

Small Grants for Scientific Activities – workshops

Final Report

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Activity Title: ***Unveiling the impact of HPC in Soft Condensed Matter***

Date: 12/04/2016 (10 am – 5pm)

Highlights of the event

25 participants took part to the workshop. Most of them were senior researchers, but a good number of young researchers (PhD students and postdocs) was also present. After registration, PC welcomed the participants, introduced the scope of the workshop, and acknowledged the sponsors (CCP5 and Royal Society of Chemistry), participants, and co-organisers. The CCP5 logo has been shown in the introductory Powerpoint slide, included in the fliers distributed to the participants, and added to the event web-site.

The event consisted of two main parts. In the first part, the five invited speakers presented their work and highlighted the impact of HPC from different perspectives resulting from their heterogeneous background. In particular, two speakers were academics (Profs Anwar and Wilding), two software (Dr Seaton) or hardware (Dr Gray) developers, and one from a British multinational company (Dr Briquet). At the end of each talk, the chairs (AP, HK, and PC) coordinated the discussion between the speaker and the audience.

The second part of the workshop consisted of a round table discussion, with the participants divided into two groups according to the themes they had proposed to discuss in the registration form. The round table coordinated by PC and AP discussed the impact of cognitive computing in Soft Matter, opportunities for students' training in HPC, challenges in multiscale modelling and impact of HPC resources, and finally the possibility of creating a national Soft Matter consortium to enhance the impact of our broad community. The round table coordinated by MB and HK commented on available funding for training UG students, maintaining simulation codes, software engineering, and centralising hardware resources for the community. Before closing, the two round tables merged and these themes were concisely summarised.

The support of N8 was crucial to arrange the registration of participants and all the technical details of the event (room booking, AV equipment, web-page, fliers, etc). A web-site has been created to promote the event and it is currently enriched with the oral contributions of the invited speakers. The web-page is accessible at:

<http://n8hpc.org.uk/n8-hpc-network-event-unveiling-the-impact-of-hpc-in-soft-condensed-matter/>

Impact

This workshop has brought together senior researchers from the UK interested in understanding the role of HPC in Soft Matter and how the current available HPC software and hardware can support/boost their research. The round table discussion was particularly useful to (1) identify the importance of consolidating the identity of the Soft Matter community in the UK, and (2) reflect on the benefits of creating a scientific consortium of computational scientists working in Soft Matter. This discussion is currently under debate.

Details on expenditure

The amount originally requested was £1,500. However, we were successful to ensure funding from The Royal Society of Chemistry (£700) to cover the travel and accommodation expenses of all the participants. Therefore, we only ask CCP5 to provide a budget to cover the expenses of catering, that is £620. The invoice issued by the catering company can be provided on request.

Details to process the payment

Bank: National Westminster Bank PLC

Sort code: 01-06-57

Account number: 47125160

Account name: University of Manchester General Account

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