CRYSTALLOGRAPHY DATA COLLECTION BY USING A WEB INTERFACE

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Platform independence and remote access are essential for modern crystallography data acquisition.

DATA ACQUISITION

X-ray crystallography is an experimental technique that exploits the fact that X-rays are diffracted by crystals. Based on the diffraction pattern obtained from X-ray scattering off the periodic assembly of molecules or atoms in the crystal, the electron density can be reconstructed.

Crystallography normally requires a short measuring time. That means users cannot spend time on complex interfaces and ideally, as more or less all data acquisition is standard, users should be able to work remotely from their own institute. With our prototype, we are testing both goals: user-friendly interface and remote data acquisition.

SOLUTION CHOSEN

Development on multiple platforms caused trouble ever since the beginning. There exist however some frameworks which allow to write a code that can be compiled or even run on different operating systems. Java is one solution if the goal is to develop a product that can run on many different systems, each solution however has it's own drawback. Java for example has problems with stability and is not always easy to deploy. We decided instead to use a different approach which consists of a web application development and lets the user work with his own browser. This simplifies also the software deployment, as the only thing needed is to update the server.

ARCHITECTURE

Data acquisition involves a lot of different hardware and software components. In order to communicate with them, we chose two protocols: HTTP, which we use mainly for image transfer, and XML/RPC [1]. XML RPC is a new standard which can replace corba or RPC (Remote Procedure Call).
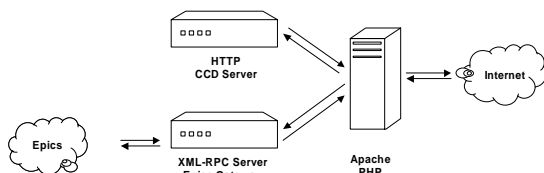

Fig. 1: Software/hardware components

In our case XML/RPC is used to bridge between the PHP code used inside the web application and our EPICS [2] control system (see Fig 1).

WORKING PROTOTYPE

In order to verify the feasibility of our project, we decided to create a first working prototype. This proto-

type allows to test all involved technologies and to clarify some concepts.

We have chosen to implement a part which requires a lot of user interaction and graphics, namely the crystal alignment tool. Crystals need to be centered in the middle of the beam in order to get good diffraction patterns. This tool allows scientists to see their crystal and interactively position the crystal.

Two main things have been implemented: image streams which allow to see in real-time the crystal and see how commands modify the position, and sliders which allow to issue some commands like rotate omega axes or change zoom factors.
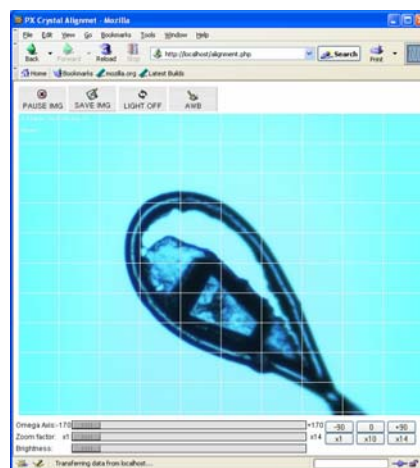

Fig. 2: Crystal alignment interface

TECHNOLOGY

We used C code to implement the XML/RPC -> Epics bridge and PHP to write the web application. Javascript has been used in order to provide silders and other buttons.

The image stream uses Netscape/Mozilla server push technology [3].

FUTURE DEVELOPMENT

The crystallography staff is planning to use this technology to provide an integrated environment. Using web-based applications, will also allow to follow the experiment remotely without the need for installing special clients.

REFERENCES

[1] http://www.xmlrpc.com/

[2] http://www.aps.anl.gov/epics

[3] http://wp.netscape.com/assist/net_sites/pushpull.html