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CONSCRIPT: a program for generating electron density isosurfaces for presentation in protein crystallography

M. C. Lawrence[a]* and P. Bourke[b]

[a]Biomolecular Research Institute, 343 Royal Parade, Parkville, Victoria 3052, Australia, and [b]Department of Astrophysics and Supercomputing, Swinburne University of Technology, PO Box 218, Hawthorn, Victoria 3122, Australia. Correspondence e-mail: mike.lawrence@bioresi.com.au

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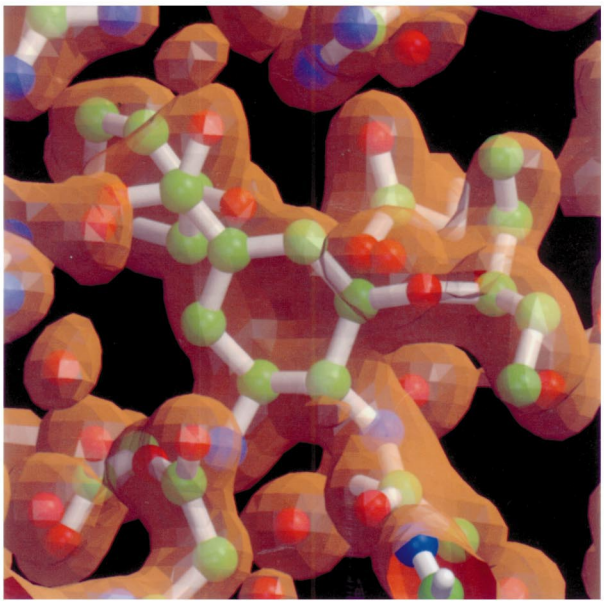
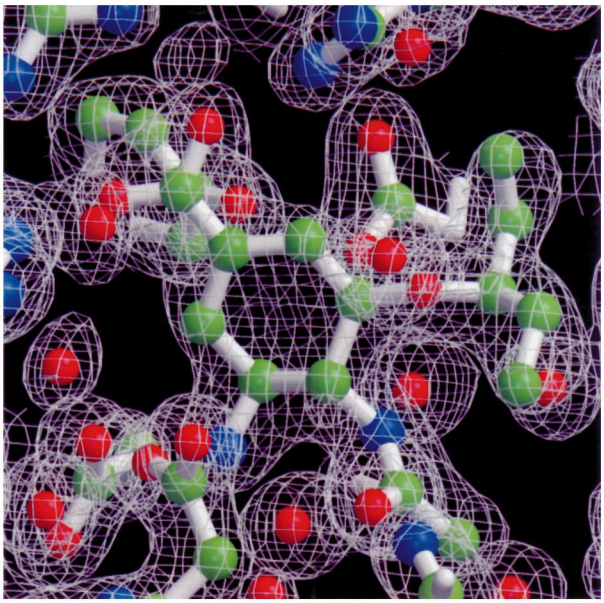
1. The crystallographic problem

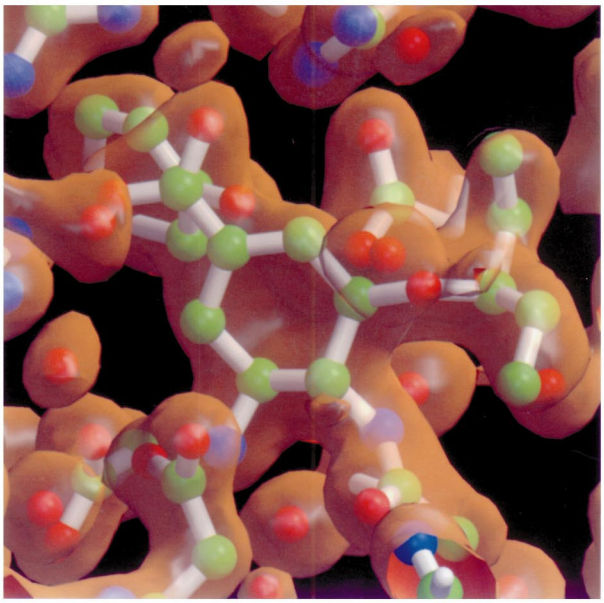
The literature presentation of electron density maps in protein crystallography is typically performed *via* the 'wire-frame' or 'chicken-wire' technique. While this method of rendering has been enormously successful in interactive atomic model building over the past two decades, it is not ideal for printed or static electronic journal display. In particular, pictures often appear cluttered with wire-frame lines and adequate illusion of depth is only achieved in combination with stereo-pair presentation. Stereo-pair viewing is still perceived as somewhat daunting to the uninitiated. Thus, while the quality of



(*b*)



(*a*)



(*c*)

Figure 1
($2F_o - F_c, \alpha_{calc}$) electron density isosurfaces in the vicinity of an inhibitor bound to influenza virus neuraminidase. (*a*) *CONSCRIPT* conventional wire-frame representation. (*b*) *CONSCRIPT* triangulated surface with uniformly shaded facets. (*c*) *CONSCRIPT* triangulated surface with Gouraud-shaded facets. The isosurface is contoured at 1.2σ and is shaded transparent brown on the outer surface and transparent orange on the inner surface. Map sampling is at 0.36 Å (1/5 resolution). Atomic coordinates were obtained from the Protein Data Bank (PDB; Bernstein *et al.*, 1977) entry 2QWK (Varghese *et al.*, 1998). Structure factors associated with this entry were obtained from the author (J. Varghese, personal communication). Images were generated using *MOLSCRIPT* and *Raster3D* as described in the text. *CONSCRIPT* surface generation times on an SGI R5000 processor running IRIX 6.5 for the three figures were 44.3, 46.4 and 52.1 s, respectively.

presentation of atomic models, molecular surfaces and protein schemes is now exceedingly high, combining these with wire-frame electron density display is somewhat anachronistic.

We have thus developed software that will allow protein electron density isosurfaces to be generated in triangulated form suitable for input into the popular *MOLSCRIPT* package (Kraulis, 1991). We propose that this method of display leads to pictures that are easier to interpret and in many cases would dispense with the need for stereo-pair presentation.

2. Method of solution

CONSCRIPT employs the marching-cube algorithm (Lorensen & Cline, 1987). This algorithm has been considered before for electron density isosurfaces (Weber, 1999), but here we integrate it directly into protein crystallography and its public domain map generation and molecular rendering software.

The marching-cube algorithm is relatively straightforward in concept and is based upon analysing in turn each unit grid block within the electron density map. Each block is defined by its eight vertex coordinates and by the electron density at those vertices. The isosurface intersects all edges of the block that have one vertex above the isosurface value and the other below. These intersection points, computed by simple linear interpolation, can be grouped into triplets to create triangular facets which approximate the isosurface itself. The grouping needs to be performed in a consistent way so that facets from adjacent grid blocks connect together correctly. The *CONSCRIPT* implementation of this algorithm allows in addition the triangulated surface to be Gouraud shaded (Gouraud, 1971) *via* assigning normals to each facet vertex.

3. Software/hardware environment

All testing of *CONSCRIPT* has been performed in combination with *MOLSCRIPT* (version 2.1.2) and *Raster3D* (version 2.5b; Merritt & Bacon, 1997) on a Silicon Graphics R5000 workstation running IRIX 6.5. Calls are made to the *CCP*4 (version 4.0; Collaborative Computing Project, Number 4, 1994) subroutine library `libccp4.a` for input parsing, memory allocation and map handling. Calls are also made to a quick-sort subroutine `qsort`; this routine is part of the Fortran 77 library currently associated with IRIX 6.5.

4. Program specification

CONSCRIPT is written in Fortran 77 plus common extensions. Memory allocation within the program is part dynamic, part static; however, critical array sizes can be increased *via* environment variables.

CONSCRIPT can read in electron density maps in either *CCP*4 or *X-PLOR*/*CNS* format (Brünger *et al.*, 1987, 1998). Both isosurface and wire-frame representations can be generated. The output is in the form of an 'object file' suitable for input into *MOLSCRIPT* wherein it can be superposed with an atomic model and/or protein scheme. While *MOLSCRIPT* offers a number of output options, *Raster3D* appears particularly suitable for final rendering of the isosurface. Examples of *CONSCRIPT*-generated isosurfaces displayed in this fashion are presented in Fig. 1.

The time required to generate an isosurface is a linear function of map size N in the absence of Gouraud shading, whereas with Gouraud shading the time required varies as $\sim N \log N$. Surface generation times for the images displayed in Fig. 1 are given in the caption.

5. Documentation and availability

CONSCRIPT and its documentation are available from http://www.bioresi.com.au/conscript and may be used subject to the terms and conditions detailed at that address.

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