MS47 New horizons in teaching crystallography in the 21st century

MS47-03
An interactive tool to explore the two-dimensional Fourier transform
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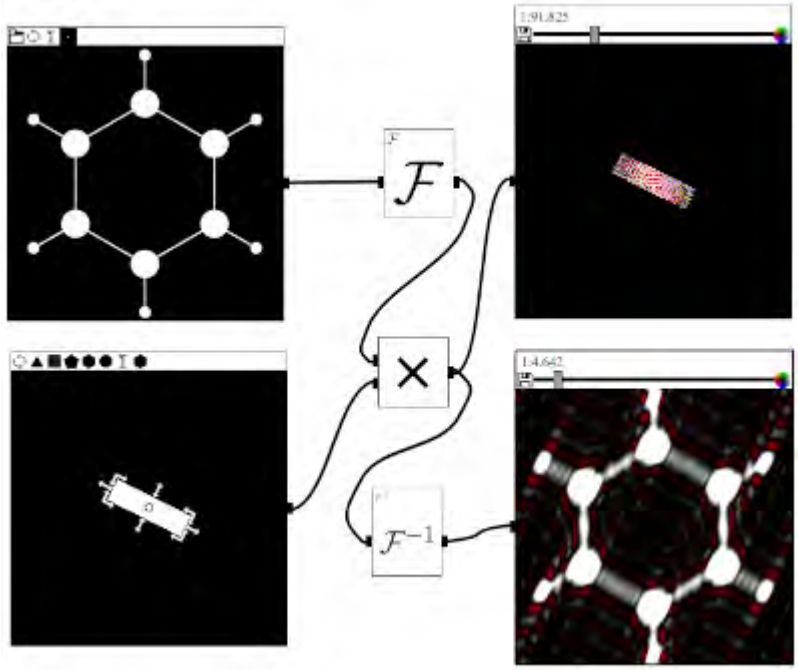
Abstract
According to the kinematic model of diffraction, the diffraction pattern of an object is the square of the norm of its Fourier transform. Therefore, understanding the Fourier transform is crucial in understanding diffraction phenomena. However, the Fourier transform is highly counterintuitive. The best and perhaps only way to come to terms with the Fourier transform is by applying it.
In this context we developed a tool that can be used to interactively explore the two-dimensional Fourier transform in the classroom and demonstrate many of its properties. Two-dimensional source data (arbitrary images, polygons, lattices, Gaussian distributions) can be processed and combined (Fourier transformed, convoluted, added, multiplied, taken to the power, rotated, split into phases and magnitudes) in arbitrary ways and finally displayed.
Thus, numerous fundamental properties of the Fourier transform (linearity, scaling, origin shift, convolution theorem, complex numbers, Fourier transform of real and/or symmetric functions) as well as properties of the diffraction pattern (termination effects, Patterson function, displacement parameters, homometry, quasi-periodicity and countless more) can be demonstrated. For example, Fig. 1 shows the effect of Fourier termination, which might be due to an extreme absorption profile, on a benzene ring. Fig. 2 shows that the inverse Fourier transform of intensity data gives the autocorrelation (Patterson) function of the object under investigation.
All parameters, such as for example the shape of the absorption profile in Fig. 1, can be modified interactively and give immediate results even on modest hardware. Thus, questions and ideas that arise in class can be experimented with spontaneously. The high speed is due to usage of the FFTW library [1]. The code is available under an open-source license.

References
[1] M. Frigo, *Proceedings of the 1999 ACM SIGPLAN Conference on Programming Language Design and Implementation (PLDI '99)*, Atlanta, Georgia, May **1999**

Truncation effect owing to absorption



Patterson function