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computer program abstracts

This category provides a rapid means of communicating up-to-date information concerning both new programs or systems and significant updates to existing ones. Submissions should follow the standard format given in *J. Appl. Cryst.* (1985). **18**, 189–190, also available from **Crystallography Journals** Online at http://journals.iucr.org/j/services/authorservices.html.

Fourier3D: visualization of electron density and solvent-accessible voids in small-molecule crystallography

Duncan M. Tooke* and Anthony L. Spek

Department of Crystal and Structural Chemistry, Utrecht University, Padualaan 8, 3584 CH Utrecht, The Netherlands. Correspondence e-mail: d.m.tooke@chem.uu.nl

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1. The crystallographic problem

Although three-dimensional electron density visualization is common in protein crystallography, it is rarely used by small-molecule crystallographers. However, in cases such as disorder and the location of hydrogen atoms, it can prove an invaluable tool in correctly interpreting and modelling a crystal structure.

The previously released *MCE* program (Hušák & Kratochvíl, 2003) excellently fulfills this role for Windows-based PCs, and has inspired us to create an equivalent program to address the needs of crystallographers using Unix (including Linux).

Fourier3D reads map files written by *PLATON* and generates colour-coded three-dimensional surfaces based on specified critical density levels. The map handling is fully interactive and controlled using a simple GUI. There are several display styles for both surfaces and molecular fragments. A screenshot or *POV-Ray* input file can be written at any time.

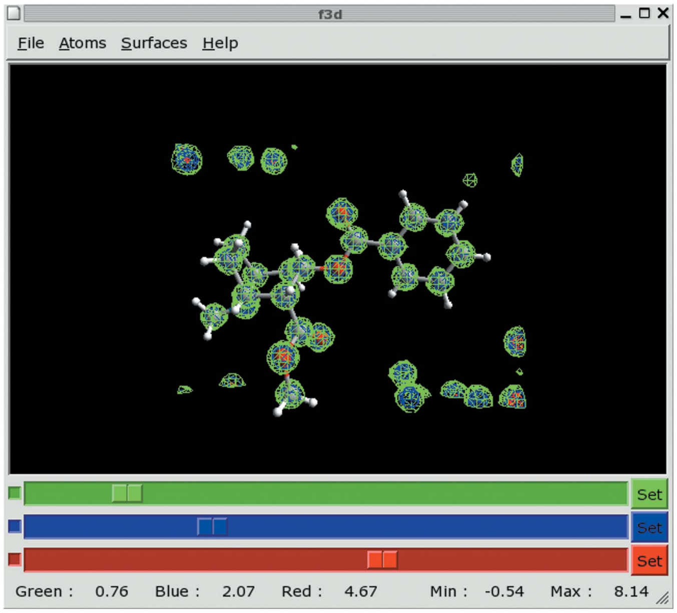
Whilst sharing a degree of common code with *MCE*, *Fourier3D* additionally introduces: a simplified intuitive cross-platform GUI; improved mouse controls; front and rear slabbing planes; high-quality molecular display styles; solid-surface modes; integrated support for visualization of solvent-accessible voids; no need to recompile for use with very large maps; quick reference help and full on-line documentation.

Other Unix software that offers similar display methods includes the powder diffraction package *FOX* (Favre-Nicolin & Cerny, 2002) and the commercially available *maXus* program (Bruker AXS).

2. Method of solution

Fourier3D reads `.fou` format Fourier maps and `.slv` format solvent-accessible void maps as generated by *PLATON* (Spek, 2003). The program is specifically designed to work hand-in-hand with *PLATON*, and is automatically launched from within the program *via* the graphical user interface.

The program generates three colour-coded three-dimensional surfaces based on specified critical density levels. These surfaces can be turned on and off individually, and the critical density levels can be changed independently. The map can be rotated, translated and zoomed, and slabbing planes can be used to restrict the amount of the



Green : 0.76 Blue : 2.07 Red : 4.67 Min : -0.54 Max : 8.14

Figure 1
The main program window. General program functions are accessed using the drop-down menus at the top, whilst surfaces are controlled using check-boxes, sliders and buttons. The status bar at the bottom gives context-sensitive information.

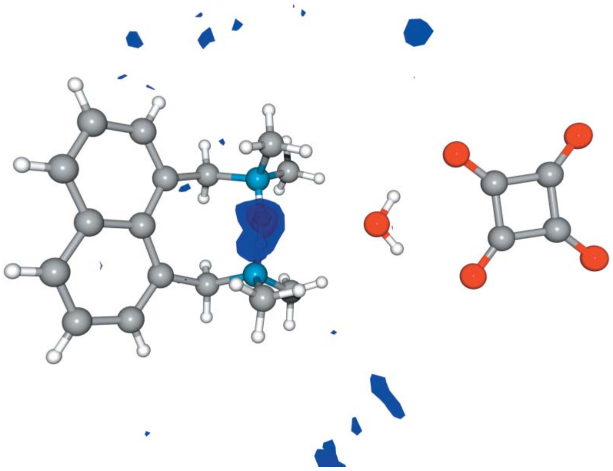


Figure 2
Example of a structure in which the detailed interpretation of hydrogen bonding is of interest. 1,8-Bis(dimethylaminomethyl)naphthalene is one of a class of molecules known as 'proton sponges', due to their ability to trap H^+ ions in a very strong intramolecular hydrogen bond. The proton is often found in a central position, but in this case examination of difference Fourier maps clearly showed two sites. The final populations were refined to a 3:1 ratio (Bouma *et al.*, 1999). $F_{\rm obs} - F_{\rm calc}$ map with partial hydrogen atoms omitted from structure factors. *POV-Ray* image generated in blue solid surface mode with ball and stick structure.

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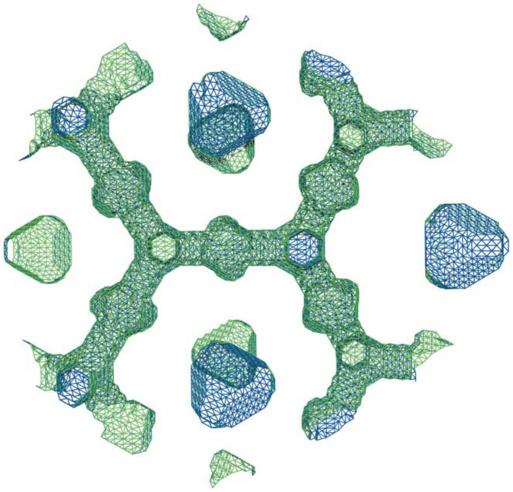

Figure 3
Slice through the solvent-accessible void of a zeolite clathrate (Choi *et al.*, 2002). The blue surfaces are inside the voids. Wireframe map with no structure displayed.

map displayed in the axis perpendicular to the screen, which allows viewing of interior details in large maps.

Several display styles for both surfaces and molecular fragments are available, and a screenshot or high-quality *POV-Ray* (http://www.povray.org) file can be made of the map at any time. *POV-Ray* files are automatically rendered on-screen if the program is installed.

Figs. 1–3 illustrate the use of the program.

3. Software and hardware environment

The program is written using C++ and OpenGL, with the free open-source version of the Qt library (http://www.trolltech.com/products/qt) used for the graphical user interface. The program will compile on any Linux or Unix computer with the relevant development libraries. Due to the cross-platform design of both OpenGL and Qt, it would be trivial to port the program to either Windows or MacOS, so long as the proper Qt licences were available.

Integration of the program into other software packages should likewise present few difficulties. The `.fou` and `.slv` files are plain ASCII, and full details of their formats are provided with the source code. Map points and atoms listed in the file are rendered 'as is', using only a transformation matrix and with no need to provide symmetry operations, and all bonds are calculated during runtime based on covalent radii. With the possible exception of minor issues concerning end-of-line characters, files produced on one platform should additionally be readable on any other.

The program will run on any platform for which it can be compiled. As with all OpenGL software, an accelerated graphics card increases performance by orders of magnitude, and can be considered almost essential for large maps.

4. Documentation and availability

The program is designed to be as intuitive to use as possible. The main window is simple and uncluttered, and the map controls are colour-coded. A quick reference window is always available, and full on-line documentation can be accessed from within the program *via* a Web browser.

The source code and a Linux executable are available free of charge *via* the author's website http://www.cryst.chem.uu.nl/tooke/fourier3d/. *PLATON* can be obtained from http://www.cryst.chem.uu.nl/PLATON.

The authors would like to thank Michal Husak for his generous permission to use an early IRIX version of his *MCE* software as a convenient starting point for the prototype of the program. Thanks also go to Louis Farrugia, Rob Hooft, Huub Kooijman and Martin Lutz for help and discussions.

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