

Minutes of CCP9 Working Group Meeting

University of Warwick, Tuesday April 6, 12:30-14:00

Present: Simon Crampin, Volker Heine, Richard Needs, Mike Payne, Paul Strange, Julie Staunton, James Annett (Chair), Emilio Artacho, Ian Morrison, Walter Temmerman (secretary)

1. The chairman presented his report. In this was stressed that in the next 6 months EPSRC proposals need submitting for CCP9 networking and CCP9 flagship.
2. The **renewal for the networking** should aim for a budget of k£ 50 to cover travel for visitors and workshops. Introduce categories for visitors depending on the duration of the visit and consider splitting costs. Contact the visitors beforehand so that we can make sure that the visits will happen. We should take into account in the planning of the workshops that the present Psi-k ESF funding will only last until the end of 2007. Also Psi-k2005 will take place on September 17-21, 2005 in Schwäbisch Gmünd. Therefore have one big CCP9 Conference in 2006 and in 2007 plus a few small ones. Networking costs could also include travel among UK institutions. Should we include help for the Psi-k newsletter? Having a summer student for the web pages was extremely beneficial. Code training days co-funded with CECAM or/and Psi-k could be included in the networking proposal. Possible codes could be SIESTA and the KKR. Also, code development meetings could be funded by the networking grant. The meeting also decided that James Annett should remain the CCP9 Chairman for this renewal proposal. Possible successors for the subsequent renewal proposal included Julie Staunton. For this renewal proposal each member of CCP9 should list 4 papers and a recent highlight.
3. Membership: New names were proposed: Chris Pickard (developer of new CASTEP software), Mike Towler (Royal Society research fellow), David Bowler (UCL), Dario Alfé (UCL), and Andrew Horsfield (UCL). A discussion took place what level seniority CCP9 members had to be. It was decided not to include post-doc, but to accept EPSRC and Royal Society research fellows. It was also decided to circulate the working group list and to perform some weeding of inactive members. A presence at some CCP9 activity in the last 3 years would be required.
4. New Flagship: Walter Temmerman presented a strategy for materials specific calculations for strongly correlated electron systems as a possible new flagship proposal. This proposal would use DMFT ideas to include dynamical correlations in the recently developed local self-interaction-corrected (L-SIC) LSD code. The meeting suggested trying to make the proposal as sexy as possible in terms of scientific applications, and to not emphasize the code development aspects. Also the paradigm shift with Hector should be taken into consideration. Should we publicize the proposal with Hugh Pilcher-Clayton?
5. CCP9 Conference 29-30 November (Daresbury): A discussion on this Conference took place. It was decided to have no parallel sessions and the poster session to be combined with lunch.
6. Psi-k2005 Conference September 17-21, 2005 (Schwäbisch Gmünd): CCP9 should have a presence at this meeting. Maybe invite also some EPSRC people?

7. E-science and Visualisation: James Annett is the spokesperson of this initiative Tony Hey. The budget is provisionally 0.5 M£. The meeting suggested that Ian Morrison and Paul Durham should be asked to form part of the steering group of the initiative.
8. Edinburgh e-science workshop: James reported on a recent meeting of all the CCP chairs at the National e-science centre. He also pointed out the opportunities to hold joint meetings of CCP9 with the e-science centre in Edinburgh.

01 August 2004

Walter Temmerman