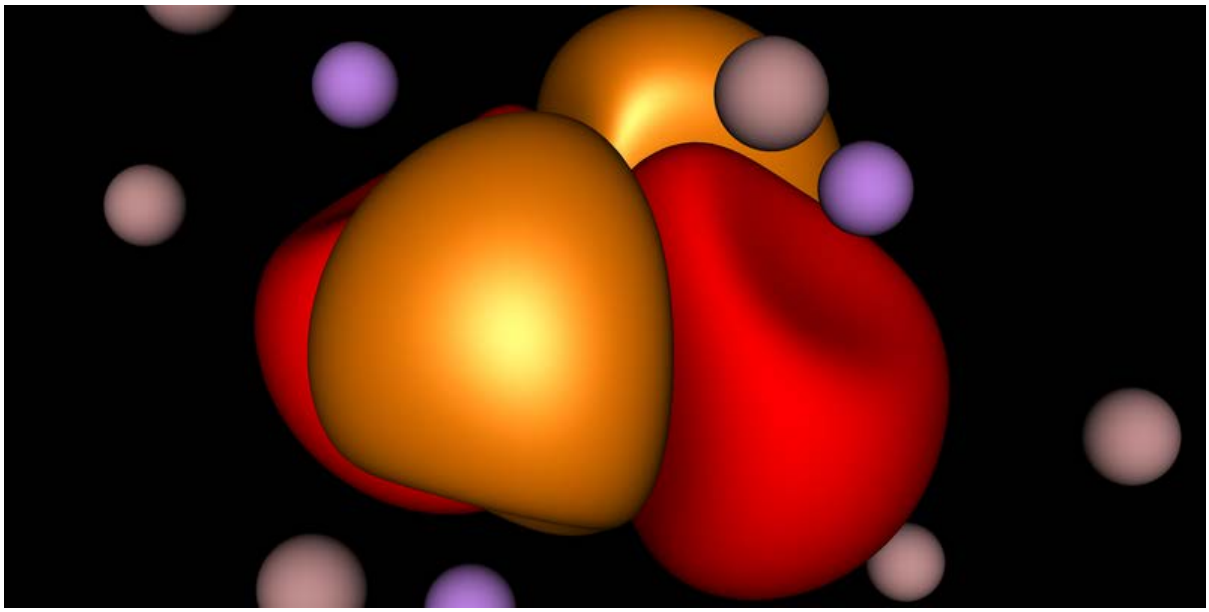
Questaal Hands-On Course

Daresbury Laboratory, 16 – 19 May 2017

Organizers: Jerome Jackson, Martin Lueders, Leon Petit, & Mark van Schilfgaarde



Daresbury Laboratory was pleased to welcome 40 scientists to the "Questaal Hands-On Course" which took place over four days between May 16th and 19th. The Questaal software suite features the first all-electron GW code and the first implementation of the quasiparticle-self-consistent GW method, which is significantly more accurate and reliable than conventional density-functional methods. The focus of the course was to introduce these advanced methods to researchers already familiar with electronic structure calculations and to teach them the practical details needed to perform such calculations for materials and systems relevant to their individual research areas.

The GW approximation (G = Green's function, W = screened Coulomb interaction) of Hedin has its origin in many-body perturbation theory: it is the first term in a perturbation around some non-interacting one-particle Hamiltonian H_0, usually LDA, i.e with $H_0 = H_{LDA}$, and GW = $G^{LDA}W^{LDA}$. Since the original paper by Hybersten and Louie, $G^{LDA}W^{LDA}$ has enjoyed great success, but it has a number of shortcomings, which can become drastic when DFT is a poor starting point. The QSGW approximation is a novel theory that overcomes the starting point dependency by iterating G to self-consistency, and which has already proven successful for the calculation of band gaps and densities of states for a wide selection of materials. It also contains, in a natural way, many-body effects missing in DFT, such as dispersion forces important in chemistry, as well as excitations such as spin waves. The Questaal suite furthermore has a new extension to DMFT.

The first day of the meeting involved introductory talks describing the LMTO basis and history of the Questaal package, and gave an overview of the wide range of different properties that can be calculated with the code, including not only GW and QSGW

calculations, but also structural relaxation, fully-relativistic and non-collinear LMTO in the ASA, calculation of magnetic exchange interactions, among many others. As part of the introduction to the Questaal package, the results of a detailed verification exercise for the full-potential LMTO code were presented, demonstrating the accuracy of the code and its relation to alternative implementations of density functional theory.

The organisation of the course for the remaining three days consisted of introductory theory sessions on each of the days, given by the principle code architects and project leaders, followed by tutorial sessions where the participants were guided through exemplary problem cases before ending each day with a "hands-on" session where the code development team were available to assist the participants in working through their own calculations. For the theory sessions, Mark van Schilfgaarde (King's College London), discussed "Comparing Density-functional Green's function methods", Myrta Gruening (Queen's University Belfast) discussed "Many body perturbation theory", while Lorenzo Sponza and Swagata Acharya (King's College London) presented "Interacting Green's functions and DMFT". The graduated approach to teaching the code, from lectures to practical sessions via tutorials, was very well received and within the limited time available many participants were able to complete calculations of direct relevance to their research.

The highlight of the course was the presentation of the newly implemented interface to Kristjian Haule's continuous time quantum Monte Carlo DMFT solver. This interface allows the union of DMFT's powerful ability to treat strong local correlation with the QSGW scheme's accurate description of non-local screening effects. Such GW+DMFT calculations represent the current state-of-the-art in electronic structure calculations for real materials and the step by step introduction to the method given in the workshop helped a little to unravel the mystery of this admittedly complicated method and help pave the way for the more routine use of this technology by the electronic structure community.

Additional information on the Questaal code can be found at https://www.questaal.org/, and the lecture notes on the presentations given at the hands-on course can be downloaded from http://www.ccp9.ac.uk/QuestHandsOn/

Lecturers:

King’s College London: Mark van Schilfgaarde, Swagata Acharya, Pooya Azarhoosh, Scott McKechnie, Dimitar Pashov, Alena Vishina, and Lorenzo Sponza
Daresbury Laboratory: Jerome Jackson
Queens University Belfast: Myrta Gruening and Brian Cunningham

Programme:

Tuesday May 16

12:30 – 14:00 registration
14:00 – 15:00 Theory: *Introduction to LMTO* (van Schilfgaarde)
15:00 – 15:30 Theory: *Validation* (Jackson)
15:30 – 16:00 coffee
16:00 – 18:00 Theory: *Overview of LM/LMF code capabilities* (McKechnie, Azarhoosh, Vishina, Cunningham, Pashov)

Wednesday May 17

9:00 – 10:30 Theory: *Comparing density functional and Greens's function methods* (van Schilfgaarde)
10:30 – 11:00 coffee
11:00 – 12:30 Tutorial & hands-on: *Guided LMF* (Jackson)
12:30 – 14:00 lunch
14:00 – 15:30 Tutorial & hands-on: *Guided LMF optics and LMGF* (Azarhoosh, Vishina)
15:30 – 16:00 coffee
16:00 – 18:00 Hands-on: *Build your own compound* (LM/LMF)

Thursday May 18

9:00 – 10:30 Theory: *Many body perturbation theory* (Gruening)
10:30 – 11:00 coffee
11:00 – 12:30 Tutorial & hands-on: *QSGW calculations* (McKechnie)
12:30 – 14:00 lunch
14:00 – 15:30 Tutorial & hands-on: *QSGW + response* (Sponza, Vishina, Cunningham)
15:30 – 16:00 coffee
16:00 – 18:00 Hands-on: *Build your own compound* (QSGW)
19:00 – 21:30 workshop dinner

Friday May 19

9:00 – 10:30 Theory: *Interacting Green's functions and DMFT* (van Schilfgaarde, Sponza, Acharya)
10:30 – 11:00 coffee
11:00 – 12:30 Tutorial & hands-on: *QSGW + DMFT* (Sponza)
12:30 – 14:00 lunch
14:00 – 15:30 Tutorial & hands-on: *DMFT + response* (Acharya)
15:30 – 16:00 coffee
16:00 – 16:45 Hands-on: *Final questions*