

MINUTES OF THE CCP3 WORKING GROUP MEETING

Diamond House Harwell Science and Innovation Campus 29/10/2008

Present	Apologies
Dr. S Crampin (Chair)	Dr S. Dhesi
Dr. M Warren	Prof. D Bird
Dr. A Wander	Dr. P Durham
Prof. NM Harrison	Dr. R Lindsay
Prof. DP Woodruff	Prof P Weightman
Dr. M. Read	Prof. A Fisher
Dr BG Searle	Prof. J Blackman
Dr. C Nicklin	Prof. R Godby
	Prof. J Blackman
	Prof. R Godby
	Prof. GP Srivastava
	Dr EA Colbourn
	Prof. G Thornton
	Prof W Flavell
	Prof. R Smith
	Prof. J Inglesfield
	Miss CL Bailey
	Prof. S Holloway
	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
	Prof. A Fisher
	Dr. RL Johnson

1 Apologies for absence

Apologies for absence were noted.

2 Minutes of the previous meeting (30/05/07)

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

Action: AW to install on web

3 Chairman's Report

Simon Crampin welcomed everyone to his first meeting as chair of CCP3. In particular, Dr Mark Read from AWE was welcomed to his first meeting. Andrew Fisher was thanked by the whole working group for his work on behalf of the CCP during his time as Chairman.

The working group was updated on the CCP steering panels that had been held since the last WG meeting. Enhancing awareness of the CCPs has been an issue, and a new glossy PR brochure detailing the work of the CCPs has been prepared and will be circulated - SC thanked those who had contributed material for him to form the basis of the CCP3 content. New review criteria for CCP flagship grants have been established, in an attempt to address the low success rate of code development grants within the peer review system. There was also some discussion of PRACE - the initiative to provide a number of European supercomputer systems.

SC also reported on his involvement on behalf of CCP3 in developing the Materials and Nanoscience case for the Next National HPC Provision (Child of Hector). This science case has been passed to the EPSRC council and signed off. It is now with RCUK.

4 Activity Reports

The CCP has been involved in a number of activities this year;

- The Spectroscopy of Nanoparticles Workshop held with CCP9, Light-net and Diamond in January 2008
- Faraday Discussion on Water in August 2008
- The CRYSTAL Training Course in September 2008

There was some discussion concerning the possibility of re-running the F90 course. The material from this course is available at <http://www.lighthouse.eu/f90.shtml>
If there is sufficient interest this course will be rerun.

Action: ALL - Notify AW of interest in this course

Action: AW - Create link to the course material from the CCP3 website

The working group requested visitor reports from GPS and AF on their recent visitors

Action: GPS and AF to submit reports to AW asap

The working group requested an update on progress with the current flagship grant.

Action: WH, AF and GT to submit to AW asap

Work has been completed on a parallel implementation of the DL_FIND package. The manual is not yet complete but a link will be circulated asap.

Action: AW to circulate relevant link

5 Hartree Centre

AW reported on progress with the proposed Hartree Centre at the Daresbury Science and Innovation Centre. Further details are available at http://www.cse.scitech.ac.uk/events/Hartree_Summary/

6 Science Round Table

MR reported on the work of his group within AWE. The group looks at issues such as radiation damage of materials, actinides, polymers and explosive compounds. Issues include gas diffusion through grain boundaries, radiation damage in filled polymers, and molecular crystals. The group uses everything from first principles simulation up to finite element analysis with codes such as Materials Studio, Castep, DMOL, Gaussian, VASP, GULP and DL_POLY. DPW talked about problems with the Lawrence Berkeley Photoelectron Diffraction Code which is not producing the same results as the German Code from Volker Fritzsche. AW had seen similar issues with the LBL code and his PR_AUGER code. DPW had also experienced problems with the

ease of use of the ROD code for surface x-ray diffraction. There is clearly a need for a new, updated version of ROD. CN was asked to produce a user specification and AW would then seek to develop and implement the required software.

Action: CN to produce user requirements for new SXR code

DPW also reported on progress with the implementation of inelastic scattering in the VEGAS code used for the analysis of MEIS data. There may be scope for an application into the NAG distributed support programme to fund further parallel developments of the VEGAS code.

Action: NMH to circulate details of the NAG DSC prior to the MEIS steering group meeting on 25th November

SC discussed his recent work on Monte Carlo simulations of electron beam induced deposition, and its application to immobilising nanoparticles. The work was producing extremely encouraging results, but outstanding issues remain concerning diffusion and charging effects, which manifest themselves in nanofabrication simulations which predict incorrect dimensions of deposited nanostructures.

NMH reported on a number of areas in which his group is active; molecular crystals, intermediate band solar cells, photocatalysis of hydrogen, defects and Mangelli phases, transparent oxides (with Roger Smith), AlF_3 , solid oxide fuel cells, chromia and peapod carbon nanotubes.

It is intended that a Science Round Table will become a standing item on future CCP3 WG meetings, in order to foster collaboration and identify areas where CCP3 can play a useful role.

7 Grants

The HECTOR proposal has not yet been submitted but will be submitted as a CCP3 flagship grant including the working group costs.

Action: AF to forward details of the last grant to SC

Action: SC to contact contributors to proposal for updated material

The joint CCP1/CCP3 grant of TD-DFT is nearing submission. Hardy Gross is involved as an overseas collaborator and AW was due to hold a telephone conference with Lucia Riening on 7th November to further discuss the proposal.

A CCP3 supported grant on the development of parallel iterative image reconstruction software was submitted with the University of Manchester and Daresbury into the EPSRC HPC Software Development grant call.

8 Medium and Long Term Priorities

Clearly, the CCPs are developing more of an HPC flavour. The proposed CCP3 HECTOR bid is therefore timely. CCP3 also has a long tradition of providing support for users of experimental facilities and it is important that the CCP continues to provide support for software running on all classes of system; from the desk top to high end machines.

9 Publicity

The web site is rather out of date. It will be important to address this by the time the HECTOR grant is submitted. Could all members of the working group review the web site and provide AW with suggestions for updates.

Action: ALL

10 AOB

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

Action: SC to contact and invite

11 Date of Next Meeting

It has tentatively been suggested that the next meeting will be held at the University of Reading during ISSC. Georg Held from Reading has been suggested as a new member of the working group.

Action: SC to contact and invite

12 Actions

1. AW to install minutes of the previous meeting on the web
2. ALL - Notify AW of interest in the F90 course

3. AW - Create link to the course material from the CCP3 website
4. GPS and AF to submit visitor reports to AW asap
5. WH, AF and GT to submit grant report to AW asap
6. AW to circulate link to DL_FIND package asap
7. CN to produce user requirements for new SXR code
8. NMH to circulate details of the NAG DSC prior to the MEIS steering group meeting on 25th November
9. AF to forward details of the last grant to SC
10. SC to contact contributors to proposal for updated material
11. ALL - review the web site and provide AW with suggestions for updates.
12. SC to contact A. Michelaidis, M. Persson and G. Held and invite them to join the working group