



UNIVERSITI SAINS MALAYSIA

Workshop on

Mathematical Methods in Macromolecular Crystallography:

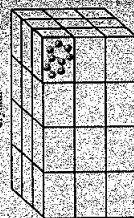
Theory and Practice

molecule



unit cell

crystal



19-22 AUGUST 2002
EUREKA COMPLEX, USAINS, USM

Organised by

School of Mathematical Sciences
Universiti Sains Malaysia, Penang

<http://www.usm.my/math/crystal>

PROGRAMME

Opening Ceremony *of* *'Mathematical Methods in Macromolecular Crystallography' Workshop*

8.50 am	Arrival of Guests
9.00 am	Speech by Dr. Noor Atinah Ahmad Chairperson
	Opening Speech by the Honorable Prof. Dato' Dzulkifli Abd. Razak Vice-Chancellor, Universiti Sains Malaysia
9.15 am	Photo session
9.20 am	Tea

INTRODUCTION

Crystallography is applicable in many different field of science and has been responsible for many discoveries such as in medicine and engineering. Realizing the importance of understanding the mathematical concept in crystallography, the school of mathematical sciences, USM has organized this workshop to bring together researchers from different discipline of science, such as Mathematics, Physics, Biology, Chemistry and others on an intellectual discourse in the hope to strengthen fundamental research in crystallography among the Malaysian scientist. Mathematics are used as a basic tools in the field and therefore sufficient background in mathematics theories and methods is crucial for the advancement of this area. Thus, this workshop is a platform to achieve a better future in the area of crystallography.

This workshop is planned in such a way that participants will have a balance input of theory and underlying concepts of crystallography as well as methods, tools and current practice. The academic leadership of Professor Alexander Urzhumtsev who has had almost 20 years of experience working in this field will be crucial to bridge the gap between mathematicians and non-mathematicians, as well as provide relevant inputs to stimulate further research in this area.

BACKGROUND

Crystallography is a branch of science that deals with determining the arrangement and bonding of atoms in crystalline solids as well as the geometric structure of crystal lattices. It involves the study of biological and chemical processes at the most basic level, that is, how atoms and molecules interact and react.

Understanding of crystallography has led to advances in many different fields of science and has been responsible for the discoveries of new drugs, understanding diseases, advancement in material engineering and many more.

Mathematics plays an important role in crystallography especially in modeling, data analysis and structure determination. Fundamental research in this field requires substantial use of mathematical theories and methods. Therefore new advancements in crystallography can be made possible through a combination of strong mathematical foundations and a thorough understanding of the underlying science.

COURSE OBJECTIVE

This workshop is aimed at providing participants with a foundation for research in the field of crystallography through sufficient exposure to mathematical theory and practice and sharing of new ideas and recent advancements in this field.

PROGRAMME

Monday 19 August 2002

10.00-11.30

Fundamentals

- field of crystallography
- basic goal of structural crystallography
- crystals; direct space; fractional coordinates;
- crystallographic symmetries
- crystallographic space groups
- diffraction by crystals; structure factors; phase problem

11.30-1.00

Fundamentals of Fourier transformation

- Fourier transformation of a periodic function
- three-dimensional Fourier transformation
- Fourier transformation of a grid function
- Fourier transformation and a convolution
- Fourier coefficients and the origin shift

1.00-14.00

Lunch Break

14.00-15.30

Model of crystal

- Atomic structure
- Ionic crystals
- Symmetry and phase transitions
- Molecular crystals: macromolecules
- Protein, nucleic acids, viruses, macromolecular complexes
- secondary and spatial structure
- model of independent isotropic atoms
- fixed-bond models for chain molecules
- anisotropic atoms
- multipolar modelling
- crystallographic solvent molecules and bulk

15.30-16.00	solvent - other models - different levels of a crystal description Tea Break	14.00-15.30	Direct methods - distribution of structure factors - sigma-2 formula - tangent-formula - MULTAN approach
16.00-17.30	Problem of structure determination - phase problem - direct methods - intermediate density calculation - density analysis and interpretation - model refinement - history and milestones	15.30-16.00	Tea Break
		16.00-17.30	Molecular Replacement - use of a particular information: approximate model - 6D-search - rotation function - translation function - rigid-body refinement
Tuesday 20 August 2002			
9.00-10.30	Patterson methods - Patterson function and its properties - Patterson function and the atomic structure - resolution of the Patterson function - superposition methods		
10.30-11.00	Coffee Break		
11.00-12.30	Fundamentals of probabilities, statistics and linked tools - Central Limit Theorem - Bayesian approach - Likelihood approach - least-squares method - Von Mises distribution; modified Bessel functions		
12.30-14.00	Lunch Break		

Wednesday 21 August 2002

9.00-10.30	Experimental methods (MIR, SIR, MAD) - experiment with modified conditions - SIR method - Hendrickson-Lattman phase distribution - MIR method - MAD method
10.30-11.00	Coffee Break
11.00-12.30	Optimisation techniques - different classes of optimisation techniques - optimisation without derivatives - gradient methods - second-order optimisation methods - numeric realisation of optimisation techniques - random search methods; Metropolis algorithm - optimisation of several criteria simultaneously - optimisation with constraints - methods of Binary Integer Programming
12.30-14.00	Lunch Break
14.00-15.30	Atomic model refinement - the problems of the refinement - Fast Differentiation algorithm - fast calculation of structure factors - crystallographic criteria and their derivatives - scheme of a refinement program - model quality
15.30-16.00	Tea Break
16.00-17.30	Model building - main information - main difficulties - basic ideas: connectivity, libraries - automated model building

Thursday 22 August 2002

9.00-10.30	Density improvement - main principles of density improvement - iterative algorithms - density modification - solvent flattening - histogram matching - atomcity
10.30-11.00	Coffee Break
11.00-12.30	Direct phasing from low resolution
12.30-14.00	Lunch Break
14.00-15.30	Other problems - data analysis, space group determination; twinning - difficult cases of molecular replacement - phase improvement - modelling at subatomic resolution - modelling at low resolution - refinement - structure analysis; docking - folding: model building by homology
15.30-16.00	Tea Break
16.00-16.30	Closing

❖ About The Instructor ...

Dr. M. Alexandre URZHUMTSEV, Professor at the University Henri Poincaré in Nancy, France, has almost 20 years of experience working in the field of crystallography including development of low-resolution macromolecular crystallography, phase determination and improvement, and atomic refinement.

Besides teaching numerous courses in mathematics, physics and crystallography, he has been dedicatedly involved in the development of teaching programs in crystallography, organization of teaching seminars for students and young researchers of the laboratory as well as development of courses in mathematics, crystallography and biophysics for physics and physical sciences students.

He has authored and co-authored over 73 articles including 46 in refereed journals, 6 invited reviews and more than 80 abstracts. In addition, he has been involved in the development of crystallographic program including the FROG program for atomic model refinement, the COMPANG program for multiple rotation analysis and a number service program distributed in a hundred crystallographic laboratories. He was also engaged the determination of macromolecular structures comprising of 15 complexes of aldose reductase, mutant Y5S of gyrase 43K, ribosomal particle 50S etc.

He has participated in industrial projects with Lyonnaise Pharmaceuticale (LIPHA, Lyon, France), IDD (New Jersey), Roussel Uclaf (Romansville, France), CRESSA (Grenoble, France), and various international meetings including 1st Int. Meeting on Structure and Chemistry of Ribonucleases, Moscow, USSR, 1998; European Workshop on Crystallography of Biological Macromolecules, Como, Italy: II, 1991; IV, 1995; Int. Crystallographic Congress: XVIII, Glasgow, Great Britain, 1999; XIX 2002, Geneva, Switzerland, to name a few.

Recent international meetings include DKG Crystallographic Meeting, Kiel, Germany, 2002; Workshop on High-throughput X-ray Structure Determination, Santa Fe, USA, 2002; ACA Crystallographic Meeting, San Antonio, USA, 2002.

He has conducted many invited seminars: at the Institute of Biophysics, Sofia, Bulgaria; Max-Planck-Institute, Hamburg, Germany; IBS, Grenoble, France; Yale University, New Haven, USA, IMPB, Barcelona, Spain and many more. The most recent ones were at Max-Planck-Institut, Hamburg, Allemagne, 2002; Institut of Pretien Research, Pushchino, Russia, 2002 and SLS synchrotron, PSI, Villigen Switzerland, 2002.

ACKNOWLEDGEMENT

PERSAMA

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