

MINUTES OF THE CCP3 WORKING GROUP MEETING

University College London 30/05/2007

Present	Apologies
Prof. A Fisher (Chair)	Prof. D Bird
Dr. A Wander	Dr. P Durham
Dr. R Lindsay	Prof. NM Harrison
Prof. P Woodruff	Prof. R Godby
Dr. S Crampin	Prof. DP Woodruff
Prof. GP Srivastava	Dr EA Colbourn
Dr. C Nicklin	Prof. J Blackman
Prof. G Thornton	Prof W Flavell
Prof. R Smith	Prof. J Inglesfield
Miss CL Bailey	Prof. S Holloway
	Dr S. Dhesi
	Prof. W Hofer
	Prof. J Jefferson
	Dr L Kantorovich
	Dr. R Lambert
	Dr. WC Mackrodt
	Prof. JAD Matthew
	Prof. M Finnis
	Prof. C. Norris
	Prof. S Parker
	Dr. S Tear
	Prof. Sir JB Pendry
	Dr. J Purton
	Dr. M Warren
	Prof P Weightman
	Dr. RL Johnson

1 Apologies for absence

Apologies for absence were noted.

2 Minutes of the previous meeting (07/07/2006)

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

Action: AW to install on web

3 Matters Arising

The report on interactions with the Software Engineering Support Project (SESP) was held over to the next meeting.

Action: RS to report to next meeting

4 Chairmanship

Andrew Fisher announced that he would be standing down as Chairman of the project. The committee thanked him for his excellent service. Simon Crampin was elected as the new chair and will take over for the next meeting.

Action: AW to update the web site

5 Visitors

Support for the following visits was agreed;

Karen Holberg will visit UCL.

Action: AF to report on visit to next meeting

H. Idriss will visit UCL and Manchester

Action: GT and RL to report on visit to next meeting

The current flagship project still has visitor money available.

Action: ALL discuss possible future visitors at next meeting

6 Workshops

It was agreed that CCP3 should hold a workshop on spectroscopy of nanoparticles covering electron and vibrational spectroscopies. The meeting will be held in collaboration with LighTneT and Diamond. CCP9 should also be approached as a possible co-organising body.

Action: AW to contact James Annett to discuss CCP9 involvement

Possible speakers include Richard Palmer (Birmingham), Rex Godby (York), Hardy Gross (Free University of Berlin), Paul Sherwood (STFC, Daresbury), Lars Peterson (??), Chris Binns (Leicester), Geoff Thornton (UCL) and W. Hofer (Liverpool).

The venue was suggested as Coesners House and the aim would be to hold the meeting in September.

Action: CN and AW to progress

Action: GT to contact TFSG of the IoP about possible contributions

Action: ALL Suggestions for speakers to be forwarded to AW asap

The project still has funds available for workshops and anyone with ideas for possible meetings should report to the next meeting.

Action: ALL

7 F90 Course Report

The F90 course was held in Edinburgh in April. The training room could only hold 26 people and the course was over subscribed. Feedback from the course had been positive. Given that there was a waiting list for the course the aim should be to re-run the course about the same time next year. It might be possible to upgrade the course to a F2003 course depending on compiler availability at that time.

Action: AW and CLB to organise

There was some discussion about the possibility of holding a course on parallel algorithms and MPI.

Action: AW to discuss with Ian Bush and report to next meeting

8 Flagship Grant Report

AJF reported that the current flagship grant was progressing well. STM-IETS had been implemented within the bSKAN program, and a range of calculations performed with metallic overlayers and individual molecules on TiO₂ (Gilberto Teobaldi, Liverpool and Nikolaos Beglitis, UCL). This complements the experimental work on OH groups on TiO₂ (Gregory Cabailh, UCL). GT, AJF and WAH were congratulated on the work to date.

9 Future Grants

The current grant expires in late 2008 or early 2009 and the committee felt that it was important to begin preparation of a future grant now to ensure continuity of funding. The CCP's are not limited to a single flagship grant and all members of the working group are strongly encouraged to come forward with suggestions and ideas for future projects.

Action: ALL

9.1 CCP1/CCP3 Grant

Huub Van Dam will visit Hardy Gross shortly to discuss possible implementations of TDDFT in the solid state although it is likely that this will require the use of current densities. The working group felt that this was an important topic to pursue and strongly supported the idea of a joint CCP1/CCP3 grant in this area.

Action: AW to progress and report to the next meeting

9.2 VEGAS and MEIS

A grant in support of the MEIS facility had been prepared and submitted into the recent HPC call from the EPSRC. This grant was unsuccessful but will be worked up as a CCP3 bid and resubmitted.

Action: AW to progress and circulate when complete

9.3 SXR

There was a clearly identified need from the Diamond community for work on direct methods in SXR to work in combination with traditional analysis techniques such as ROD. DLV provides a natural platform for the interfacing of these methods.

Action: CN to discuss with AW and Barry Searle

10 DLV & DL_EXCURV Status Report

AW reported that 475 DLV licences have now been issued (215 in the last 12 months) and that 384 DL_EXCURV licences have now been issued with 151 in the last 12 months. Barry Searle and Stanko Tomic were congratulated on their efforts. AW reported that STFC had agreed to continue to provide a small effort in support of the DL_EXCURV code.

11 CCP3 HPCx Bid

This grant had not yet been submitted and needed updating. The working group felt that this should now target Hector.

Action: AW to circulate current version and request updates

12 AOB

AF suggested that A. Michelaides and Mats Persson should be invited to join the working group.

Action: SC (as new chair) to contact and invite

13 Date of Next Meeting

CN reported that Diamond would be keen to host the next working group meeting. It was suggested that this could be held in conjunction with the planned workshop on Spectroscopy of Nanoparticles.

Action: CN and AW to fix dates and venue when the workshop dates are finalised

14 Actions

1. AW to install minutes of the previous meeting on the web
2. RS to report on SESP to next meeting
3. AW to update the web site with details of the change of chairman

4. AF to report on K. Holberg visit to next meeting
5. GT and RL to report on H. Idriss visit to next meeting
6. ALL develop ideas for possible visitors and report to next meeting
7. AW to contact James Annett to discuss CCP9 involvement in workshop
8. CN and AW to progress workshop
9. GT to contact TFSG about possible contributions to the workshop
10. ALL Suggestions for speakers at the workshop to be forwarded to AW asap
11. ALL Suggestions for possible future workshops to the next meeting
12. AW and CLB to organise F90/F2003 workshop in April 2008
13. AW to discuss possible parallel workshop with Ian Bush and report to next meeting
14. ALL to report to next meeting on possible future CCP3 grant and projects
15. AW to progress CCP1/CCP3 grant and report to the next meeting
16. AW to progress and circulate VEGAS grant when complete
17. CN to discuss SXR and DLV with AW and Barry Searle
18. AW to circulate current version of HPCx bid and request updates
19. SC (as new chair) to contact A Michelaidis and M Persson and invite them to join
20. CN and AW to fix dates and venue for next meeting when the workshop dates are finalised