ccp B

# Collaborative Computational Project for Biomolecular Simulation

# What is CCPB?

- officially started in March 2006
- supports biomolecular simulation community in UK
- managed by a team of 9 UK academics and a community development officer
- key mission

"to build and strengthen the capacity of the UK community that makes use of biomolecular simulation methods in its research"

# What does CCPB do?

- annual residential meeting
- specialist training workshops
- annual lecture tour by a prominent overseas academic
- quarterly newsletter to keep biomolecular simulation community up to date
- bulletin board for problem solving

# CCPB Management

**Management Group:**

- Charlie Laughton (Chair)
- Leo Caves (York)
- Jon Essex (Southampton)
- Guy Grant (Cambridge)
- Sarah Harris (Leeds)
- Richard Henchman (Manchester)
- Adrian Mulholland (Bristol)
- Mark Sansom (Oxford)
- Mike Sutcliffe (Manchester)

**Community Development Officer: Chris Grindon**

**International Advisory Board:**

- Nicholas Foloppe (Vernalis)
- Fabrizio Gagliardi (IBM)
- Andrew Leach (GSK)
- Andrew McCammon (Scripps)
- Modesto Orozco (Barcelona)

# Membership

- membership is free
- application form on website
- benefits include
  - quarterly newsletter
  - access to bulletin board
  - free attendance at workshops (UK students and academics only)
  - subsidised registration at annual meeting (UK students and academics only)
- CURRENT MEMBERSHIP: 164

# Website

www.ccpb.ac.uk

- manifesto
- meetings calendar
- newsletter
- bulletin board
- links to software, funding bodies etc.
- details of members research interests to promote collaboration
- job adverts

# Annual meeting

**Biomolecular Simulation 2007**

- theme: Faster, Bigger, Better
- dates: Wed 3th – Fri 5th January 2007
- venue: University of Nottingham
- Five international keynote speakers + proffered papers and poster session
- ‘Technology showcase’
- 80 delegates from 16+ different UK institutions + from US, Portugal, France, Germany, Eire and Spain.

# Specialist training workshops

- workshops are generally hands-on with around 20-30 attendees
- recent workshops:
  - The analysis of MD simulation data
  - How to set up a protein MD simulation
  - reviews on website, including software downloads
- forthcoming workshops:
  - QM/MM simulations
  - An introduction to protein docking

# Other activities

- 1 day meeting as satellite to European Biophysical Society (EBSA) meeting in London in July
  - Modelling single-molecule biophysical experiments
  - Joint with NSCCS and BBS
- The CCPB Lecture Tour
  - Tour of 3 UK universities by a distinguished international scientist
    - '2006 lecturer': Jiali Gao
    - 2007 lecturer: Wilfred van Gunsteren
    - 2008 lecturer: Andrew McCammon

# Supporting Research

- no ‘flagship’ research project
- Approach:
  - Add ‘badge’ and letters of support to appropriate research projects from members
  - Provide opportunities for members’ networking/collaboration
  - Provide a mechanism for disseminating research outputs
  - Provide a repository for community resources

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