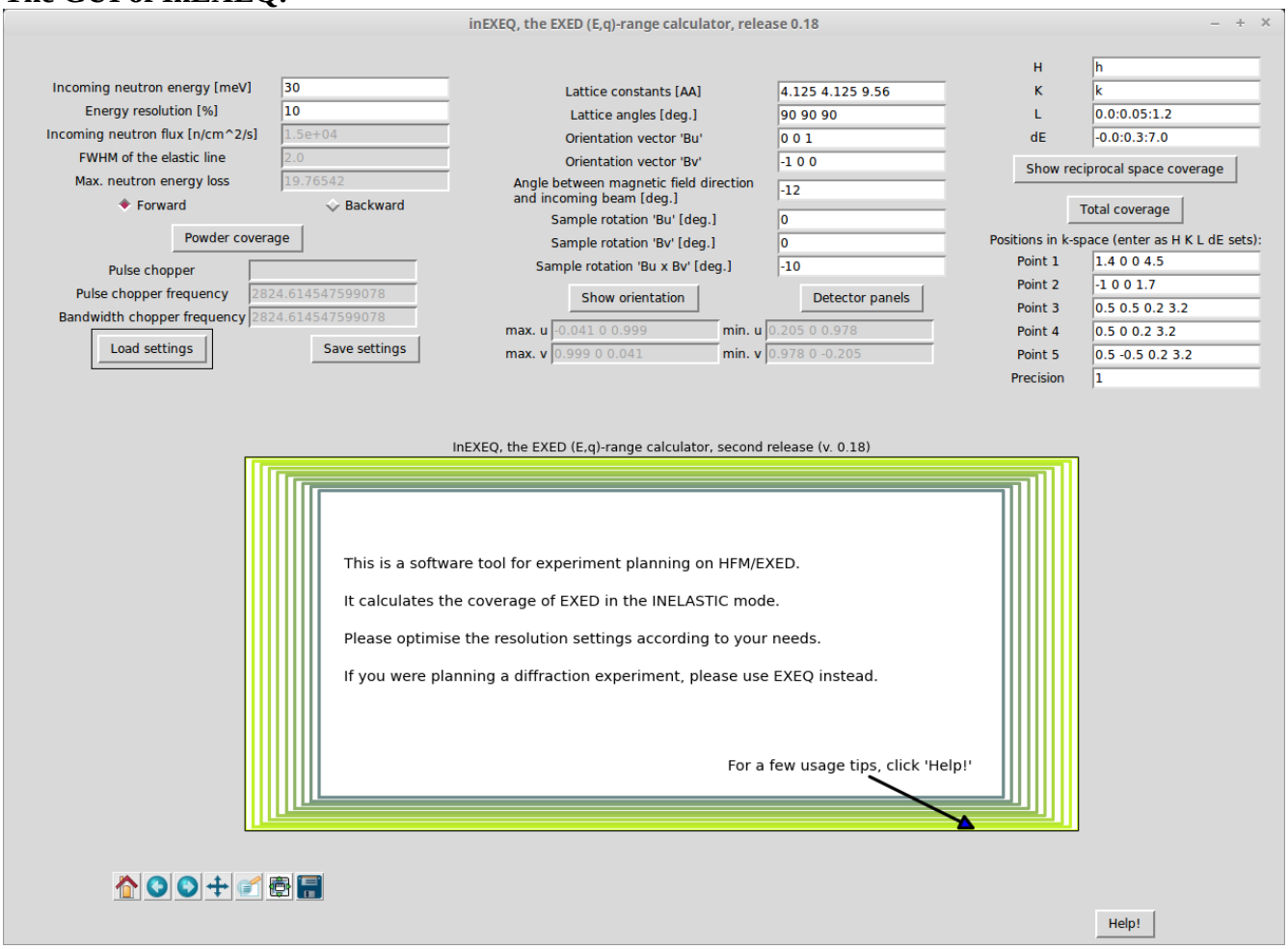
InEXEQ release 2
List of features.

The GUI of InEXEQ:



The sample has to be defined by the user.
The orientation vectors are defined in respect to the magnetic field direction, contrary to the traditional definition. **Bu** and **Bv** vectors are identical to **u** and **v** when the magnet is at 0º rotation angle.

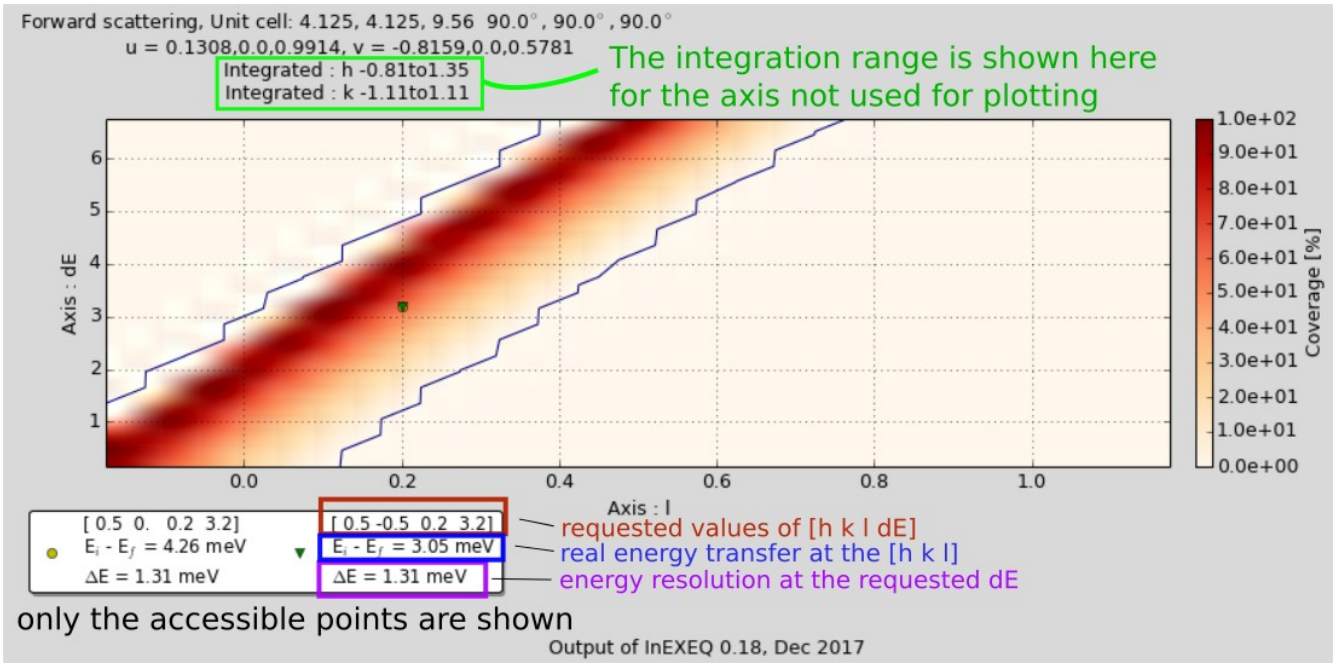
Incoming energy and energy resolution define the chopper speed and incoming neutron flux. The wavelength spectrum is taken from Vitess simulations of EXED.

The calculation of coverage is performed on a rectangular grid. The percentage of the coverage corresponds to how much of the volume in the integration range is accessible by the instrument.

The number of the grid points is proportional only to **PRECISION** parameter. If you need more points along h, reduce the number of points along k, OR increase precision. **Do not increase precision above 2 if you have a computer with low RAM.**

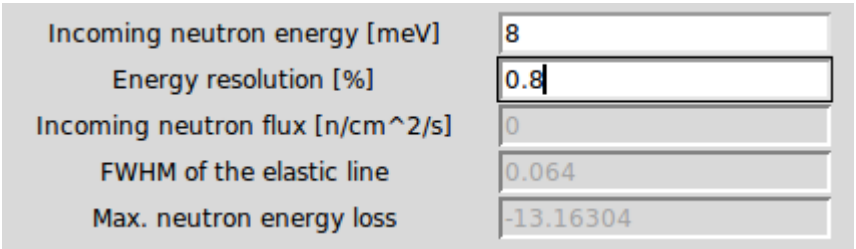
All the input parameters can be **SAVED to a file**, and **LOADED from a file.** This way it is possible to store the sample definition and orientation for later, or send the settings to the EXED instrument scientists.

Coverage maps:
"Show reciprocal space coverage" button creates a map of the reciprocal space, shown below.



Since l and dE are the axes where the **range and step size** were specified (in the previous page), they are the axes used for plotting. The coverage along h and k is integrated, and the range is shown in the map header (highlighted in green.)

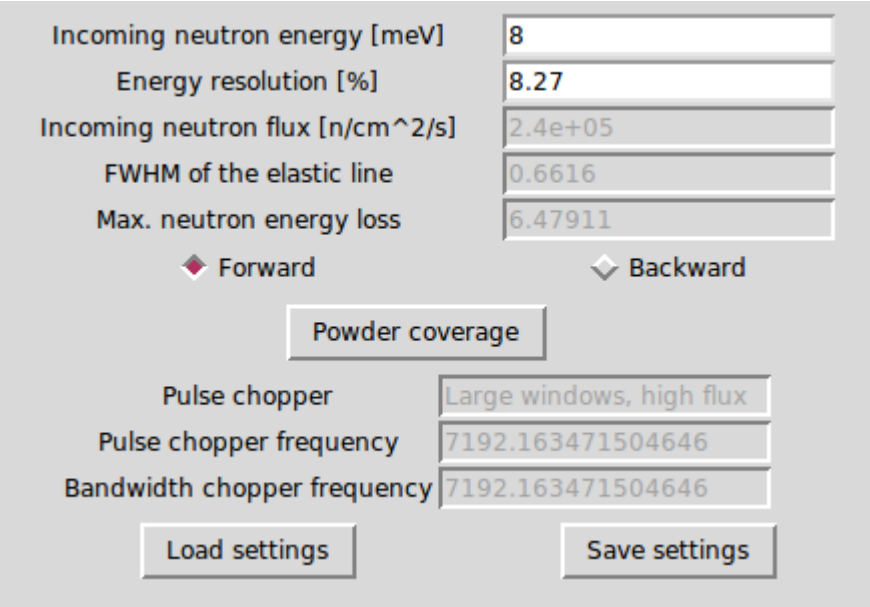
The interface contained marker points. This are the points that the user wants to access; in the map only the points that are accessible with the current sample orientation are shown. Since for one set of E_i, h k and l only one E_f is possible, the real energy transfer is shown for each point. If the difference between the needed and real energy transfer values are within the instrument's energy resolution, the point is considered to be visible.



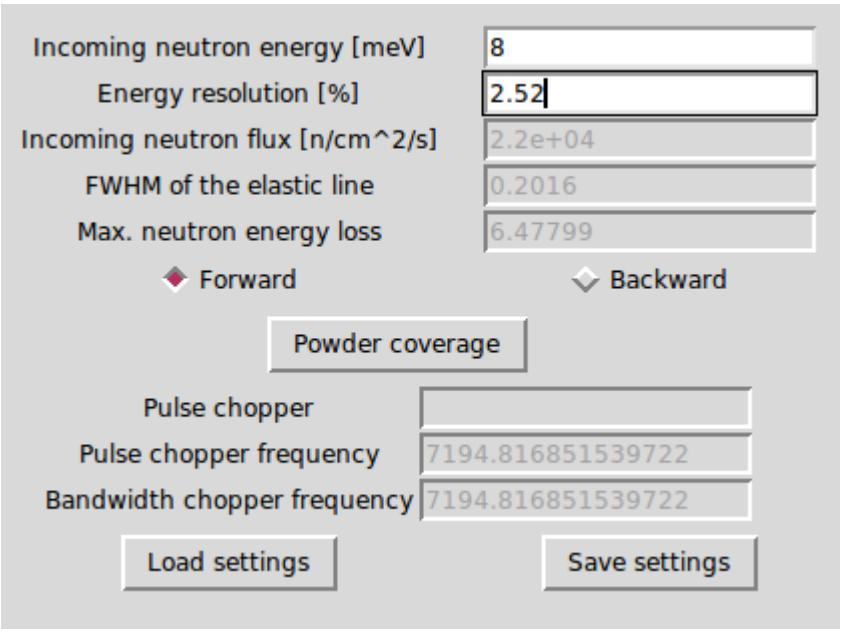
If the energy resolution is outside of the instrument's range, the neutron flux for this setting is shown as 0.

Resolution tuning

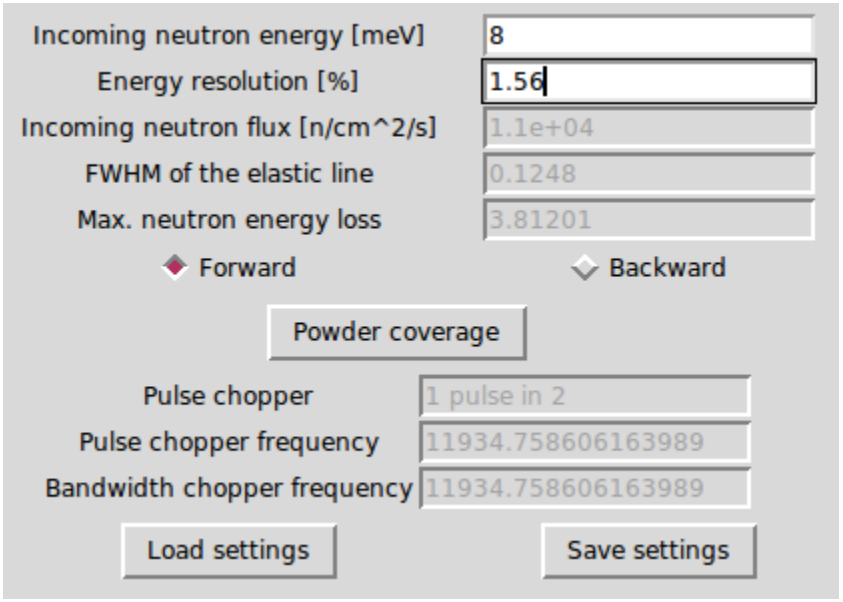
1. If the resolution is relaxed enough to use the large chopper windows, InEXEQ will calculate the incoming flux accordingly. Once the “Large windows, high flux” mode has been reached, there is no way to further improve the flux, and it is not necessary to relax the resolution any further.



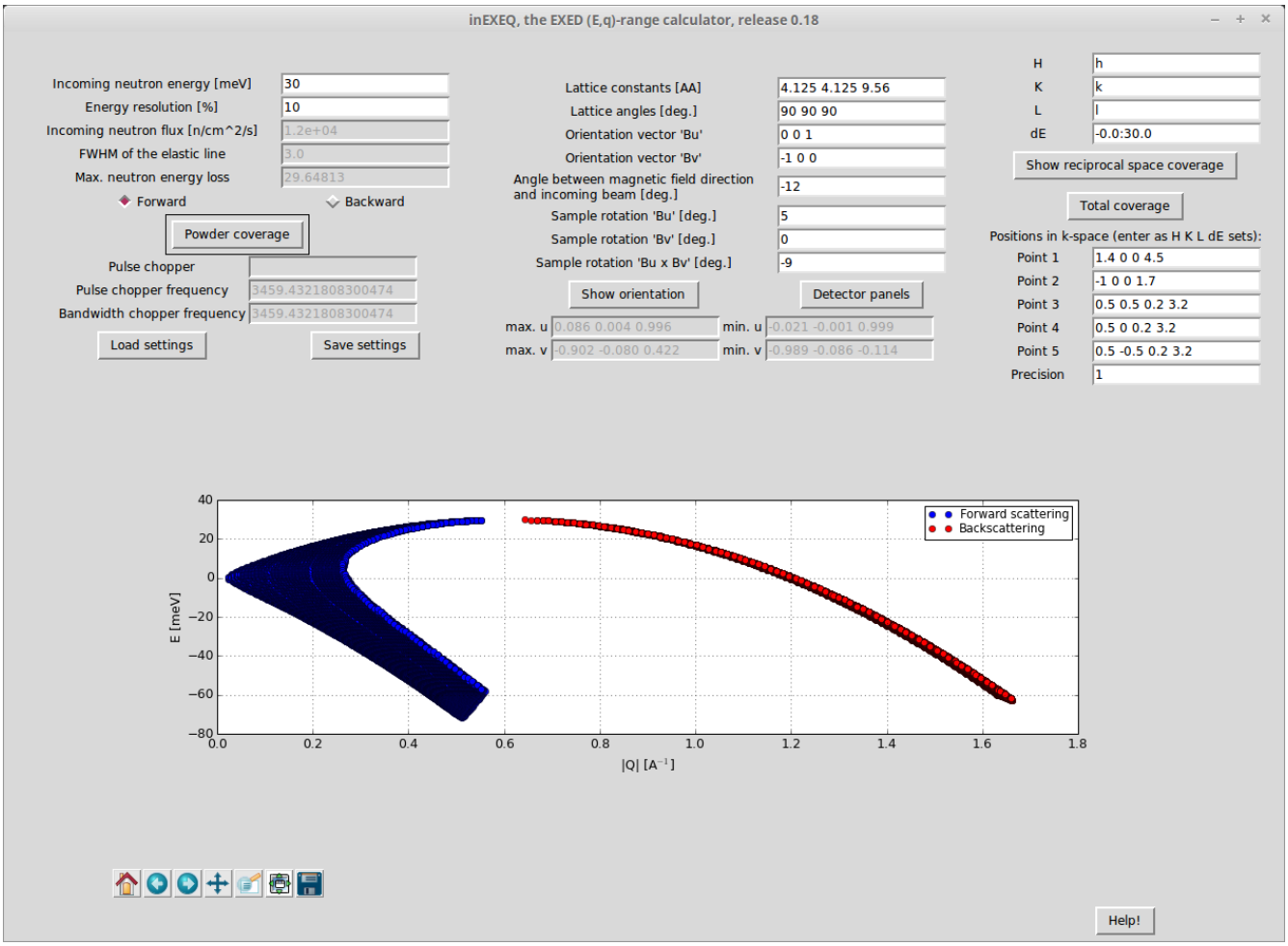
When a better resolution is necessary, the small chopper windows are used. This reduces the instrument flux by an order of magnitude.



Maximum resolution can be reached by increasing the chopper speed to 12000 rpm. This speed cannot be reached by intermediate choppers, and therefore 1 pulse in 2 is discarded, halving the flux further. There is no way to increase the resolution any further beyond this point.



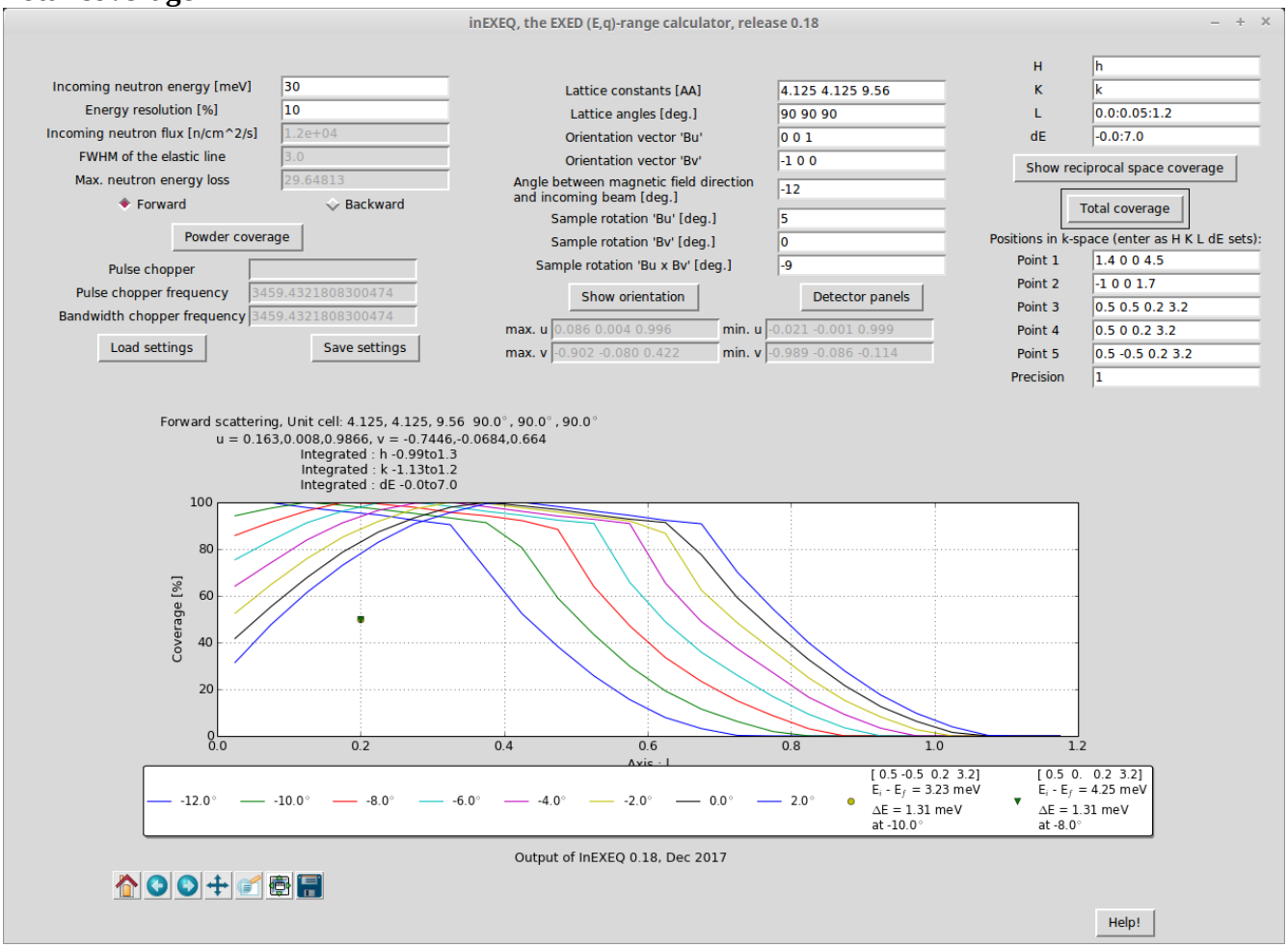
Powder coverage



The powder coverage is the map of the instrument (E,q) range for the current parameters. It depends on the incoming energy. It is always calculated for the maximum magnet rotation angle. The results of the calculation still depend on the h, k, l range in the interface, unless the values are given as 'h', 'k' and 'l'; then the entire covered range is shown.

The negative part of the energy transfer shows the neutron energy gain processes.

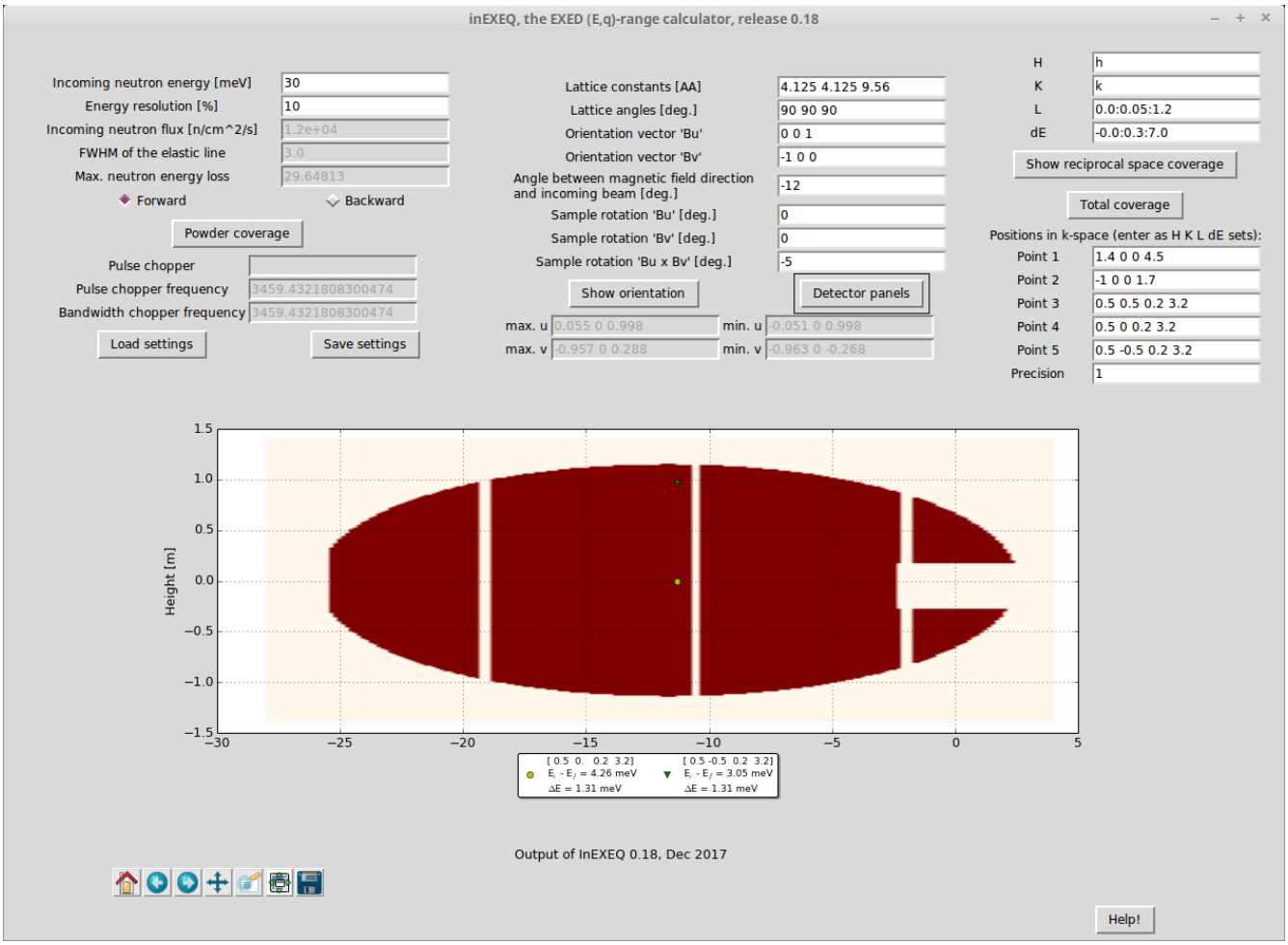
Total coverage



“Total coverage” calculates the accessible E,q range for the current settings at different magnet rotation angles, from -12º to +2º in steps of 2º, and plots them together.

If some marker points were specified, the “Total coverage” option calculates also which angle is optimal for each point. The criterion here is how far the requested energy transfer is from the real one at each angle.

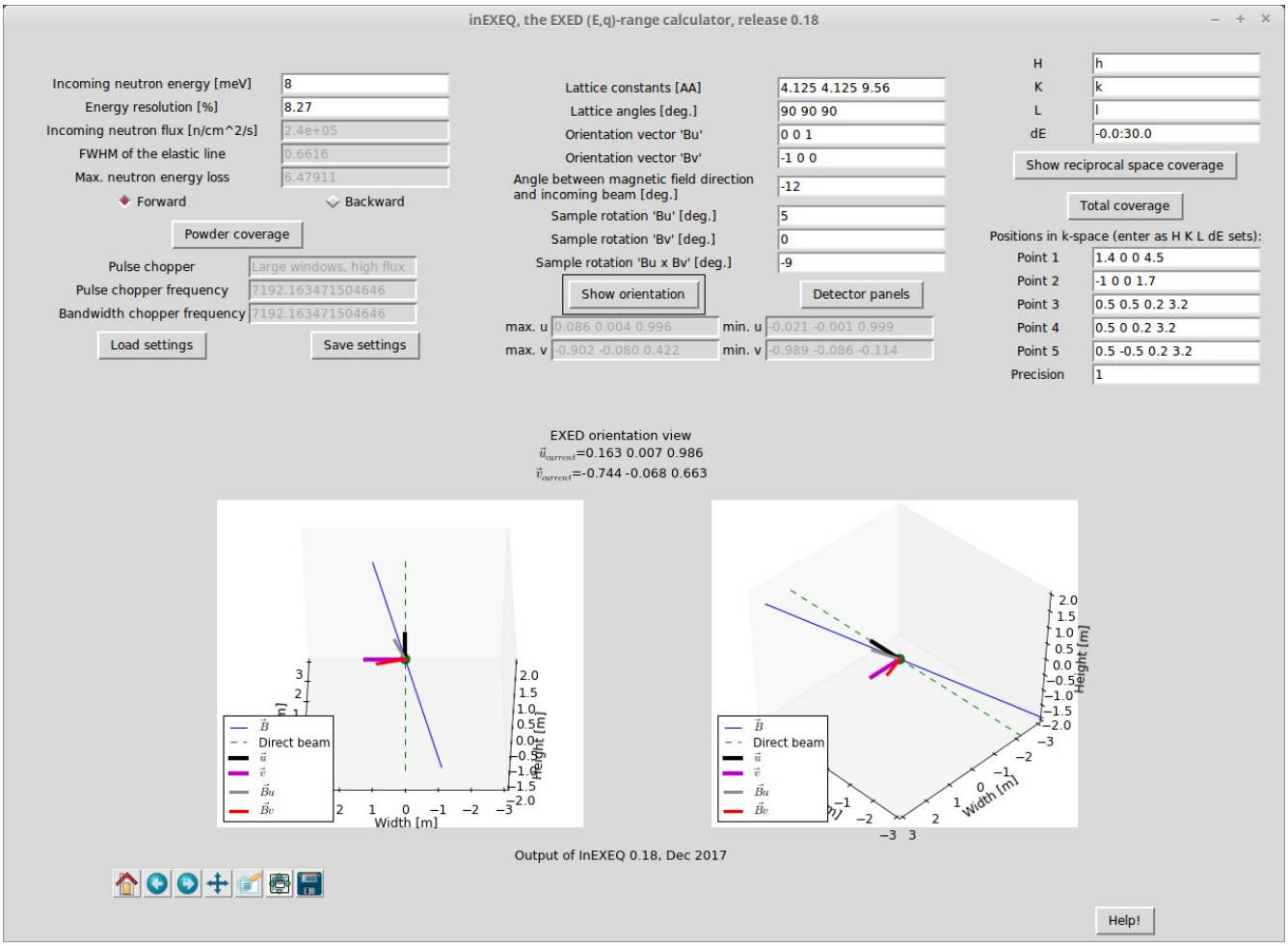
Detector view



Detector view shows the real-space view of the detector panels. The shadow of the magnet cone, beamstop and the gaps between the panels are included in the plot.

If some marker points were specified AND are within range for the current settings, the position of these points on the detector will be marked. This is useful in predicting technical difficulties, e.g. if the region of interest in the reciprocal space turns out to be cut in two by a gap between detectors.

Sample orientation view



Here the direction of the **Bu** and **Bv** vectors is shown in real space, relative to the neutron beam and magnetic field directions.
The classical **u** and **v** vectors are also calculated.

This plot is useful for checking the direction of the sample rotation angles, and the magnet rotation angle. It is recommended to make sure that the positive direction of each angle is the same on your goniometer as it is on EXED, before you orient your sample based on InEXEQ results.

More features?

If you find some missing feature particularly important, please let the EXED instrument scientists know about it. If enough users ask for the same feature to be implemented, it could be added to the next release.