

# MINUTES OF THE CCP3 WORKING GROUP MEETING

Daresbury Laboratory

Tuesday 23<sup>rd</sup> September 2003

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Present	Apologies
Dr. AJ Fisher (chair)	Dr. JF Annett
Prof. W Flavell	Prof. D Bird
Dr. A Wander	Dr. J Blackman
Dr. BG Searle	Prof. NM Harrison
Dr. P Durham	Dr EA Colbourn
Dr. M Finnis	Prof. R Godby
Dr. J Purton	Dr. J Gale
Prof. GP Srivastava	Dr. S Holloway
Prof. P Weightman	Dr. R Lambert
Prof. DP Woodruff	Dr WC Mackrodt
Dr. S Tomić	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

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## 1 Apologies for absence

Apologies for absence were noted.

## 2 Minutes of the previous meeting (16/01/2003)

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

**Action: AW to install on web**

## 3 Matters Arising

### 3.1 Vibrational Spectroscopy of Single Molecules

AJF reported on the status of this grant. It will be circulated to NMH and GPS for comments and will hopefully be submitted within the next six weeks. It is intended to include the working group costs for the period following the expiry of the current flagship project into this grant. This will hopefully provide rolling funds for the project.

**Action: AJF to circulate the grant to NMH and GPS for comments**

**Action: AJF to coordinate costings with AW**

### 3.2 Clusters Grant

There was a wide ranging discussion of the possible application areas of the clusters grant which include supported metal particles on oxides, gas phase clusters, semiconductor clusters, magnetic clusters and problems involving the growth and assembly of clusters. The working group felt that it is important that the proposed grant has clearly identified experimental targets.

**Action: NMH and MF to report to the next meeting**

### 3.3 Dynamics and Excited States

AJF circulated material on TDDFT prior to the meeting. The working group felt that the area of dynamics and excited states is a clear target for CCP3 particularly in view of the range of experiments being proposed for the 4GLS facility. CCP3 will hold a workshop on this topic within the next six months (Q2 2004). A working group of WF, AW, MF, RG and PWe was established to drive this forward. The theoreticians need to identify clear targets, and the experimentalists will then suggest relevant speakers to attend.

**Action: WF, AW, MF, RG, PWe**

### 3.4 DIAMOND

It is not clear if there are currently areas of joint interest between CCP3 and DIAMOND. This needs to be clarified before discussions can be taken forward.

**Action: AJF to contact CN following the next DIAMOND SAC Meeting**

### 3.5 Non-linear Optics

As both JI and SC were unable to attend this meeting this discussion was postponed until the next meeting.

**Action: JI and SC to report to the next meeting**

## 4 CCP Steering Panel and the JCSR Review

AJF reported on the JCSR review. JCSR is a subcommittee of JISC and has indicated that a joint CCP bid on software technology developments would be welcome. Robert Harrison from Oak Ridge National Laboratory was asked to perform a scoping study of the CCP's. His report has identified a number of suggestions for focussed projects including:

- A common and extensible framework and technology set for CCP GUIs and data visualisation (possibly integrating current activity in CCP1, CCP3, CCP5).
- Component architectures and other mechanisms for increasing code interoperability and for managing and transitioning legacy codes.
- Establishing a common "SourceForge-like" resource.
- Refreshing the software skills and tools employed by the wider CCP communities including the standards of academic code development.
- The performance of scientific applications on parallel computers and parallel programming tools and paradigms.
- Problem-solving environments and work-flow management (possibly building on joint GUI).

The working group felt that these were all important projects. In particular it was felt that some progress could be made on two items prior to a decision from JCSR on funding - namely the coordination of GUI developments and the establishment of a SourceForge like environment. It was suggested that a cross CCP working group could investigate these options.

**Action: AJF to recommend the establishment of working parties to the CCP steering panel**

## 5 Student Bursaries and Visitor Support

The meeting agreed that in future the following guidelines would be followed when deciding on support:

## 5.1 Visitors

- Visitors to interact with at least two CCP3 centres.
- A report on the visit to be submitted to AW for inclusion in the CCP newsletter as soon as possible after the visit is complete.

**Action: GPS, JI, SC, NMH to provide reports on their visitors for the next newsletter**

**Action: ALL - requests for visitor support to be submitted to AW**

## 5.2 Student Bursaries

- Each working group meeting will decide on a few conferences for which bursaries will be available and set a deadline for requests for funding.
- A total of six hundred pounds will be made available for bursaries to attend those meetings. The expected level of support is 150-200 pounds per student which will allow us to provide 3 or 4 bursaries per period.
- Following the deadline all requests received will be considered and evaluated and funding decided upon.
- Students applying for bursaries should be involved in projects that have at least a tie-in to computational projects.
- Following the meeting, students will be required to produce a report on the conference for the CCP3 newsletter

For the next period bursaries will be available for

- IUVSTA - Venice 28th June - 2nd July 2004
- VUV14 - Cairns, Australia 19th - 23rd July 2004
- ECSCD - Spain, July 2004

The deadline for receipt of requests for funding is 25th February. All bursary requests should be sent to [ccp3@dl.ac.uk](mailto:ccp3@dl.ac.uk)

**Action: ALL**

## 6 Flagship Grant Update

The committee welcomed Dr Stanko Tomić to his first working group meeting. Stanko reported on his first six months of work and was congratulated for the excellent start he has made.

## 7 DLV Status Report

BGS reported on the current status of DLV and announced that version 2.3 will be available within the next month.

## 8 CRYSTAL Status Report

AW reported on the current status of CRYSTAL and presented preliminary results for a 33,000+ basis set calculation of a protein. The MPP CRYSTAL binary is installed on HPCx and any members of the working group who require access to it should contact AW.

## 9 CCP3 HPCx Bid

There was further discussion of a possible CCP3 HPCx bid. Several members of the working group were interested in applying for Class II time to test applications. The relevant forms are available at <http://www.epsrc.ac.uk/hpc>

**Action: ALL - reconsider a possible bid at the next meeting**

## 10 AOB

AJF proposed that Werner Hofer should be invited to join the working group.

**Action: AJF to contact WH and invite him to participate**

AW reported that JG has asked to stand down from the working group due to his impending move to Australia. JG was thanked for his contributions to the project.

**Action: AJF to write to JG and thank him for his contribution**

The next meeting will be held during CMMP in Warwick in April 2004.

## Action List

1. AW to install minutes on web site
2. AJF to circulate Vibrational Spectroscopy Grant to NMH and GPS and liaise with AW over costs
3. NMH and MF to report on cluster grant at next meeting
4. AW and WF to report on dynamics and excited states workshop at next meeting
5. AJF to contact CN regarding interactions with DIAMOND
6. JI and SC to report on non-linear optics at the next meeting
7. AJF to progress the outcome of the JSCR review with the CCP steering panel
8. GPS, JI, SC and NMH to provide reports on visitors for the next newsletter
9. CCP3 HPCx bid
10. Invite Werner Hofer to join the working group
11. AJF to thank JG for his participation with CCP3