

## Report of the visit by Juerg Hutter

(Max-Planck-Institut fuer Festkoerperforschung Stuttgart).

### Visit of Juerg Hutter to Queen's University, Belfast

Mike Finnis. Belfast

We were interested in advances made by Juerg and the Stuttgart group led by M. Parrinello who work mainly on *ab initio* molecular dynamics. Juerg presented a talk entitled "Gaussian basis sets in large scale condensed matter simulation". This was of technical interest, representing an attempt to develop an *ab initio* code for MD which scales linearly (an "O(N)" method) with the number of atoms. It is a departure from the use of plane-waves as a basis, which has been a characteristic of the Car-Parrinello MD used in Stuttgart up to now. It seems too soon to judge if it will be successful. There are other efforts in this direction, e.g. in Mike Gillan's group at Keele, using an entirely different approach, which appear to be at least as promising. At present, however, the ("O(N<sup>3</sup>") methods are still ahead of the game for routine applications. Juerg is also intimately acquainted with the code we use at Queen's, called FEMD, because he designed and wrote much of the CPMD package within which it now runs. His technical expertise was extremely useful in helping us to improve this code. Together with Ali Alavi, they implemented a block version of the Lanczos diagonalisation method used in FEMD. This change resulted in a greatly improved code, largely because of reducing data movement during execution. Depending on the machine and size of problem, speedups of factors of 2 to 5 have been obtained. This new code is now routinely used in our work.

### Visit of Juerg Hutter to University College London

Andrew Fisher. UCL London

The CCP5-sponsored visit of Juerg Hutter to UCL took place on 30 April 1998. He spent the day in the Condensed Matter and Materials Physics Group and gave a seminar entitled "Large-scale condensed matter calculations with Gaussian basis sets", which was attended by colleagues from the Royal Institution, Imperial College, Oxford and Keele Universities as well as members of the UCL group.

Dr Hutter described his work on applying Gaussian basis sets to *ab initio* calculations using density functional theory. This research was of great interest to the UK groups present, and after his seminar there were extended discussions with Professor M. J. Gillan and his group (Keele, now at UCL, with interests in O(N) calculations using other localized basis sets); with Dr I. Oleinik (Oxford, with interests in modelling of oxides); with Dr A. L. Shluger and his group (interests in modelling processes in oxides and in developing "embedding" codes using localized orbitals);

and with Dr A. J. Fisher and his group (interests in excitations and transport theory). Dr Hutter remained at UCL until the evening, when he left for Cambridge.

This was a valuable visit which brought us up to date with work which is relevant both for fundamental developments in computational algorithms, and for many applications of interest to the UK computational physics community.

### **Visit of Juerg Hutter to Cambridge**

Mike Payne TCM Cambridge

Dr. Hutter's visit to Cambridge was marked by a power cut across most of Cambridge ten minutes before his seminar was supposed to begin. While this would have reduced most speakers to blithering wrecks, Dr. Hutter proceeded to give a blackboard (in blackened room, as the weather was so dull) version of his talk which amazingly managed to convey most of the ideas and methodology of his new computational scheme for performing large scale calculations using Gaussian basis sets. Dr. Hutter managed to speak to a number of people in both the Physics and Chemistry Departments in Cambridge and his 'black in black' seminar attracted a good number of people from Chemistry which is pretty unusual given the vast, in Cambridge terms, distance between the departments. Dr. Hutter's seminar finished just in time for our regular Friday afternoon drinks in the Theory of Condensed Matter Group.

### **Visit of Juerg Hutter to Exeter**

Bob Jones Exeter

Juerg Hutter arrived at Exeter on Monday 4 May and gave a talk to the Theoretical Physics Group on May 5 entitled "Large scale condensed matter calculations with Gaussian basis sets".

These basis sets are also used by the Exeter group of Dr. Jones but primarily in cluster calculations. Dr. Shrivastava's group, who use supercell methods, also attended the talk. He then held detailed discussions with both groups where discussion focussed on the pseudo-potentials and techniques that he uses to perform these large scale supercell calculations and the problems in implementing  $O(N)$  techniques. He left in the afternoon of May 5.

Altogether, the visit was a useful one especially in getting access to the pseudo-potentials used by the MPI group.