DARESBURY LABORATORY

# INFORMATION QUARTERLY for PROTEIN CRYSTALLOGRAPHY

An Informal Newsletter associated with Collaborative Computational Project No. 4 on Protein Crystallography

Number 14

April 1985

## Contents




| | | |
|---|---|---|
| **Editor:** | Pella Machin | Science & Engineering Research Council, Daresbury Laboratory, Daresbury, Warrington WA4 4AD, England |
| **Deputy Editor for Imperial College:** | Dr. Alan Wonacott | Imperial College of Science & Technology, The Blackett Laboratory, Prince Consort Road, London SW7 2BZ |
| **Deputy Editor for Birkbeck College:** | Dr. David Moss | Department of Crystallography, Birkbeck College, University of London, Malet Street, London WC1E 7HX |

## Editorial

As you may have noticed, it is some time since the last edition of this newsletter appeared, and it was clearly a mistake to call it the Information Quarterly! Contributions have not been very forthcoming, partly because the latter part of 1984 was filled with international meetings and was generally busy.

I must therefore begin by apologising to those, in particular the York group, who sent articles for this edition of the newsletter relatively early. I am sure that they are still very useful and interesting contributions, though I know the authors are concerned that the information is now a couple of months old.

I would again like to thank those who have contributed to this newsletter and encourage them and all other readers to continue to support it by sending articles (of any length) to me for the next issue, which I hope will follow on schedule in 3 months time.

Pella Machin

21 March 1985

## YORK PROTEIN CRYSTALLOGRAPHY NEWS

Guy Dodson

The protein crystallographers in York have been doing a great deal of travelling over the last four months. Rod Hubbard has been visiting (and we hope it stays that way) Harvard University and Bob Liddington has just settled down from his very active six months in Daresbury. Eleanor and I visited India, New Zealand and Australia and had a wonderful time. There are greetings from Vijayan, Viswamitra, Siv Ramasechan at Bangalore, Kannaw at Bombay, Neil Isaacs, Peter Coleman at Melbourne, Ted Baker at Palmerston North and John and Sue Cutfield at Dunedin. From Poland, Zygmunt Derewenda has reappeared with his family for three months in order to accelerate the T state met-haemoglobin refinement. And Spicek Dauter, also from Poland, will be returning from Gdansk in February. If travel is a good thing and a sign of a healthy laboratory, then York is in excellent condition!

Colin Reynolds will be moving to Liverpool Polytechnic to join John Baldwin's Biophysics Group. We will miss Colin for every reason but we hope and expect to continue collaboration in his new environment. The research plans look very promising with studies on ubiquinone:nucleosome complexes, histones and insulin all ready to begin.

Finally, David Fincham has joined the group as ICL Research Lecturer. David was formerly in the DAP Support Unit at Queen Mary College where much of his work was concerned with the use of the DAP for dynamical simulation of liquids. This type of work lies in the area of interest of CCP5. As this group extends their work to more complicated systems, their interest in graphics is growing and David is organising a workshop for them in the New Year. An example of the application of graphics in this field is provided by a project on which David is currently working in collaboration with Martin Dove in Cambridge. Martin has carried out a simulation study of the transition to an orientationally disordered phase in the crystalline form of sulphur hexafluoride. Now they are working on producing a movie so they can study the dynamical processes involved in this phase transition. David is keen to extend the technique of dynamical simulation to macromolecules, and advocates the closest possible integration between graphics and energy and dynamics calculations.

News from the Graphics Group at York by Rod Hubbard

1. Harvard 84

I spent the summer ( April to October ) working in the Chemistry Department at Harvard University with Martin Karplus' group. The original intention was to learn about molecular dynamics and energy calculations. Although I did pick up quite a bit about these techniques the main result of the trip was a new graphics program which is called HYDRA. On arrival in Harvard I was astounded to find that with two vaxes and two Evans and Sutherlands at their disposal the only programs they had to look at protein structures was FRODO. This is fine for fitting electron density maps and looking at single molecules but is obviously not appropriate for structure comparison or analysis of the thousands of datasets that come from dynamics calculations. So the only techniques available for looking at dynamics was to make a movie ( frame by frame ) or to look at plots of the variations of parameters such as torsional angles etc throughout the trajectory.

This seemed to be ridiculous and so I started to write HYDRA. Its initial construction was designed to exploit the PS300 and allow interactive display and interrogation of dynamics datasets. This is achieved by downloading into the PS300 pictures of many datasets from a trajectory. These can then be viewed by turning a dial or automatically changed by an internal clock. From this initial idea I found that I had to construct a complete new program for structure representation to allow the flexibility and features that are required.

HYDRA stands for Harvard York DRAwing program and is an appropriate name because the program can be considered as a loose collection of heads where each head has particular functions associated with it. ( I could also say that I fancy myself as Hercules but delete *.* is enough

for any mortal to kill the beast ). There follows a very brief outline description of the program.

Central to HYDRA is flexible atom selection and colouring which should allow any choice of atoms and colours to be specified. Different bonding algorithms are available so that for example such diagrams as CA plus side chain can be created. Also I have incorporated a hydrogen bond generator so that hydrogen bonds can be displayed for the atoms selected. This feature is particularly useful for looking at and rationalising protein structures.

So far there are ten heads in HYDRA.

CHAT

Like in FRODO this is the part of the program where the global parameters are set.

MAIN

In this head one dataset can be displayed and interrogated.

COMPARE

In this head two datasets can be compared with interactive and flexible nomination of atoms to be used in least squares overlap and various visual cues for the atoms chosen for overlap and reporting the "goodness of fit".

MOLCUL

This head is at present the same idea as in FRODO, that is generating background objects. Currently dot and contoured surfaces, colouring and radius determined by a fourth parameter and flexible labelling is supported.

CHARMM

An extremely narrow interface exists to CHARMM, the macromolecular

mechanics package written at Harvard ( for energy calculation, minimisation, dynamics, normal mode analysis, modelling and structural analysis ).

MOVIE

This head contains all the commands to allow movies to be made in which the ps300 is driven by a script.

DATA

A data interface so that various types of formatted files can be converted and used in HYDRA.

RASTER

This head is the most recent addition and allows shaded pictures or stick diagrams to be drawn on a raster device.

DYNAMICS

This is the head for looking at multiple datasets such as from a dynamics run, but could easily be any other series of "identical" files.

MODEL

Work is in progress on this head which will allow interactive modelling ( similar to FBRT and TOR hopefully with some of the restrictions of FRODO lifted ) with continuous distances and energy evaluation. This part of the program will be developed further when I return to Harvard early next year.

This is only a brief description. At the moment the program is not ready for general release - mainly because it is likely to change violently over the next 4 months and the documentation is incomplete.

2. Other News

While at Harvard I saw a lot of the work of the groups of Bill Lipscomb, Steve Harrison and Don Wiley. Don Wiley's studies on haemaglutinin in particular seems to be entering an exciting phase as he

now has 30 - 40 mutants ( NOT engineered ) and is starting a study to correlate their biology and structure with the changes in sequence.

Also while in the States I went to San Diego ( courtesy of Spectragraphics ) to work for a few days on the Spectragraphics. It is actually quite a nice graphics device for many applications except fitting electron density maps where its vector drawing speed means it is way behind the PS300. Apart from a few bugs ( hopefully now fixed ) that I found in the system it is very easy to adapt programs to run on it.

Rod Hubbard
7/12/84

## Biological Structures Group Autumn Meeting
12th November 1984

The Biological Structures Group of the BCA held a very successful one-day autumn meeting at Birkbeck College, London on the subject of Position Sensitive Electronic Detectors. The meeting was organised by Peter Lindley and John Helliwell. Papers were presented on detectors and their application in single-crystal studies, small-angle- and fibre diffraction and time-resolved studies at both conventional and synchrotron radiation sources.

Single-crystal work requires the highest spatial resolution two-dimensional detectors; it also needs the most elaborate software. The two types of detectors which are in current use are television systems, such as the one in use in the commercially available FAST diffractometer, and multi-wire chambers. The principles of the former were described by Arndt; Papiz and Helliwell reviewed preliminary results obtained with the FAST diffractometer now installed at the SRS.

The full benefits of single-crystal area detector diffractometers are realised only with software which can predict exactly when and where diffraction spots appear on the detector as the crystal rotates, and which can then carry out a profile analysis of the spots. Two approaches to these problems were described by Thomas, for the FAST diffractometer, and by Durbin, for the Xentronics multi-wire chamber installed at Harvard. Bartels concentrated mainly on the equally important problem of determining the initial orientation of the sample.

Fourme described the multi-wire detector with a spherical drift space which has been in use for some time at LURE. An improved detector was being commissioned; the area-detector diffractometer is intended largely for tuned-wavelength work.

Small-angle studies generally allow the spatial resolution requirements to be relaxed somewhat; many applications only need one-dimensional linear detectors. The biggest problem is often that of the very high counting rates which arise, especially at SR sources. Bordas reviewed the general problems in this field. Mochiki gave an account of a gas-filled linear position-sensitive detector which works in an analogue or integrating mode and, therefore, does not suffer from the same counting-rate limitations as a true counter.

Very challenging problems are now being tackled, especially at SR sources, which involve time-slice one- and two- dimensional data collection on muscle and other fibres, often associated with the simultaneous measurements of other physical quantities such as a stretching force. Faruqi described some of the muscle work which is being carried out at Daresbury and at DESY, and Nave described the multi-wire area detector which has been developed for this type of work at the SRS.

There was an interesting trade exhibition at which position-sensitive detectors from several manufacturers were on display. The well-attended meeting demonstrated the general interest among crystallographers at large in the use and application of the new devices; the audience was by no means confined to detector specialists or even those specifically concerned with biological structures.

U.W. Arndt

# SRS Timetable information

Gordon Locke-Scobie (Daresbury Laboratory)

Experience has shown that printed SRS-timetables sent out some weeks before a cycle starts quickly become out of date. Typically Protein Crystallography (PX) users have many short beam line allocations, for example 3 shifts is common, thus timetable changes are invariably relatively complex and are important to many users. Thus a computer readable timetable that was easily read by users and easily updated by a PX manager was suggested.

SRSINFO is a menu driven program which displays up to date beamline timetable information on screen, specifically for the Protein Crystallography group. It has recently been installed on the DLVB VAX 750 computer at Daresbury Laboratory (DL). SRSINFO provides options to view a long term general SRS timetable, a detailed timetable of the current SRS cycle and a detailed timetable of the next cycle. It also has options to view "News-items" and a self-help facility.

Each PX-user group has been provided with a username on DLVB as well as directions on how to log on from remote sites. SRSINFO is automaticlly invoked each time a user Logs on, and the most recent "News-Item" automatically displayed. Thus each user group is able to quickly gain access to up to date timetable information.

Although the primary function of SRSINFO was to display timetable information, the opportunity was taken to provide more general information, thus a "News-Item" facility was included. This facility allows a PX-manager at DL to give short textual messages that can be read by each other user group.

Timetable and News Item information is stored in several text data files, therefore several programs were introduced to enable a PX manager to update these files. There is a program to produce a blank table (including correct dates) for detailed timetable files. This process produces a text file with 3 separate columns marked off. The first column contains day, date and shift information. The second and third columns are left blank and are intended for port 7.2 and port 9.6 allocations (these two ports are used by PX-users). The VAX EDT editor, after having several key functions redefined, makes a passable table editor and is used to fill in, or alter information in these columns. Also a simple news file editor has been written to delete and input news items.

# Current Computing Work in Protein Crystallography at Birkbeck College

D. S. Moss
March 1985

The following notes indicate the scope of the computing work on proteins being carried out by the research groups in the Labortory of Molecular Biology. The names quoted are only those of people who are most directly concerned with the computing work. Machines used are the ULCC Amdahl V8 and Cray 1, the Daresbury AS 7000 and the College VAX 11/750.

## Aspartic Proteinases

(Frank Watson, Galib Khan, Ian Tickle)

Several aspartic proteinases (36000 daltons) are in various stages of structure determination. The enzyme from the chestnut fungus endothia parasitica has been refined to 1.9Å and mucor pusillus enzyme is currently in the early stages of refinement.

The mammalian enzyme hog pepsin is being studied by molecular replacement. Cross rotation functions are being computed using the refined enzyme as search fragments.

## Hormones

(Anne Cleasby, Anne-Marie Treharne and Jasmine Tickle)

Proinsulin (9000 daltons) is being studied by molecular replacement in order to determine the position of the molecular two-fold axis relating the dimer components. Isomorphous replacement is also progressing.

The cyclic hormone oxytocin (nine residues) has been refined in several crystal forms, including structures showing disorder at a disulphide bridge.

Isomorphous replacement work is also being carried out on neurophysin and nerve growth factor.

## Molecular Graphics

(Janet Mahoney, Lawrence Pearl, Andrew Hemmings)

Program development for surface representation and energy calculations is underway.

## Plasma Proteins

(Beatrice Gorinsky, Susan Bailey)

A 3.5 Å map of the iron binding protein transferrin (78000 daltons) has been calculated using three isomorphous derivatives. The molecule consists of one polypeptide chain and consists of two domains. Electron density of each domain has been isolated and the position of the suspected two-fold axis relating the domains is being calculated in the crystal space.

## Molecular Dynamics of Ribonuclease

(Brendan Howlin, Gillian Harris and Alan Pevy)

A 24 ps molecular dynamics simulation of a unit cell of ribonuclease has been carried out and the results are being compared with results of an X-ray refinement of side groups. Diffraction data on a dinucleotide complex are being collected to high resolution in order to study in detail the effect of liquid binding on enzyme mobility.

## Eye Lens Proteins

(Huub Driessen, Helen White, Daruka Mahadevan)

X-ray structure determinations of the β and γ crystallins (20000-32000 daltons) are being carried out. γ-II crystallin is being refined at 1.5Å resolution and its structure has been used to solve γ-IV crystallin using molecular replacement. The latter is being refined at 2.3Å resolution. The structure determination of a β-crystallin with four molecules in the asymmetric unit is in progress using both isomorphous and molecular replacement.

## Protein Structure Prediction

(Janet Thornton, Willie Taylor, David Barlow)

Techniques for the analysis and prediction of protein structures are being developed on our College VAX 11/750 and PDP 11/60 computers. Templates for use in structure prediction are being developed.

## Protein Data Base Design

(Mike Sternberg, Jane Nyakavin)

Collaboration with the SERC Protein Engineering Club and Leeds University is taking place in order to establish a database of protein sequence and structure for use in modelling and prediction.

Work with the Imperial Cancer Research Fund on use of PROLOG in Expert Systems is also taking place.

# MOLECULAR REPLACEMENT MEETING

Pella Machin (SERC, Daresbury Laboratory)

CCP4 organised a meeting on the Molecular Replacement method, which was held at Daresbury in February 1985. We are indebted to Eleanor Dodson who suggested the topic and who was instrumental in the subsequent organisation. Approximately 85 delegates attended the meeting including several European participants.

As well as giving an introduction to the theory of the technique, speakers presented details of many case studies, which helped to highlight the practical aspects involved in obtaining a meaningful result using molecular replacement. The programme of the meeting is given here and proceedings will be issued in due course.

We are grateful to all those who contributed and attended this discussion meeting, for helping to make it a very timely, and profitable 2 day meeting. As well as helping to illuminate molecular replacement, the meeting served as a useful forum for informal discussions amongst protein crystallographers.

Science and Engineering Research Council
Daresbury Laboratory

MOLECULAR REPLACEMENT
TWO-DAY MEETING: 15-16 FEBRUARY, 1985

PROGRAMME

FRIDAY 15 FEBRUARY

| | | | | |
|---|---|---|---|---|
| 10.45 | Transport leaves Lord Daresbury Hotel for Laboratory | | | |
| TIME | TOPIC | SPEAKER | | CHAIRMAN |
| 11.00-11.30 | COFFEE | | | |
| 11.30-13.00 | Theory Overview | | | G Dodson (York) |
| | Introduction | G Dodson (York) | | |
| | Introduction to Rotation and Translation Functions | D M Blow (Imperial) | 40 mins | |
| | Symmetry problems of rotation function | D S Moss (Birkbeck) | 40 mins | |
| | Relationship between Eulerian and spherical polar co-ordinates | P R Evans (MRC Cambridge) | 10 mins | |
| 13.00-14.00 | LUNCH | | | |
| 14.00-15.30 | Translation Function | | | D M Blow (Imperial) |
| | Limitations of a rotation function and a translation function | W G J Hol (Groningen) | 30 mins | |
| | Translation function variants | I J Tickle (Birkbeck) | 30 mins | |
| | Molecular replacement and the crystallins | H Driessen (Birkbeck) | 30 mins | |
| 15.30-16.00 | TEA | | | |
| 16.00-17.30 | Case Studies | | | E J Dodson (York) |
| | Problems of applications and general rules of thumb | E J Dodson (York) | 30 mins | |
| | 6PGDH from Bacillus stearothermophilus | P Carr (UMIST) | 10 mins | |
| | Gramicidin | M M Harding (Liverpool) | 10 mins | |
| | PFK | P R Evans (MRC Cambridge) | 10 mins | |
| | Multi-dimensional search methods | D. Rabinovich (Weizmann Inst.) | 20 mins | |
| 17.45 | Coach leaves Laboratory for Lord Daresbury Hotel | | | |
| 19.30 | Dinner in the 'Bridge Room' at the Lord Daresbury Hotel | | | |

SATURDAY 16 FEBRUARY

| 08.40 | Coach leaves Lord Daresbury Hotel for the Laboratory | | | |
|---|---|---|---|---|
| TIME | TOPIC | SPEAKER | | CHAIRMAN |
| 9.00-10.30 | Real Space Techniques | | | |
| | Application of Patterson search methods in citrate synthase, chymototrypsinogen and c-phycocyanin | R Huber (MUnich) | 45 mins | A C T North (Leeds) |
| | Real space v reciprocal | M Buehner (WUrzburg) | 45 mins | |
| 10.30-11.00 | COFFEE | | | |
| 11.00-12.30 | Case Studies and Subsequent Refinement | | | |
| | Phase extension by density averaging: Haemacyanin | W G J Hol (Groningen) | 30 mins | M Adams (Oxford) |
| | A new approach to molecular replacement and angular correlation in reciprocal space | R Karlsson (Basle) | 30 mins | |
| | Corels - how rigid is your molecule? | A Leslie (Imperial) | 30 mins | |
| 12.30-14.00 | LUNCH | | | |
| 14.00-15.30 | Refinement of haemoglobin | Z Derewenda (York) | 30 mins | T L Blundell (Birkbeck) |
| | Discussion session | T L Blundell (Birkbeck) | 60 mins | |
| 15.30-16.00 | TEA AND CLOSE OF MEETING | | | |

8502-84/525

# Calculation of the Polarization State of the X-ray Beam at the Sample on the SRS Wiggler PX 9.6 Station

by M. Z. Papiz (Physics Department, Keele University)
and J. R. Helliwell (SERC, Daresbury Laboratory)

The protein crystallography station (9.6) on the wiggler beam line has now been in operation for over a year. The installation and commissioning of a focussing pre-mirror, in December 1984 has emphasized the need to know oscillation film polarization factors more accurately.

An additional complication is that owing to the variety of project requirements there has not been a standard monochromator wavelength setting for the station; monochromatic data have been collected over the wavelength range 0.6Å $<\lambda<$ 1.73Åand Laue data using 0.2 $<\lambda<$ 3Å.

The aim here is to calculate polarization $\tau$ and $\tau'$ correction factors for all likely conditions encountered on station 9.6.

## Basic Theory

### 1. Angular Aperture

#### a. without pre-mirror

The vertical angle subtended ($\gamma v$) at the protein crystal or collimator (c), which ever is smaller, from a synchrotron source of vertical size(s) is

$$\gamma v = \frac{(S + C)}{D} \quad \ldots\ (1)$$

where D is the distance from S to C

b. with pre-mirror

A focussing pre-mirror is used, inter alia, to collect a large angular aperture of radiation and image the source at the sample. In so doing a larger percentage of vertically polarized light is brought to the sample (ie. the beam is less polarized overall)

Equation 1. becomes

$$\gamma_v = \frac{(A + C)}{D_c} \quad \ldots\ldots (2)$$

where A is the spatial aperture of the mirror and $D_c$ is the distance of the mirror to the collimator.

2. Polarization Factor

If the parallel and perpendicular intensities, integrated over the angle $\gamma_v$, are $I_{ll}$ and $I_{\perp}$ respectively then $\tau$ (the polarization ratio) can be defined as

$$\tau = \frac{I_{ll} - I_{\perp}}{I_{ll} + I_{\perp}} \quad \ldots\ldots (3)$$

This is the quantity needed for Laue work. The polarization ratio after reflection from a single crystal monochromator becomes

$$\tau' = \frac{\propto I_{ll} - I_{\perp}}{\propto I_{ll} + I_{\perp}} \quad \ldots\ldots (4)$$

where $\alpha$ = cos 2$\theta$m and 2$\theta$m is the Bragg angle of the cylindrically bent single crystal monochromator. The polarization factor P (Kahn et. al (1982) working from Azaroff (1955)) is then;

$$P = \frac{(1 + \cos^2 2\theta)}{2} - \frac{\tau'}{2} \cos 2\varrho \, \sin^2 2\theta \quad \ldots\ldots (5)$$

where 2$\theta$ is the protein crystal Bragg angle and $\varrho$ the azimulthal angle in the plane of the film, which is placed normal to the X-ray beam. ($\varrho = 0^\circ$ is the axis mutually perpendicular to the beam and the horizontal rotation axis). In equation 5. for Laue work $\tau'$ is replaced by $\tau$ .

Calculation of $\tau$ and $\tau'$

The 'without mirror' calculation of $\tau$ and $\tau'$ assumes a 5$\sigma$ source size of S = 1.0 mm and a source to collimator distance D = 22000 mm. In the pre-mirror case, since the mirror is set at a critical angle of 3 mrad it projects A = 2 mm source size onto the vertical plane, which is a distance Dc = 11000 mm from the collimator. Calculations of $I_{11}$ and $I_{\perp}$ were made with a program based on that of Poole (1976) as a function of machine energy, wiggler magnetic field, wavelength and collimator size (Table 1). $\tau'$ and $\tau$ are shown for a Si (111) monochromator. In the range of $\lambda$ relevant to the use of Ge(111) (ie $\lambda > 1.28$), the calculations do not differ significantly from those made for Si (111) and only deviate by 1% at $\lambda = 2.9 A^\circ$

The variation of $\tau$ and $\tau'$, as a function of the sample size c, is linear to better than 0.2%. Interpolation to intermediate sample sizes is therefore straight forward.

This note is based on a Daresbury Laboratory Technical Memorandum by the authors.

References

Azaroff L. (1955) Acta Crystallogr 8 701-4

Kahn R, Fourme R, Gadet A, Janin J, Dumas C and Adre D (1982.c) J Appl, Crystallogr 15, 330-7

Poole J, Daresbury Laboratory Technical Memorandum DL/SRF/TM4 revised (1978) and DL/SRF/TM4 (1976) and DL/SRF/TM6 (1976)

Table 1

POLARIZATION CALCULATION AT 2.0 GEV 5.0 TESLA
WITHOUT A MIRROR

| LAMBDA | | (1) TAU | (1) TAUP | | (2) TAU | (2) TAUP | | (3) TAU | (3) TAUP |
|---|---|---|---|---|---|---|---|---|---|
| 0.10 | * | 0.979 | 0.979 | * | 0.973 | 0.973 | * | 0.966 | 0.966 |
| 0.20 | * | 0.979 | 0.979 | * | 0.971 | 0.971 | * | 0.963 | 0.963 |
| 0.30 | * | 0.979 | 0.979 | * | 0.971 | 0.971 | * | 0.962 | 0.962 |
| 0.40 | * | 0.979 | 0.979 | * | 0.971 | 0.971 | * | 0.962 | 0.962 |
| 0.50 | * | 0.980 | 0.979 | * | 0.972 | 0.971 | * | 0.963 | 0.962 |
| 0.60 | * | 0.980 | 0.980 | * | 0.972 | 0.972 | * | 0.964 | 0.963 |
| 0.70 | * | 0.981 | 0.980 | * | 0.973 | 0.972 | * | 0.965 | 0.964 |
| 0.80 | * | 0.981 | 0.981 | * | 0.974 | 0.973 | * | 0.966 | 0.964 |
| 0.90 | * | 0.982 | 0.981 | * | 0.974 | 0.973 | * | 0.966 | 0.965 |
| 1.00 | * | 0.982 | 0.981 | * | 0.975 | 0.974 | * | 0.967 | 0.965 |
| 1.10 | * | 0.983 | 0.981 | * | 0.976 | 0.974 | * | 0.968 | 0.966 |
| 1.20 | * | 0.983 | 0.982 | * | 0.976 | 0.974 | * | 0.969 | 0.966 |
| 1.30 | * | 0.983 | 0.982 | * | 0.977 | 0.975 | * | 0.969 | 0.966 |
| 1.40 | * | 0.984 | 0.982 | * | 0.977 | 0.975 | * | 0.970 | 0.967 |
| 1.50 | * | 0.984 | 0.982 | * | 0.978 | 0.975 | * | 0.970 | 0.967 |
| 1.60 | * | 0.984 | 0.982 | * | 0.978 | 0.975 | * | 0.971 | 0.967 |
| 1.70 | * | 0.985 | 0.982 | * | 0.979 | 0.975 | * | 0.972 | 0.967 |
| 1.80 | * | 0.985 | 0.982 | * | 0.979 | 0.975 | * | 0.972 | 0.967 |
| 1.90 | * | 0.985 | 0.982 | * | 0.979 | 0.975 | * | 0.973 | 0.966 |
| 2.00 | * | 0.986 | 0.982 | * | 0.980 | 0.975 | * | 0.973 | 0.966 |
| 2.10 | * | 0.986 | 0.982 | * | 0.980 | 0.974 | * | 0.973 | 0.966 |
| 2.20 | * | 0.986 | 0.981 | * | 0.980 | 0.974 | * | 0.974 | 0.966 |
| 2.30 | * | 0.986 | 0.981 | * | 0.981 | 0.974 | * | 0.974 | 0.965 |
| 2.40 | * | 0.986 | 0.981 | * | 0.981 | 0.973 | * | 0.975 | 0.964 |
| 2.50 | * | 0.987 | 0.981 | * | 0.981 | 0.973 | * | 0.975 | 0.964 |
| 2.60 | * | 0.987 | 0.980 | * | 0.982 | 0.972 | * | 0.975 | 0.963 |
| 2.70 | * | 0.987 | 0.980 | * | 0.982 | 0.971 | * | 0.976 | 0.962 |
| 2.80 | * | 0.987 | 0.979 | * | 0.982 | 0.970 | * | 0.976 | 0.961 |
| 2.90 | * | 0.987 | 0.978 | * | 0.982 | 0.969 | * | 0.976 | 0.959 |

SI(111) MONOCHROMATOR 2D(H,K,L) = 6.271 A

(1) COLLIMATOR 0.2 MM, GAMMA(VER) =0.0031 DEG

(2) COLLIMATOR 0.4 MM, GAMMA(VER) =0.0036 DEG

(3) COLLIMATOR 0.6 MM, GAMMA(VER) =0.0042 DEG

Table 1 continued

POLARIZATION CALCULATION AT 1.8 GEV 4.5 TESLA
WITHOUT A MIRROR

| | | (1) | | | (2) | | | (3) | |
|---|---|---|---|---|---|---|---|---|---|
| LAMBDA | | TAU | TAUP | | TAU | TAUP | | TAU | TAUP |
| 0.10 | * | 0.983 | 0.983 | * | 0.978 | 0.978 | * | 0.973 | 0.973 |
| 0.20 | * | 0.982 | 0.982 | * | 0.976 | 0.976 | * | 0.969 | 0.969 |
| 0.30 | * | 0.982 | 0.982 | * | 0.976 | 0.976 | * | 0.968 | 0.968 |
| 0.40 | * | 0.982 | 0.982 | * | 0.975 | 0.975 | * | 0.968 | 0.968 |
| 0.50 | * | 0.982 | 0.982 | * | 0.976 | 0.975 | * | 0.968 | 0.968 |
| 0.60 | * | 0.983 | 0.983 | * | 0.976 | 0.976 | * | 0.969 | 0.968 |
| 0.70 | * | 0.983 | 0.983 | * | 0.977 | 0.976 | * | 0.969 | 0.969 |
| 0.80 | * | 0.984 | 0.983 | * | 0.977 | 0.976 | * | 0.970 | 0.969 |
| 0.90 | * | 0.984 | 0.983 | * | 0.978 | 0.977 | * | 0.970 | 0.969 |
| 1.00 | * | 0.984 | 0.984 | * | 0.978 | 0.977 | * | 0.971 | 0.970 |
| 1.10 | * | 0.985 | 0.984 | * | 0.979 | 0.977 | * | 0.972 | 0.970 |
| 1.20 | * | 0.985 | 0.984 | * | 0.979 | 0.977 | * | 0.972 | 0.970 |
| 1.30 | * | 0.985 | 0.984 | * | 0.979 | 0.977 | * | 0.973 | 0.970 |
| 1.40 | * | 0.986 | 0.984 | * | 0.980 | 0.978 | * | 0.973 | 0.970 |
| 1.50 | * | 0.986 | 0.984 | * | 0.980 | 0.978 | * | 0.974 | 0.970 |
| 1.60 | * | 0.986 | 0.984 | * | 0.980 | 0.978 | * | 0.974 | 0.970 |
| 1.70 | * | 0.986 | 0.984 | * | 0.981 | 0.978 | * | 0.974 | 0.970 |
| 1.80 | * | 0.986 | 0.984 | * | 0.981 | 0.977 | * | 0.975 | 0.970 |
| 1.90 | * | 0.987 | 0.984 | * | 0.981 | 0.977 | * | 0.975 | 0.970 |
| 2.00 | * | 0.987 | 0.984 | * | 0.982 | 0.977 | * | 0.976 | 0.969 |
| 2.10 | * | 0.987 | 0.983 | * | 0.982 | 0.977 | * | 0.976 | 0.969 |
| 2.20 | * | 0.987 | 0.983 | * | 0.982 | 0.976 | * | 0.976 | 0.969 |
| 2.30 | * | 0.988 | 0.983 | * | 0.982 | 0.976 | * | 0.977 | 0.968 |
| 2.40 | * | 0.988 | 0.983 | * | 0.983 | 0.976 | * | 0.977 | 0.968 |
| 2.50 | * | 0.988 | 0.982 | * | 0.983 | 0.975 | * | 0.977 | 0.967 |
| 2.60 | * | 0.988 | 0.982 | * | 0.983 | 0.974 | * | 0.978 | 0.966 |
| 2.70 | * | 0.988 | 0.981 | * | 0.983 | 0.974 | * | 0.978 | 0.965 |
| 2.80 | * | 0.988 | 0.981 | * | 0.984 | 0.973 | * | 0.978 | 0.964 |
| 2.90 | * | 0.988 | 0.980 | * | 0.984 | 0.972 | * | 0.978 | 0.962 |

SI(111) MONOCHROMATOR 2D(H,K,L) = 6.271 A

(1) COLLIMATOR 0.2 MM, GAMMA(VER) =0.0031 DEG

(2) COLLIMATOR 0.4 MM, GAMMA(VER) =0.0036 DEG

(3) COLLIMATOR 0.6 MM, GAMMA(VER) =0.0042 DEG

Table 1 continued

POLARIZATION CALCULATION AT 2.0 GEV 5.0 TESLA
WITH A FOCUSSING PRE-MIRROR

| LAMBDA | | (1) TAU | (1) TAUP | | (2) TAU | (2) TAUP | | (3) TAU | (3) TAUP |
|---|---|---|---|---|---|---|---|---|---|
| 0.10 | * | 0.944 | 0.944 | * | 0.944 | 0.944 | * | 0.944 | 0.944 |
| 0.20 | * | 0.904 | 0.903 | * | 0.903 | 0.903 | * | 0.902 | 0.902 |
| 0.30 | * | 0.877 | 0.877 | * | 0.874 | 0.873 | * | 0.872 | 0.871 |
| 0.40 | * | 0.865 | 0.864 | * | 0.858 | 0.856 | * | 0.853 | 0.852 |
| 0.50 | * | 0.855 | 0.853 | * | 0.854 | 0.843 | * | 0.838 | 0.836 |
| 0.60 | * | 0.849 | 0.946 | * | 0.837 | 0.834 | * | 0.827 | 0.824 |
| 0.70 | * | 0.846 | 0.842 | * | 0.831 | 0.827 | * | 0.820 | 0.815 |
| 0.80 | * | 0.844 | 0.839 | * | 0.828 | 0.822 | * | 0.814 | 0.809 |
| 0.90 | * | 0.843 | 0.836 | * | 0.826 | 0.819 | * | 0.811 | 0.804 |
| 1.00 | * | 0.843 | 0.835 | * | 0.824 | 0.816 | * | 0.809 | 0.799 |
| 1.10 | * | 0.843 | 0.833 | * | 0.824 | 0.814 | * | 0.807 | 0.796 |
| 1.20 | * | 0.844 | 0.832 | * | 0.824 | 0.811 | * | 0.807 | 0.793 |
| 1.30 | * | 0.845 | 0.831 | * | 0.824 | 0.810 | * | 0.806 | 0.790 |
| 1.40 | * | 0.846 | 0.830 | * | 0.825 | 0.809 | * | 0.807 | 0.787 |
| 1.50 | * | 0.847 | 0.829 | * | 0.826 | 0.806 | * | 0.807 | 0.785 |
| 1.60 | * | 0.848 | 0.827 | * | 0.827 | 0.804 | * | 0.808 | 0.782 |
| 1.70 | * | 0.849 | 0.826 | * | 0.828 | 0.802 | * | 0.809 | 0.779 |
| 1.80 | * | 0.851 | 0.824 | * | 0.830 | 0.799 | * | 0.809 | 0.776 |
| 1.90 | * | 0.852 | 0.822 | * | 0.831 | 0.797 | * | 0.810 | 0.773 |
| 2.00 | * | 0.854 | 0.819 | * | 0.832 | 0.794 | * | 0.812 | 0.769 |
| 2.10 | * | 0.855 | 0.817 | * | 0.833 | 0.790 | * | 0.813 | 0.765 |
| 2.20 | * | 0.856 | 0.814 | * | 0.835 | 0.787 | * | 0.814 | 0.761 |
| 2.30 | * | 0.858 | 0.810 | * | 0.836 | 0.782 | * | 0.815 | 0.756 |
| 2.40 | * | 0.859 | 0.806 | * | 0.838 | 0.778 | * | 0.817 | 0.750 |
| 2.50 | * | 0.860 | 0.802 | * | 0.839 | 0.773 | * | 0.818 | 0.744 |
| 2.60 | * | 0.862 | 0.797 | * | 0.840 | 0.766 | * | 0.819 | 0.737 |
| 2.70 | * | 0.863 | 0.791 | * | 0.842 | 0.760 | * | 0.821 | 0.729 |
| 2.80 | * | 0.864 | 0.784 | * | 0.843 | 0.752 | * | 0.822 | 0.720 |
| 2.90 | * | 0.866 | 0.776 | * | 0.844 | 0.743 | * | 0.823 | 0.710 |

SI(111) MONOCHROMATOR 2D(H,K,L) = 6.271 A

(1) COLLIMATOR 0.2 MM, GAMMA(VER) =0.0115 DEG

(2) COLLIMATOR 0.4 MM, GAMMA(VER) =0.0125 DEG

(3) COLLIMATOR 0.6 MM, GAMMA(VER) =0.0135 DEG

Table 1 continued

POLARIZATION CALCULATION AT 1.9 GEV 4.5 TESLA
WITH A FOCUSSING PRE-MIRROR

| | (1) | | | (2) | | | (3) | |
|---|---|---|---|---|---|---|---|---|
| LAMBDA | TAU | TAUP | | TAU | TAUP | | TAU | TAUP |
| 0.10 * | 0.957 | 0.957 | * | 0.957 | 0.957 | * | 0.957 | 0.957 |
| 0.20 * | 0.924 | 0.924 | * | 0.923 | 0.923 | * | 0.923 | 0.923 |
| 0.30 * | 0.900 | 0.900 | * | 0.898 | 0.897 | * | 0.896 | 0.896 |
| 0.40 * | 0.887 | 0.886 | * | 0.882 | 0.881 | * | 0.879 | 0.878 |
| 0.50 * | 0.877 | 0.876 | * | 0.869 | 0.868 | * | 0.864 | 0.862 |
| 0.60 * | 0.871 | 0.869 | * | 0.861 | 0.858 | * | 0.853 | 0.850 |
| 0.70 * | 0.867 | 0.864 | * | 0.855 | 0.851 | * | 0.845 | 0.841 |
| 0.80 * | 0.864 | 0.860 | * | 0.850 | 0.846 | * | 0.839 | 0.834 |
| 0.90 * | 0.862 | 0.857 | * | 0.847 | 0.841 | * | 0.835 | 0.828 |
| 1.00 * | 0.861 | 0.855 | * | 0.846 | 0.838 | * | 0.832 | 0.824 |
| 1.10 * | 0.861 | 0.853 | * | 0.844 | 0.835 | * | 0.830 | 0.820 |
| 1.20 * | 0.861 | 0.851 | * | 0.844 | 0.832 | * | 0.828 | 0.816 |
| 1.30 * | 0.861 | 0.849 | * | 0.844 | 0.830 | * | 0.827 | 0.813 |
| 1.40 * | 0.862 | 0.848 | * | 0.844 | 0.828 | * | 0.827 | 0.810 |
| 1.50 * | 0.863 | 0.846 | * | 0.844 | 0.826 | * | 0.827 | 0.806 |
| 1.60 * | 0.863 | 0.844 | * | 0.844 | 0.823 | * | 0.827 | 0.803 |
| 1.70 * | 0.864 | 0.843 | * | 0.845 | 0.821 | * | 0.827 | 0.800 |
| 1.80 * | 0.865 | 0.841 | * | 0.846 | 0.819 | * | 0.827 | 0.797 |
| 1.90 * | 0.866 | 0.838 | * | 0.847 | 0.815 | * | 0.829 | 0.793 |
| 2.00 * | 0.867 | 0.836 | * | 0.847 | 0.812 | * | 0.829 | 0.790 |
| 2.10 * | 0.868 | 0.833 | * | 0.848 | 0.809 | * | 0.830 | 0.786 |
| 2.20 * | 0.869 | 0.830 | * | 0.849 | 0.805 | * | 0.830 | 0.781 |
| 2.30 * | 0.870 | 0.826 | * | 0.850 | 0.801 | * | 0.831 | 0.776 |
| 2.40 * | 0.871 | 0.822 | * | 0.851 | 0.796 | * | 0.832 | 0.771 |
| 2.50 * | 0.872 | 0.818 | * | 0.852 | 0.791 | * | 0.833 | 0.764 |
| 2.60 * | 0.873 | 0.813 | * | 0.853 | 0.785 | * | 0.834 | 0.758 |
| 2.70 * | 0.874 | 0.807 | * | 0.854 | 0.778 | * | 0.835 | 0.750 |
| 2.80 * | 0.875 | 0.801 | * | 0.855 | 0.770 | * | 0.836 | 0.741 |
| 2.90 * | 0.876 | 0.793 | * | 0.856 | 0.762 | * | 0.837 | 0.731 |

SI(111) MONOCHROMATOR 2D(H,K,L) = 6.271 A

(1) COLLIMATOR 0.2 MM, GAMMA(VER) =0.0115 DEG

(2) COLLIMATOR 0.4 MM, GAMMA(VER) =0.0125 DEG

(3) COLLIMATOR 0.6 MM, GAMMA(VER) =0.0135 DEG

# STOCHASTIC DYNAMICS AND MACROMOLECULES

University of York

September 11th - 13th 1985

## CALL FOR CONTRIBUTIONS

Contributions are invited for the second CCP5 meeting of 1985. The title of the meeting will be interpreted broadly. There are likely to be sessions on polymers, colloids and biological macromolecules, not necessarily limited to stochastic methods. Theoretical developments in stochastic methods would also be appropriate. Invited speakers who have already accepted include:

H.J.C. Berendsen/W. van Gunsteren (Groningen)
- Stochastic dynamics of proteins

G. Bossis (Nice)
- Colloids

C.L. Brooks (Harvard)
- Stochastic boundary methods

As always with our meetings the proceedings will be fairly informal, and accounts of work in progress or discussion of computational techniques will be welcome.

If you would like to contribute a talk or poster please send a title, and if possible a short abstract, to one of the undersigned organisers. A registration form will be included in the next CCP5 mailing.

Eric Dickinson
Procter Department of Food Science
University of Leeds
Leeds LS2 9JT

David Fincham
Department of Chemistry
University of York
York YO1 5DD

## GROUP COMPUTERS AND NETWORK ADDRESSES

It was suggested that a summary of computers used by UK protein crystallographers would provide useful information for those trying to implement CCP4 and related programs. Also with the increasing availibility and reliability of computer networks, communication by electronic MAIL is becoming the easiest way of talking to people, so a summary of the relevant network addresses is given here. Note that as well as the specific site addresses given here, most PX users of the SRS at Daresbury have a username on the DLVB vax computer and may be contacted via it. In the near future these numbers will be transferred to the new Vax at Daresbury which will be dedicated to PX use.

I hope that the network addresses given here will be useful for reference purposes. The network system is very clever but also very complicated and there are often different local settings of mnemonics. I understand that the addresses may be composite - the address of a site central packet switch (CPSE) which is usually 12 digits plus 2 subaddress digits, and the specific machine address which is also 12 digits. Examples of this occur for Sheffield and Edinburgh.

SURVEY OF COMPUTERS AND NETWORK ADDRESSES

| Site | University Mainframe | In-house | Others | JANET address for mail or FTP |
|---|---|---|---|---|
| Sheffield | ICL1906S | Perkin Elmer 3240 | Prime | 000012200041 SHGA 0000122000C004 CPSE-Sheffield |
| Leeds | Amdahl 580/60 | Pdp 11/45 | Cyber 176 CDC 7600 (UMRCC) | 000001080500 LEVA |
| York | Dec 10 | Perqs Microvax | Vax 11/750? | 0000060000087 ~~YKXA~~ YKQB |
| Oxford | ICL2988 Vax 11/780 | Vax 11/750 | ULCC Cray UMRCC Cyber | 000050250200 |
| MRC Cambridge | IBM3081 | Vax 11/780 | ..... | ..... |
| Imperial College | ULCC Amdahl Cray | Vax 11/750 | AS/7000 (Daresbury) | 000000000048 ZIVA(=HEPvax) |
| Birkbeck | " | Vax 11/750 Pdp 11/60 | " | 000005161000 BBK.CU |
| Bristol | Honeywell Multics | Perq | Vax 11/750 | 000060210002 (Vax) 000060110000000 (Honeywell) |
| Liverpool | IBM3083 | ..... | DL AS7000 DL Vax11/750 | 000010500101 LIVIBM |
| Edinburgh | ICL2976 ICL2988 | Perq Pdp11/70 | Vax 11/750 | 000015000001 (2976=EMAS) 000015000003 (2988) 000007001004O4 CPSE Edinb'h |
| SERC, Daresbury | ..... | AS7000 (MVS, TSO) | Vax 11/750 Perq | 000001003000 DLVB |

0000 1200 5000 VAX
UK.AC LEEDS.BIOVAX
UK.AC.YORK.CHEMVAX

## PROGRAM BUG REPORT

Many protein crystallography programs are widely distributed, and numerous versions result. When bugs are identified it is difficult to know which versions are immune and which suffer from the fault. By detailing here information about possible bugs, we hope to draw your attention to their existence and to give you an opportunity of checking your code. The editor would be pleased to receive information about any other similar errors for inclusion in future issues.

The code shown here is part of the subroutine SDIAD from the FFT program. The incorrect version is shown first, with the important lines marked, and the hopefully correct version is shown second. This bug was kindly detailed by Phil Evans (MRC Cambridge) who may be contacted if further information is required.

```
      IF (K .LT. I) GO TO 300
      IF (K .EQ. I) GO TO 400
      J = (K - I)*D2
      KO = I*D2 + 1
      DO 350 K1 = KO, D1, D3
      K2 = K1 + D4
      DO 350 K = K1, K2, D5
      L = K + J
      A = X(K)
      X(K) = X(L)
      X(L) = A
      A = Y(K)
      Y(K) = Y(L)
      Y(L) = A
  350 CONTINUE
  400 CONTINUE
C
      CALL CMPL FT (X, Y, N, DIM)
C
      M = N OVER 2 - 1
      DO 600 I = 2, M
      ANGLE = TWO PI*FLOAT(I-1)/TWO N
      C = COS(ANGLE)
      S = SIN(ANGLE)
      KO = (I - 1)*D2 + 1
      FOLD = .TRUE.
      GO TO 500
C
  450 CONTINUE
      C = -C
      KO = (N + 1 - I)*D2 + 1
      FOLD = .FALSE.
C
  500 CONTINUE
      DO 550 K1 = KO, D1, D3
      K2 = K1 + D4
      DO 550 K = K1, K2, D5
      A = Y(K)/C
      X(K) = X(K) + S*A
      Y(K) = A
  550 CONTINUE
      IF (FOLD) GO TO 450
  600 CONTINUE
C
      M = N OVER 2*D2
      KO = M + 1
      DO 650 K1 = KO, D1, D3
      K2 = K1 + D4
      DO 650 K = K1, K2, D5
      J = K - M
      L = K + M
      A = 2.0*X(L)
      X(K) = X(K) + A
      Y(K) = A
      X(L) = X(J)
      Y(L) = -Y(J)
  650 CONTINUE
C
      RETURN
C
  700 CONTINUE
      WRITE (6, 1000) N
      STOP
C
 1000 FORMAT (18HOSDIAD N ODD.   N =, I10)
C
      END
```

INCORRECT

```
      IF (K .LT. I) GO TO 300
      IF (K .EQ. I) GO TO 400
      J = (K - I)*D2
      K0 = I*D2 + 1
      DO 350 K1 = K0, D1, D3
      K2 = K1 + D4
      DO 350 K = K1, K2, D5
      L = K + J
      A = X(K)
      X(K) = X(L)
      X(L) = A
      A = Y(K)
      Y(K) = Y(L)
      Y(L) = A
  350 CONTINUE
  400 CONTINUE
C
      CALL CMPL FT (X, Y, N, DIM)
C
      M = N OVER 2 - 1
      DO 600 I = 1, M
      ANGLE = TWO PI*FLOAT(I)/TWO N
      C = COS(ANGLE)
      S = SIN(ANGLE)
      K0 = I*D2 + 1
      FOLD = .TRUE.
      GO TO 500
C
  450 CONTINUE
      C = -C
      K0 = (N - I)*D2 + 1
      FOLD = .FALSE.
C
  500 CONTINUE
      DO 550 K1 = K0, D1, D3
      K2 = K1 + D4
      DO 550 K = K1, K2, D5
      A = Y(K)/C
      X(K) = X(K) + S*A
      Y(K) = A
  550 CONTINUE
      IF (FOLD) GO TO 450
  600 CONTINUE
C
      M = N OVER 2*D2
      K0 = M + 1
      DO 650 K1 = K0, D1, D3
      K2 = K1 + D4
      DO 650 K = K1, K2, D5
      J = K - M
      L = K + M
      A = 2.0*X(L)
      X(K) = X(K) + A
      Y(K) = A
      X(L) = X(J)
      Y(L) = -Y(J)
  650 CONTINUE
C
      RETURN
C
  700 CONTINUE
      WRITE (6, 1000) N
      STOP
C
 1000 FORMAT (18HOSDIAD N ODD.   N =, I10)
C
      END
```

CORRECT