MINUTES OF THE WORKING GROUP 1
MEETING OF CCP4
HELD AT YORK ON JANUARY 4, 2004

Present:

Jim Naismith (Chairman)	St Andrews University
Keith Wilson	York University
Martyn Winn	Daresbury Laboratory
Robert Esnouf	Oxford
Dave Stuart	Oxford
Peter Artymiuk	Sheffield
Randy Read	Cambridge
Lindsay Sawyer	Edinburgh University
Jennifer Littlechild	Exeter University
Simon Phillips	Leeds University
Samar Hasnain	Daresbury Laboratory
Elspeth Garmen	Oxford
Jane Endicott	Oxford
Martin Noble	Oxford
Phil Evans	MRC, Cambridge
Eleanor Dodson	York University
Rick Lewis	Newcastle
Peter Moody	Leicester University
Andrew Leslie	MRC-LMB
Neil Isaacs	Glasgow University
Louise Johnson	Oxford
Katy Brown	Imperial College
Katherine McAuley	Daresbury
Daniel Holloway	Bath
Christine Cardin	Reading University
Richard Pauptit	AstraZeneca
Nick Keep	Birkbeck
Vilmos Fulop	Warwick University
Colin Nave	Daresbury Laboratory
Stephen Prince	UMIST
Miroslav Papiz	Daresbury Laboratory
David Brown	Pfizer
Charles Ballard	Daresbury

Apologies: Ian Tickle

1. Minutes of last meeting

The minutes of the meeting of 3rd Jan 2003 were accepted. There were no matters arising. These minutes (and for previous years) can be obtained from http://www.ccp4.ac.uk/wg/

2. **Chairman's report (see Appendix 1)**

Study Weekend

Airlie McCoy and Neil McDonald were thanked for their organisation of the 2003 Study Weekend.

Anastassis Perrakis and Martin Noble were thanked for their organisation of the 2004 Study Weekend. There had been 394 registrants this year.

We are unable to book Leeds for 2005, and CCP4 staff are looking into a number of possible venues. The meeting agreed that CCP4 staff could be flexible over the precise timing of the Study Weekend, although it was noted that participants from abroad usually needed to stay a Saturday night to get cheap flights.

There has been a request from Chick Wilson that the Study Weekend is moved to run in conjunction with the BCA Easter meeting. After some discussion, it was decided to retain the current time slot.

CCP4 grant

The grant was successfully renewed for 5 years from 1st October 2003. The DL staff were thanked for their help in the grant preparation. The grant funds Harry Powell, Eugene Krissinel, Martyn Winn, Alun Ashton and Maeri Howard-Eales.

Executive

Jim had suggested that he ends his term as Chairman in January 2007, giving the new Chairman time to prepare the next grant for submission in October 2007 (with a start date of October 2008). Thereafter, the Chairmanship will run with 5 year terms. This was agreed.

Other CCP4 posts have a faster turnover, and this was thought to be a good thing. There were no elections this year, but it was noted that Garib's term ended at the next meeting and members of WG1 should consider possible replacements.

Finances

The Executive aim to keep a reserve of between 75k and 150k. Industrial income continues to increase, resulting in a tendancy for the reserve to increase. It was noted that the "reserve" is in fact a yearly contribution from the CCLRC SRD budget, calculated on the basis of previous years' underspends.

Ongoing Projects

The Executive received a report on the progress of the CCP4 Molecular Graphics project "ccp4mg" at a meeting in November. A beta release is planned in the next couple of months, with the release of 1.0 as soon as possible after that. Progress has been good with a solid foundation for future developments, and the Executive recommended funding for an extra 3 years. This was agreed.

Martin Noble's postdoc on ccp4mg began on 1st October.

New Projects

At the full developers meeting in April 2003, a number of concerns were raised. One of these was on IPR and commercialisation. York developers have reached an agreement with the University to enable distribution of code through CCP4. Keith is unable to distribute the agreement itself, but will distribute a summary of the arguments used.

Action: Keith

It was reiterated that users must cite individual authors, as well as the general CCP4 reference, in order to support career progression of CCP4 developers. It was pointed out that members of WG1 acting as referees can help to ensure this happens.

CCP4 needs to address automation. Charles Ballard has submitted a proposal for two posts to develop automated tasks together with the underlying enabling infrastructure. A scientific advisory board (Charles Bond, Airlie McCoy, Tadeusz Skarzynski, Paul Emsley) will ensure that the project is applicable to real-life situations. The automated tasks will include non-CCP4 programs.

Geoff Battye has begun work with Andrew on the Mosflm GUI. There will be an initial release in the next few months, after which they will actively seek feedback from user groups. Geoff will also help with more general promotion of Mosflm, through visits to labs, companies and meetings. (N.B. DL staff have in the past done general CCP4 training visits to groups, and are happy to respond to such requests.)

Maria Turkenburg is being funded part-time to develop documentation, tutorials etc. In particular, she will liaise closely with the automation and mosflm projects.

The Exec have funded these projects on behalf of WG1. The meeting agreed these decisions.

Licensing

The licence has been re-written to be more robust, while retaining the spirit of the previous version. This licence will apply to version 5.0 It has been agreed by the Exec, CCP4 developers, external developers, and some companies. There are distinct academic and commercial version of the licence. Existing academic users do not need to sign again.
We have also confirmed with current contributors our non-exclusive right to distribute their code. Source code banners will acknowledge authors.

Diamond

Jim, Keith and Charles visited Diamond in October. DLS are keen to host CCP4. Jim asked for a costing of the move, to assess affordability. This costing depends partly on deals for individual staff, and the DL staff were asked to begin negotiations with DLS. However, it transpired that DL staff are not permitted to negotiate directly with DLS and all negotiations must go through CLRC management at RAL. Transfer of staff from DL to DLS would come under the TUPE regulations. There are currently no precedents for this, as existing Diamond staff have taken new jobs through open competition.
The plan would be to locate CCP4 staff in the planned Research Hotel.   The Hotel is now likely to be smaller than originally planned, and unlikely to open before 2008. Based on these uncertainties, Jim proposed that there be no move within the lifetime of the current grant. This would also give stability to existing DL staff, and would allow the automation project to run uninterrupted at DL.
Colin Nave presented a paper on behalf of SRD management at DL. The paper argued that the CCP4 group should not be moved for the next few years, due to existing synergies and on-going developments. The longer-term position depends on how plans for the DL Campus develop.

There was a general discussion of possibilities. Siting the core group of CCP4 at a university is still a possibility. It is considered important to keep the core group intact at a single location. The CCP4 grant can be moved if necessary. CCP13 are also considering a possible move.

The meeting agreed that the Exec should continue to negotiate with Diamond on a possible move, and report on progress at the next WG1 meeting. However, the DL staff were to be guaranteed that there would be no move before the end of 2006.

Other funding commitments

CCP4 are funding 5% of a secretary at St Andrews. Any comments can be sent to Neil.

The meeting agreed to renew Keith's position for a further year.

Neil told the meeting that, following meetings with Shanghai and Beijing development groups, there was a strong desire to hold CCP4 workshops in China. Money is available from various sources, and what is needed is people's time.

3. Keith's report (Appendix 2)

Keith gave a report on finances (see distributed documents). The finances are looking healthy. Exec are aiming to bring down the "reserve", see comments above.

CCP4 currently employ 5 staff on the grant, and 15 through commercial receipts. In addition, there is one CCP4-associated person on the EU Temblor grant, one to be appointed on the EU Bioxhit grant, and one on the BBSRC e-HTPX grant. Each CCP4-funded person had filled out a one-page summary of their current and future activities, and these were distributed at the meeting. There will be an All Hands meeting of CCP4 staff early in the year, followed by a series of monthly group meetings. These meetings will aim to keep cohesion between CCP4 developers following the recent expansion.

Keith suggested that Colin Nave act as an ex-officio member of the Exec to provide a link with CCLRC management. This was agreed.

4. Year 4 Diamond beamlines

Andrew described the proposal for a year 4 beamline optimised for long wavelengths. He asked for letters of support by 9th February.

5. AOB

Thanks were given for Jim's work on the grant renewal.

Appendix 1 Chairman's report on behalf of the Executive

1 Study weekend
The first item is to thank last years study weekend organisers Neil McDonald and Airlie McCoy for a very successful meeting.

We also need to thank the otherwise thankless, Martin Noble and Anastassis Perrakis for putting together what looks to be a fascinating program.

The final attendance is 394 (down about 20).

2 Grant
On a house keeping note, the CCP4 operating grant was renewed with flying colours. To re-iterate the grant funds the following for five years

Harry Powell with Andrew Leslie at MRC-LMB for MOSFLM
Eugene Krissinel with Kim Henrick at EBI on new automated methods of analysing structures
Martyn Winn at DL on renewing core libraries and refinement
Alun Ashton providing core programming support
Maeri Howard-Eales secretary
 V5 scheduled for February

3 Executive
The new grant began in October 2003. This means it expires in Oct 2008, which means we will have to renew in Jan 2008, which implies a submission Oct 2007. I suggested by email that we begin to alter the chairman's term of office to reflect the move to a five year term.

My suggestion is that my term will end Jan 2007 giving me a four year term. This arrangement means that if a new chair is elected they have time before writing the renewal. All future terms will be five years with the next running from Jan 2007 to Jan 2012.

4 Finances
Keith will present a detailed update on our position. The Executive aim to maintain a reserve of between 75 and 150K. This absolutely requires we overspend in some years.
Industrial 150 licences, still a year on year increase.

5 Major project: Ongoing

The graphics viewer: The Executive at a full day meeting in November saw first hand the level of progress on the Graphics viewer. The project was funded for an initial three year period which is due to expire around now. A full report of progress in the form of powerpoint will be made available this year. Liz Potterton and Stuart McNicholas have made excellent progress, a viewer is rapidly coming into focus that will be free and have a high degree of functionality. The Executive are mindful of competition from many sources but were absolutely convinced that the CCP4 viewer will be better than anything currently available. Martin Noble has managed to hire a

very talented post-doc in the autumn. The Executive have funded a detailed proposal for a further three years for both Stuart and Liz. It appeared to the Executive that the viewer has been designed very carefully and this strength will now pay off with more visible rapid progress over the next 18 months. The viewer is here and please take time to test it.

6 Major project: New
The Executive met with all CCP4 programmers, grant holders and interested parties in February. This was a very interesting and informative meeting in which strong views were aired. There is a strong feeling amongst some of the programmers who collaborate with CCP4 that the Executive is unaware of the problems facing them and is not properly exercising management. This is a long term issue of what CCP4 is about and there is no easy answer. There will be an annual meeting.

What came out clearly was there is pressing need for CCP4 to get serious about automation. The DL staff indicated a strong willingness to lead this project. Charles Ballard fronted a proposal from the DL staff for a three year period. The Exec has asked Charles Bond (Dundee), Airlie McCoy (Cambridge), Tadeusz Skarzymski (GSK) & Paul Emsley (York) to act as mini science advisory board. This is to try to help the DL staff by acting a sounding board and a filter for suggestions. The initial plan is to set up intelligent tasks which make decisions based on outputs from CCP4 programs. Very quickly after that tasks will be created to interface seamlessly to non-CCP4 programs such as SOLVE, SHELX etc (provided user has appropriate licences).

As part of this effort, we have funded an additional post at MRC-LMB. The aim here is to develop a new GUI for MOSFLM, create a windows version and proselytise. This new person will be able to visit companies /big labs and give training days. The Exec are convinced MOSFLM is one of the best programs available but it needs to be pushed a little by us by making a nicer interface and providing training.

An additional part time post (Maria Turkenburg) will oversee development of tutorials and manuals for CCP4 and assist with MOSFLM.

7 Licence issues
This has absorbed a huge amount of time for little pay off in benefit to the suite. The trigger was our appearance on legal divisions of a company's radar. They 'helped' us re-write an illegal & confused licence (or they would not sign). We have been iterating since then to what we now think a final final licence. En passant we have identified the principal authors and backdated permission to distribute. The new document will hopefully prove to be robust and has the blessing of legal affairs at CCLRC. The Executive has engaged with programmers who contribute to the suite.

8 Diamond
An oral update will be given.

9 Other funding commitments
5% secretary St Andrews
St Andrews summer school
Galashiels workshop

SW workshop
Part time support for GUI for PHASER
Co-funding of BIOXHIT proposal
LIMS development

10 Keith Wilson has been a superb asset to CCP4. The Exec requests a further years contract.

CCP4 WG1 Meeting Jan. 4th 2004

NAME: Alun Ashton, Daresbury Laboratory

PROJECT TITLE: CCP4 core group member and CCP4 LIMS.

2003 ACTIVITIES:
- User and developer support: Ongoing activity, user/developer support rota. Specialist help on Windows and Linux. Administrator for CCP4 Server. CVS repository for CCP4mg, DNA and other developers on request. Web pages CVS, and ftp for main CCP4 project as well as MAXINF and AUTOSTRUCT EU projects.
- CCP4 Package: Assist with releases and new libs mainly with $CPROG and with Linux and windows issues/compilations/binaries.
- CCP4 Publicity: BCA-York, poster, April 2003; AsCA, Australia – CCP4 stand and workshop August 2003; Galasheils Sept 2003; St Andrews Summer School September 2003
- Line Management; Maeri Howard-Eales, Peter Wood till July 2003, Chris Morris since Dec 2003.
- LIMS application - Secured CCP4 funding for further development of LIMS application – MOLE. A number of other applications for resources and involvement in/support for initiatives are also underway.
- LIMS initiative – CCP4 has a key role in data management initiatives both in the UK and throughout Europe. I am personally coordinating an EU initiative – LIMGRID (http://www.ccp4.ac.uk/limgrid/) which with other partners is involved in coordinating resources to produce a data management package for the whole of the structure solution process.

2004 PLANS:
- User and developer support.
- CCP4 Package development.
- CCP4 Publicity.
- Continue with the leading role for CCP4 in data management and the development of the data management application and initiatives.

PRESENT COLLABORATORS: General CCP4 suspects, EBI, OPPF, ESRF (+others on Grenoble Campus),

POTENTIAL COLLABORATORS: UK SPoRT initiatives.........

NAME: Charles Ballard, Daresbury Laboratory

PROJECT TITLE: CCP4 programmer

2003 ACTIVITIES:

Release 5.0 lead by P. Briggs (itanium/linux port)

Initiation of automation project

Study weekend organiser, with Maeri Howard-Eales, at Leeds 4-5 Jan 03

CCP4 staff representative for move to Diamond investigation.

Working with Maeri Howard-Eales on CCP4 finances

Helpdesk support – specialising in Mac OS X, x-windows programs.

Introduced bugzilla for bug tracking during CCP4 release procedure

2004 PLANS:

Bringing automation project up to speed, including recruiting and line managing two additional staff members.

Initial phase of structural solution data model, along with John Ionides, Gerard Bricogne and others (K. Cowtan and E. Dodson ?) [SPINE and BIOXHIT]

Helpdesk support – specialise in Mac OS X, x-windows programs.

PRESENT COLLABORATORS:

POTENTIAL COLLABORATORS:

Tassos Perrakis/Serge Cohen, Steven Ness/Raj Pannu, CCPN/EBI, Peter Briggs

NAME: Peter Briggs, Daresbury Laboratory

PROJECT TITLE: CCP4 (core Daresbury group)

2003 ACTIVITIES:

- **Technical Support** (in rotation with AWA & CCB)
- **Coordination of CCP4 Releases** (currently version 5.0)
- **Update of CCP4 commercial and academic licence** (with KSW, MHE and Jackie Potts/CCLRC)
- **CCP4i Development and Support**
- Continued development of Database Handler, MTZ hierarchical viewer (with Anne
- Baker), MOSFLM-CCP4i (with Harry Powell)
- **New CCP4 Libraries**
- Performed testing & debugging
- **Publicity and Education**
- ACA 2002 (Cincinnati): spoke in CCP4 workshop, manned exhibition stand
- Talks at: Intro to CCP4 (Study Weekend Jan 03), EBI eHTPX-SPINE Data Management meeting (Mar 03), SR User meeting (Sept 03).
- **BioXHIT FP6 Proposal**
- Successfully coordinated CCP4 contribution to BioXHIT proposal (with assistance from MDW and Colin Nave) to fund 1 person to work on data management in CCP4i.
- **Assisted CCB in developing DL-CCP4 Automation proposal**

2004 PLANS:

- **Continue technical support role**
- **Complete release of CCP4 5.0 and subsequent patch releases**
- **CCP4i Development and Support**
  - Continue development of MapSlicer, MTZ hierarchical viewer (with Anne Baker)
  - Investigate development of CCP4I in context of CCP4 Automation project (supertasks, workflow presentation)
- **Publicity and Education**
  - Exhibition and workshop at ACA 2004 (Chicago)
- **BioXHIT**
- Recruit and supervise new staff member to work on Data Management in CCP4i.
- **Participate in CCP4 Automation project** (with CCB)

PRESENT COLLABORATORS: CCP4i: Anne Baker, Harry Powell, Liz Potterton, Eleanor Dodson. Other DL CCP4 staff & externals via technical support.

POTENTIAL COLLABORATORS: CCP4i: Maria Turkenburg; LIMS project (AWA); partners in BioXHIT project & CCP4 automation project

NAME: Martyn Winn, Daresbury Laboratory
PROJECT TITLE: CCP4 core staff

2003 ACTIVITIES:

CCP4 library development.
Extension to MTZ format, and changes to programs to use this.
Work towards 5.0 (incorporate bulk, ncont, pdbcur; polarrfn interface; program extensions; testing; fixes)
Work on e-htpx, especially parallel computing.
Contributions to autostruct, temblor
DL admin, CCP4 admin, miscellaneous form-filling.

2004 PLANS:

TLS / normal modes developments (as promised in grant)
Continued library developments.
Increased use of scripting interface to library, e.g. in ccp4i procedures and in automation schemes.
Data Harvesting (Temblor)
Parallelisation / task farming / parametric applications.
Roll-out other e-htpx advances, e.g. web services.

PRESENT COLLABORATORS: York, Cambridge, CSE @ DL, ESRF

POTENTIAL COLLABORATORS:

NAME: Chris Morris, Daresbury Laboratory
PROJECT TITLE: MOLE
2003 ACTIVITIES: I started work at CCP4 on the 1st December. The aim of the post is to extend the MOLE LIMS following extensive consultation with users and evaluation of the ongoing field trials. Before starting here I was the senior web developer at an ISP, Supanet, with responsibilities including security and training.
2004 PLANS: Continuing the development of the MOLE LIMS. The first stage will be to get it into full working order for use at York, Daresbury, Grenoble, and other sites upon request. Following that will come a review of architectural options to make it metadata driven and customizable, and a new release incorporating updates to the data model, with extensive consultation with EBI and others. Extending the LIMS to support more lab activities will follow, and APIs for automatic data collection and the control of robots.
PRESENT COLLABORATORS: Laboratories in CCP4
POTENTIAL COLLABORATORS: Other protein laboratories

NAME: Maeri Howard-Eales, Daresbury Laboratory

PROJECT TITLE:
Administrator/Executive Assistant (never quite sure!)

2003 ACTIVITIES:

- Co-ordinate the arrangements and operation of the annual Study Weekend. To organise and liaise with other SRD staff, CCB and external Scientific Organisers.

- Act as a co-editor for the Study Weekend edition of ActaD.

- Maintenance of files and corresponding databases for all commercial companies using CCP4.

- Supply financial information on CCP4 at agreed times during the month/year. Continue to keep KSW informed and visit York when required to maintain regular communication.

- Maintain all mailing lists as needed.

- Create a commercial newsletter on an annual basis.

- Development and updating of marketing and publicity material, including CCP4 industrial web pages, as needed.

- Assist other CCP4 group members and attend, where necessary, exhibitions and small meetings to publicise CCP4 activities.

To attend Executive, Working Group 1 and 2 meetings as required and produce minutes of the me publication on web in a timely fashion.

2004 PLANS:
as above as well as the following
- Secure a venue for both 2005 and 2006 Study Weekends.
- Look to produce the 2004 Study Weekend ActaD by June 2004.
- Responsible with Peter Briggs for the co-ordination with PDB to produce a CCP4/PDB workshop at the ACA in 2004.
- Obtain a course on using Quark as well as Photoshop with the idea to re-design CCP4 marketing materials.

PRESENT COLLABORATORS: n/a

POTENTIAL COLLABORATORS:
N/a

NAME: Pryank Patel, Daresbury Laboratory
PROJECT TITLE: EC Contract No. QLR1-CT-2001-00015 for TEMBLOR

2003 ACTIVITIES:

Aims:
- Extend the basic harvesting ideas to allow for complete automatic collection of data for X-ray structure determination.
- Develop tasks in order to handle sequence information.

How achieved:
- 'Data Harvesting Manager' has been written to help user manage harvest files. Can do basic cross-validation of harvest files to check for consistent data. Will also be able to convert files from mmCIF to XML.
- Currently integrating PDB_EXTRACT into suite via 'Data Harvesting Manager' interface. Updated to handle new version of PDB_EXTRACT.
- Begun adding extra code for some CCP4 programs, i.e. DM, to write harvest files containing data items requested by PDB for deposition.

2004 PLANS:

- Continue to integrate PDB_EXTRACT into suite, as well as modifying more of the current CCP4 programs to produce missing data items in harvest files.
- Further develop functionality of the harvesting manager – merging harvest files, communication with EBI deposition centre, etc. Need to look at various methods of communication with databases, e.g. SOAP.
- Cross validating harvest information with original data files (mtz)
- Possible interaction with LIMS project

PRESENT COLLABORATORS: EBI, RCSB

POTENTIAL COLLABORATORS:

NAME: Keith S. Wilson, University of York
PROJECT TITLE: Scientific secretary of CCP4. 20% post funded by CCP4

2003 ACTIVITIES:
1. Regular planning meetings with Daresbury and York CCP4 staff.
2. Preparation of revised Licence (with Peter Briggs). Formal assignment of authorship to CCP4 program suite modules (done by MW).
3. Revised spreadsheet for CCP4 finances incorporating forward look (with MHE and CB).
4. Discussions regarding possible move to Diamond (with JN and CB).
5. Plans for continuation of Molecular Graphics project, and initiation of LIMS and Automation posts (with Daresbury team and LP).
6. Involvement of CCP4 in EC funded and BIOXHIT, with funds coming to CCP4 for eight man years.
7. Meetings with other groups such as SPINE and e-HTPX to try and coordinate activities.

2004 PLANS:
1. Arrange more formal planning meetings with Daresbury, York and other CCP4 staff. This will involve a meeting with al CDCP4 staff and the executive in January or February to discuss the years work and try to attain a more strategic overview.
2. Set up a steering committee for the Automation project.
3. Finalise the Licence discussion and get it sent out with the new release early 2004. The revised Licence, both commercial and academic versions will be posted on the CCP4 web site.
4. Initiate preparation of a new CCP4 program manual. This topic has been on the agenda for some time. Hopefully I will make a start during 2004.

PRESENT COLLABORATORS:
All CCP4 staff and many associates.

POTENTIAL COLLABORATORS:

NAME: Maria Turkenburg, University of York

PROJECT TITLE: 1) Autostruct: tutorials, test data; 2) CCP4 Automation

2003 ACTIVITIES:
Test data for Autostruct website;
Tutorials for CCP4 (HTML/XHTML), as update for tutorial2000;
Update of some CCP4 program documentation;
Update of CCP4 roadmaps;
Some new teaching material

2004 PLANS:
Learn Python;
Incorporate CHART into CCP4/CCP4i directly (with Paul Emsley);
Tcl/Tk tutorials inside CCP4i (templates are ready);
Evaluate crystallographers' use of CCP4i, and their approaches to and protocols for macromolecular structure solution, starting with people in York, in order to facilitate high-througput/automatic structure solution within CCP4;
Update CCP4 MAD tutorial to accurately reflect contents of data for GerE;
More new teaching material (e.g. Atomic Scattering Factor Plots – use of CROSSEC)

PRESENT COLLABORATORS:
Eleanor Dodson, Alun Ashton, Peter Briggs, Harry Powell, Thomas Schneider, Andrew Leslie, Anastassis Perrakis, Clemens Vonrhein, Randy Read, George Sheldrick, Andrea Schmidt, Martyn Winn

POTENTIAL COLLABORATORS:
Paul Emsley, Kevin Cowtan, Charles Ballard, Johan Turkenburg, Jan Dohnalek, others at York

NAME: Fei Long, University of York
PROJECT TITLE: The refinement method for low resolution data, based on the combination of molecule dynamics and fast local minimisation techniques.

2003 ACTIVITIES:

1. Continue to optimise the efficiencies of the existing local minimisation algorithms such as the conjugate gradient and eigenvalue filtering method combined with line minimization techniques in both the Cartesian and torsion angle spaces.

2. Add some new global optimization techniques such as the genetic algorithm to the codes.

3. Search for intelligent algorithms that combine molecular dynamics with local minimization.

4. Start to build a C++ template class library on the global minimization using UML.

5. Test the codes on entries in DICTIONARY.

2004 PLANS:

1. Finish to test codes for DICTIONARY.

2. Test all dctionary entries

3. Start testing codes for X-ray diffraction data especially at low resolution and early stages of structure analysis

4. Including the effects of electrostatic interaction in the codes.

PRESENT COLLABORATORS:

Garib Mushudov, Alexei Vagin

POTENTIAL COLLABORATORS:

Kevin Cotwan, Paul Emsley, Liz Poterton, Stuart MacNicholas and other ccp4 people

NAME: James Foadi, University of York
PROJECT TITLE: Automated Evaluation of Crystallization Trials
2003 ACTIVITIES: From 01/01/2003 to 30/06/2003 I have been working, mainly as an external consultant, for Millenium Pharmaceuticals Inc, based in Cambridge. My main activity during those six months has been the application of molecular replacement techniques to attempt the *ab initio* solution of a protein structure with data at 4 angstroms resolution. The work was under the supervision of Keith Wilson. From 01/07/2003 onward I have started a collaboration with Julie Wilson on the automated evaluation of crystallization trials. My main activity is to create ideas and implement them into a software for the preprocessing of images coming from various robot systems. The present programming language is still Fortran 77, but work has started to convert the software in C.
2004 PLANS: My present contract with CCP4 will terminate on June 30th. I will carry on with the ideation and implementation, as described above. More specifically, I have a project of delving more deeply into various Computer Vision techniques, in order to find with a higher precision the boundaries of a drop in the crystallization trials.
PRESENT COLLABORATORS: Julie Wilson
POTENTIAL COLLABORATORS: Some help from people at the Computer Science department

NAME: Dan Zhou, University of York
PROJECT TITLE: Bayesian Statistics in Twin Problem
2003 ACTIVITIES: I am working with Dr Garib Murshudov on a thesis entitled "Bayesian Statistics in Twin Problem"   1) We have programmed equations to determine the twin fraction more accurately using Bayesian statistics to find the proper weights for the experimental data.   2) The twinning operators for some space groups are derived within the program, and when there are several options, each is tested in turn to determine the correct operator. With the help of Dr Andrey Lebedev we have written a subroutine to extend the detection of possible twin operators to any cell and spacegroup.   3) We have derived the equations needed to add a twinned refinement option to REFMAC5, and have begun to code these.
2004 PLANS: 1) I aim to complete the detwinned program, and to test it thoroughly against a wide range of problems.   2) We will scan the RSCB data bank for structures where experimental data is available, and which have the potential to be twinned to extend our test set of data.   3) We aim to complete the implementation of refinement against twinned data.   4) Write paper and thesis
PRESENT COLLABORATORS:
POTENTIAL COLLABORATORS:

NAME: Liz Potterton, University of York

PROJECT TITLE:CCP4 Molecular Graphics

2003 ACTIVITIES:

In the last year Stuart and I have greatly extended the functionality of the program so that it is nearly ready for release. Particularly I have extended the functionality for analysing structures and written or extended the GUI and interface tools for molecule superposition, display of maps and crystals, creating movies and molecule selection and colouring options. We have put out an initial alpha test version.

Small enhancements to Sketcher (CCP4i).

2004 PLANS:
Release 1.0: intended for Feb.
Release 1.1: mid-2004 improvements to 1.0 - priorities determined by user feedback
but probably enhanced movie interface. Work with Martin Noble and Jan Gruber to include display of surfaces.
Release 2.0 late 2004: Crystallographic model building (not *ab initio*). Incorporate functionality from Paul Emsley and Tassos Perrakis. Interface smoothly to Refmac, evaluation of quality of structure, automatic and manual tools for editing structure.
I will work mostly on the GUI and Stuart will work on algorithms and any new graphics that is required.

Beyond 2004: Kevin Cowtan and Tassos are developing automated *ab initio* methods. MG will do whatever is necessary to support and build on their programs. We will probably still need manual model building tools as well!

PRESENT COLLABORATORS: Stuart McNicholas, Martin Noble (& Jan Gruber), Tassos Perrakis (& Serge Cohen), Kevin Cowtan and Paul Emsley.

POTENTIAL COLLABORATORS: Garib Murshudov

NAME: Stuart McNicholas, University of York

PROJECT TITLE: CCP4 Molecular Graphics

2003 ACTIVITIES: Further work on the Molecular Graphics project to the point of being almost ready for release. My contribution over the year has been to speed up sections of the program. Develop methods for dealing with molecule rotamers easily. Add many methods the the maths library used by the program. Port the program to Windows NT/2000/XP and Mac OS X. The program now runs on these operating systems and Linux, IRIX and SunOS. Added support for many more file formats. Improved clipping planes, depth cueing, line smoothing, text and image overlays. Made many imprvements to Python/C++ interfacing, including vastly simplifying MMDB Python interface. Created framework for making distributable packages for all OSes, eg. self-extracting archives for Windows, RPMs for Red Hat and SuSE Linux.

I also demonstrated the program at the CCP4 Workshop at the ACA meeting in Northern Kentucky.

2004 PLANS:
Release 1.0: intended for Feb.
Release 1.1: mid-2004 improvements to 1.0 - priorities determined by user feedback but probably enhanced movie interface. Work with Martin Noble and Jan Gruber to include display of surfaces.
Release 2.0 late 2004: Crystallographic model building (not *ab initio*). Incorporate functionality from Paul Emsley and Tassos Perrakis. Interface smoothly to Refmac, evaluation of quality of structure, automatic and manual tools for editing structure.

Beyond 2004: Kevin Cowtan and Tassos are developing automated *ab initio* methods. MG will do whatever is necessary to support and build on their programs. We will probably still need manual model building tools as well!

I expect to work mostly on algorithms and the Open GL side of things.

PRESENT COLLABORATORS: Liz Potterton, Martin Noble (& Jan Gruber), Tassos Perrakis (& Serge Cohen), Kevin Cowtan and Paul Emsley.

POTENTIAL COLLABORATORS: Garib Murshudov

NAME: Jan Gruber, Oxford University
PROJECT TITLE: Computational approaches to molecular model building and analysis in CCP4 molecular graphics Suite.

2003 ACTIVITIES:

Looking forward to starting work on this project. Reading some papers, Bought a new computer for Xmas   …

2004 PLANS:

Macromolecular surface representations/Visualisation:

Development/ implementation of fast and stable surface algorithm.

Implementation of algorithm for solving Poisson-Boltzmann equation and visualisation of local electrostatic potential as contours/mapped onto surface

GRID to CCP4MG interface for visualisation hydrophobicity character of surfaces by mapping of local hydrophobicity onto protein surface.

Work towards CCP4MG native hydrogen bonding potential for analysis of protein surface character.

PRESENT COLLABORATORS: Martin Noble, Elizabeth Potterton, Stuart McNicholas

POTENTIAL COLLABORATORS:

NAME: Eugene Krissinel, EBI, Hinxton
PROJECT TITLE: CCP4: *Analysis, fingerprinting and recognition of protein-protein interfaces*

2003 ACTIVITIES:

The mmDB library is now effectively finished and the associated Sbase package has been made available CCP4mg and other interested parties.

The protein matching system, SSM (http://www.ebi.ac.uk/msd-srv/ssm/), is now in a mature state and an XML/Soap interface has been completed. The system is available for distribution via the SSM Download Center at http://www.ebi.ac.uk/msd-srv/ssm/cgi-bin/ssmdcenter . An extensive survey of the literature concerning algorithms and methods for protein protein recognition and protein surface characterisation has been completed. A preliminary software development, "PI_Process" for finding protein interfaces from a PDB file has been written and is under test.

A collaboration with Jacqueline Cherfils cherfils@lebs.cnrs-gif.fr, where the work carried at GIF on protein interactions focuses on 'multispecificity', which is the ability of a protein surface
to recognize different ligands without sequence or structure relationship. This work is using the small GTP-binding protein family as examples. The software, PI_Process will in part use this family and the associated data from Cherfils as a test case.

Three manuscripts have been submitted and are in press:
New CCP4 Coordinate Library as a toolkit for designing the coordinate-related applications in protein crystallography. Krissinel, E.B., Winn, M.D., Ballard, C.C., Ashton, A.W., Patel, P., Potterton,E.A., McNicholas, S.J., Cowtan, K.D. and Emsley, P. *Acta Cryst*. **D,** in press
Common subgraph isomorphism detection by backtracking search E.B. Krissinel & Henrick, K. *Software Practice and Experience* in press
Secondary Structure Matching (SSM), a new tool for fast protein structure alignment in 3D. Krissinel, E.B. & Henrick, K. *Acta Cryst*. **D** in press

2004 PLANS:

To fully develop the PI_Process software into an automatic interface recognitiona and characterisation system with future work to lead to a database and search system for sequence and common interface geometries.

Work will also begin on the sub-project *Chemical-Topology Analysis of Electron Density Maps, Ligands and Protein Structures,* once CCP4's approach to map display and model building software has been decided.

PRESENT COLLABORATORS: CCP4 associated partners and Jacqueline Cherfils (GIF Paris)

POTENTIAL COLLABORATORS:

NAME: Geoff Battye, LMB Cambridge
PROJECT TITLE: Development platform independent GUI for Mosflm
2003 ACTIVITIES: Developing new widget set for Mosflm GUI. Producing a GUI with a user-friendly look and feel. Currently, this has the ability to directory browse, pick spots on images and use these in autoindexing. While the underlying communications code (*i..e* the Mosflm server-client model developed by Graeme Winter) has been retained, the GUI itself has been re-designed with the end-user in mind. It is much easier to get started and has behaviour that is more similar to other modern graphical interfaces.
2004 PLANS: Work will proceed to produce a pre-release version of the GUI by around the middle of the year, which will be suitable for critical evaluation by local users in the LMB and by users elsewhere. All important functionality of the current GUI will be implemented in the new one, *e.g.* modules for autoindexing, prediction, zooming, post-refinement, integration, strategy calculations. Some of these require changes to the Mosflm core code, which will be done by Harry Powell. Once a prototype is available, it is likely that Geoff will demonstrate it at meetings in the Crystallographic community.
PRESENT COLLABORATORS: Andrew Leslie & Harry Powell (MRC-LMB).
POTENTIAL COLLABORATORS: It is likely that some work in conjunction with Graeme Winter (who is the current expert on the Mosflm server code) will take place.

NAME: Harry Powell, LMB Cambridge
PROJECT TITLE: Development and Maintenance of Mosflm
2003 ACTIVITIES: Many bug fixes and general code tidying in Mosflm. Addition of new features including buffered i/o to scratch files (improves performance across Linux NFS networks), exclusion of spots near ice rings for indexing, improved autopicking of an index solution, ellipses on swung-out detectors can now be used for determining beam coordinates. Improved support for new detectors. Produced executable which runs under MS-Windows. Many small changes to help implement automated data integration in DNA project. Suitable output is now produced for Popov's BEST program for intelligent strategy determination. Released version 6.2.3. Updated documentation, helped Maria Turkenburg to produce a CCP4 style tutorial. Helped Pete Briggs in writing a Mosflm integration ccp4i task. Gave talks at several meetings and workshops about Mosflm, data collection and data processing - ACA, AsCA, ECM, BCA, St Andrew's, CCP4 study weekend.
2004 PLANS: More of the same. Mosflm is continuing to develop into the data integration program of first choice. Over 3700 copies of version 6.2.2 have been downloaded from the LMB ftp and http servers. A large number of *ad hoc* changes and improvements will be made when found to be necessary. Two important projects under way currently will be pursued. (1) An initial version of the next generation version of Mosflm (which will use a new GUI written by Geoff Battye) will be released around the middle of the year. (2) The spot positions on the detector will be incorporated in a more robust post-refinement procedure.
PRESENT COLLABORATORS: Andrew Leslie & Geoff Battye (MRC-LMB), Pete Briggs & Charles Ballard(CCP4-DL), Maria Turkenburg (CCP4-York), members of the DNA project (SRS & ESRF). Sasha Popov & co-workers at EMBL, Hamburg. Some interactions with detector manufacturers. Other programmers at MRC-LMB.
POTENTIAL COLLABORATORS: Other members of CCP4 team. Expanding DNA to other synchrotrons (DESY, SLS, diamond).

NAME: Anne Baker (*in absentia,* presented by Airlie McCoy), Cambridge University
PROJECT TITLE: Phaser GUI
2003 ACTIVITIES: Completed GUI for MR component of *Phaser* Tested Phaser in many combinations of input and found many bugs Corrected errors and ommissions in the documentation (documentation released with *Phaser* executable)
2004 PLANS: Release GUI for MR component for *Phaser* (though Cambridge website) Develop and release GUI for experimental phasing component of *Phaser* HTML documentation for *Phaser* Work towards release of *Phaser* in CCP4 5.x   MTZ crystal/dataset selection with Peter Briggs
PRESENT COLLABORATORS: Peter Briggs
POTENTIAL COLLABORATORS: