

POWGEN User Manual to Data Acquisition

DAS

The Data Acquisition System (DAS) consists of a set of computers and electronics controlling the acquisition and storage of data collected at each instrument at SNS. The das-opi computer is the main computer and most of the work for setting up runs occurs on this computer. There are two monitors for the das-opi computer towards the right side of the hutch (Figure 1). On the extreme left and right sides of the hutch are computers for data reduction, visualization and analysis, which are discussed in the document *POWGEN User Manual for Data Reduction*.

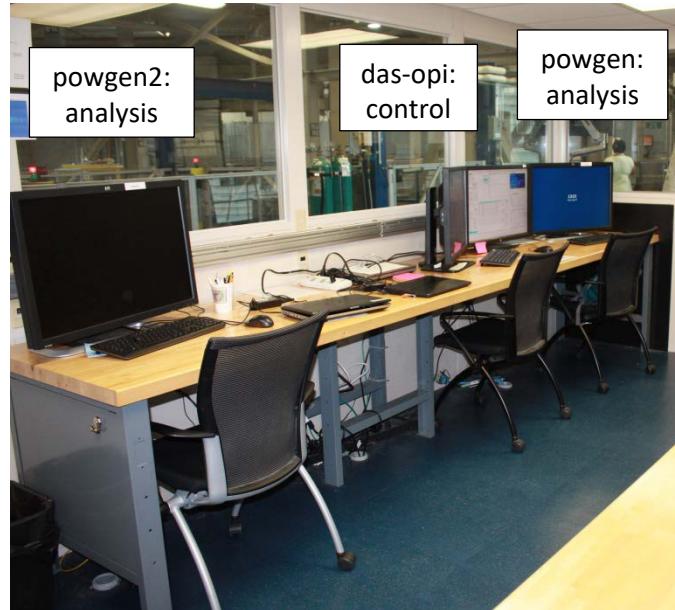


Figure 1. Powgen hutch, showing the analysis and control computers.

Dashboard

The right monitor of the das-opi control computer displays the instrument dashboard (Figure 2). The dashboard contains all the information and controls a typical user will need for their experiment.

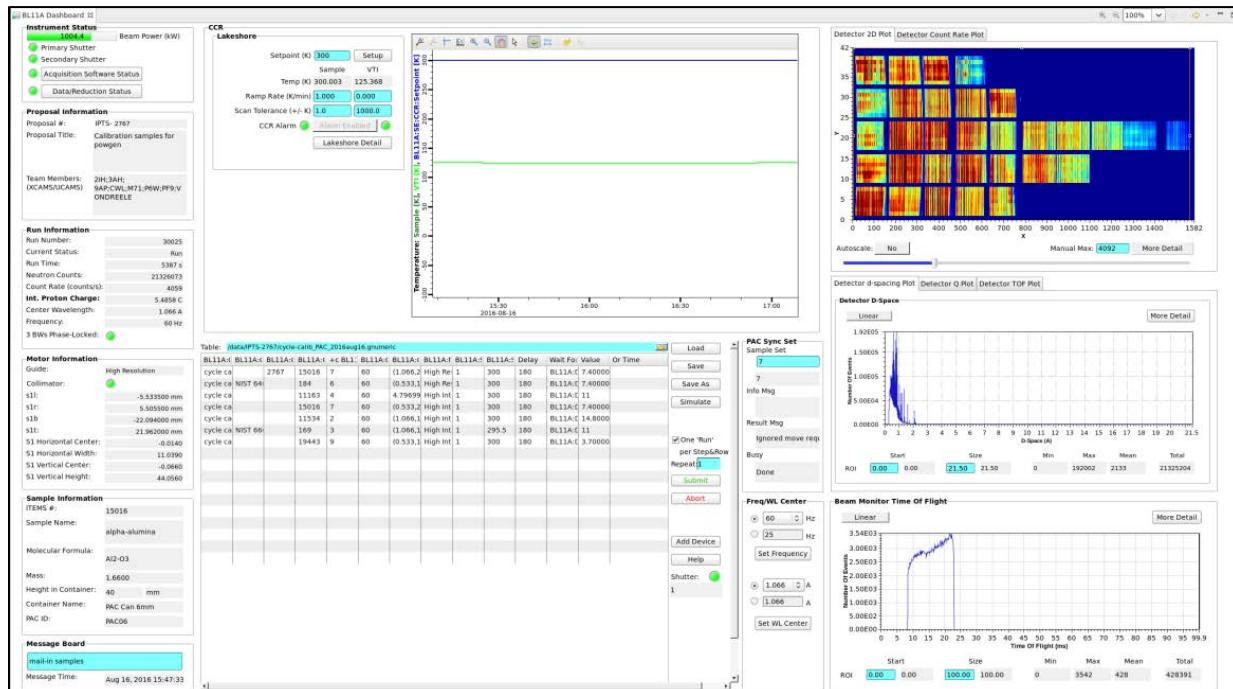


Figure 2. Dashboard overview. See

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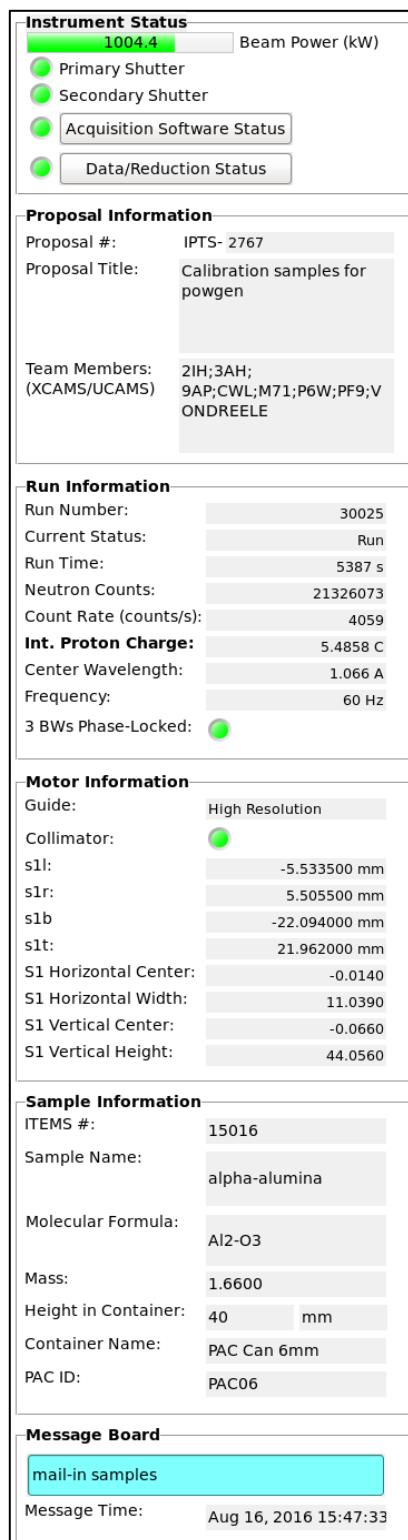


Figure 3. Instrument Status Display

Instrument Status Display The left column (Figure 3) of the dashboard displays instrument status, including the beam power and shutter status indicators at the top. The Proposal Information box indicates the currently selected proposal. The total time and collected beam proton charge of the current run are shown in the Run Information box. In the same box is the status of the bandwidth choppers, including the selected center wavelength and frequency. The Motor Information box displays the current guide setting and slit positions. The sample name, composition and other details are shown in the Sample Information box.

Sample Environment and Table Scan Controls The center section (Figure 4) of the dashboard displays a plot of the sample temperature and sample environment controls, including the setpoint, ramp rate and tolerance. Underneath the temperature plot are the table scan controls, used for automating data collection. The use of table scans will be discussed later. To the right of the table scan controls, the PAC Sync Set box may be used to select a sample when using the sample changer (PAC). The Freq/WL Center box may be used to change the bandwidth chopper settings. Most user experiments will be with a frequency of 60 Hz and a center wavelength option from the dropdown menu. In each case, you must first select the desired value, then press the appropriate Set button.

Data Plots The right section (Figure 5) of the dashboard displays data plots. At the top is the Detector 2D Plot, which displays the total counts across each detector face. This plot should correspond to the expected picture posted in the hutch. If one of the detectors displays no intensity, please contact beamline staff or the IHC (after hours). The middle plot shows the diffraction data, summed across all detectors, as a function of d-spacing, Q (=2π/d) or time-of-flight. The bottom plot shows the beam monitor spectrum. Plot options are available by right-clicking in the plot area and selecting Show/Hide Graph Toolbar (Figure 6). By default the plot will autoscale in both the x- and y-axes. In order to zoom in, you must disable autoscale by clicking the Configure Settings button on the left end of the graph toolbar, going to the Axes tab, selecting the desired axis from the dropdown menu and then unchecking the Auto Scale Enabled option. Once autoscale is disabled, you may click the Rubberband Zoom button in the graph toolbar and then click and drag on the plot to zoom in. Clicking the Perform Autoscale button in the graph toolbar will zoom the plot back full.

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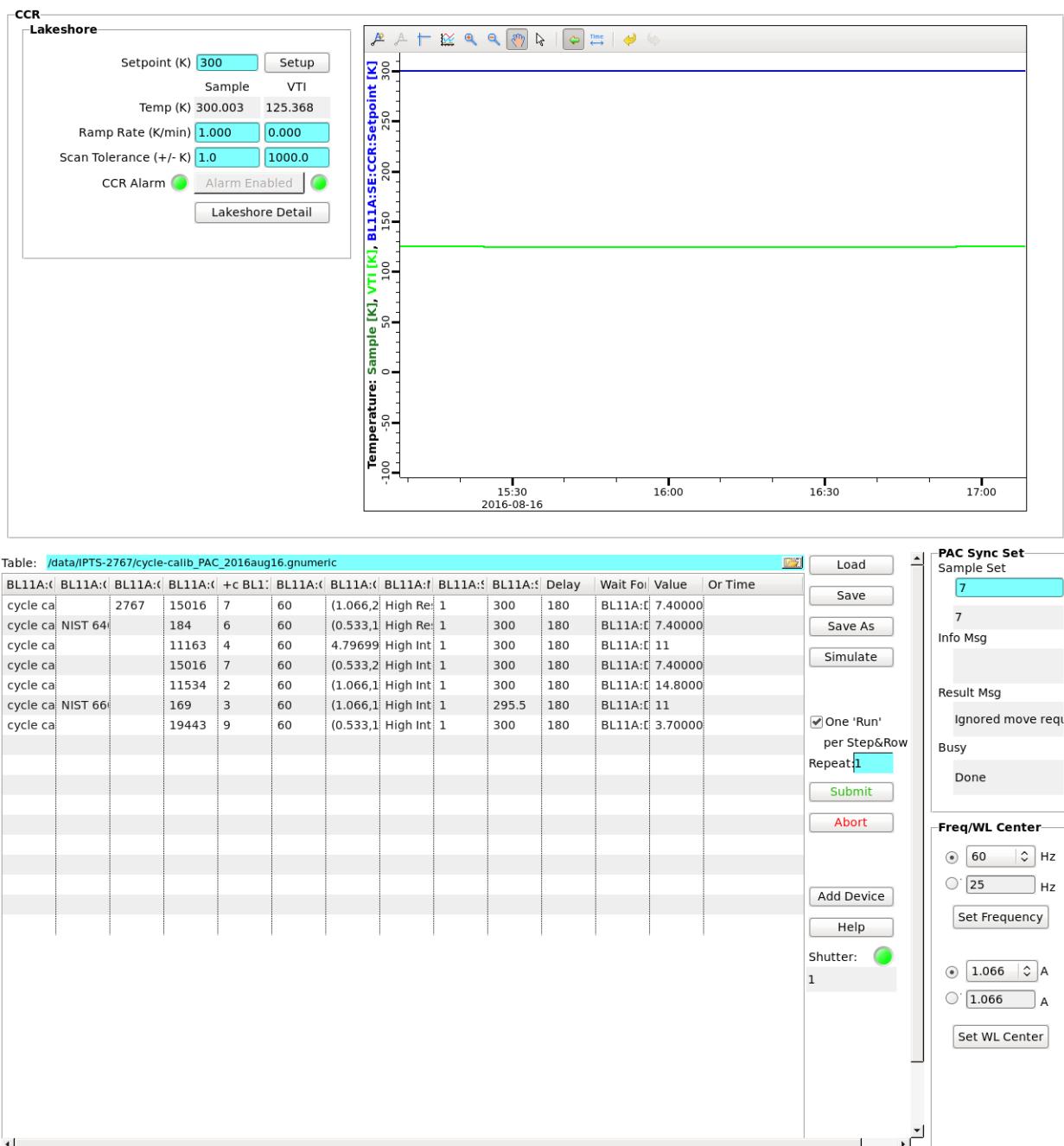


Figure 4. Center area of the dashboard, showing temperature controls at top and table scan controls at the bottom.

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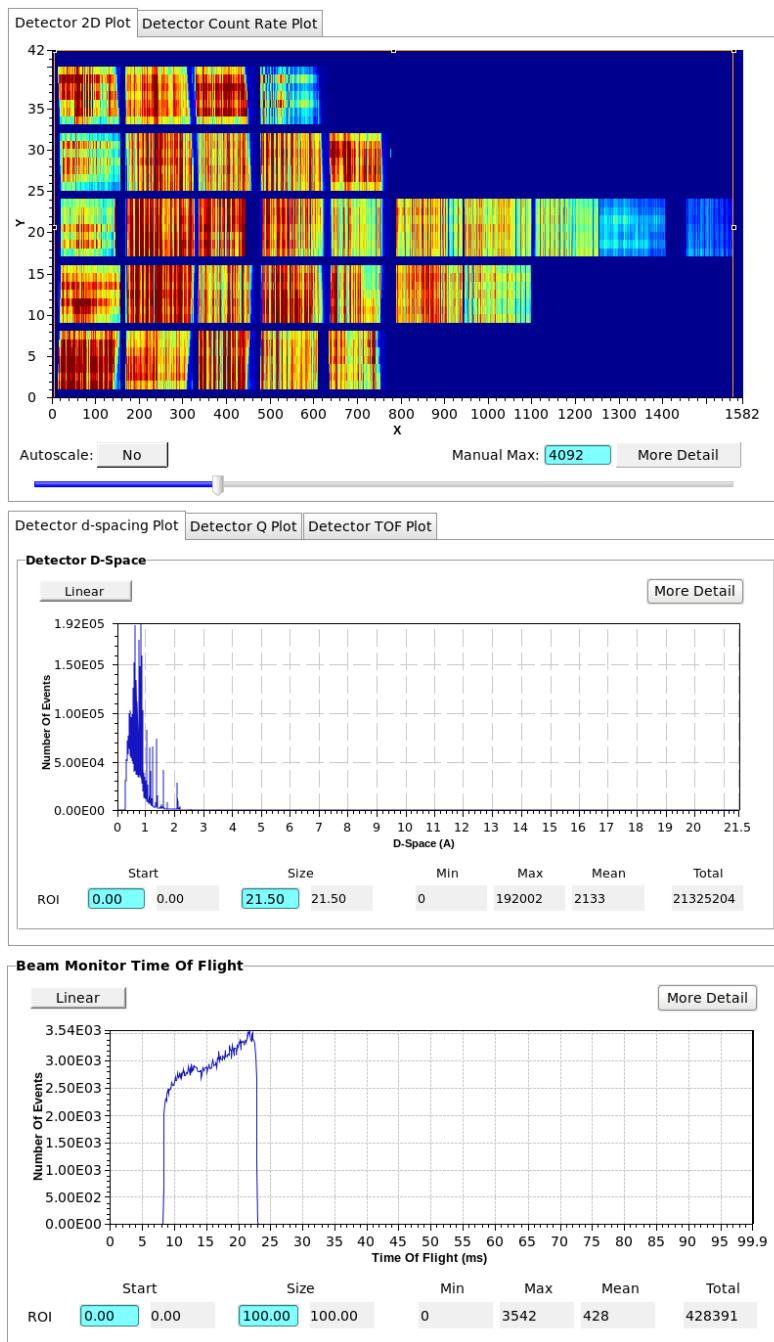


Figure 5. Right column of the dashboard, showing plots of detector and beam monitor data.



Figure 6. Graph Toolbar, with the Configure Settings, Perform Autoscale and Rubberband Zoom buttons highlighted (left to right).

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Additional Screens

Additional screens (Figure 7) are available on the left monitor with more instrument information. The Navigator pane on the far left displays the file structure. Files may be opened from the Navigator pane by double-clicking. To the right of the Navigator pane is the Scan Simulation/Editor pane, which will be discussed in more detail later, along with the Scan Monitor pane at the bottom. The upper right section of the monitor contains several tabs with more information about the beamline equipment. The BL-11A POWGEN User Home tab has indicator lights for the status of each piece of beamline equipment. All status lights should be green when functioning properly. The Table Scan tab contains similar table scan controls as are in the Dashboard (Figure 4). The BL11A_Skf_Chop_User tab shows status lights for each of the three bandwidth choppers, along with the frequency and phase settings. The PAC Seq tab shows the status of the sample changer, with the sample currently in beam highlighted in orange. The BL11A CCR tab shows the temperature controls and plot, as in the Dashboard (Figure 4). Other tabs may be present depending on the sample environment equipment installed at the beamline.

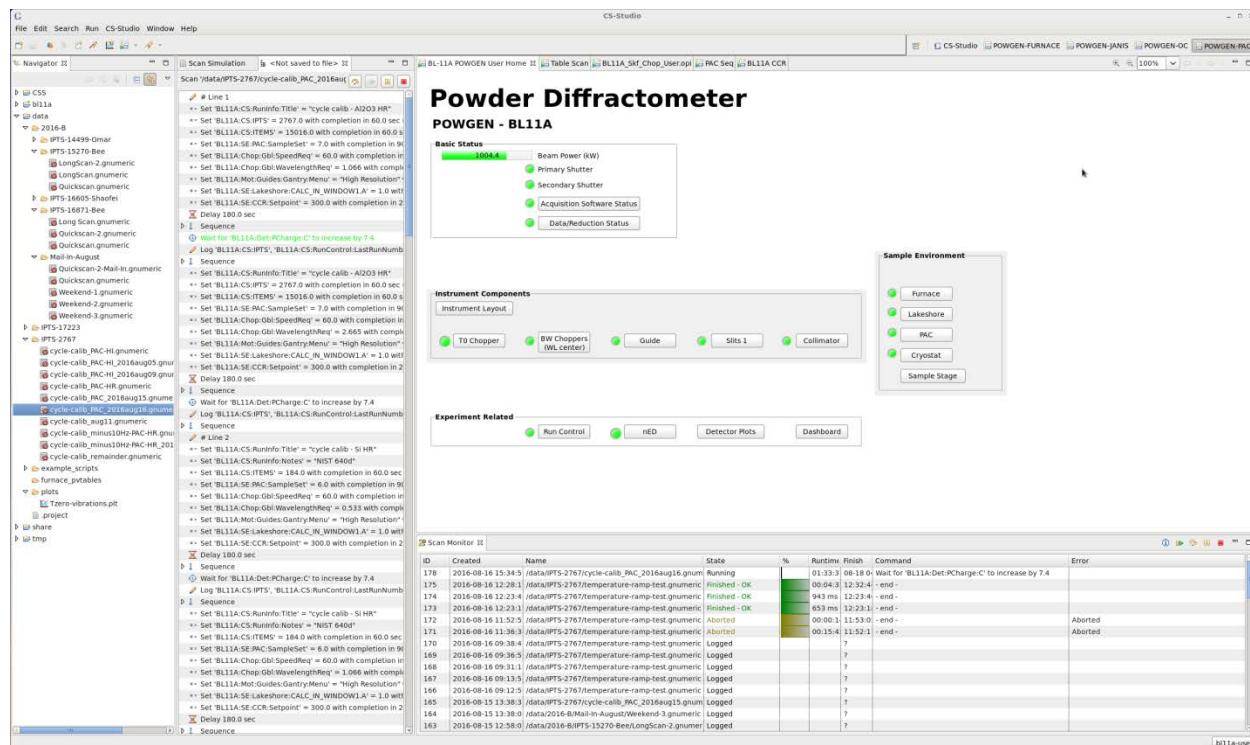


Figure 7. Additional screens shown on the left monitor of the control computer.

Table Scan Scripts

The preferred mode of data collection is using table scans, which are spreadsheet files that lay out the desired data collection and instrument steps, e.g. count time, sample temperature and sample changer position. User table scans are saved in the folder data/cycle/IPTS-XXXXX, where cycle is the run cycle (e.g. 2016-B) and XXXXX is the proposal number. Example scripts for each instrument setup are in the data/example scripts folder. They may be opened and changed with the Gnumeric program.

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Preparing a Script To prepare a table scan, copy the appropriate example script into your proposal folder and rename it appropriately. Open the script in Gnumeric and replace the example values with your desired values. Each line contains the instrument and data collection parameters for one scan (or one set of similar scans). Table 1 describes the meaning of each column heading. Each line of the table will be executed successively.

Table 1. Table scan script column headings.

Column Heading	Description
General Settings	
title	title for the run
comments	additional information about the run
ipts	your proposal number
Items	ITEMS number of the sample being measured
frequency	chopper speed in Hz, typically 60
wavelength	desired center wavelength in Å
guide	selectable guide setting, either "High Resolution" or "High Intensity"
Delay	wait time in seconds before data collection
Wait For	criteria to use to signal the end of the run, typically "pcharge"
Value	value of criteria to signal the end the run
temp_INIT	initial temperature, used only in simulations to estimate script times
Email and Text Notification Settings	
NotifyEmail	email addresses or phone numbers to which to send notifications
NotifySubject	text of the notification
NotifyTrigger	enter a value of 1 to send a notification
PAC Sample Changer Settings	
pac	sample position (1-24) to place in the beam position
temp_LKS	sample temperature in K
ramp_LKS	ramp rate in deg/min
tol_LKS	temperature tolerance window in K
Janis Cryofurnace Settings	
SetPoint1	sample temperature in K
Ramp1	ramp rate in deg/min
Tol1	temperature tolerance window in K
SetPoint2	VTI temperature in K
Orange Cryostat Settings	
temp_CRYO	sample temperature in K
ramp_CRYO	ramp rate in deg/min
tol_CRYO	temperature tolerance window in K
Furnace Settings	
temp_FURN	sample temperature in °C
ramp_FURN	ramp rate in deg/min
tol_FURN	temperature tolerance window in °C
AGES Gas Flow Settings	
gas types, e.g. O2	flow rate of that gas in sccm, see example script for valid gas names

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Data is typically collected either for a specified time or a specified cumulative beam power (known as pCharge). At Powgen, we routinely collect on pCharge. When collecting on pCharge, data collection time will be extended if the neutron beam goes down during a run, in order to reach the same beam exposure. The expected amount of pCharge per hour depends on the beam power, as in Table 2.

In certain columns of the table scan script, such as center wavelength and sample temperature, you may include multiple values, either as comma separated values enclosed in parentheses or as Python-compatible range commands. That line in the script will be repeated for each value. For example, if `(0.7, 2.665)` is entered in the wavelength column, two runs will be collected, one with a center wavelength of 0.700Å and one with 2.665Å. Or, if `range(100, 301, 10)` is entered in the temperature column, runs will be collected every 10deg between 100 and 300.

Simulation Once your table scan file is prepared, you may simulate it. The program will run through the script, line-by-line, without actually changing any parameters, and estimate the total time. To simulate a script, it must first be loaded into the EPICS software. On the central area of the dashboard (Figure 4), click on the folder icon. Browse to and select your file. Once the correct path and filename are displayed to the left of the folder button, press the Load button. The table below should automatically be filled with the entries from your script. Finally, press the Simulate button. On the left monitor, in the center section, the simulation output will be displayed. Each change of an instrument setting will be outlined, along with the estimated time to execute each line of the script, and at the bottom, the total estimated time to execute the entire script. Check the simulation output carefully to ensure that everything is as expected.

Submitting a Script Once your script is ready and the simulation output has been verified, you may run your script by pressing the Submit button (Figure 4). A line will be added to the top of the Scan Monitor pane (Figure 7), representing that script. The Scan Monitor shows the filename, status (Aborted, Failed, Finished or Running), runtime, estimated finish time and which command is currently executing. Double clicking a script in the Scan Monitor pane displays the Scan Editor, which shows the list of commands to be executed, with the current command highlighted in green text.

Separate table scan scripts may be queued. While the first script is running, load and submit the second script. It will be added to the top of the Scan Monitor pane and will automatically be executed once the first script finishes. To abort a currently running script, you may press the Abort button on the dashboard (Figure 4) or the abort button on the Scan Monitor Pane (Figure 7), which looks like a red square. You may also pause and resume a currently running script by pressing the appropriate buttons on the Scan Monitor Pane.

Table 2. Accumulated beam exposure per hour, as a function of beam power.

Beam Power (MW)	pCharge per hour (coulomb/hr)
0.85	3.3
1.0	3.7
1.1	4.3
1.2	4.5
1.3	4.7
1.4	5.4