

Semper 6 Command Reference

flc

keys:	[from]	<number>	source picture
	to	<number>	output picture, fitting <i>all peaks</i>
	size	<x>, <y>	dimensions of output picture
	radius	<number>	maximum radius considered in <i>all peaks</i> mode (radius given in pixels)
	position	<x>, <y>	position of single peak to be fitted in picture coordinates
	lline	<n1>, <n2>	position of single peak to be fitted in terms of base vectors <i>u</i> , <i>u2</i> and <i>v</i> , <i>v2</i>
	snr	<number>	threshold intensity signal-to-noise ratio below which peaks are discounted
	mark	<number> <yes or no>	mark fitted sites
	mkmode	<number>	mark mode
	mksize	<number>	mark size
options:	wiener		perform <i>Wiener</i> -optimised least squares peak fit
	verify		print information about fit at the console

Use **flc** (*fourier lattice component*) to perform lattice averaging by the transform peak profile fitting method. **flc** fits lattice (fourier) components to the isolated peaks found in the transform of a periodic image, discommensurate with the sampling lattice.

Examples

```
flc position 52.6, 20.9
```

This command, given a half-plane *Fourier* current picture, fits a transform peak at the indicated position, returning the component value as *t*, *t2*.

```
u=20.3, 2.5 v=1.2, 16.8; flc line 3, -1
```

This command fits the peak with indices 3,-1 on the lattice defined by *u* and *v*.

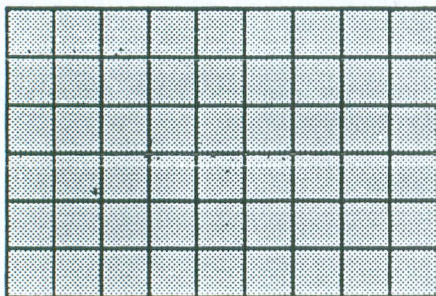
```
fourier 1; u=..., ... v=..., ...; flc to 2 size 65, 128; image
```

This command transforms picture 1, fits all sites on the lattice defined by *u* and *v*, and recovers a single unit cell of the image. *u* and *v* might be fitted more accurately using **xwires list**; **library lattice**; **base 999** after displaying the power spectrum (*ps*).

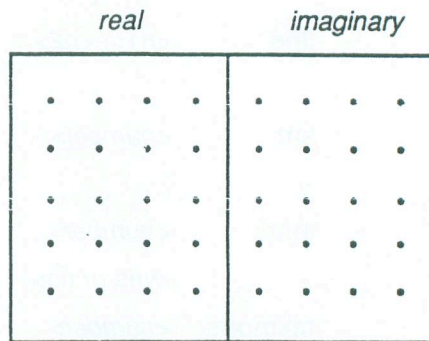
flc

Description

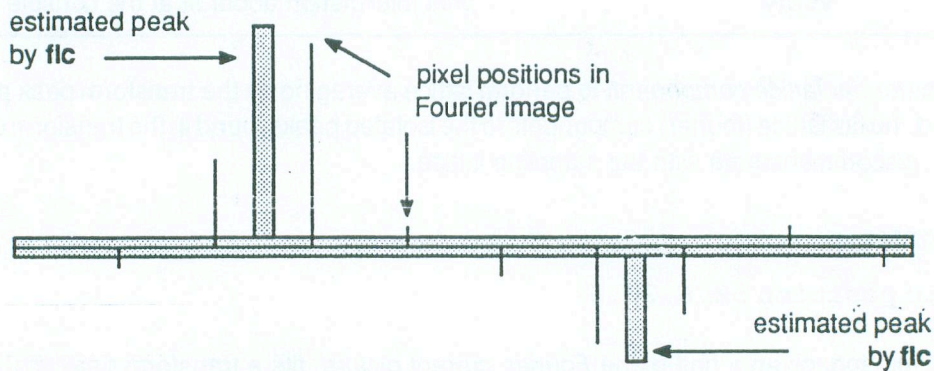
The *fourier* transform of a 2-D periodic image consists of an array of isolated peaks at positions forming a lattice that is reciprocal to the real space lattice. Unless the signal periodicity is an exact multiple of the sampling lattice in both directions, the peaks fall between the transform sampling values and (ideally) have a crossed sinc profile. **flc** allows you to recover the peak values by fitting the samples. The diagram below illustrates the stages of the **flc** command.



Stage 1. 2-D periodic image

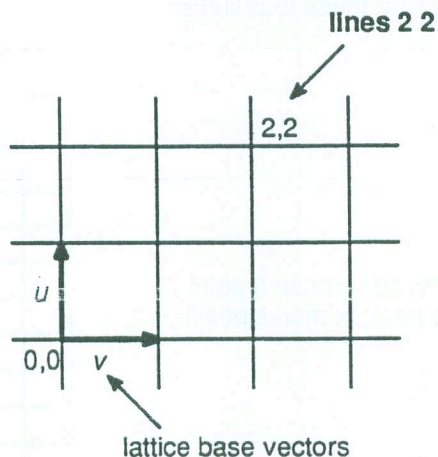


Stage 2. Fourier transform – regular lattice of points



Stage 3. Peaks extrapolated by flc

If you do not specify an output picture using **to**, only one peak is fitted and its values are returned in the variables **t** and **t2**. You can determine that the position is fitted directly using **position** or indirectly using lattice indices specified by **linc**, as is shown in the following diagram. The source (and output) must be a half-plane *Fourier* picture.



Reference by **lines** key using the lattice index

If you specify an output picture, all sites on the lattice defined by u and v are fitted and the resulting values are stored in an output picture. The output picture is a half-plane *Fourier*, size 17 by 32, unless you specify different dimensions using **size**. Note that you can exclude peaks beyond a cut-off radius from the origin using the **radius** key.

Pixel (h,k) receives the value for the site with indices (h,k) etc. so that on inverse transformation the output yields one unit cell of the structure, sampled on a lattice exactly subdividing the unit cell. You can restore normal cartesian (square) sampling using the command **extract uv..** (Use **library reciprocal** and **library Invert** in turn to convert the *fourier* plane base vectors u and v to suitable values for **extract**).

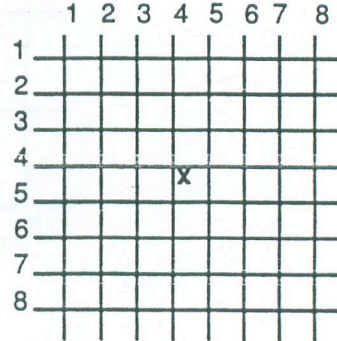
The **verify** option causes details of the fitting to be reported at the console.

The following steps are performed for each peak that is fitted:

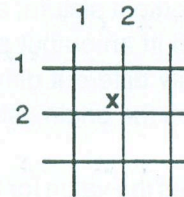
- Step 1** The mean noise intensity is estimated from the peripheral values of an 8 point square region around the peak.
- Step 2** The signal intensity is estimated via the integrated intensity in a 2 point square region, subtracting the estimated noise intensity.
- Step 3** If the resulting signal-to-noise intensity ratio is less than 3 (or the value of the key **snr**), the peak is discarded (with a warning message in single peak mode).
- Step 4** A simple estimate of the lattice *fourier* component is made by combining a modulus given by the square root of the estimated signal intensity with a phase given by the phase of the average of the 4 points around the peak position. (2 or 1 points as necessary if one or both of the peak coordinates is in fact integral).

The following diagrams illustrate these four steps:

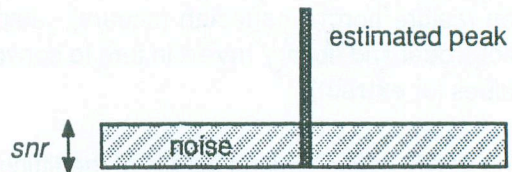
Step 1. Mean noise estimated from an 8 point square region around the peak (x marks peak)



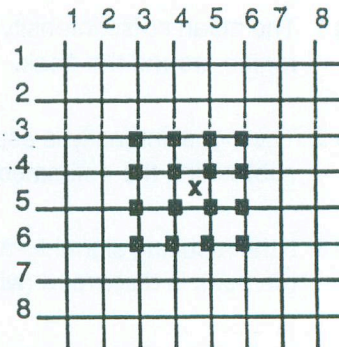
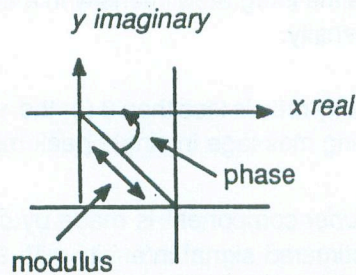
Step 2. $snr = \text{integrated intensity from a 2 point square region minus estimated noise intensity}$ (x marks peak)



Step 3. If signal-to-noise intensity is less than 3 or value of snr , discard the peak



Step 4. Estimate of fourier lattice component by combining modulus and phase – phase from the average of the 4 points around the peak position. (x marks the peak)



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If you specify the **wiener** option, **flc** performs two further steps:

- The ideal crossed sinc profile values are generated for a 4 point square region and a better value for the lattice component is obtained from the corresponding data samples d using an expression of the form:

$$t = \text{sum}(s.d) / [\text{sum}(s.s) + nu / \langle |t|^2 \rangle]$$

where nu denotes the mean noise intensity as estimated earlier, and $\langle |t|^2 \rangle$ the expected signal intensity, estimated using an initial evaluation with nu set to zero.

- The extent to which the local data conform to the expected crossed sinc profile is assessed using a *Chi-squared* difference between predicted and actual transform values, for report on the console.

Do *not* use the **wiener** option under the following conditions:

- the periodic signal does not fill the entire original image field
- the periodic signal is imperfect so that the peak profiles are distorted
- you do not accurately know the reciprocal lattice

If these conditions do not apply, **wiener** provides a more reliable estimate of the lattice fourier component than the usual mode.

If you indicate a display using the **mark** key, **flc** marks the fitted sites in the style and size specified by **mkmode** and **mksize**. Refer to *Appendix C, Semper Keys and Options* for details of the keys **mkmode** and **mksize**.

Notes

display marking:	sites fitted
multi-layer pictures:	faulted
forms used internally:	complex
variables used:	$u, u2, v, v2$ (fourier space lattice base vectors when peak position is specified using line)
variables set:	$t, t2$ (real, imaginary parts of fitted fourier component (single peak modes))
see also:	base, extract, lattice

Defaults and Ranges

keys/options	defaults	range
[from]	current picture, held in the variable <i>select</i>	valid picture number
to	<i>none</i>	valid picture number
size	picture size 17, 32	positive integers
radius	<i>none</i>	positive real number
position	<i>none</i>	within bounds of picture (real numbers)
line	<i>none</i>	within terms of lattice index
snr	ratio 3	positive real number
mark	mark off	see <i>Appendix C</i>
mkmode	1 (upright cross)	integer in range 1 to 5
mksize	2	positive integer
verify	verification off	