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Transformation of X-ray Server from a set of WWW-accessed programs into WWW-based library for remote calls from X-ray data analysis software

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Abstract

X-ray Server [x-server.gmca.aps.anl.gov] is a public project providing a collection of online software tools for modeling data in the fields of surface X-ray scattering and grazing-incidence X-ray diffraction from thin solid films and multilayers with account for the effects of crystal lattice strains, magnetization and interface roughness. This paper reports on recent developments that are addressing numerous requests to expand the Server access beyond plain web browser sessions and facilitate batch processing, remote fitting and integration of Server programs into users' data analysis software.

Keywords: X-ray diffraction; X-ray scattering; X-ray theory; Web-based computations

1. Introduction

A typical cycle of developing a theory, at least in the X-ray scattering field, is (1) working out a model, (2) deriving respective equations, (3) writing a simulation or data analysis software, (4) comparing numerical data to an experiment, and, provided the above steps were successful, (5) writing a paper. After this cycle is accomplished, the question arises, how to share the software into which one has invested significant effort and know-how expertise? There are several known ways for that. Here we are not considering commercial applications because not all leading-edge studies may be of immediate commercial interest. Then, the most common approach is to give the software away in some way using the principle: 'use it on your own risk and do not blame me'. Many researchers choosing this way either post links at some common repositories like SINCRIS [1] or invite to download their software through personal web pages, e.g. [2,3]. Some of such donated X-ray and neutron scattering software is collected under the roof of sponsored projects like XOP [4] and DANSE [5] where the programs are supplied with graphical interfaces for an easier use.

X-ray Server [6] launched in 1997 suggests another mechanism of sharing software that helps to maintain close links between the researcher developing models and software on one hand and the end users on the other. The software is not given away, but operates directly on developer's web server available for immediate use through the Internet without downloading. This has proven to be the most efficient technology for having feedback from users and thus refining the software and extending the models. The advantages on the users' side are also essential since there is no installation, the software is always at hand and the most recent version is used. These advantages are confirmed by the project's success: more than 130,000 job requests from ~5500 sites have been served with the base of ~1500 regular users who performed 10 or more calculations. X-ray Server was inspired by the WWW interface to some X-ray simulation software provided through the Center for X-ray Optics [7] at the Laurence Berkeley National Laboratory. However, while CXRO is a sponsored project, the aim of X-ray Server is to explore efficient ways for an individual willing to deliver his/her scientific results and software to the community.

Section 2 provides a short overview of software tools available through the Server. Section 3 describes recently developed software wrappers and mechanisms that can help to facilitate automated access, remote fitting and integration of Server programs into users' data analysis software. In

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Table 1
The list of software operational at X-ray Server

No	Name	Description	Usage
1	*X0h*	A program interpolating dielectric susceptibilities χ_0 and χ_h for some crystals and other materials in wide range of X-ray wavelengths with the option to compare data from different databases.	61,601
2	*X0h+*	A tool based on *X0h* that can help to plan X-ray experiments by providing search for Bragg planes in crystals under various conditions.	
3	*GID_sl*	Software that calculates X-ray diffraction curves from strained crystals and multilayers for any Bragg-case diffraction with scans around arbitrary axes. It can be used for usual symmetric and asymmetric diffraction, for extremely asymmetric diffraction, as well as for grazing incidence and other Bragg-case diffraction geometries.	34,351
4	*TER_sl*	Software calculating X-ray specular reflection and respective X-ray standing waves from multilayers with interface roughness. It uses a new algorithm converging faster than Parratt's recursions.	13,180
5	*TRDS_sl*	Software for modeling X-ray diffuse scattering from interface roughness in multilayers. It implements several different models of roughness and can calculate such effects as skew roughness transfer in multilayers, dependence of interface–interface roughness correlations on lateral size of roughness and X-ray scattering from atomic steps.	10,383
6	*MAG_sl*	A program that calculates X-ray resonant specular reflection from magnetic multilayers with interface roughness and transition layers	8789
7	*BRL*	A program that models multiple Bragg diffraction of X-rays by perfect crystals. Can simulate up to 12-wave dynamical Bragg diffraction of X-rays from a plate-shaped crystal including the cases of X-ray waves grazing along the plate surface and Bragg angles close to 90°.	1861

The usage statistics is given as of July 7, 2006 (the total number of calculation equals 130,165).

Conclusions we briefly summarize some of experience gained from the X-ray Server development.

2. X-ray Server structure

The list of software operational at X-ray Server is shown in Table 1. At present seven programs are available. They are based on about 17 research papers by the author where respective models were suggested and scattering equations derived. The programs can help to model X-ray curves primarily in the fields of surface X-ray scattering and grazing-incidence X-ray diffraction from thin solid films and crystalline as well magnetic multilayers with account for effects of lattice strain and interface roughness. Modeling constitutes about 55% of Server requests while the rest are the database interpolations for calculations of X-ray scattering amplitudes and related services for planning X-ray experiments.

The technical details of making the scientific software available through the X-ray Server are discussed elsewhere [8]. In brief, the implementation of the WWW interface is illustrated by Fig. 1. In this example *GID_sl* is a program calculating Bragg curves, i.e. scientific software resulted from a research project. To start the calculations, it expects input data in the form of a file passed as a command line argument. At the end *GID_sl* produces a data file containing the dependence of X-ray reflection coefficient on a scan angle. The web browser interface to *GID_sl* consists of an HTML form for entering the input parameters by a remote user and an additional program *GID_form* parsing these parameters and converting them into the input file of *GID_sl*. The wrapper program *GID_form* receives data from a web server (e.g. Apache [9]) and calls *GID_sl*. After the execution of *GID_sl* is finished, *GID_form* produces an HTML page with the link to the *GID_sl* output file. Additionally, *GID_form* uses freeware software Gnuplot [10] and InfoZIP [11] to generate a plot for the HTML page and compress the output data, respectively. In this scheme *GID_sl* does not need any special modifications for the remote access and the only software needed is thin wrapper layer *GID_form*. Thus, the effort of making WWW access to modeling software is very affordable.

3. Advanced access to X-ray server

Being a well established and reliable resource of X-ray modeling with a nearly 10-year history, X-ray Server has received numerous requests to expand beyond plain web browser sessions and facilitate automated access, remote fitting and integration of Server programs into users' data analysis software. As an example, a diffraction program written by a user could remotely access X-ray structure amplitudes provided by the *X0h* program (see Table 1 for *X0h* description). This would make the user's code much more lightweight and the effort much smaller since sorting out the task of calculating structure factors could be left out to the Server. Another example could be the need to calculate a series of structure factors or diffraction and reflectivity curves as a function of a parameter. It would be

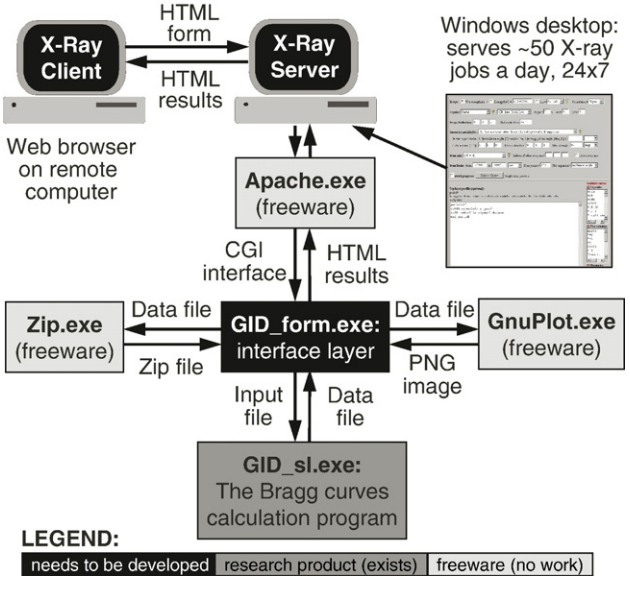

Fig. 1. Scheme of adding WWW interface to scientific software. The only pieces to be developed are the HTML form and the input data parsing layer *GID_form.exe*.

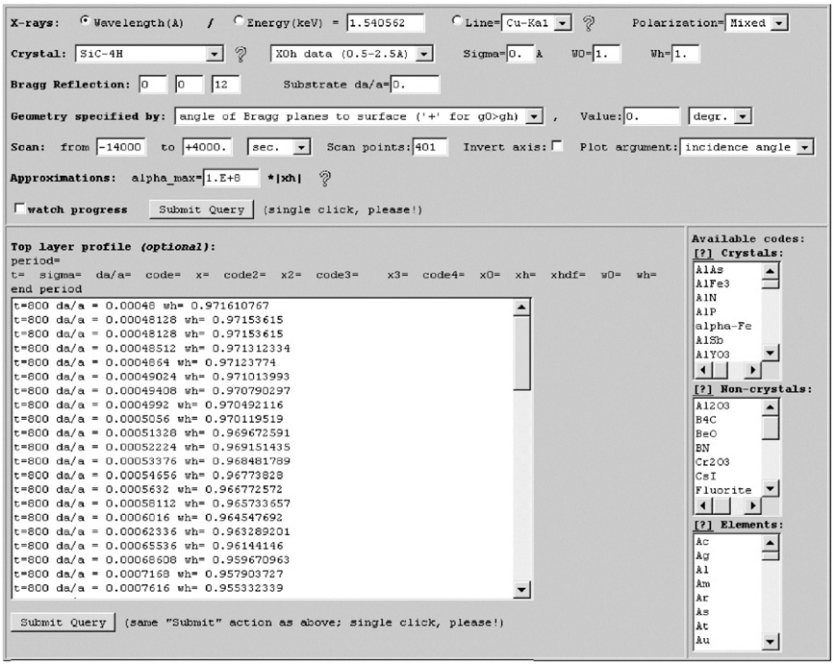

Fig. 2. Web interface input form of *GID_sl* program containing more than 200 parameters in the description of strained crystal surface layer.

much more preferable to have such operation scripted than running a session in a web browser several hundred times and manually varying a parameter at each calculation. Finally, one more interesting task requested by many users is remote fitting of experimental data at X-ray Server. The main challenge here is the number of parameters: for example, the Bragg curves calculated with the *GID_sl* program can be specified with hundreds or even thousands of parameters describing the surface layer. The input form presented in Fig. 2 corresponds to a typical material science application. It describes the surface layer of SiC approximated by 72 sublayers and containing more than 200 parameters like thickness, strain and structure factor. With so many input parameters, the approach to choose a subset of what could be fitted would tailor software for a specific task, i.e. lead to the loss of general Server applicability. On the other hand, implementing fit option for everything would obviously make the programs and the interface impractically heavy. Besides, when it comes to fitting, often the simulated curves need to be convoluted with the geometry of the experiment; for example, with the incident beam divergence after the monochromator or slits, and etc. Given the diversity of geometries at synchrotrons and lab sources, incorporation of generic account for experimental resolution function and geometrical corrections does not seem to be feasible.

Therefore, it has been suggested to move the choice of fitted parameters as well as the account for experimental corrections to the client side. In other words, the server can solve the physical problem of X-ray interaction with model media, while the specifics of experiment are left to the client-side software. This is presented in Fig. 3. A fitting routine written by a user runs in a loop on his client computer. It fits experimental data by requesting model data from the server via a wrapper script at each step of the fitting loop. If necessary, the simulated curves returned by the wrapper are convoluted with experiment in user's software. This is expected to be an optimum share of responsibilities between the Server and the users. Although some programming is required on the users' side, it grants users the maximum flexibility in analyzing their data without any need to program scattering models.

The examples of wrapper scripts are downloadable from the Server. These are mostly PERL scripts not exceeding 100 lines of code and containing detailed comments for easy learning.

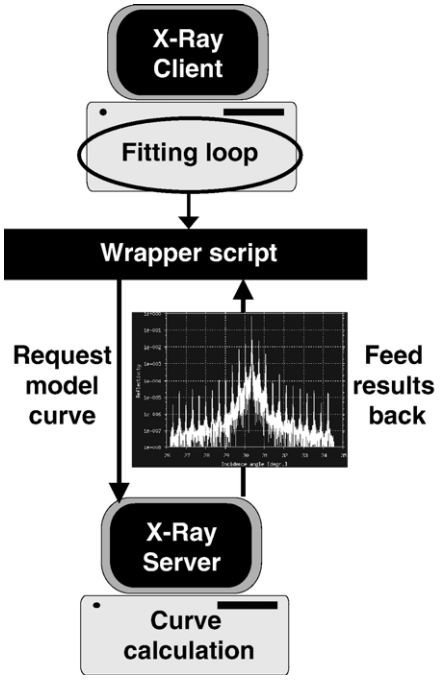

Fig. 3. Scheme of remote fitting at X-ray Server with the help of wrapper scripts.

The wrappers can be called from user's software written in any language using the *system()* function. Varying parameters can be passed to the scripts as command line arguments.

4. Conclusions

The experience gained from the X-ray Server development extends much beyond the scope of programs presented through it, i.e. beyond the field of surface X-ray scattering. The solutions how to maintain the link between the developer and users, how to efficiently expand models and refine scientific software based on user's feedback are quite common not only for X-ray and neutron scattering, but for many other fields of research. Therefore, the automation solutions suggested in this paper are believed to benefit a wide scientific audience.

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