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Molray – a web interface between *O* and the *POV-Ray* ray tracer

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A publicly available web-based interface is presented for producing high-quality ray-traced images and movies from the molecular-modelling program *O* [Jones *et al.* (1991), *Acta Cryst.* A**47**, 110–119]. The interface allows the user to select *O*-plot files and set parameters to create standard input files for the popular ray-tracing renderer *POV-Ray*, which can then produce publication-quality still images or simple movies. To ensure ease of use, we have made this service available to the *O* user community *via* the World Wide Web. The public *Molray* server is available at http://xray.bmc.uu.se/molray.

1. Introduction

One of the problems when presenting structural work in a journal is how to best represent a three-dimensional structure in a two-dimensional medium. Stereo pairs are commonly used, but one can assume that most people do not look at these with stereoviewers unless they have a specific interest in the molecule. For this reason it is important that the mono images give as much depth information as possible even when viewed separately. Realistic rendering and particularly ray-tracing techniques is a means to this end. There are many high-quality rendering programs available for molecular modellers (Merrit & Murphy, 1994; Kraulis, 1991; Esnouf, 1997), but most are independent systems whose operation must be mastered alongside the operation of the interactive map-fitting system that the crystallographer uses daily.

More recently, some web-based services have become available, for example at IMB Jena (Sühnel, 1996; http://www.imb-jena.de/IMAGE.html), where a VRML viewer can be used to select viewpoints for renderings of a complete protein.

Given the infrequency with which most workers publish, preparing figures for manuscripts is usually a time-consuming relearning exercise. The program *O* (Jones *et al.*, 1991) provides a broad range of capabilities for creating molecular objects as well as contoured electron densities. The program can generate a metafile of drawing instructions and this can now be used to produce publication-quality images *via Molray*.

2. Design

The main design aim was to develop a system that was extremely simple to use for beginners and infrequent users, since few people need to make high-quality images often enough to remember a complicated command system. The system should also be web based to avoid the need to install and maintain the program at every site.

In the simplest case, the user need only point their browser at the *Molray* web page (Fig. 1), enter the name of the *O*-plot metafile and click on 'Make Image' in order to obtain a first-draft image. Often, the only parameters that need to be changed from that point are the quality of the rendering and the size of the image. These parameters are highlighted so that nervous users can ignore the more advanced features if they wish. The web page is divided into four panels, each used for a different step in the rendering process, but for users with limited screen space one window with a single panel can be reused.

Because all the calculations are performed on the remote server and all communications with the user's browser are implemented in pure HTML, the user does not need to download any plugins or helper applications and the service can be used with any combination of client machine and browser. A minor exception to this is the progress monitor, which requires JavaScript to be enabled before it will operate, but image generation is not affected if the progress monitor is not enabled.

3. Use

O has an extensive set of options to make molecular images and these can be saved as a metafile of drawing instructions. The first panel of *Molray* then prompts for the name of such an *O* metafile and gives the option of stepping to another panel to select objects that are in

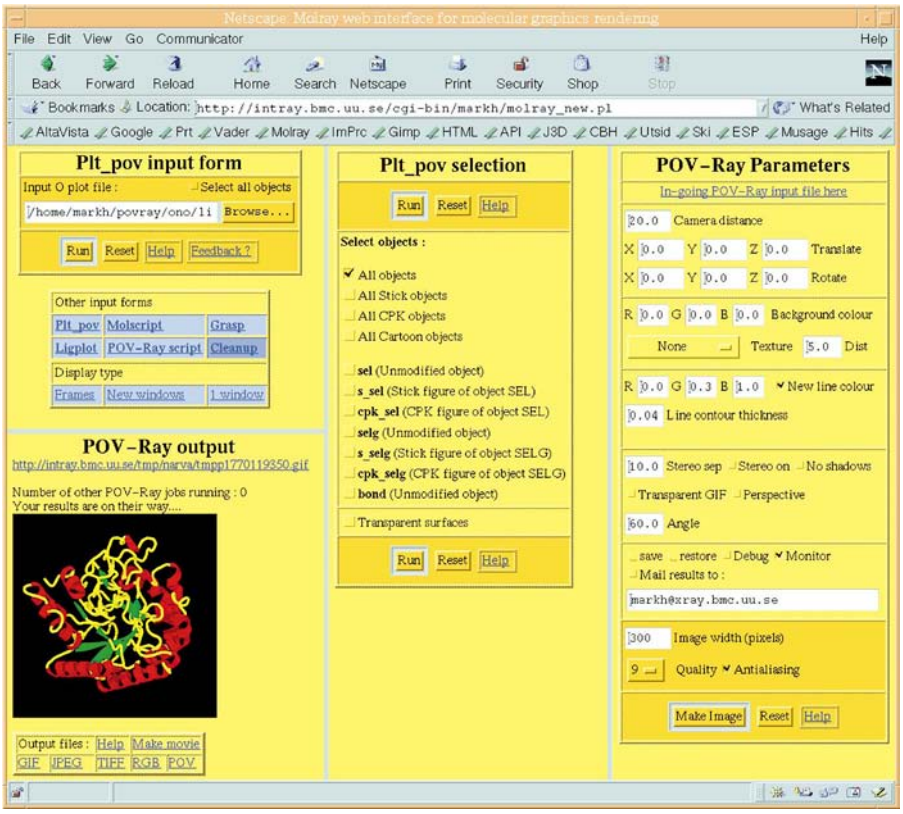

Figure 1
The *Molray* user interface.

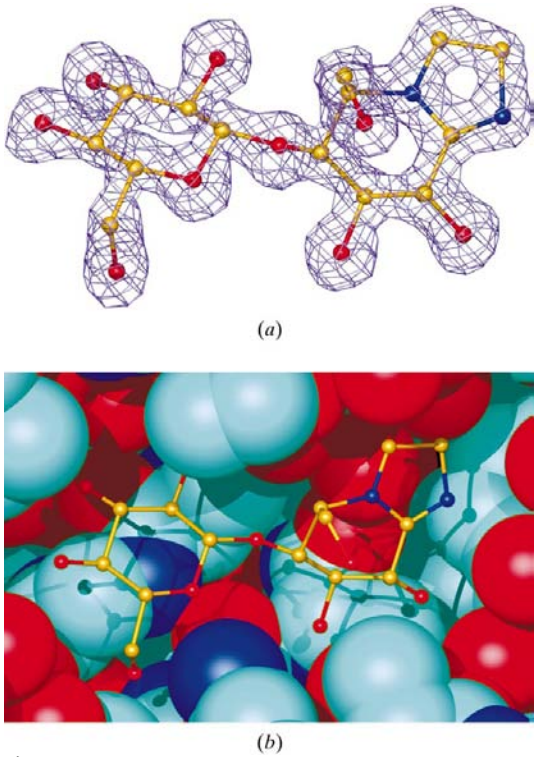

Figure 2
(*a*) Electron density around the Cel6A/cellobiono-imidazole complex (Ståhlberg *et al.*, manuscript in preparation). (*b*) Ball-and-stick figure of cellobiono-imidazole binding to CPK surface of Cel6A (Ståhlberg *et al.*, manuscript in preparation). More examples of *Molray* results can be found at http://xray.bmc.uu.se/molray.

the metafile but which may or may not be wanted in the current rendering. After selection, the main rendering panel appears, where the user can choose the size and quality of the rendering, background colour or texture and map contour-line thickness, along with stereoscopic and perspective options. It is also possible to make adjustments to translations and rotations of the scene, although these would normally be optimized in *O* before writing out the metafile.

Once these parameters have been chosen (or the defaults are used), the user clicks on 'Make Image' and when rendering is finished a small copy of the image appears in the third panel. Parameters can then be adjusted and new images created *ad nauseam*. Once optimized, the full-sized image can be picked up with one click in TIFF, GIF, JPEG or RGB formats. An example image showing contoured electron density is shown in Fig. 2(*a*); Fig. 2(*b*) shows a ball-and-stick representation superimposed on a CPK model of an enzyme active site. If desired, the 'Make Movie' option can also be selected, in which case the fourth panel is filled by an interface similar to the main rendering window, with the exception that starting and ending values can be entered for the rotation and translation values and these are used to produce a movie scene. There is an option to then append other scenes to this one to make a more complex movie. Output formats for the movies are currently GIF89a and MPEG-1.[1]

4. Implementation

The web interface is a 'cgi' script written in Perl-5, the metafile is interpreted and converted to *POV-Ray* input format by a Fortran-77 program called *plt_pov* and the rendering is performed by the publicly available program *POV-Ray*, written by the POV-Ray Team (The POV-Ray Team, 2000). All these programs reside on the server in Uppsala, but each component can be run separately and on any local machine. Each panel of the interface corresponds to a different section of code within the Perl script. Separate scripts could have been used, but the overhead of a monolithic program was considered worthwhile to avoid the pitfalls of maintaining many different scripts. The code associated with the first panel uploads the user's metafile to the server and then runs *plt_pov* to produce a simple *POV-Ray* input file. The code in subsequent panels then performs 'sed' operations on that initial file in order to produce new input files with different values for parameters. Because there are no intermediate formats within the *Molray* system, individual steps can be performed on different machines if desired. For example, evaluation of parameter settings can be performed using the interface, but *POV-Ray* can be run locally to exploit faster dedicated machines or previously created *POV-Ray* files can be fed into *Molray* for rendering.

For users wishing to set up their own service, any server that supports Perl-5 and on which *POV-Ray* and the support programs can be installed can be used as a host. The code is available free of charge from the *Molray* website.

Molray has been installed on a Compaq XP1000 running True64 V4.0f and the

[1] Examples of movies are available as MPEG and GIF files from the IUCr electronic archive (Reference: gr2147) and can be viewed in the online version of this paper. Details on how to access these data are available at the back of the journal.

Apache web server 1.3.9 and on a Dell Dimension L733R running Mandrake Linux 7.3 and Apache 1.3.14.

This service is supported in part by hardware provided by Compaq.

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