How to start an experiment at BT7

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- 1. To start JICE, find the "JICE-month-date-year.jar" icon (for example, ^{7372008,jar}) 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".

| | Premonocoll OPEN Instrument: BT7 | |
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| File Edit Window | Help Analyzer Mode FLAT | |
| - The East Window | Detector Mode SD Instrum | ent State: PAUSE 🙆 🚱 |
| / Server Queue) Samp | Experiment Configuration | د ا |
| | Sample Environment \ Experiment Details \ Device Details \ | |
| Alghment Wode. | | 1 |
| -Setting Up the O | | |
| Input the lattice co | | |
| Approximate latti | 4 | |
| For reference. u i | 9 | |
| a: 6.2832 Å | | |
| α: 90.0 * | | |
| | | Apply Reset |
| | Setup for adding, removing, and updating a controller for the sample environment. | |
| -Scattering Plane | Devices on System | |
| Enter two non-col | | |
| plane. | | |
| h1: 1.0 k | · | Apply |
| | Controller Type Controller Alias | |
| h2: 0.0 k | Temp 🔹 lakeshore331 🔹 Temp | Keset |
| | Properties | |
| Move Devices | WARNING!! Damage to the instrument or equipment may occur if inappropriate tilt limits are entered! | |
| Device | | Jog Step |
| Ei | List of Maggurament - C Kable - C Calcius | - 0.1 + |
| 42 | | |
| | | |
| FAlign Sample at L | Add Device Update Device Remove Device | |
| To define the scatt | | |
| Drive to the lattice Repeat this for any | | |
| plane is defined. | | |
| Elastic scattering a | | |
| h: | | |
| | | |
| | | nent Position |
| | | 5(AS).11/A |
| a) Run a O (A3) pe | Red indicates a required field OK Cancel | |
| c) run an Upper T | | |
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| 😻 🛛 Server Que | eue - JICE | |

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

| | | Premonacoli OPEN Filter Focus (DUT Mono Focus(HIV) FLAT/SGTTL Analyzer Mode FLAT Detector Mode ED ICP Data on |
|-----------|----------------------|--|
| | | Internal we |
| 🗏 Conso | le - JICE | |
| File Edit | Window Help | |
| | Console | Instrument State: PAUSE 😡 😒 |
| 📮 Consol | Device Status | Data |
| ⊂Instrume | Live Data | |
| Inches | Move Device | Instrument Timer Tue See 16 10:50:24 EDT 2009 |
| instru | Peak Scan | Instrument nine, nde sep 10 10.30.34 EDT 2000 |
| Currei | Resource Editor | 12 |
| Curre | Resource Manager | 4) |
| | Sample Alignment | Scan Progress: No scan running. |
| | Server Queue | |
| | | |
| Log Mess | ages Dry Run Results | etailed Error Messages |
| 10:50:2 | 21 AM> ask GETFITE | SULTS getnewlattice |
| | | |

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.

| Mon Sep 15, 17:37 | Premonocoll OPEN | Instrument: BT7 | 3🕹 🕙 84 °F 🕕 | 🦲 🛃 🖄 👟 🖑 İndiv |
|---|--|------------------------|--------------|-----------------|
| | Filter Focus OUT | PAUSE | | |
| | Analyzer Mode FLAT | | | |
| Sample / | Alignment - Detector Mode SD | | | |
| ile Edit Window Help | Instrume | nt Stoto: BALISE 🙃 🕥 | | |
| Server Queue ' Sample Alignment \ 🖃 Console \ 🛪 Move | Device \ Lve Data \ Peak Scan \ Resource Edit | or \ | | |
| Nignment Mode: UB Matrix disabled 👻 | | · | | |
| | | | | |
| Setting Up the Orientation Matrix for the Sample — | | | | |
| Input the lattice constants and angles that describe the Approximate lattice spacings can be entered and later For reference: α is the angle between a and b, β is the | structure of the crystal lattice for your sample. refined after scanning 20. angle between b and c, and γ is the angle betwe | encanda | | |
| a: 62832 Å b: 62832 Å c: 62832 Å | | | | |
| a 0.2002 A 0. 0.2002 A C. 0.2002 A | | | | |
| | | | | |
| | | Apply Reset | | |
| | | | | |
| Scattering Plane Definitions | | | | |
| Enter two non-collnear reciprocal lattice vectors to defin plane. | he the scattering | | | |
| h1: 1.0 k1: 0.0 l1: 0.0 | | Apply | | |
| | | Apply | | |
| h2: 0.0 k2: 0.0 l2: 1.0 | | Reset | | |
| | | | | |
| Move Devices | | | | |
| Device CurrentPosition | TargetPosition | Jog Step | | |
| Ei 4.874meV | 4.87407493384 Gol - | 0.1 + | | |
| A3 35.915° | 35.9146 Gol - | 0.1 + | | |
| | | | | |
| Align Sample at Lattice Reflection(s) | | | | |
| To define the scattering plane, a minimum of two reflect Drive to the lattice reflection desired and fine tune the lo | ions must be found. Incation using the steps below. | | | |
| Repeat this for any number of reflections until you are co | onfident the desired | | | |
| plate is defined. | | | | |
| Elastic scattering assumed: Ef = El | | | | |
| h: k: l: | Drive A4 Drive Q (A3/A | Ð | | |
| | Calculated Angular Alignm | ent Position | | |
| | 20(A4):N/A | 0(A3):N/A | | |
| a) Pup a Q(A2) peak crap | b) Pup a Q/2Q/A2 (A4) peak cran | | | |
| c) run an Upper Tilt or Lower Tilt peak scon | oy run a 0/20(AS/AH) peak scan | 233 | | |
| cyrun an opper rin or cower rin peak scan | | <u> </u> | | |
| | | | | |
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- 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".

| Console - JICE | | |
|-----------------------|---------------------------|---|
| File Edit Window Help | | |
| New | Angle Scan | Instrument State: PAUSE 😣 🤄 |
| Open | Vector Scan | |
| Close | Environment Scan | |
| Save | Motor Scan | Instrument Time: Tue Sep 16 10:52:37 EDT 2008 |
| Save As | Sequence | |
| Print | run by N/A) | |
| Reconnect | Scan Progress | No scan running. |
| Change Instrument | | |
| Change Experiment | | |
| Administrative Mode | s Detailed Error Messages | |
| Exit | TRESULTS getnewlattice | |

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.

| iample Alignment | Live Data 💌 *Untit | led1 | | | Instrument 5 | itate: |
|---|--|--|---|------------|--------------|--------|
| strument | | | | | | |
| 1 | Mode: 💿 Ir | ntial/Final C |) Initial/Step 🔘 🕻 | enter/Step | | 1 |
| | Initial | Final | Center | Step | Units | |
| A1 | | | N/A | N/A | | |
| A2 | | 1 | N/A | N/A | | |
| A3 | | 1 | N/A | N/A | | |
| ₩ A4 | 10 | 20 | 15 | 0.2 | | |
| A5 | | 10 | N/A | N/A | | |
| A6 | | 1 | N/A | N/A | | |
| Additional Devices | | | | | | |
| Include Amother De | svice in Scan | | | | | |
| Scan Parameters | | | | | | |
| | Number of Points: | 51 | Data of Interest: | Detector 💌 | | |
| | Base Count: | 1 | Count Against: | The v | | |
| | Prefactor: | 1 | Timeout: | | | |
| vironment wironment paramete vy device with fields e current position is | r will be set to target va left blank will not be mov at run time. | ilue before sc red and will st | an is started. Jay at whatever | h | | |
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| nvironment nvironment paramete nvironment paramete vidente vakh fields ne current position is controller Type: Properties | r will be set to target va left blank vill not be mov at run time. ease Select Device | ilue before sc red and will st | an is started. ay at whatever | | | |
| vironment ny device with fields e current position is Controller Type: Properties | r will be set to target va left blank will not be mov at run time. ease Select Device | alue before sc red and wall st | an is started. Jay al whatever | | | |
| vironment nvironment paramete nvironment paramete e current position is Controller Type: Pr Properties ago Buffer o center scan on a pr d press Populate File any field is left blank | r will be set to target va left blank will not be mov at run time. ease Select Device | ilve before so red and will st ppropriate ar ored. | an is started. Iay at whatever below ngles. | | | |
| Invironment Invironment paramete invironment paramete invironment position is Controller Type: Pe Properties agg Buffer to center scan on a po ind press Populate Iblani any field is left blani It=(E)-EF) | er will be set to target va left blank vill not be mov at run time. nase Select Device v disk in reciprocal space, e disk button to calculate a these values will be ign meV Fixed EF v | eved and will st enter values b ppropriate ar ored. | an is started. ay at whatever below ngles. meV | | | |
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| witonment nitronment paramete nitronment paramete e current position is Controller Trype: Pie Properties agg Buffer o center scan on a pie of press Populate File any field is left blank Rt=(E+EF) | r will be set to target va left blank will not be mov at run time. ease Select Device v disk button to calculate a (these values will be ign meV Fixed EF v | eved and will st enter values b appropriate ar ored. Populate I | an is started. ay at whatever below ngles. meV Fields | | | |

- 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 (0:20) 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

|) *Untitled2) | Instrument State: F | AUSE 🥹 |
|-----------------|---|----------|
| rver Queue 58 | pre Aughment () Console () Move Device () Le Live Data (reak scan (Resource Editor () or other position in reciprocal space) along a vector direction. | onuted |
| | Instrument | |
| | Fixed Energy Fixed Ef 🔹 14.7 meV | |
| | Mode: Mode: Initial/Final Initial/Step Center/Step | |
| | Initial Final Center Step Units | |
| | h 2.0 2.0 2 0 rlu | |
| | k 0.0 0.0 0 rlu | |
| | | |
| | | |
| | Ele(EleC) 0.0 15.0 7.5 0.5 mev | |
| | Scan Parameters | |
| | Number of Points. 31 Data of Interest. Detector V | |
| | Base Count: 170000.0 Count Against: Monitor - | |
| | Prefactor: 1.0 Timeout: | |
| | | |
| | Environment | |
| | Any device with fields left blank will not be moved and will stay at whatever | |
| | the current position is at run time. | |
| | Controller Type: Please Select Device | |
| | Properties | |
| | | |
| | Scan Description | |
| | Scan Name: Q2 | |
| | Data File Prefix: YHoMnO3 | |
| | Comments: | |
| | | |
| | ✓ | |
| | Clear Dry Run Scan Save Scan Save and Run Scan | |
| | | |

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 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.

| Server Oueue \ Sample Align | ment 🔪 🖃 Console 🖓 🐴 Move Device 🖓 📴 Live D | Data \ Peak Scan \ Resource Editor \ |
|---|---|---|
| iles | | |
| Files | Current Point: N/A Total Points: 1 | Monitor Count: N/A Detector Count: N/A |
| Q2 Q3 Q4 Q4 Q4more Q4test align Sequences Sequences Silli seq.txt Python Scripts XML Files Common | 2:scan runscan Q2 3:scan runscan Q2.5 4:scan runscan Q3 | |
| | | |

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 <u>\charlotte.ncnr.nist.gov</u> 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 <u>http://www.ncnr.nist.gov/dave/download.html</u> 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.