

MINUTES OF THE CCP3 WORKING GROUP MEETING

Daresbury Laboratory

Thursday 16th January 2003

Present	Apologies
Dr. AJ Fisher (chair)	Dr. JF Annett
Prof. W Flavell	Prof. D Bird
Dr. A Wander	Dr. J Blackman
Dr. BG Searle	Dr. P Durham
Prof. NM Harrison	Dr. M Finnis
Dr EA Colbourn	Prof. R Godby
	Dr. J Gale
	Dr. S Holloway
	Dr. R Lambert
	Dr WC Mackrodt
	Prof. J. Inglesfield
	Dr. S Crampin
	Prof. G Thornton
	Prof. J A D Matthew
	Dr. C Norris
	Dr. RE Palmer
	Dr. S Parker
	Prof. JB Pendry
	Dr. J Purton
	Prof. R Smith
	Prof. GP Srivastava
	Dr. S Tear
	Prof. P Weightman
	Prof. DP Woodruff

1 Apologies for absence

Apologies for absence were noted.

2 Minutes of the previous meeting (17/04/2002)

The minutes were approved as an accurate record of the last meeting.

Action: AW to install on web

3 Matters Arising

3.1 Joint CCP3/CCP5 Meeting

AF reported on the joint meeting held on Modelling and Simulation of Nanostructures. A report on this meeting is available on the CCP3 web site.

3.2 Vibrational Spectroscopy of Single Molecules

AF and GT have begun to develop this grant. The possibility of broadening this proposal was discussed. In particular the grant will require calculations of vibrational modes to be performed. The meeting felt that this proposal could be extended to include GPS, NMH, AW, Andrea Russell (Southampton), Barbara Montanari (Imperial College) and Andy Horn (Manchester). This would lead to the grant covering areas such as RAIRS, EELS, RAMAN as well as STM activities.

Action: AJF to co-ordinate activity

3.3 Code Training Workshop

The next code training workshop will be held as a satellite of the ESRF user meeting in Grenoble.

4 Report on CCP Steering Panel Meeting

AJF reported on the meeting held in October 2002.

- Mike Allen was keen to raise the profile of the CCP's via creation of 'glossy' publicity material. AJF and AW had prepared and submitted a contribution on behalf of CCP3.
- The CCP e-Science bid was not funded. However, the e-Science Centre at Daresbury is able to provide advice and help with grid software and services to the CCP's. As part of this activity DLV is being 'gridised' in collaboration with the e-Science Centre.
- The CCP web pages have been revamped. The main page can now be found at www.ccp.ac.uk. As part of this process the CCP3 web pages have been overhauled and redesigned. The new pages are available at www.ccp3.ac.uk

5 Flagship Grant

The flagship grant started on 01/01/2003. Dr. Stanko Tomić has been appointed as the PDRA and will start on 03/03/2003. The committee welcomed him in advance.

AW reported on the initial stages of the grant work plan. The first task for the PDRA will be to provide a code release of EXCURV including an interface to DLV in order to utilise its powerful graphics. It is hoped that this will be complete by the end of the year. WF welcomed this plan as the need to run EXCURV on DL based machines has led to problems in the analysis of experiment data.

6 New Grant Proposals

6.1 Clusters Grant

The clusters grant submitted as a Flagship Grant proposal in 2001 was discussed. This grant was based on the combined use of *ab initio* methods, self consistent tight binding theory and empirical models for the study of metals clusters on surfaces. The grant was not funded. The referees comments were in general very positive but included; (i) in general, it is very difficult to parameterise semi-empirical quantum mechanical methods to yield sufficient reliability for modelling such systems, (ii) the code development aspects of the project did not lead clearly to a methodology that would allow the CCP3 community to study this class of system. The working group therefore felt that this grant should not be resubmitted.

However, it was felt that the advent of the HPCx facility now made *ab initio* calculations of such systems possible if suitable initial geometries could be generated. In addition the Daresbury group has worked with Julian Gale at Imperial College to develop a variable charge model of ZnO surfaces. It was therefore proposed that a new grant should be developed based on a combination of density functional theory and modelling with variable charge models (as implemented in GULP). For systems of most current interest - involving surface clusters with many tens of atoms - this requires the development of an order N version of CRYSTAL. It is already apparent from calculations performed with of order 1000 atoms per cell that this is both necessary and feasible. The project will benefit from the previous flagship grant in which analytic energy gradients were implemented by Klaus Doll. The suggested composition of this grant is NMH, MF, Barbara Montanari (Imperial), RML, and GT. The grant could also consider small metal clusters on semiconductor surfaces.

Action: NMH to progress and co-ordinate

6.2 4GLS

WF provided an overview of the current status of the 4GLS project. There will certainly be a need for theoretical developments around the proposed experimental programme on this facility. Given CCP3's role as an SR support CCP, it was felt that we should be taking a proactive approach to the potential needs of this community. WF stressed that many of the proposed experiments involved dynamics including pump probe type experiments. In addition there are many proposals for two photon experiments such as SFG and SHG.

AJF suggested that time dependent DFT was probably the best methodology for tackling problems such as the interaction of high intensity radiation fields with molecules and suggested that CCP3 should consider the development of such methods for surface studies.

Action: AJF to circulate literature on TDDFT

The working group should consider the literature with a view to either organising a workshop or a series of visits in order to progress this subject towards development of a grant proposal.

Action: ALL

There are also opportunities for development of theoretical tools for the treatment of non-linear optics which could be developed.

Action: JEI and SC to explore non-linear optics and report to next meeting

6.3 DIAMOND

There are certainly also theoretical needs around the new third generation facility, DIAMOND, to be constructed at RAL. Again CCP3 should be taking a proactive role in fostering links with this community and it was suggested that a workshop on theory for DIAMOND could be held at RAL to explore possible collaborative opportunities.

Action: AJF to contact CN and PWO to explore possibility of a CCP3/DIAMOND Workshop

7 HPCx

AW reported that the HPCx facility is now operational. CRYSTAL has been ported to the new platform and thanks to the efforts of IJ Bush at DL the code performs very well. Scaling data for a Cr₂O₃ surface modelled as a 2D slab with 700 atoms per unit cell and 14850 basis functions and for the simulation of a protein crystal (crambin, with 1284 atoms per cell, and about 12000 basis functions) were presented. For systems of this size excellent parallel scaling has been achieved allowing 512 processors to be used and an energy force calculation performed in a few hours. The current version of CRYSTAL is installed on HPCx and available to any member of CCP3 who wishes to utilise it.

The UKCP and Materials Consortia grants have been funded in full and both involve electronic structure calculations on surfaces.

There is the possibility that CCP3 could develop and submit a consortium bid for time on the new machine. If any members of the working group have codes or projects that they would like to run on the facility they should contact AW asap who will coordinate submissions and investigate the possibility of forming a new consortium.

Action: ALL

8 DLV Status Report

DLV 2.2 is in beta release and provides the following new features:

- A web interface to the inorganic crystal structure database
- An interface to the current version of CRYSTAL
- An interface to GULP
- The ability to animate phonon modes

The last two items have been used as a teaching package at IC. The materials used are available from NMH. In addition, an interface to the grid is being developed.

9 Other Codes

The LEED package is currently being used to investigate the role of self consistent phase potentials in studies of oxide surfaces. In addition, the photoelectron diffraction package forms the basis of a grant proposal between AW and R Lindsay.

10 Requests for Funding

With the start of the new flagship grant funds are available for visitors, workshops and student bursaries. Suggestions to AW.

Action: ALL

The following requests were received:

- NMH requested 400-00 for his student Miss K Yeowell to attend the IWOX meeting in Japan which was approved. NMH was reminded that students attending conferences should provide a report on the conference for the next newsletter.

Action: NMH

- AW requested 500-00 for a visit by Anne Chaka of NIST. This was approved. The dates will be finalised and circulated to the committee so that arrangements for her to visit other institutions during her visit can be made.

Action: AW

- AJF mentioned that CCP3/CCP5 were planning to further joint workshops as discussed in the April 2002 meeting.

11 Newsletter

The working group felt that the newsletter should be prepared and circulated by the end of March. AW pointed out that there was a lack of contributed material for the newsletter and mentioned that anyone wishing to make a contribution would be warmly welcomed. The following suggestions were made:

- WF to contribute a progress report on 4GLS
- K. Yeowell to contribute a report on the IWOX meeting
- NMH to contribute an article with K. Refson and B. Montanari on the calculation of vibration modes within CASTEP.
- B. Montanari to be asked to contribute a report in the forthcoming SRRTNet workshop on Theoretical Needs of the Biological SR Community to be held in Frascati in February.

- AW to provide a short note on the performance of CRYSTAL on the HPCx facility in collaboration with IJ Bush.
- Stanko Tomic to provide a short introduction to himself as the new PDRA.

Action: WF,NMH,AW

12 Any Other Business

The poor attendance at the current meeting due to clashes with the start of term was discussed. It was felt that the next meeting should be held in conjunction with a conference. The next meeting will therefore be held during ISSC which will be held in Liverpool during June.