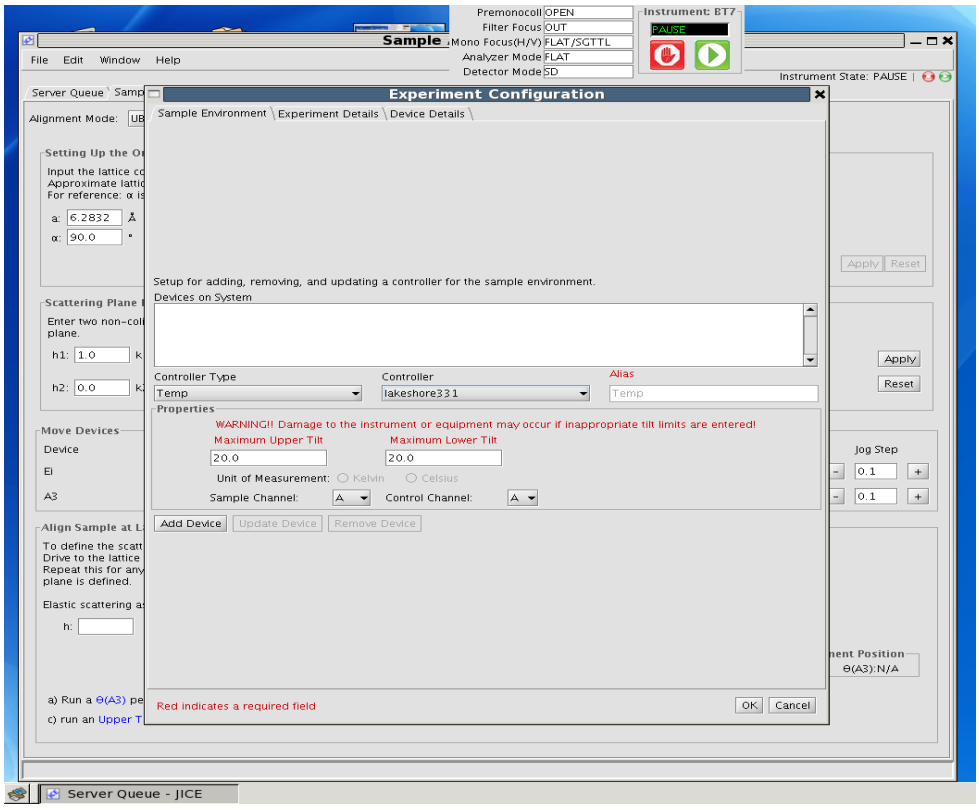
How to start an experiment at BT7

1. To start JICE, find the "JICE-month-date-year.jar" icon (for example, 

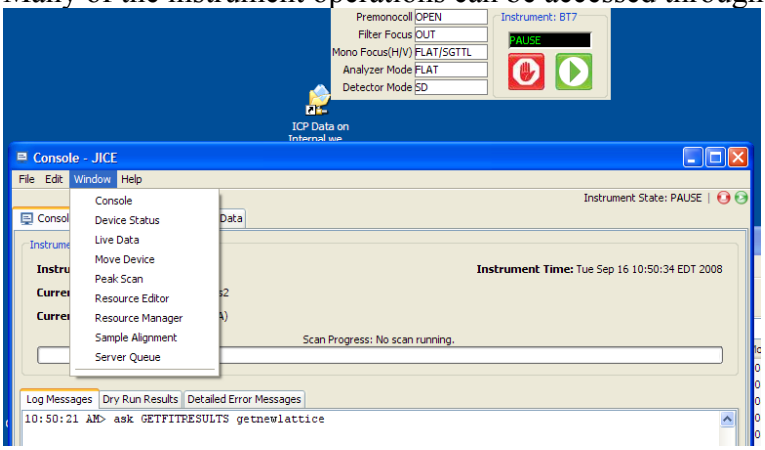
) on the BT7 desktop. Double-click the icon to start the client. All commands to the instrument are executed from the JICE program.

2. The BT-7 *Instrument Scientist* (as a 'superuser') can set up a subdirectory for the experiment. In the JICE window, under "File", choose "new experiment" and a pop up window will open. (S)he will enter the proposal ID of the new experiment. Then the "experiment configuration" window pops up with the "Experimental details" tab open (there are three tabs). Under the "Experimental details" tab, you can enter "experiment name", "participants" and "experiment details". Under the "sample environment" tab, you can set up the temperature and/or magnetic field controllers for your particular sample environment. Click on "controller type", pick "Temp" or "Magfield", for example, then click on "controller" to see a list of controllers, then Press "Add Device". You can also "update device" if some 'under-the-hood' device parameters need to be changed, or "remove device". You also can change software limits under the "device details" tab, but this must be done with great caution; these limits are there to protect the instrument, so please do not increase the limits unless you are absolutely certain that no problems can occur. In general, you should NOT increase the limits.

   Users can access the experimental configuration information under "Edit", then "Experiment configuration".



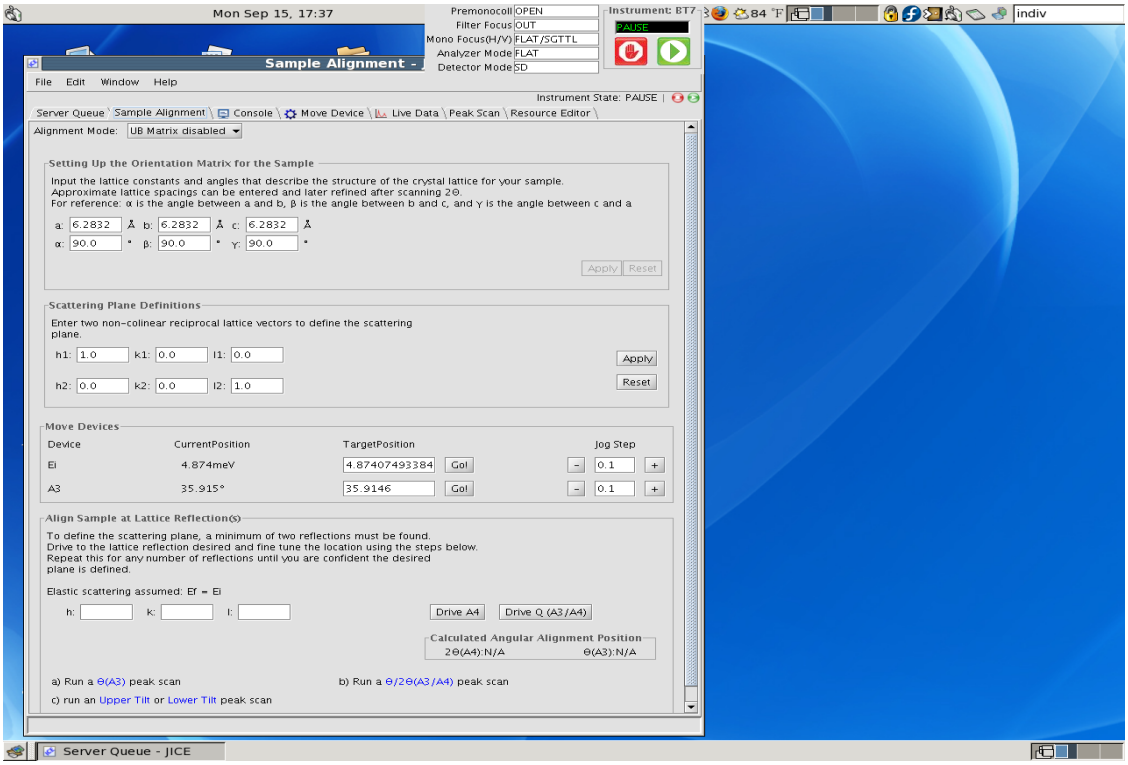
3. Many of the instrument operations can be accessed through the various windows. Requesting a



window, such as "Live Data", will create a new tab with that window active in the Console. These tabs can also be dragged out onto the desktop as a stand-alone window, if desired.

The icon at the top of the desktop gives some basic instrument information, and can be used to ***pause and resume,*** or ***stop*** the instrument command sequence. This icon appears on all the desktops and is forced to the front so that it is always available. The keyboard command "ALT-F12" can also be used to stop the instrument.

4. To input lattice parameters and align your sample, choose the "sample alignment" tab.



a) Enter "*a*", "*b*","*c*", "α", "β" and "γ" and click on "**apply**" to define crystal lattice.
b) Enter "*h1*", "*k1*", "*l1*" and "*h2*", "*k2*", and "*l2*" and click on "**apply**" to define the scattering plane.
c) Enter "*h*", "*k*" and "*l*", and JICE will calculate and display the A4 (diffraction angle), and A3 (sample rotation) values. If this is your first peak, press "drive A4" to move the analyzer system to the correct Bragg angle. Then go to the "move device" window to drive "A3"

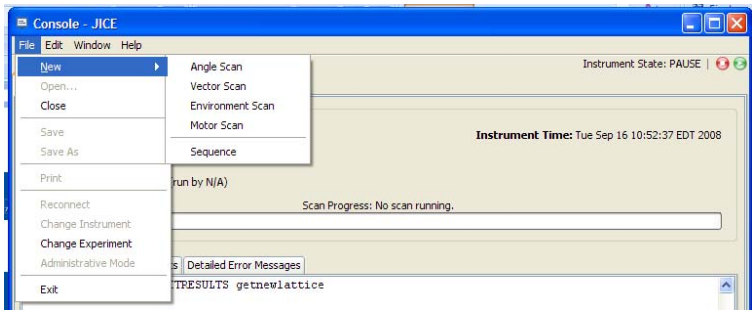
around until you find your peak.

d) To do a rocking scan, open the "peak scan" window. Then choose device "A3", and enter values for "range", "step size", "duration" and click on "findpeak". You can "move to fit" and then "redefine A3" to the calculated value shown in the "sample alignment" panel. You determine the actual d-spacing by doing an "A3-A4" (θ:2θ) and then update the appropriate lattice parameter(s), and adjust the goniometer tilts by scanning "smplutilt" or "smpltilt" [sample upper tilt, sample lower tilt] in the peak scan panel.

e) Once your first peak is properly aligned, input the (*h,k,l*) for the second peak and go to the 2nd peak via the "sample alignment" panel (enter "*h*","*k*","*l*" and press "drive to Q"). Adjust the tilt (peak scan on "smplutilt" or "smplltilt") and adjust the lattice parameter(s) for this peak ("peak scan" on "A3-A4").

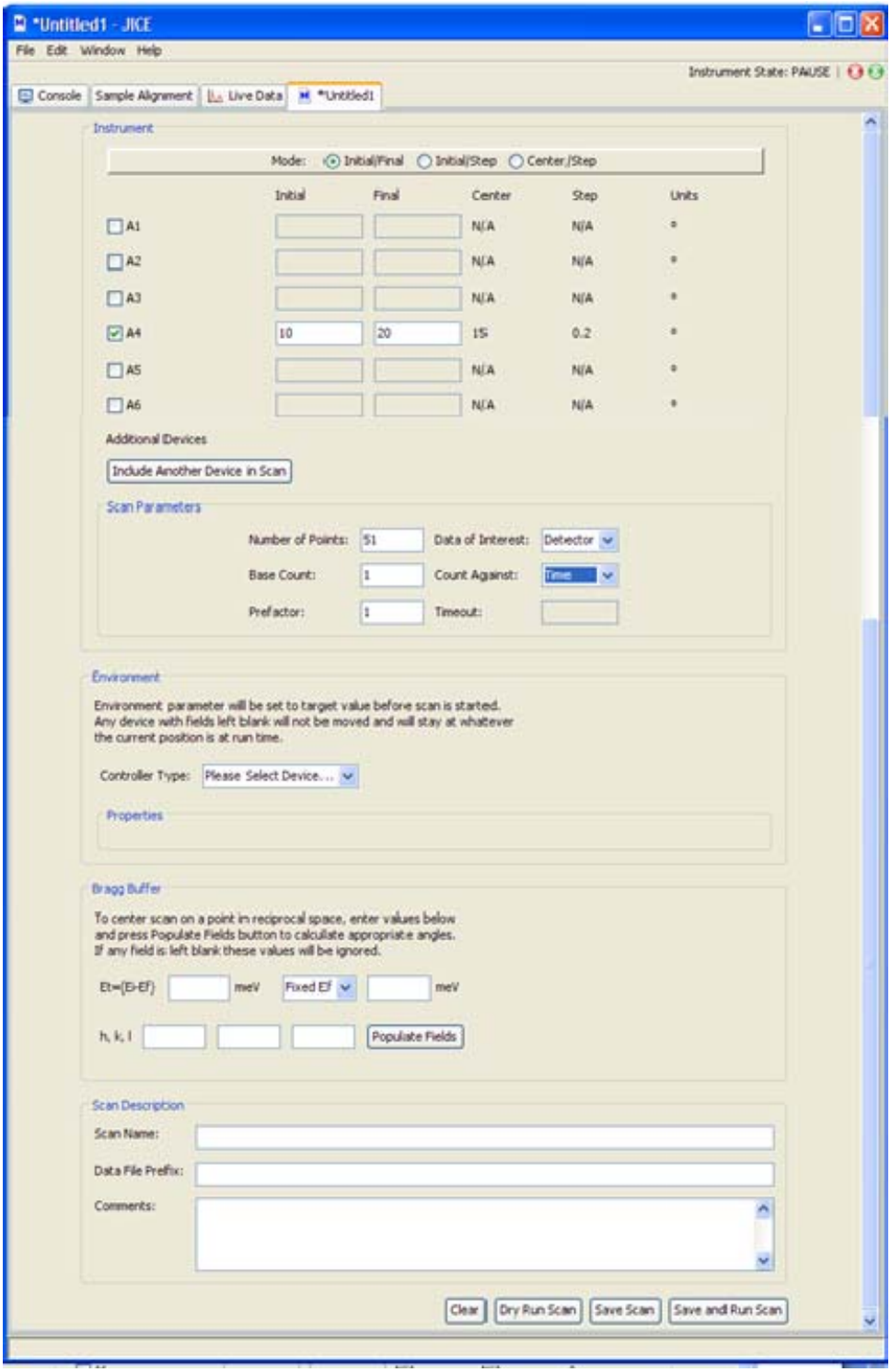
5. Once sample is aligned, you can adjust the width and height of slits before the sample ("smplwdth" or "smplhght") and after the sample ("bksltwdth" or "bkslthght") ("peak scan" these four motors one by one), to reduce your background.

6. To set up a scan, go to "File", and "New". Choose either "Angle scan", "motor scan", "vector scan" or "environmental scan".



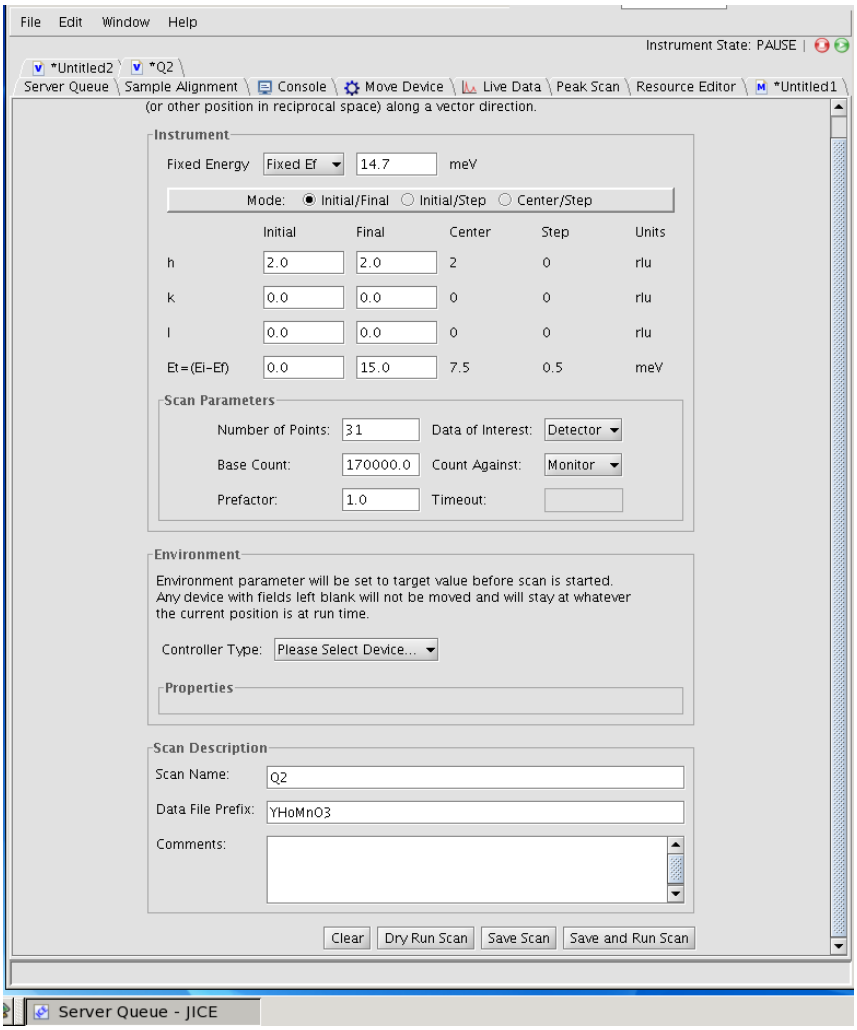
A new tab will open to allow you to set up that type of scan. You can choose either to enter "initial/final", "initial/step" or "center/step" values.

a) To do a "motor scan", click on the little square before the motor of interest, enter "scan ranges", "number of points", and "base count" (to measure the monitor rate go to "console panel" and type "rate" at the command line) and "prefactor", then give your scan a "scan name"; The scan name will be used to actually execute the scan. The data file will be saved using the "data file prefix" as the filename prefix plus a number. Enter "comments" if desired. Press "save scan" to save it, "dryrun scan" to calculate the angles and check angle limits, and "save and run scan" to run the scan manually. Dryrun will open a pop-up window to view the angles and error messages (if any), and the results of the Dryrun will also appear in the Console Tab. Running the scan puts the command in the server queue (explained below) to be executed.



b) To do a scan of a Bragg peak (a.k.a. Bragg Buffer in ICP), in "motor scan" choose "center/step" mode, go to the section called "Bragg Buffer", enter "Et=ei-ef" 0 meV and enter the value for "fixed Ei/Ef". Enter "*h,k,l*" then press "populate fields" and all the values for the angles are populated. To do an A3 (rocking) scan, click on the square before A3; To do an A3:A4 (θ:2θ) scan, click on the square before A3 and A4, and enter the steps for A3 and A4 in a 1:2 ratio.

c) To do a constant-**Q** or contant-E scan, go to "vector scan" and enter values for "*h*","*k*","*l*" and "E", enter "scan name", "data file prefix" and "comments". Press "save

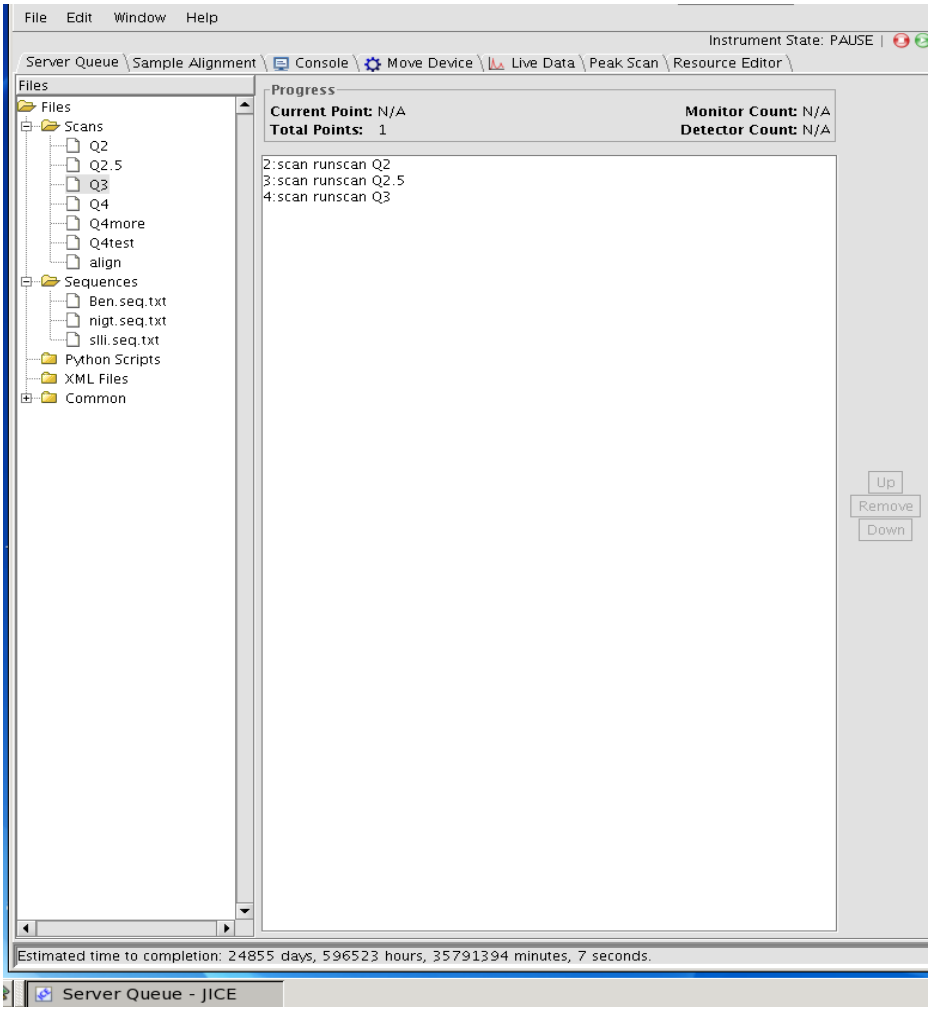


scan" to save it, "dryrun scan" to "dry run" or press "save and run scan" to run the scan.

d) To do an environment scan such as scanning the temperature or magnetic field, choose "environment scan". Select either "Temp" or "Hmag". Enter the appropriate ranges, and go to "properties" to enter the values for "tolerance", "wait between the points", "wait before the points". **NOTE: Make sure to move to the correct A4 value or Bragg position of interest before running the environment scan.**

7. To run a sequence of scans, go to "window", then "server queue". On the left of the server queue window, there is folder called "scans" and your scans are saved there. To execute a scan you can either 1) click on the scan of interest, then drag to the right window, OR 2) right click on the scan and the choose "add to queue". "scan runscan <scanname>" will show up in the server queue in the right pane of the window. If this is the first scan in the queue, then this scan will start running and "scan runscan <scanname>" becomes bold. Drag additional scans into the queue in the order you want. Any other commands that you want to execute, such as "move temp 231.0", can be executed from the console command line, or any of the other command windows such as in "move device" or "find peak", and these will be added to the queue in the order in which they are given. You can change the order in the queue by highlighting a command or multiple commands in the right window and then move them up or down by pressing the "up" or "down" buttons, or remove them with the "remove" button.
8. Alternatively, you can write a sequence file. Go to "file", then "new", then "sequence", then a sequence tab will open. You can write all the commands in this file, then go to "File", then "save" or "save as" to the filename of your choice. Then go to the "server queue", and in the

left pane there is a “sequence” folder and your sequence file is saved there. Drag the sequence file to the right pane, or right click and choose “add to queue” to run the sequence file. Current data are displayed in the “live data” panel.



9. To get your experimental data onto your own computer, you can use a memory stick at BT7 to copy your data. The data directory is located at /usr/local/ice/usr/<proposalID>/data . Alternatively, if you are on the visitor’s network in the user room, you can find your data on the charlotte computer. You can get to charlotte by typing \\charlotte.ncnr.nist.gov in the address bar of any window. All data are archived here and are organized in subdirectories by the year and month that the cycle started. auto-mounted on your computer (if not, open network places, and go to charlotte.ncnr.nist.gov). Go to the “ICP data” subdirectory, go to “BT7”. Then go to the latest folder (e.g. 200807, for the cycle that started July, 2008), then to the folder with your proposal ID number. You can copy (select and drag/copy) your data to your own computer. DAVE can be downloaded at http://www.ncnr.nist.gov/dave/download.html onto your laptop to view and analyze your data, or you can use your own software. All triple axis data are stored as simple ascii files.