



Issue 7 - September 2008

newsletter

contents:

- annual conference
- US Partnership Award
- software repository
- workshops
- Interface special Issue



This years conference venue:
The Yorkshire Museum and Gardens

website:

www.ccpb.ac.uk

chairman's comments



Dear All,

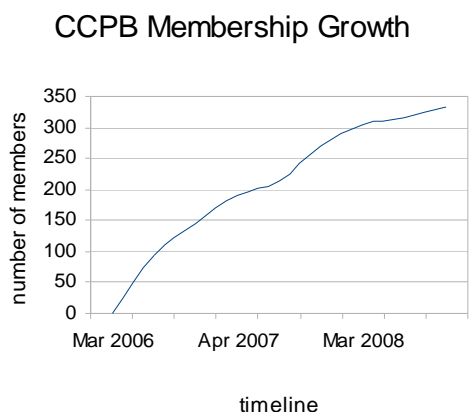
Welcome to the latest edition of the CCPB newsletter. It's hard to believe that CCPB has only been in existence for two and a half years, but the time has come to prepare our application to BBSRC for the renewal of our funding. We have asked for your support for this, and have been delighted with the response - more details about this below. Meanwhile its business as usual – we have a full program of events and activities planned for the autumn and winter. The highlight of course will be the annual conference, which this year will be in York on the 6th-8th January. In addition we are initiating our US partnering programme: you will find details of the scheme to support short training visits to US labs, and we welcome Nathan Baker who is coming over from the Washington University in St Louis to run a specialist 1-day training workshop on electrostatics in biomolecular simulation. The CCPB website now features a software repository, and we will be running a workshop this autumn (final date to be confirmed) in conjunction with the National Grid Service to introduce CCPB members to this large (and “free”!) computing resource. We hope you will be able to make as much use as possible of these opportunities, and look forward to seeing you in York in January for what should be another very enjoyable annual conference.

Charlie Laughton
Chairman

ccpb grant renewal

The current CCPB grant is due to run out at the end of February 2009. The management committee are currently in the process of putting together our grant renewal, which will hopefully see CCPB funded for a further 5 years. If funded, we will continue with all our current events and activities and will be adding even more.

During this renewal process, we recently surveyed our members to find out how well you think we are doing. We would like to thank everyone who responded – we had over 100 responses - and this has helped us immensely with our plans for the next 5 years.



It is clear that the events we have organised over the last few years have been very well received. The survey results show that 89% of those who attended one or more of our conferences said that they had made new contacts by doing so and nine respondents said that new collaborations had resulted.

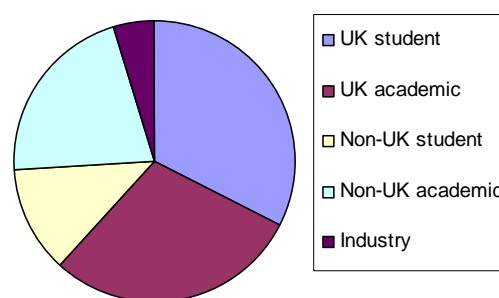
Of those who had attended one or more of our training workshops, nine reported that they had been able to use the training in partial fulfillment of their University's graduate training programme. One respondent who attended the *Analysis of Biomolecular Simulation Data* workshop reported that the techniques learnt had contributed to published research. The most popular of our courses is the *How to set up a protein simulation* course, which has been oversubscribed both times we have run it. Due to this popularity we intend to run this course on a regular basis.

Of those who had attended one or more of the CCPB's Peripatetic Lecturer's events, 95% said it had given them a clearer picture of the latest international research in the area.

These results are all very encouraging and so we will be continuing to run all these events and hopefully adding even more!

We were also very encouraged by the survey results regarding our website. It is clear that this is a much used resource, with almost all respondents indicating that they found the website useful. Almost 90% of respondents used the website to find out about relevant conferences and training courses and 47% had downloaded our workshop training material to help them learn a new technique. This training material is currently available for download 'as is' but in future we hope to turn this data into more user friendly online training.

Current member types



While these core activities will continue, CCPB's aim for the next five year period is to increase the impact of biomolecular simulation on UK science. We will be aiming to do this by an increased focus on bridge-building activities with related areas of experimental science, and increased engagement with other organisations, both in the UK and abroad.

annual conference

We are pleased to announce our third annual conference – Biomolecular Simulation 2009 – which will be held at the Yorkshire Museum and Gardens, from Tuesday 6th until Thursday 8th January 2009. The meeting has a broad theme, highlighted by the research interests of our invited speakers:

- Nathan Baker (University of Washington, US)
- Peter Tieleman (University of Calgary, Canada)
- Paolo Carloni (SISSA, Italy)
- Jed Pitera (IBM Research, US)



(left - right: Nathan Baker, Peter Tieleman, Paolo Carloni, Jed Pitera)

More names will be added shortly to this impressive list of invited speakers, keep an eye on our conference website (www.ccpb.ac.uk/events/conference/) for updates.

Of course we are also looking for offers of oral and poster presentations from our members, details of how to submit your abstract can be found on the conference website. The deadline for abstract submission is 14 November 2008.

Registration is now open with an early bird deadline of 14 November and final registration deadline of 28 November 2008.

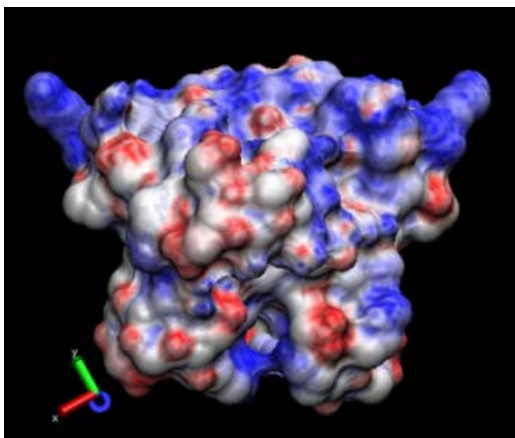
US Partnership Award (USPA)

We have recently been successful in gaining funding to set up links with the National Biomedical Computational Resource (NBCR) in the US. Over the next 4 years we will be involved in 3 activities with our friends in the US, this will involve: interchanging our training activities (see below for details of our first workshop); promoting the exchange of young researchers between the UK and the US (see below for details of our exchange funding); and holding community building and strategic workshops with key researchers from both the US and UK.

USPA Workshop on Electrostatics calculations

We are pleased to announce that Nathan Baker, from Washington University, will be giving the first of our USPA Workshops. He will be demonstrating the use of the APBS software to study the electrostatic properties of biomolecular systems.

APBS (Adaptive Poisson Boltzmann Solver) is a software package for modelling biomolecular solvation through solution of the Poisson-Boltzmann equation (PBE), one of the most popular continuum models for describing electrostatic interactions between molecular solutes in salty, aqueous media. Continuum electrostatics plays an important role in several areas of biomolecular simulation, including:



- simulation of diffusional processes to determine ligand-protein and protein-protein binding kinetics
- implicit solvent molecular dynamics of biomolecules
- solvation and binding energy calculations to determine ligand-protein and protein-protein equilibrium binding constants and aid in rational drug design
- biomolecular titration studies.

The workshop will take place on Friday 9th January at the University of York, as a satellite event to our annual conference, at which Nathan Baker is also an invited speaker. More details on how to register are available from the workshop pages of our website.

CCPB Early-Stage Researcher Short Visits Scheme to the USA

This year, CCPB is running a new funding scheme for UK-based scientists to carry out research for up to two months in leading laboratories in the USA.

Objectives: The purpose of the award is to give young researchers the chance to learn new techniques in biosimulation, and to expand collaborative activity between UK and USA research groups.

Eligibility: The scheme is open to all UK-based scientists. Priority will be given to those at the postdoctoral and postgraduate levels.

Expenses: The award will cover travel and living expenses up to £2000.

To apply for this award, please email Dr Chris Grindon (chris@ccpb.ac.uk) enclosing:

- 1 page research proposal
- 2 page CV
- Two letters of support, one from your UK supervisor and the other from the laboratory in the USA

Deadline: the submission deadline this year will be 21 November, 2008. Winners of the awards will be notified by mid December. The research visit must be completed by the end of 2009.

Up to two awards will be made this round. Awardees will be invited to present their research at the CCPB Annual Meeting and to contribute an article to the CCPB Newsletter.

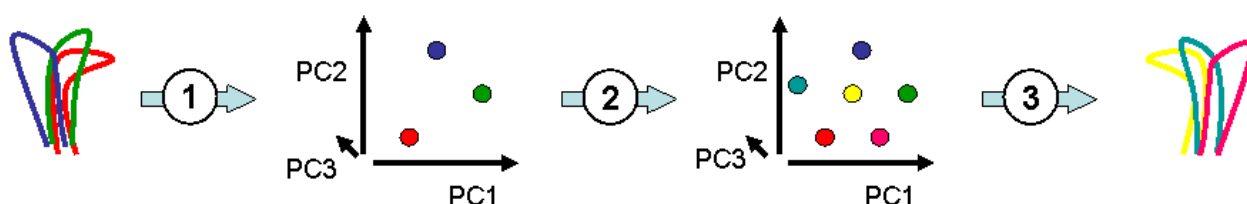
software repository

We have recently set up a software repository to allow CCPB members to share software they have created or developed. This can be anything relevant to biomolecular simulation ranging from small utility scripts to large programs – basically, if you have developed something that has made your life much easier, and could do the same for others, we would be very pleased to know about it!. You may upload it onto our server using the 'upload software' link on the website: www.ccpb.ac.uk/software/ .

All of the software listed on the page is available for download in GZIP-compressed Tar format. Further details about each piece of software, including the License Agreement covering usage and how to install the software can be viewed in the accompany README file.

We hope that you all find this repository useful, and let us know if you can think of ways it could be developed further.

On the web page you will also see a link to the web service COCO (Complementary Coordinates), a project resulting from an informal collaboration between CCPB and CCPN. COCO takes a user's ensemble of structures and through a PCA based method generates further structures that fill 'gaps' in the distribution – the process is illustrated below.



If you too have created a web resource that you are interested in perhaps being hosted by CCPB, please get in touch.

workshops

We re-ran our *How to set up a protein simulation* workshop back in April and again, this workshop was oversubscribed. Due to the popularity of this workshop we intend to make this a regular event on the CCPB calendar running every 12-18 months.

We are still planning to run a *Free Energy* workshop but due to factors out of our control this will now be put off until 2009.

However, before Christmas we plan to run a joint workshop with the National Grid Service to help users get access to their computational resources. We are currently putting together the details for this workshop, which we hope will take place in November, and more information will be available soon.

We are also planning to run a similar workshop next year in association with NAG to help users get access to HECToR, the UK national supercomputer service.

Keep checking the workshop pages of our website for updates on these courses: www.ccpb.ac.uk/events/workshops/ .

interface special issue

A special Themed Supplement of the *Journal of the Royal Society: Interface* on Biomolecular Simulation is about to appear. *Interface* is a cross-disciplinary journal, focusing on work at the interface between the physical and biological sciences.

The issue includes a review of the field of biomolecular simulation by van der Kamp *et al.* (<http://journals.royalsociety.org/content/x567628k61075173/fulltext.html>), freely accessible via the web from the Royal Society. This issue covers a range of biomolecular simulation methods and applications, including atomistic molecular dynamics simulations, coarse-grained MD and combined quantum mechanics/molecular mechanics (QM/MM) methods. The papers include MD investigations of the effects of DNA oxidative damage, and the role of water molecules in ligand binding to Heat Shock Protein 90 (Hsp90); QM/MM studies of enzyme-catalysed reaction mechanisms (including lactate dehydrogenase and aromatic amine dehydrogenase); tests of QM/MM methods for modelling biomolecular interactions; QM/MM methods for modelling electron transfer pathways in proteins; and modelling of DNA-lipid interactions by coarse grained MD, in particular to study the self assembly of DPPC and DPPC/DMTAP lipid bilayers in the presence of a DNA dodecamer.



The *Interface* special issue, organized by Adrian Mulholland, arose from the 2nd Annual CCPB Conference 'Biomolecular Simulation 2008: Frontiers of Biomolecular Simulation' held in Bristol, January 7th-9th 2008. The conference, sponsored by Clearspeed (www.clearspeed.com), highlighted state-of-the-art applications and methodological developments across the whole growing field of biomolecular simulation. There were over one hundred delegates, from industry and academia.

The meeting featured presentations across the range of biomolecular simulation, including talks by Johan Åqvist (Uppsala, Sweden), Inaki Tunon (Valencia, Spain), Siewert-Jan Marrink (Groningen, the Netherlands), Marcus Elstner (TU Braunschweig, Germany), Jan Jensen (Copenhagen, Denmark), Ian Williams (Bath), Mike Sutcliffe (Manchester), Victor Guallar (Barcelona, Spain) and Rebecca Wade (EML Research, Heidelberg, Germany). There were also oral and poster presentations from more junior scientists, in keeping with CCPB's remit. There were also a number of presentations from resource providers, including talks on using the new UK supercomputer, HECToR, for biomolecular simulations.

Poster prize winners were Juan Fernandez-Carmona (University of Southampton) and Leon Harrington (University of Oxford), with runners up of Kitiyaporn Wittayanarakul (University of Strathclyde), Heike Meiselbach (University of Erlangen), Jon Mujika (University of Bristol) and Anna Anastasi (University of Warwick).

barcelona workshop review

On the 10th and 11th July this year, CCPB joined forces with the Barcelona Supercomputer Centre and the Spanish Institute for Research in Biomedicine to run a two-day workshop on biomolecular simulation techniques. Hosted by Modesto Orozco (University of Barcelona) and with thirty six attendees from six different countries, the workshop featured material drawn from CCPB one day specialist workshops (“how to set up a protein simulation”, and “the analysis of biomolecular simulation data”) mixed with material from the Spanish group’s own training courses. The event was a great success and we hope it will be the first of many international training collaborations. We are very grateful to the European Science Foundation (ESF), SimBioMa, and the BBVA Foundation for extra support for this.



other interesting meetings

Other upcoming meetings you may be interested in are highlighted below. A full list can be found on our events webpage: <http://www.ccpb.ac.uk/events/>

Enzyme mechanisms: fast reaction and computational approaches

Manchester, UK

9-10 October 2008

http://www.biochemistry.org/meetings/programme.cfm?Meeting_No=SA088

National Grid Service (NGS) Innovation Forum '08

MoSI, Manchester, UK

4th - 5th November 2008

<http://www.ngs.ac.uk/innovationforum>

MGMS Young Modellers Forum

London, UK

28 November 2008

<http://www.mgms.org/YMF2008/YMF2008.html>

Ab Initio Modelling in Applied Bio-Sciences: Structure, Dynamics & Function

Uppsala University, Sweden

11-12 December 2008

<http://people.sissa.it/~alema/conference/index.htm>

Computer-aided Molecular Design

Jolly beach Resort, Antigua

18-21 March 2009

<http://www.zingconferences.com/z.cfm?c=61>

job vacancies

Postdoctoral Positions in Computational Biophysics

Several postdoctoral research positions are now available in the Theoretical Molecular Biophysics group at the Max Planck Institute of Biophysics, Frankfurt am Main, Germany. The successful candidates will utilize molecular simulations and other computational approaches in the areas of structural immunology, signaling and/or membrane proteins.

Candidates are expected to have a doctoral degree in (bio)chemistry or molecular (bio)physics. A basic understanding of protein structure and physical chemistry is absolutely required. Training and experience with molecular simulation methods are also essential. The following are not required but would be advantageous: the capacity to improve or develop simulation methodologies; scientific programming skills; experience with force-field development via quantum-mechanical and/or statistical methods.

Postdoctoral Position in Bioinformatics and MD Simulation

A postdoctoral position is available in the BMAD group in the Bioinformatics Institute Singapore. The projects combine Bioinformatics knowledge, building models and carrying out MD simulations to work on a range of proteins, establishing mechanisms of action, predicting testable hypotheses which include designing peptide/small molecule inhibitors of specific interactions.

Projects are carried out in close association with experimental groups. The candidate must have good knowledge of physical chemistry and structural biology. Experimentalists from structural biology labs who secretly desire to change careers to more realistic computational studies are encouraged to apply too. Experience with any of the systems we work with (p53, kinases, eif4e) will be an advantage.

- A PhD in related discipline
- Some background in structural biology and biochemistry will be desirable
- Candidates from all fields of natural sciences are encouraged to apply
- A good team player with an interdisciplinary approach is a must

Further details of these jobs and who to contact if you are interested can be found on our jobs webpage – <http://www.ccpb.ac.uk/jobs/>.



contact us

centre for biomolecular science
university of nottingham
university park
nottingham ng7 2rd

email: info@ccpb.ac.uk
tel: 0115 8468544
fax: 0115 8467983