

MINUTES OF THE CCP3 WORKING GROUP MEETING

University of Cardiff 29/06/2005

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

1 Apologies for absence

Apologies for absence were noted.

2 Minutes of the previous meeting (17/01/2005)

The draft minutes had some minor typographical errors. The minutes were approved as an accurate record of the last meeting.

Action: AW to correct and install on web

3 Matters Arising

3.1 DIAMOND Interactions

AJF has contacted Colin Norris and arranged a meeting to discuss possible CCP3/DIAMOND interactions.

Action: AJF to continue discussions

3.2 Changes to the Working Group

Lev Kantarovich has agreed to join the working group.

Action: AW to contact and update web site

3.3 Visitors

Gard Röpke will visit Kings/UCL and Daresbury to talk about non-equilibrium statistical mechanics.

3.4 Grant Updates

AJF reported that the 'Single Molecule Spectroscopy' grant had been successful. This includes the administrative funds for CCP3 from Jan 2006 following the termination of the current flagship grant.

Action: AW to install news on web site

AW provided feedback on the LighTnet proposal. The review comments on this grant are very good and a formal announcement of the outcome is expected in September.

In the absence of NMH and MF detailed discussion of the clusters grant was postponed until the next meeting.

Action: NMH and MF to report to the next meeting

The CCP HPCx bid is nearing completion and is expected to be submitted shortly.

Action: AJF to submit science case to AW asap

In preparation for possible future grant submissions we need to update the publications lists, visitor lists and workshop lists.

**Action: ALL submit updated lists to AW. The current
publication list is available via
<http://www.ccp3.uk/Coordination/CCP3/pubs.htm>**

4 CCP Steering Panel Report

Peter Coveney is the new chair of the CCP steering panel. It was announced at the CCP steering panel meeting that there will be a new call for eScience projects that should concentrating on science and it was felt that the CCP's are ideally placed to bid into this call. The total budget is expected to be 9 Million with three projects being funded at a level of around 3 Million. It is anticipated that an outline submission (2 pages) will need to be submitted by September. The meeting agreed that AJF should seek to include CCP3 in any cross CCP bid into this call.

Action: AJF to progress

4.1 Visitor Reports

AW has still to receive reports on visitors from NMH, GPS, JI and SC.

Action: NMH, GPS, JI and SC to provide short reports to AW asap

5 Workshops

It was decided that there were several workshops that CCP3 could organise.

- **Excited States** AW to liaise with RG and organise a two day workshop on excited states for late 2005 or early 2006. This could be held in conjunction with 4GLS activities.

Action: AW and RG to organise

Action: PWe to suggest key experimental speakers

- **Low Dimensional Magnetic Systems** AJF has held discussions with Walter Temmerman who is also interested in this subject. There is clear scope for a joint CCP3/CCP9/PsiK workshop in this area.

Action: AW to liaise with WT and progress. WH suggested as possible CCP3 organisor

- **Growth of Soft Nanostructures** AJF has had discussions with John Harding and there is interest in this topic from both CCP's. The suggestion is that the workshop should be held in early 2006.

Action: AJF to progress

- **Wet Minerals** MW had suggested this as a possible theme at the last working group meeting.

Action: AW to discuss with MW

6 DLV Status Report

BGS reported in the current status of DLV including the release of v2.5 and the current work preparing for v3.0. BGS was thanked for his work.

7 DL_EXCURV Status Report

AW reported on current work on DL_EXCURV. The working group congratulated ST on his efforts so far. The key deliverable from this work is the release of self-consistent phase shifts. Initial testing and validation of possible methodologies is currently underway.

Full details of the DL_EXCURV package are available via

<http://www.cse.clrc.ac.uk/cmng/EXCURV/>

Since the codes release in August 2004 over 100 licences have been issued which is an impressive take up of the new code.

8 AOB

8.1 Student Bursaries

It was suggested that CCP3 should provide student bursares for the ECOSS meeting in 2006 if that takes place. It was agreed that we would provide three bursaries at the level of 150-00. Preference would be given to those presenting work at the conference.

Action: ALL - submissions and a short letter of support to AW if you have a student who wishes to apply

Action: ALL - suggestions for other conferences to support during 2006 to the next meeting

8.2 Date of Next Meeting

It was suggested that the next meeting should be held at UCL in the week following the CCP steering panel meeting. The suggested date is Tuesday 17th January.

Action: AJF to organise room

Action List

1. AW to correct minutes and install on web
2. AJF to continue discussions with Colin Norris
3. AW to contact LK and update working group on web site
4. AW to update latest news on web site with grant success
5. NMW and MF to report to next meeting on clusters grant
6. AJF to submit HPCx science case to AW. AW to prepare and circulate HPCx bid.
7. ALL - submit updated publication lists to AW
8. AJF to progress CCP3 involvement in possible cross CCP eScience bid
9. NMH, GPS, JI and SC to provide shorty visitor reports to AW asap
10. AW and RG to investigate excited states with view to organisation of a workshop
11. Pwe to submit details of key experimental speakers for excited state workshop
12. AW to liaise with WT and WH re low dimensional magnetism workshop
13. AJF to liaise with CCP5 re soft nanostructures workshop
14. AW to liaise with MW re wet minerals workshop
15. ALL - suggestions for conferences to support during 2006 to be submitted for discussions at next working group meeting
16. AJF to organise room at UCL for meeting on 17th January 2006