

MINUTES OF THE CCP3 WORKING GROUP MEETING

University College London 17/01/2006

Present	Apologies
Prof. A Fisher (Chair)	Prof. D Bird
Dr. A Wander	Dr. P Durham
Dr. BG Searle	Prof. NM Harrison
Prof. J Inglesfield	Prof. R Godby
Dr S Tomic	Prof. DP Woodruff
Prof. GP Srivastava	Dr EA Colbourn
Prof. MW Finnis	Dr. J Blackman
Dr. M Warren	Dr. S Crampin
Prof. G Thornton	Prof. W Flavell
	Dr. S Holloway
	Dr L Kantorovich
	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
	Dr. J Purton
	Dr. J Blackman
	Prof. R Smith
	Prof P Weightman
	Dr. RL Johnson

1 Apologies for absence

Apologies for absence were noted.

2 Minutes of the previous meeting (29/06/2005)

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

Action: AW to install on web

3 Matters Arising

3.1 DIAMOND Interactions

AJF has contacted Colin Norris. However finding a convenient date or a meeting was proving difficult.

Action: AJF to continue discussions

3.2 Administration

AW to add LK to the mailing list and add details of the grant success to the web pages. JI and GPS both need to provide details of their visitors in a manner suitable for inclusion in the final grant report as soon as possible.

Action: AW to update web site and mailing list

Action: GPS and JI to provide AW with reports

3.3 HPC Grant

AF has provided a section for the CCP3 HPCx bid. AW to edit and circulate to all asap.

Action: AW

4 CCP Steering Panel Report

AF updated the meeting on the last CCP steering panel meeting. The international review of UK research using HPC was on the whole favourable. Issues that were highlighted of concern to the CCP's including training of new graduates.

It was noted that High End Computing Studentships are available via responsive mode grants from the EPSRC. These are four year studentships leading to a Doctorate and to a Master's degree in Computational Science. Details of this scheme are available at <http://www.epsrc.ac.uk/ResearchFunding/FacilitiesAndServices/HighPerformanceComputing/HECTrainingCentres.htm>

In addition, AW and Ian Bush delivered an F90 course in South Africa in 2005. It was suggested that they should repeat this course in the UK badged as a CCP/HPC training event as soon as possible, funded by CCP3.

Action: AW to arrange dates and venue and contact Peter Coveney for permission to call the course a CCP training event

A joint CCP1/CCP5/CCP12 bid on multiscale modelling had been made as the CCP's bid into the latest eScience call. This bid was unsuccessful. There is an opportunity for CCP3 to seek collaborative projects with eScience groups but it is not clear how to progress this. Particular areas that should be considered include computational steering, visualisation, and data storage.

Action: ALL - to provide feedback to the next meeting

JSCR has funded Visnet based at the University of Loughborough and a Sourceforge environment for code development across the CCP's. CCP3 needs to be involved in these process and it was agreed that AW would act as the CCP3 representative on SourceForge discussions.

Action: AW to investigate Visnet and report to next meeting

5 Grant Updates

AW provided feedback on the LighTnet proposal. Contract negotiations are ongoing and we are awaiting details of the level of funding for this project. MF reported that there were no plane to persue the clusters grant. Discussion of any possible future bids arising from the CCP3/CCP9 workshop on 'Topics in Nanomagnetism' were postponed until the next meeting in WH's absence. Following on from that meeting it was proposed that John Jefferson of QinetiQ should be invited to join the working group.

Action: AF to contact JJ

The planned workshop on 'Excited States' has been cancelled due to a very similar meeting being held it Munich in March 2005. It was agreed that CCP3 would provide bursaries for people wishing to attend that meeting.

Action: AW to install details of bursaries on web

There is a clear, growing need for the development of methods of calculating excited states within the UK. This will naturally link to some activities planned for DIAMOND and more strongly couple to experiments proposed for 4GLS. In addition, there is a substantial body of work being performed using table top laser systems. One possible would be the development of TDDFT within the CRYSTAL code. This could be linked to experimental programmes underway including GT's work on photocatalysis using TiO₂.

Action: AW to progress and report to next meeting

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>

6 Workshops

AW reported on the 'Topics in Nanomagnetism' workshop held at DL in November. This was a very successful meeting held jointly with CCP9.

MW reported on progress with the organisation of a workshop on 'Wet Minerals' in collaboration with Keith Refson (RAL).

Action: MW to arrange dates and circulate asap

7 Visitors

Karen Hallberg will visit London and Oxford to discuss work on 1D wires on surfaces. A sum of 500 was allocated for this visit.

Maria Grillo will visit IC and UCL to discuss water on magnetite. A sum of 250 was agreed for this visit.

GPS reported that his visitors had not managed to visit since the last meeting. It was agreed that the sum of 1000 allocated for these visits at the last meeting would be carried forward.

GT reported that Scott Chambers and Ignatias Tsong will visit him this year.

Action: GT to finalise dates and request funds at next meeting

8 DL_EXCURV Status Report

ST reported on current work on DL_EXCURV. To date 125+ licences have been issued for the latest version of the code. Work is progressing well on the self consistent phase shift module which should be completed before the end of ST's appointment. The working group congratulated ST on his efforts.

Full details of the DL_EXCURV package are available via <http://www.cse.clrc.ac.uk/cmng/EXCURV/>

9 DLV Report

BGS reported on the latest contract negotiations with AVS. As a result of this process we are now able to freely distribute DLV to the community. v2.5 of the code is now released and v3.0 will be put on limited beta release in Q2 2006. This will include greatly enhanced project management tools and support for semi-infinite surfaces.

10 AOB

10.1 Web Site

There was some discussion about tools that are available to convert input files between formats. If anyone is aware of such tools they are requested to let AW know.

Action: ALL inform AW of useful tools and links. AW to update web site

In addition AW asked all members of the committee to provide any news, links, conference details etc. to him for inclusion on the web site.

10.2 Chair of the Working Group

AJF announced that he would like to stand down as Chair of the working group and invited suggestions for a new chair.

Action: ALL - forward suggestions to AF asap

Action List

1. AW to install minutes of the last meeting in the web site
2. AJF to continue discussions with CN
3. AW to update web site and mailing list to include LK
4. GPS and JI to provide AW with visitor reports
5. AW to edit the HPCx bid and circulate asap
6. AW to arrange dates and venue for the F90 course and contact Peter Coveney for permission to call the course a CCP training event
7. ALL - to provide feedback on possible CCP3/eScience projects to the next meeting
8. AW to investigate Visnet and report to next meeting
9. AF to contact John Jefferson and invite him to join the working group
10. AW to install details of bursaries to the Excited States workshop on the web
11. AW to progress TDDFT within CRYSTAL and report to next meeting
12. ALL submit updated publications list to AW. The current publication list is available via <http://www.ccp3.uk/Coordination/CCP3/pubs.htm>
13. MW to arrange dates for the Wet Minerals Workshop and circulate asap
14. GT to finalise dates for his visitors and request funds at next meeting
15. ALL inform AW of useful tools and links. AW to update web site
16. ALL to provide AJF with suggestions for a new chair of the project