

ONED
Version 2.00
(X Windows version)

ONED is useful for illustrating, in one-dimension, the principles of diffraction theory. One can build simple 1D motif structures by Fourier summation and perform various Fourier analysis operations on a single motif or a periodic array of motifs. ONED requires the use of a workstation with X Windows display capability. This program allows the building and display of theoretical arrays of motifs in one dimension. The program begins with the building up of a 1D motif structure. This is accomplished either by reading in an existing motif stored as a disk file or by constructing one with the interactive graphics device.

RUNNING ONED

Logon to a Linux workstation (Virion01 locally here at Purdue) using the following username:

```
Username: wshop  
Password: <Given in class>  
(Wait approximately 1-2 minutes)
```

Then issue the following commands:

```
% mkdir rob (Or whatever subdir you want to  
create for your files)  
% cd rob  
% oned  
(Wait approximately 20 seconds)
```

This will cause the ONED program to display to your screen. If for some reason this fails contact Rob Ashmore (rwa@purdue.edu).

THE MODEL BUILDING SCREEN

The Model building screen consists of two parts, the left for drawing the curves and the right for setting the values for amplitude, phase and wave number. What follows is a description of how one uses the scrollbars/toggles on the right to build the curves on the left. The Total model is a summation of all curves thus configured and is displayed at the bottom of the left part of the screen.

CONSTRUCTING A MOTIF INTERACTIVELY

To build a new motif, one needs to define the amplitude and phase for each of the wave numbers (frequencies) 0-10 in the model building screen. Turn the appropriate wave number on or off using the toggle button to the left of the ModelBuilding screen to have this curve included in the "Total" motif. The total motif is displayed in WHITE at the bottom of the curve display screen (to left of model building screen).

As a simple example one might set the scroll bars to give the following values:

| Wave # | Amplitude | Phase |
|--------|-----------|-------|
| 0 | 100 | -- |
| 1 | 100 | 0 |
| 2 | 50 | 90 |
| 3 | 50 | 180 |

NOTE: Wave #0 just adds a constant density to the motif, consequently its phase is meaningless.

Continue adding as many waves as you like (you may even remove specific waves by toggling the "Wave #" toggle).

At this point you have the option of saving your work of art as a disk file to show friends and family at an appropriate later date, or you can start over (and over and over) to get the desired result, or you can continue with what you have built. Choose the "File/Write" menu choice and enter the filename.

USING AN EXISTING MOTIF

If you already have a motif stored in a disk file, Choose the menu choice "File/Read" and then type the name of the file.

THE 1D-FFT SCREEN

On this screen an Original perfect sampled crystal is displayed in WHITE at the top of the drawing area, a BACK-transform of the current Fourier transform (with all of the noise/temperature/filters applied) is displayed below that in RED, and the Fourier Transform

(abs(Amps)) itself is displayed at the bottom in GREEN. To the right are the scrollbars that modify the perfect Crystal or the Transform and descriptions of their actions follows.

SAMPLING THE MOTIF

Each motif is stored in computer memory or on disk as a discrete (sampled) function consisting of 256 evenly-spaced points (pixels). The intensity at each pixel is the density of the motif at that point.

ONED allows you to construct large, periodic objects (1D crystals), up to 512 pixels wide by concatenating multiple copies of the motif. You must first decide how coarsely or finely to sample the 256-point motif (NSAMPL: initial default=64). Typically, one might sample the motif with 16.0 or 32.0 points (this involves simple interpolation of the 256-point function). Use the scroll bars on the 1D FFT screen to choose how coarse or fine you want to sample the motif.

SPECIFYING THE NUMBER OF REPEATS

Use the "# Motifs in crystal" scrollbar to choose how many motifs you desire in your "crystal".

NOTE: The number of motifs (NMOTIF) is entered as a floating point value, so crystals with a non-integral number of unit cells can be made. Note also that your crystal can not exceed 512 pixels in length. Depending on what value you choose for NSAMPL, a DEFAULT value for NMOTIF will be given that produces a crystal of 512 points. Only values of NMOTIF that are less than or equal to the DEFAULT are acceptable.

FLOATING THE DATA

You have the option of floating or not floating the data. Toggle between these two choices with the "Float the data" toggle button on the 1D FFT screen. Floating refers to the process of subtracting from every point in the object the average background value. Floating is generally necessary in computing FTs from discrete data otherwise spurious ripples occur in the Fourier transform as a result of strong diffraction from sharp discontinuities in the object. The DEFAULT state is to float the data.

APPLYING A TEMPERATURE FACTOR

A temperature factor (TFAC) multiplies the Fourier transform with a smooth exponential falloff. Click the toggle button and adjust the to the temperature factor you desire. Values of TFAC are in units of inverse pixels. This specifies at what point the temperature factor function reduces the FT amplitude to $1.0/\exp$ (≈ 0.368) of its original value. For TFAC = 2.0, the amplitudes in the object Fourier transform will be downweighted by $1.0/\exp$ at the edge of the transform. For TFAC = 4.0, the amplitudes drop to $1.0/\exp$ of their original values half-way out in the transform.

ADDING NOISE TO THE DATA

To add shot noise to the crystal, toggle the "Add noise to data" button and use the scroll bar to set the signal-to-noise ratio (SN_RATIO) within the range 0.01 to 50.0.

FILTERING THE DATA

You have several options for generating filtered FT data and, hence, averaging the object data.

| Scrollbars: | Meaning: |
|----------------------|---|
| Spacing of Mask | Distance (pixels) between mask holes |
| Size of Hole in Mask | Distance (pixels) of each "hole" in the mask that allows data through |

The mouse is used to set lower (low pass) and upper (high pass) limits of the FT data.

| Mouse Button: | Meaning: |
|---------------|---------------------------------------|
| Left | Inner resolution limit (low pass) |
| Middle | Outer resolution limit (high pass) |
| Right | Cancel resolution limits (i.e. reset) |

A 1D "mask" is used to zero or block out values in selected portions of the Fourier transform. The mask consists of a lattice of holes of diameter, HOLE_DIAM (Initial default = 1.0 pixel) that are evenly spaced LSPACE transform pixel units (1 TPU is one step in the discrete, 512-point transform). The program gives a DEFAULT value for LSPACE that positions the holes with respect to the IDEAL positions of the reciprocal lattice of the crystal. By altering LSPACE you can generate bizarre effects. As HOLE_DIAM is

reduced, the amount of averaging increases. "Infinite" averaging occurs when HOLE_DIAM = 1.0 (DEFAULT).

The mouse is used to impose RESOLUTION limits on the Fourier transform data and define an annulus (inner and outer limits) within which the Fourier transform is zeroed. High-pass filtering knocks out low-resolution terms and enhances high resolution features (but may create bizarre effects!).