# Collaborative Computational Project for Electron cryo-Microscopy (CCP-EM)

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*Leeds, Feb 7th 2013*

# Aims of meeting

- Introduce CCP-EM
- Begin to involve the community (you!)
- Begin the discussion on priorities
- Establish formal structures

| 11:00 | Martyn Winn (STFC) | Welcome to meeting, and introduction to CCP-EM project |
|---|---|---|
| 11:20 | Chris Wood (STFC) | First steps in CCP-EM |
| 11:40 | Ardan Patwardhan (EBI) | EMDB |
| 12:00 | David Bhella (Glasgow) | Case Study 1 |
| 12:30 | All (led by Richard) | 1st discussion |
| 13:00 | | Lunch |
| 14:00 | Ariel Blocker (Bristol) | Case Study 2 |
| 14:30 | Ed Morris (ICR) | Case Study 3 |
| 15:00 | All (led by Helen) | 2nd discussion |
| 15:30 | Martyn Winn (STFC) | Key outcomes, CCP-EM management, CCP-EM constitution, wrap-up |
| 16:00 | | Close |

# Housekeeping

- Lunch at 1pm

- Aim to finish by 4pm

- Travel claim forms
  - return now to me or Chris (with receipts)
  - post later

# Collaborative Computational Projects

Exist to support the computational needs of particular UK science communities.

- Carry out code development projects
- Maintain and distribute code libraries
- Organise training
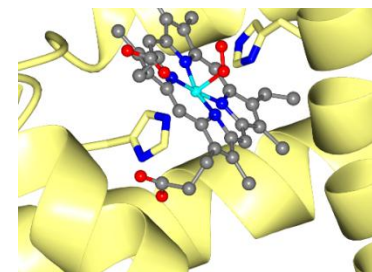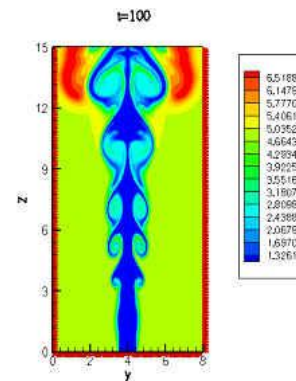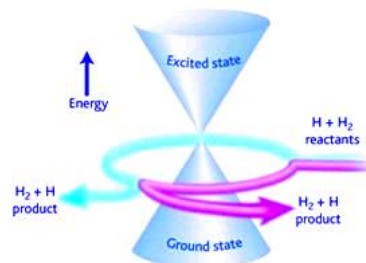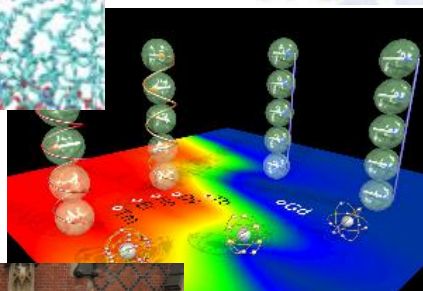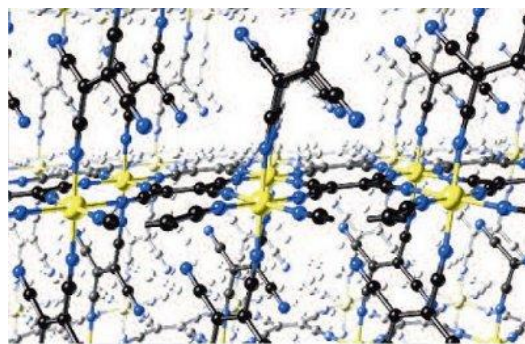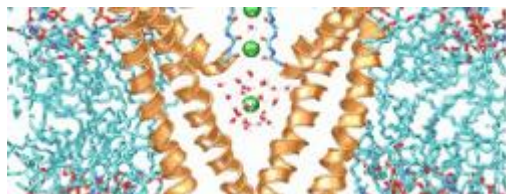- Hold meetings and workshops

First one started in 1977. New ones still being created.

Many (but not all) supported by the Scientific Computing Dept of STFC.

Often division of labour between core activities and research-orientated projects.

Mainly physical sciences, but also some biological



Training always a major part.

# Collaborative Computational Projects

- CCP2: Quantum dynamics in Atomic Molecular and Optical Physics
- CCP5: The computer Simulation of Condensed Phases
- CCP on Computational Electronic Structure of Condensed Matter
- CCP12: High Performance Computing in Engineering
- CCP-BioSim: Biomolecular simulation at the life sciences interface
- Algorithms and Software for Emerging Architectures (ASEArch)
- CCP on NMR Crystallography (Jonathan Yates)
- CCPI: Tomographic Imaging (Phil Withers)
- CCP4: Macromolecular Crystallography
- (CCPN: Macromolecular  NMR)
- CCP-EM: Macromolecular EM

**EPSRC**

**BBSRC** bioscience for the future

MRC | Medical Research Council

EPSRC have specific CCP Programme.

CCP  Steering Panel chaired by Peter Coveney, UCL

# CCP-EM

MRC Partnership Grant:

*"Towards a Collaborative Computational Project for Electron cryo-Microscopy (CCP-EM) and bridging the gaps between structure determination methods"*

Running August 2012 - August 2015.
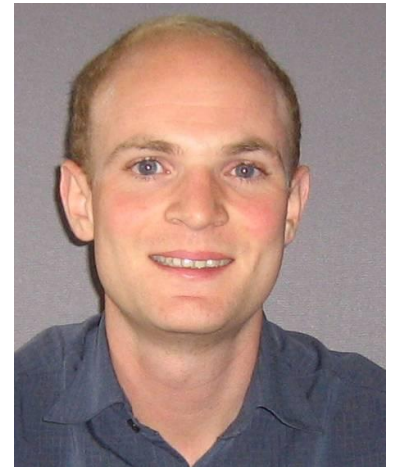
Will fund:

2 developers co-located with CCP4 at RCaH

<span style="color:red">Chris Wood + A.N.Other</span>

1-day discussion workshop in the first year

meetings of Working Groups

3 training schools

1 mini-conference

# CCP-EM

- Build a UK community for computational aspects of cryo-EM. Forum for developing a roadmap for future software developments. Focus for the cryo-EM community to interact with CCP4 / CCPN / CCPBioSim.

- Support the users of software for cryo-EM through dissemination of information on available software, and directed training. Where feasible, usability of specific codes will be addressed.

- Support for software developers, including porting and distribution of software. Coordinate and improve existing software to make it more accessible to practising scientists.

What we will do:

• Provide helpdesk, web site, mailing lists

• Gather requirements from community on gaps in functionality and usability issues

• Develop software library of useful routines

• Repository and redistribution of community codes and scripts

• Address training needs of EM labs

• Facilitate trial use of software packages

• Collaborate on standards

What we won't do:

• Reinvent wheels

Limited resources $\Rightarrow$ we will not write complete and perfect software suite

Options:

• We adopt an existing package as the CCP-EM standard

• We provide an infrastructure (workflows + GUI) on top of existing software

• We provide software that fills gaps, and complements existing software

• We focus on a particular area, such as data management, or validation

• We focus just on user support

# Longer term strategy

- Single-particle vs crystallography vs tomography

- Overlap with X-ray tomography

- Overlap with physical sciences EM

- 3 year Partnership Grant is to establish CCP

- At end, we need to be in position to get funding for a production service.

# Links to CCP4

- Winn, Krissinel involved with CCP4.

- CCP-EM developers co-located with CCP4

- CCP-EM can take technologies / codes from CCP4, and benefit from expertise

- Scientific overlap e.g. in fitting to "high-res" EM maps or "low-res" xtal maps

## CCP-EM ≠ CCP4-EM

CCP-EM should have its own ideas and direction

- Develop in line with EMDB requirements (Gerard Kleywegt, Ardan Patwardhan)

- Collaborate with international community (package developers, EM Validation Task Force, standardisation efforts of Jose-Maria Carazo)

- Interface with Instruct (ESFRI project providing infrastructure for structural biology in Europe)

# Constitution

- Purpose
  - scope of project
- Membership
  - open to all
- Management
  - WG1 / Assembly
  - WG2 / developers group / user forum
  - Executive

- Software licensing
  - Open Source (but which)
- Commercialisation
  - Not now, but later?
- Training
  - Sponsorship rules

- Will set up general mailing list. Do attendees want to be on it?

- Helpdesk. For the moment, email me or Chris.
  - Friendly
  - Helps to build up knowledgebase
  - Software specific help is also available of course

- Working parties
  - CCP-EM data models and standards
  - interface with EMDB