ivo Souza of the Centro de Fisica de Materiales (CSIC), Universidad del Pais Vasco, is one of the original developers of the MLWF formalism [Souza *et al.*, *Phys Rev B* **65**, 035109 (2001)]. Since the last major release of Wannier90 in 2010, Prof Souza's group has developed MLWF-based methods to calculate a number of advanced electronic properties such as Berry curvature, anomalous Hall coefficients, and orbital magnetization. It is now timely for these developments to be implemented in the main Wannier90 code.

The purpose of this visit was for the principal developers (Mostofi and Yates) to collaborate with Prof Souza in order to prepare the ground for a new, improved and MPI-parallelized release of the Wannier90 code, including Prof Souza's developments, for the benefit of the wider electronic structure community. We were also joined by Dr Giovanni Pizzi (Ecole Polytechnique Federale de Lausanne), who has been developing electronic transport algorithms for Wannier90.

Start date: 07/07/2012; *duration:* 8 days

Description of work carried out during the visit:

Several major additions were made to the Wannier90 code during the course of this visit, enumerated below:

1. a new utility to calculate van der Waals energies using MLWFs, based on earlier work by one of the developers [*J. Chem. Phys.* **135**, 154105 (2011)];

2. a new module to calculate electronic transport properties within the semiclassical Boltzmann formalism, based on earlier work [http://arxiv.org/abs/1112.1749];

3. new modules for calculation of Berry curvature, anomalous Hall coefficients, and orbital magnetization, based on earlier work by the developers [*Phys. Rev. B* **85**, 014435 (2012), *Phys. Rev. B* **75**, 195121 (2007), Phys. Rev. B 76, 195109 (2007)];

4. new algorithms for adaptive Fermi-level smearing;

5. implementation and testing of the above developments within an MPI-parallelised environment;

6. new documentation for the above functionality;

Description of the main results obtained:

The visit was productive, and a number of key functionalities were implemented. Importantly, we were able to implement MPI-parallel versions of the algorithms and verify, through comprehensive testing, that the parallel code produces the expected results.

Furthermore, we were able to begin the important task of writing clear documentation for the new functionality within the code, as well as start to prepare a suite of simple, demonstrative examples. This is essential for dissemination and widespread uptake of these algorithms within the community.

Future collaboration with host:

There are still a number of things to add, further develop and test prior to the new release of the code. The opportunity provided by this ESF Short Visit Grant has enabled us to discuss these things together and to develop an outline of how to achieve this. We will, therefore, be working together over the coming months to finalise the release and make it available to the community.

Projected publications:

We are considering writing an article describing the new developments in the code, similar in style to our original *Comput Phys Commun* paper of 2008, but focusing on the most recent developments, namely the calculation of advanced electronic properties and parallelism. We would expect that this paper would receive a large number of citations from members of the community who use it to generate results for their own research papers.

Wannier90 developers at Universidad del Pais Vasco, San Sebastian. From left to right: Giovanni Pizzi (EPFL), Arash Mostofi (Imperial College London), Ivo Souza (host), Jonathan Yates (University of Oxford).