Java Based Developments for Protein Crystallography

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Introduction

This article briefly describes a library of PX related Java classes and two Java programs based on these which have similar functionality to the CCP4 programs ROTGEN and IPDISP. An associated documentation preparation program is also available.

The Java Development Library

The Java Development Library (JDL) is a set of Java classes written for developing Java based software for Protein Crystallography. It contains four main sections of classes as follows:

1. ***JdlLib***

   This is a set of general purpose classes which are used in the implementation of the other sections of the library. These include classes and methods for handling strings, files, data conversions and manipulating bits. In addition, there are classes and methods for handling 3 element vectors, 3x3 matrices and 4x4 matrices and a class which carries out general non-linear least squares refinements using the Levenberg-Marquardt algorithm.

2. ***JdlView***

   JdlView is a package for use in developing windows based programs based on an older X-windows based toolkit XDL_VIEW. The JdlView classes basically fall into two categories. These are the general purpose JdlView classes which are written without any particular application in mind (e.g the menu area class or the I/O window class) and those which are written with a particular application or group of applications in mind, particularly for Protein Crystallography. They are primarily intended to be used in programs which use the JdlView management class which forms part of the package but they can also be used independently of that if required to fit within some alternative programming context.

3. *JdIPX*
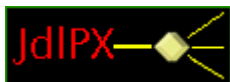
This is a set of classes specifically written for use in protein crystallography. It includes classes for holding various sets of crystallographic data, symmetry handling, reading and manipulating diffraction images. There are classes and methods for predicting Rotation, Laue and Unique reflection data and classes for storing and manipulating the predicted reflection lists. There is also a class which implements a [Diffraction Data Module (DDM)]

4. *JdIKDM*

This is a set of classes for defining and handling Keyworded parameter files and their associated data.

[Detailed documentation] of the JDL classes may be found on the CCP4 website.

The PXSim Program

PXSim is a program for carrying out simulations of Protein Crystallographic diffraction images and analysing the unique data coverage for one or more crystal settings and series of diffraction images. It is intended primarily as a teaching tool to enable the user to investigate, in some depth, the nature of X-ray diffraction patterns and the amount of data which may be collected using various settings or methods. The program may be used for simulating diffraction patterns for the Rotation, Weissenberg and Laue methods of data collection and analysing the extent of data which may be measured using those methods. The predictions are based on the set of parameters defined in a [Diffraction Data Module (DDM)].

The use of Java was chosen so that the program could be made available for use across the internet as well as being in a form suitable for porting to any Java supporting platform.

The basic screen layout is shown below:

Figure 1: Main Screen of PXSim

| Input Mode							
Display Menu		**Main Parameter Items**					
		Set no.	1	crystal	1	spot_size	0.9
		Img no.	1	wavelen	1.0		
Display		title	Yeast P	resolution	1.75	lam_min	0.5
		type	Rotation	mosaicity	0.3	lam_max	1.5
Remove		numsets	1	distance	138.70	synch	Yes
		system	Monocli	rmax	90.0	disp	0.001
		lattice	C			divv	0.025
		symm	5	phi_x	39.1721	divh	0.15
Return to Main Menu		a	96.15	phi_y	-30.2525	delcor	0.00
		b	85.80	phi_z	7.4183	pol	0.0
		c	81.90	rotstart	340.0		
		alpha	90.0	rotend	390.0	det_geom	flat
Input Mode		beta	120.54	osc/inc	2.0	weiss_c	0.00
Current Option		gamma	90.0	nwmax	3		
Orient	default						
Multfac	2.00						

The main options of the programs are as follows:

1. Rotation/Weissenberg/Laue Simulations

    Two basic types of simulations are available, standard colour simulations and interactive colour simulations. In each case a window is created with a display area for the simulation, an area to list details of a selected reflection, a control panel and a button used for requesting printer or file (JPEG or PNG) output of the simulation. The standard colour simulations show the show the patterns with the spots colour coded in a number of different ways. The interactive simulations have a slider which allow the user to investigate the effects of changing various parameters such as the oscillation range and mosaicity (or Lambda-min, dmin for Laue); spot labelling is also available and it is possible to search for reflections by their indices.

    An example of an 'interactive' simulation is shown below:

Figure 2: Example of an Interactive Rotation Simulation
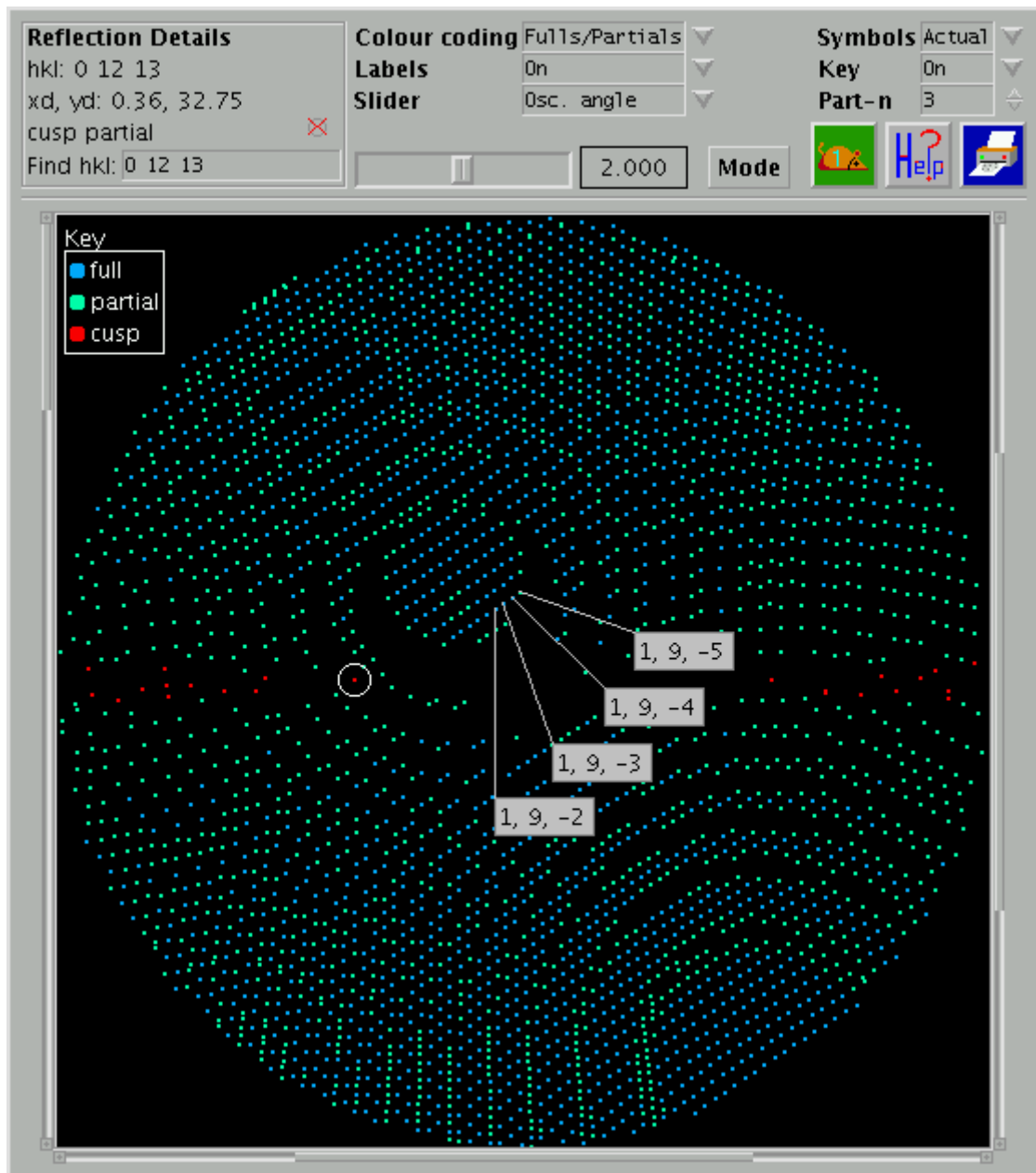
2. Unique Data Coverage

This option enables the prediction of the reflections which would be recorded for the defined crystal sets and to analyse the data coverage in terms of the unique data for the space group, cell and resolution. The analysis may be done for either the current crystal set or for all crystal sets within the data set. The results may be presented in the form or histograms describing the data coverage, in terms of a pictorial representation of the reciprocal lattice sections or as a three dimensional (rotatable) view of the reciprocal lattice.

As an example, I have chosen one of the three dimensional views as this is an option which has been newly developed for this program.
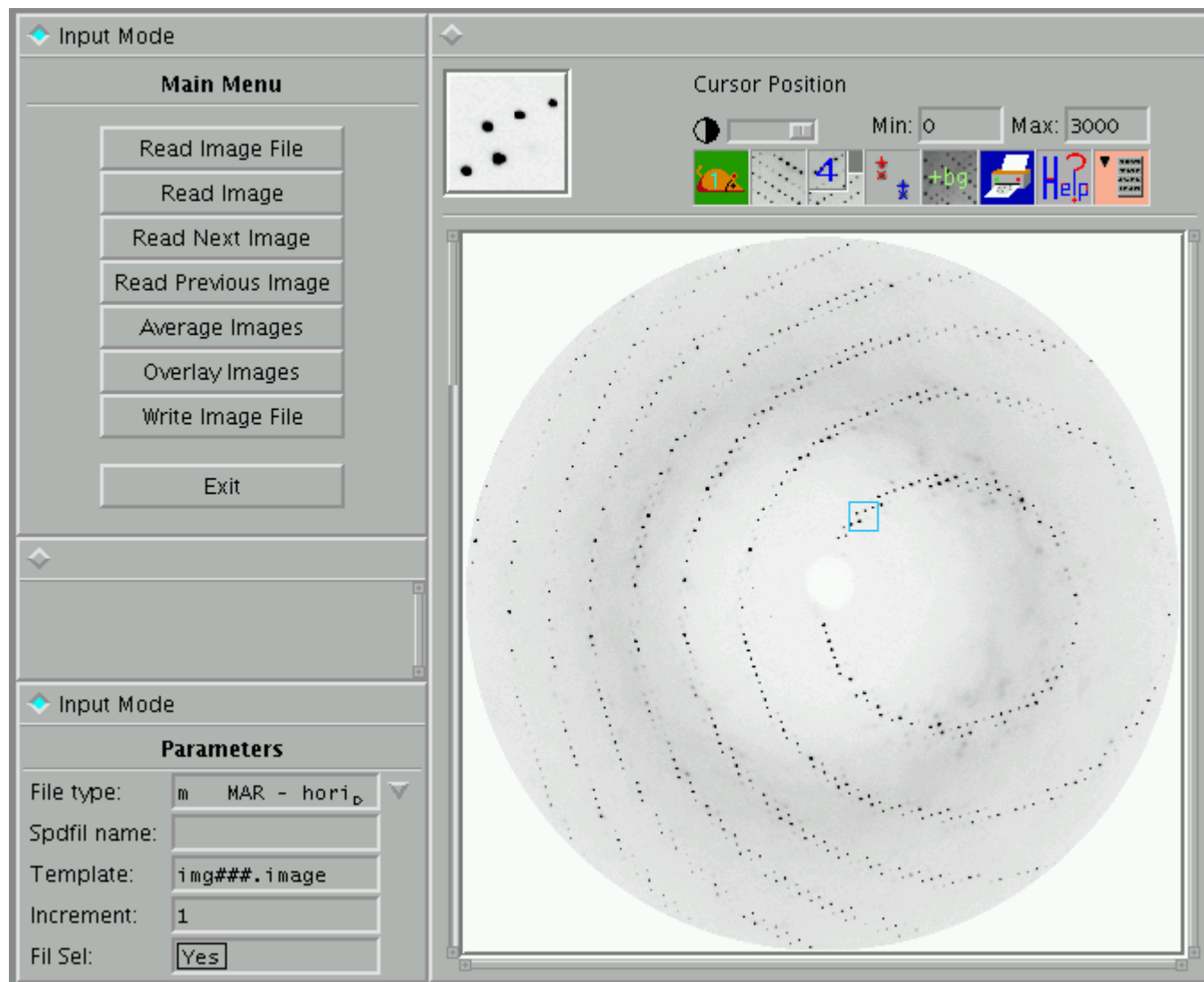
Figure 3: Unique Coverage - 3D Plot
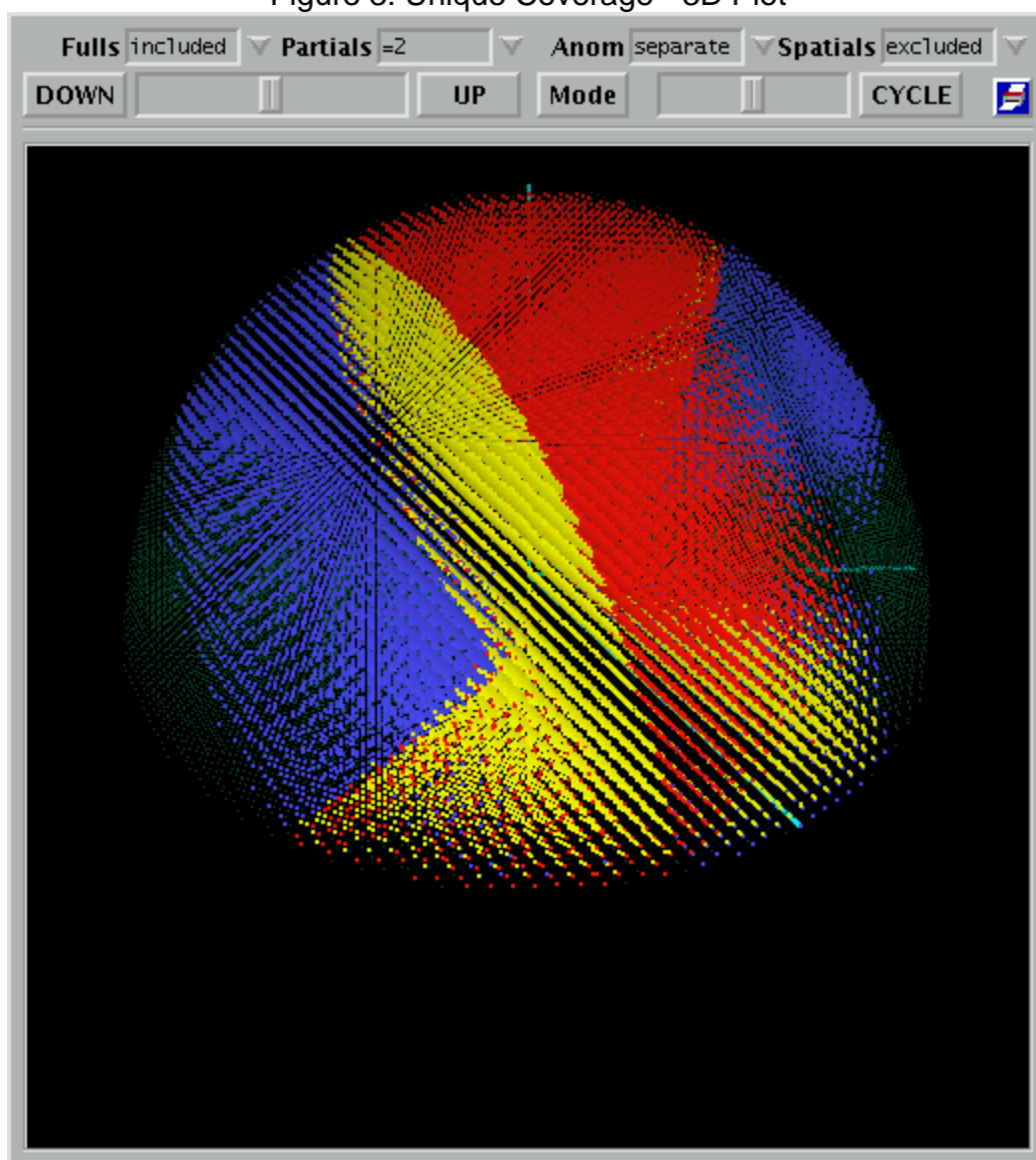
The program is available in applet form on the CCP4 web site. Detailed documentation is also available there.
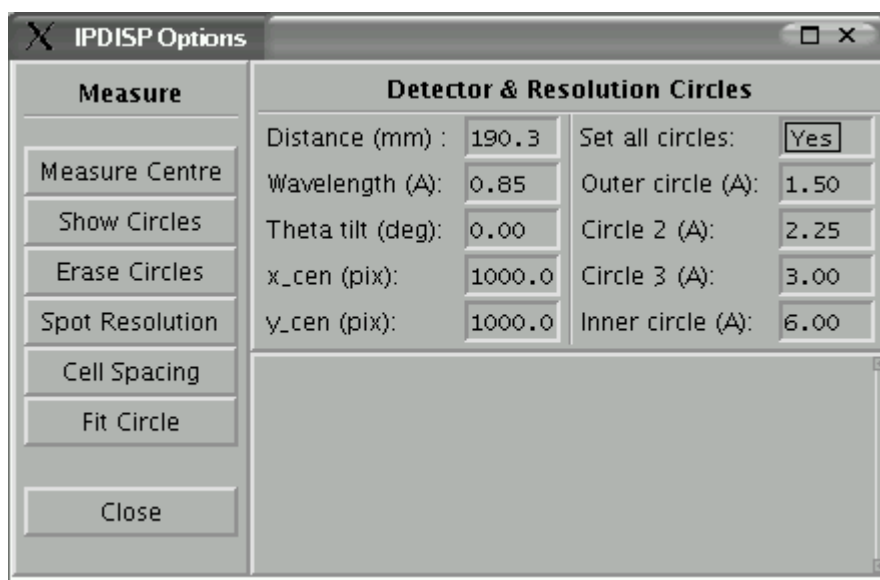
The PXimage Program

This program incorporates most of the functionality of the program IPDISP. An example is shown below:

Figure 4: PXImage program - main screen

Some of the options for measuring the image are available via a drop down menu and a dialogue window as shown below:

Figure 5: PXImage program - measurement options dialogue

This program is still under development and is not yet available via the CCP4 web site though there is an image display applet based on the image JdlPXImage class which contains many of the available functions.

The DocExtractor Program

This program is used to prepare documentation files from in a 'pre-xhtml' format or by extracting documentation sections from Java code source files. The output files will normally be in XHTML format. Documentation may be prepared from a single file or a set of linked document files. All internal links (and an optional contents page) are generated automatically by the program. This program has been used to prepare the documentation for the Java Development Library, the Diffraction Data Module and the PXSim program.