

# CCP9 WORKING GROUP

## Minutes of Meeting 8 April 2003 Queen's University, Belfast

Present: James Annett, Matt Probert, Ian Morrison, Stuart Clark, Gillian Gehring, Paul Strange, Tony Paxton, Rex Godby

### 1 Chair's Report

**1. Funding.** CCP9 has about 35k funding from EPSRC for 3 years, from 1 April 2002, therefore we are 1 year into the current grant. We do not currently have a 'flagship project', the last successful one having been the KKR ab initio Bloch wall project (Bristol). Attempts to obtain funding with GW and O(N) projects have both been unsuccessful. Although we can continue for the time being without a flagship project, we should definitely aim to have one in place before the next renewal of our core network funding.

**2. Workshops and Visitors.** Workshops supported over the past year include:

- Symposia at CMMP/CMD in Brighton April 2002
- The International Nanoelectronics Conference, Lancaster, Jan 2003
- Order and Disorder in Solids: Alloys Magnetism and Superconductivity, Bristol, April 2003.
- Workshop on the Bogoliubov de Gennes equations, Bristol, May 2003
- Dynamical Mean Field Theory workshop, Trieste, Aug 2003.

Possible future workshop include "Magnetic Oxides" (Sheffield), and Order N methods (possibly Newton Institute).

We have still had very few requests for travel for visitors. In the proposal we had allocated up to £700 per visit from the USA or Japan and £400 per visitor from the EU. We can spend more per visit if we have fewer visitors than originally planned. If you wish to request funds for a visitor, send an Email to James Annett or Walter Temmerman outlining the reasons for the visit and the expected budget.

**3. Membership.** The working group currently has about 35 members throughout the UK (list on [http://psi-k.dl.ac.uk/ccp9/CCP9\\_Working\\_Group.html](http://psi-k.dl.ac.uk/ccp9/CCP9_Working_Group.html)). We should update the list as appropriate.

**4. Web site.** The group web site <http://psi-k.dl.ac.uk/ccp9> has been updated. In particular we have added a new page listing various electronic structure codes and resources available on the internet. If you would like to add your own code, please send a brief description and a URL link to Walter Temmerman. We plan further updates to the web site over the coming summer.

In particular we want to add a resource page for code developers, modelled on the sourceforge.net site used by many OpenSource software development projects (eg a CVS server, space for uploading/downloading revisions to codes). Other suggestions for the web site are also welcomed.

**5. Brochure.** Mike Allen, chair of the CCP Steering Panel, is preparing a glossy brochure about the CCPs and their recent achievements. Thanks to those who supplied pictures for this. It will be circulated as soon as it is available.

**6. E-science.** James Annett recently attended a meeting with Tony Hey, the national E-science coordinator, together with other CCP representatives. It is proposed to undertake a ‘scoping study’ of the computational needs and expertise of the CCPs to determine how they may best take advantage of national E-science centres and software developed by existing E-science pilot projects.

A number of CCP9 members have led a proposal to the EPSRC E-science initiative based on modelling materials and devices for Nanotechnology (the nanoGRID).

## 2 Future workshops

A number of ideas were discussed, including

- Magnetic Oxides, possibly jointly with the EPSRC CMR Oxides network (Gehring).
- Order N methods, possible at Newton Institute (Gillan/Bowler)
- Symposia at CMMP 2004
- Quantum Impurities, for summer 2004 (Annett).
- Hydrogen storage materials (Morrison)
- Photonics/Optoelectronics (possibly jointly with IoP)
- Many-body perturbation theory (Godby)

Workshop proposers should send a short summary of the workshop objectives and key speakers to James Annett or Walter Temmerman.

Also several possible hands on courses were discussed

- GW and QMC hands on course

- E-science software techniques (eg Globus, Unicore, OGSA). To be organized jointly with E-science experts from the other CCPs, Regional and National E-science centres and relevant UK E-science pilot projects.

### **3 Working Group Membership**

A number of names were suggested for new members to join the working group.

Dr.J.F. Annett, 23 April 2003