

Running cohere phasing with GUI

Before using the cohere tools make sure that the installation of cohere package is completed, and that conda environment where it was installed is activated. Refer to <https://cohere.readthedocs.io/en/latest/installation.html> for installation instructions. The user's scripts should be installed.

The cohere software processing uses configuration files to control the flow of execution. The GUI effectively edits the configuration file parameters. Refer to <https://cohere.readthedocs.io/en/latest/configuration.html> for detailed description of the parameters.

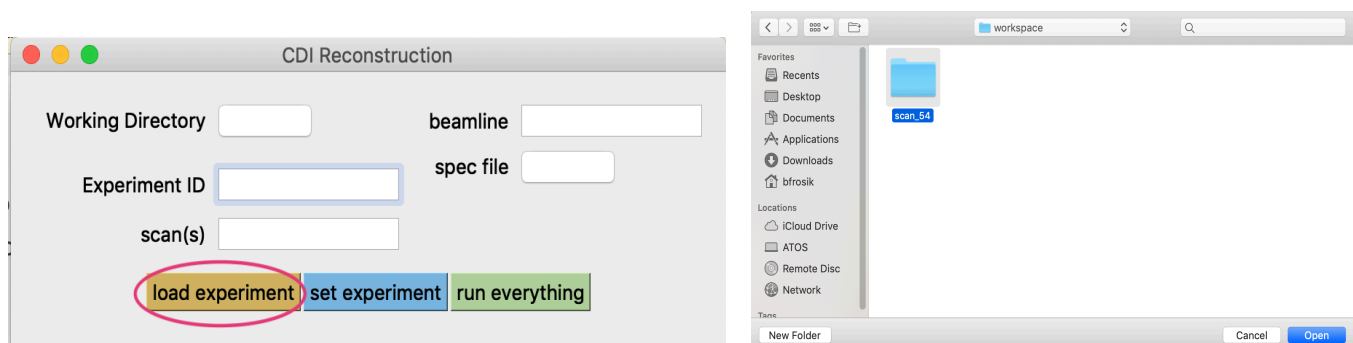
The following pages show how one can use the GUI to configure and execute a phase retrieval run. This phasing retrieval execution is called an Experiment throughout this document. It is assumed the user's current directory is cohere-scripts-main that is parent to "scripts" directory. The configuration files all use paths relative to the cohere-scripts-main directory, so one must be in this directory when one starts the GUI. The cohere-scripts package contains an example that is used in this tutorial.

To start the GUI type:

```
python scripts/cdi_window.py
```

1. Load the example experiment.

To load the example experiment included in cohere-scripts click the "load experiment" button and select the scan_54 directory under the workspace subdirectory of the cohere-scripts-main directory. In the selection dialog press "Open" or "Choose" button and the GUI will display configured parameters as shown in the next figure.



After the example experiment is loaded:

In this example an experiment in /temp/cohere-scripts-main/workspace directory will be loaded. The location of cohere-scripts-main may be different in your case. The first tab is open displaying parameters used in file preparation script.

On the top, in main window there are experiment elements:

- Working Directory
A directory where the experiment working directory is located
- Experiment ID
An arbitrary literal that combined with the scan(s) entry will form an experiment name as follows: <Experiment ID>_<scan(s)>. A directory with this name will be created in the Working Directory and all files related to the experiment analysis will be in that directory tree.
- scan(s)
A single scan, or scan range separated by “-”, which specifies raw data directories that will be included in the experiment analysis.
- beamline
A beamline that originated the experiment.
- spec file
A spec file recorded during the experiment.

The parameters in the tabs will be filled as well, but only if the configuration files existed in the chosen directory.

Note: if the beamline is not configured, the “Prep Data” and “Disp” tabs will not show up in the window.

2. Prepare experiment data for reconstruction.

Select the “Data prep” tab in the GUI.

Working Directory: /Users/bfrosik/cohere-scripts/workspace beamline: aps_34idc
Experiment ID: scan spec file: /Users/bfrosik/cohere-scripts/example/example.spec
scan(s): 54

load experiment set experiment run everything

Prep Data Data Reconstruction Display

separate scans ☐

data directory: /Users/bfrosik/cohere-scripts/example/exp_data
darkfield file: /Users/bfrosik/cohere-scripts/example/dark.tif
whitefield file: /Users/bfrosik/cohere-scripts/example/whitefield.tif

Imult:
detector: 34idcTIM2
detector area (roi): [0, 256, 0, 256, 1]
min files in scan:
exclude scans:

Load prep conf from prepare

A blue text indicates the parameter was read from the spec file

In this example a /temp/cohere-scripts-main/scan_54/prep/prepare_data.tif will be created after script is executed by clicking the “prepare” button.

Set the configuration parameters in the Data prep tab and press the “prepare” button. This will start the script that prepares raw data for reconstruction. The prepared file is in “tif” format and can be viewed with tools, such Fiji.

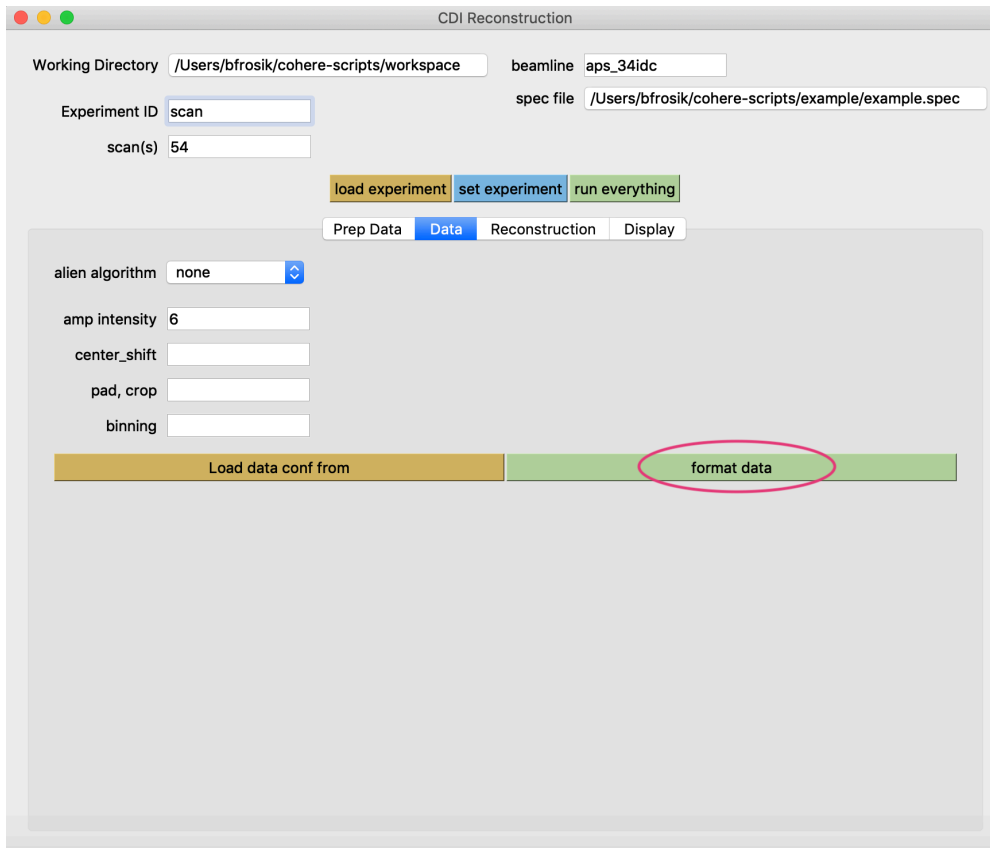
For parameters description refer to https://cohere.readthedocs.io/en/latest/config_prep.html.

The parameters will be saved in the “<ExperimentID>/conf/config_prep” file and will show up in the experiment window the next time this experiment is loaded.

Additionally, the parameters can be loaded from another experiment file by pressing “Load prep conf from” button and selecting the config_prep file from whichever experiment directory you like.

3. Format data.

Select the “Data” tab in the GUI.



In this example a formatted data file /temp/cohere-scripts-main/scan_54/data/data.tif will be created after the script is started by clicking the “format data” button.

Set the configuration parameters in the Data tab and press the “format data” button. This will start the script that formats the prepared data. The formatted data file is in “tif” format and can be viewed with tools, such as Fiji.

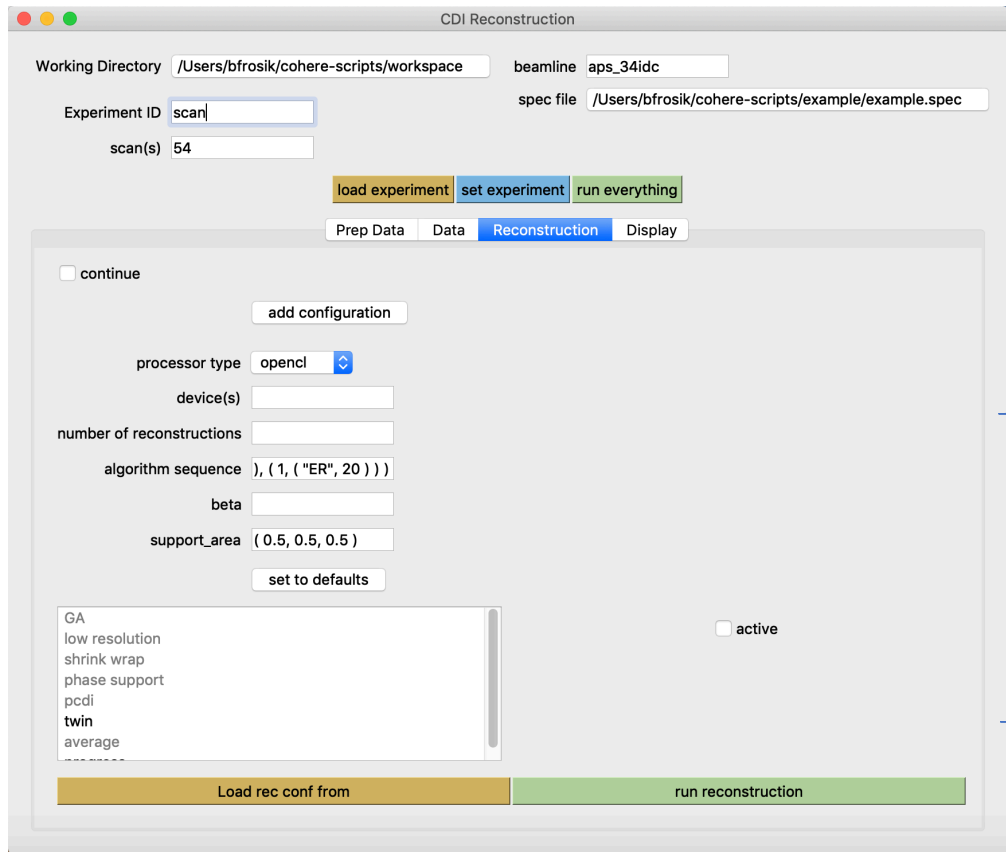
For parameters description refer to https://cohere.readthedocs.io/en/latest/config_data.html .

The parameters will be saved in the “config_data” file and will show up in the experiment window the next time this experiment is loaded.

The parameters can be loaded from another configuration file by pressing “Load data conf from” button and selecting a config_data file.

4. Run reconstruction

Select the “Reconstruction” tab in the GUI.



Reconstruction parameters which are always applicable.

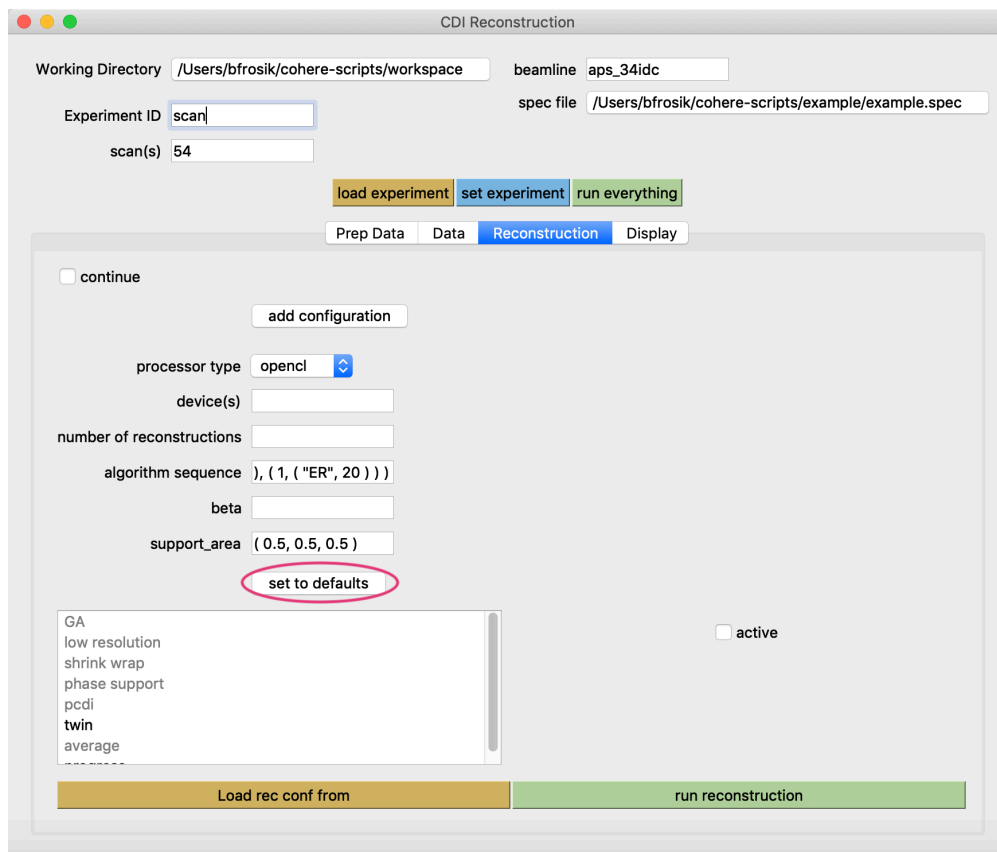
Feature list activated separately. Feature's parameters are displayed when it is activated. Active features are displayed in black letters. Disabled features appear gray in the list.

This tab has a main area where reconstruction parameters are set and a list of features that can be activated/deactivated.

For parameters description refer to https://cohere.readthedocs.io/en/latest/config_rec.html.

There are three ways to set the reconstruction parameters:

- By typing values in the boxes
- By loading from another config_rec file. Press the “Load rec conf from” button and navigate to the file.
- By using the “set to defaults” push button. This is shown in the figure below.



After the command is executed the default configuration is displayed in GU, as shown below.

CDI Reconstruction

Working Directory beamline

Experiment ID spec file

scan(s)

☐ continue

processor type

device(s)

number of reconstructions

algorithm sequence

beta

support_area

GA
low resolution
shrink wrap
phase support
pcdi
twin
average

☐ active

In this example above the basic parameters are set to default values after pressing the button.

The active features are listed in black, and the inactive features are grey. As you can see the feature shrink wrap is not active. Adding this feature and setting values to defaults is shown below.

CDI Reconstruction

Working Directory beamline

Experiment ID spec file

scan(s)

☐ continue

processor type

device(s)

number of reconstructions

algorithm sequence

beta

support_area

GA

low resolution

shrink wrap

phase support

pcdi

twin

average

progress

☒ active

shrink wrap triggers

shrink wrap algorithm

threshold

sigma

Select the “shrink wrap” feature from the list and check “active” box. A list of parameters related to shrink wrap shows up on the right, but the fields are empty. It is convenient to fill the fields with the “set to default” button, as shown below. The parameters can be then edited.

CDI Reconstruction

Working Directory beamline

Experiment ID spec file

scan(s)

☐ continue

processor type

device(s)

number of reconstructions

algorithm sequence

beta

support_area

GA
low resolution
shrink wrap
phase support
pcdi
twin
average
progress

☒ active
shrink wrap triggers
shrink wrap algorithm
threshold
sigma

User can activate/deactivate features using this window and set parameters to different values.

After setting the shrink wrap parameters the feature will be processed during reconstruction.

Press the “run reconstruction” button to run the reconstruction process as shown below.

CDI Reconstruction

Working Directory beamline

Experiment ID spec file

scan(s)

☐ continue

processor type

device(s)

number of reconstructions

algorithm sequence

beta

support_area

GA
low resolution
shrink wrap
phase support
pcdi
twin
average
progress

☒ active

shrink wrap triggers

shrink wrap algorithm

threshold

sigma

Make sure the processor type is the correct choice for your hardware. If cuda choice can't be used, try opencl. The cpu option offers the worst performance but could be the only option for some hardware.

After initiating reconstruction by pressing the "run reconstruction" button, the reconstructed files will be created in the /temp/cohere-scripts-main/workspace/scan_54/results directory in this example.

The reconstruction results are files in "npz" format: image, support, and optionally coherence. The results subdirectory contains also other files, such as summary that contains the reciprocal space error of the reconstruction for each iteration. The file plot_errors.py is an executable that will plot the errors when you type: plot_errors.py.

5. Process visualization

CDI Reconstruction

Working Directory: /Users/bfrosik/cohere-scripts/workspace beamline: aps_34idc spec file: /Users/bfrosik/cohere-scripts/example/example.spec

Experiment ID: scan scan(s): 54

load experiment set experiment run everything

Prep Data Data Reconstruction Display

results directory: /Users/bfrosik/cohere-scripts/workspace/scan_54/results

diffractometer: 34idc crop: (0.5, 0.5, 0.5) ramp upscale: 1 energy: 9.0 delta (deg): 32.174 gamma (deg): 12.6346 detdist (mm): 500.0 theta (deg): 0.2200042 chi (deg): 90.0 phi (deg): -5.0 scan motor: th scan motor delay: 0.005 detector: 34idcTIM2

Load disp conf from process display

Directory that will be recursively searched for the reconstructed images, supports and coherence. The images will be processed for the visual interpretation in the VTK vts file format and stored along with the reconstructed images.

A blue text indicates the parameters were parsed from spec file

In this example vts files: image.vts and support.vts will be created in the /temp/cohere-scripts-main/workspace/scan_54 directory after script is started with “process display” button.

Set the configuration parameters in the Display tab and press “process display” button. This will start the script that processes reconstructed image(s) for visual interpretation. The created files are: image.vts, support.vts, and optionally, if pcdi feature is active, coherence.vts. Since the files are in vts format they can be viewed with tools, such Paraview.

For parameters description refer to https://cohere.readthedocs.io/en/latest/config_disp.html .

The parameters will be saved in the “config_disp” file and will show up in the experiment window the next time this experiment is loaded.

The parameters can be loaded from another configuration file by pressing “Load disp conf from” button and selecting the file.

6. Create new experiment based on existing one.

To create a new experiment with the existing experiment simply replace the Experiment ID with a new string for example “tst”, and click the “set experiment” button. A new experiment directory will be created with copies of the configuration files from the original experiment (config_prep, config_data, config_rec, config_disp) copied to the new experiment conf directory. Now all actions will affect the tst_54 experiment space.

CDI Reconstruction

Working Directory: /Users/bfrosik/cohere-scripts/workspace beamline: aps_34idc

Experiment ID: **tst** spec file: /Users/bfrosik/cohere-scripts/example/example.spec

scan(s): 54

load experiment **set experiment** run everything

Prep Data Data Reconstruction Display

separate scans ☐

data directory: /Users/bfrosik/cohere-scripts/example/exp_data

darkfield file: /Users/bfrosik/cohere-scripts/example/dark.tif

whitefield file: /Users/bfrosik/cohere-scripts/example/whitefield.tif

lmult:

detector: 34idcTIM2

detector area (roi): [0, 256, 0, 256, 1]

min files in scan:

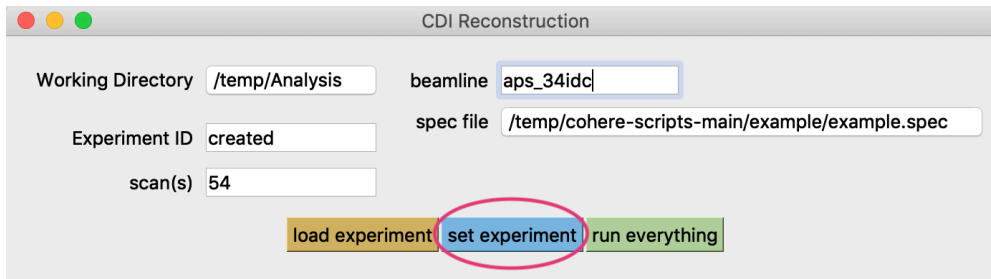
exclude scans:

Load prep conf from prepare

Replace the Working Directory, and/or Experiment ID, and/or scan(s) and create new experiment by pressing “set experiment” button

7. Create new experiment from scratch.

A new experiment space can be created through GUI by filling the parameters in the GUI window.



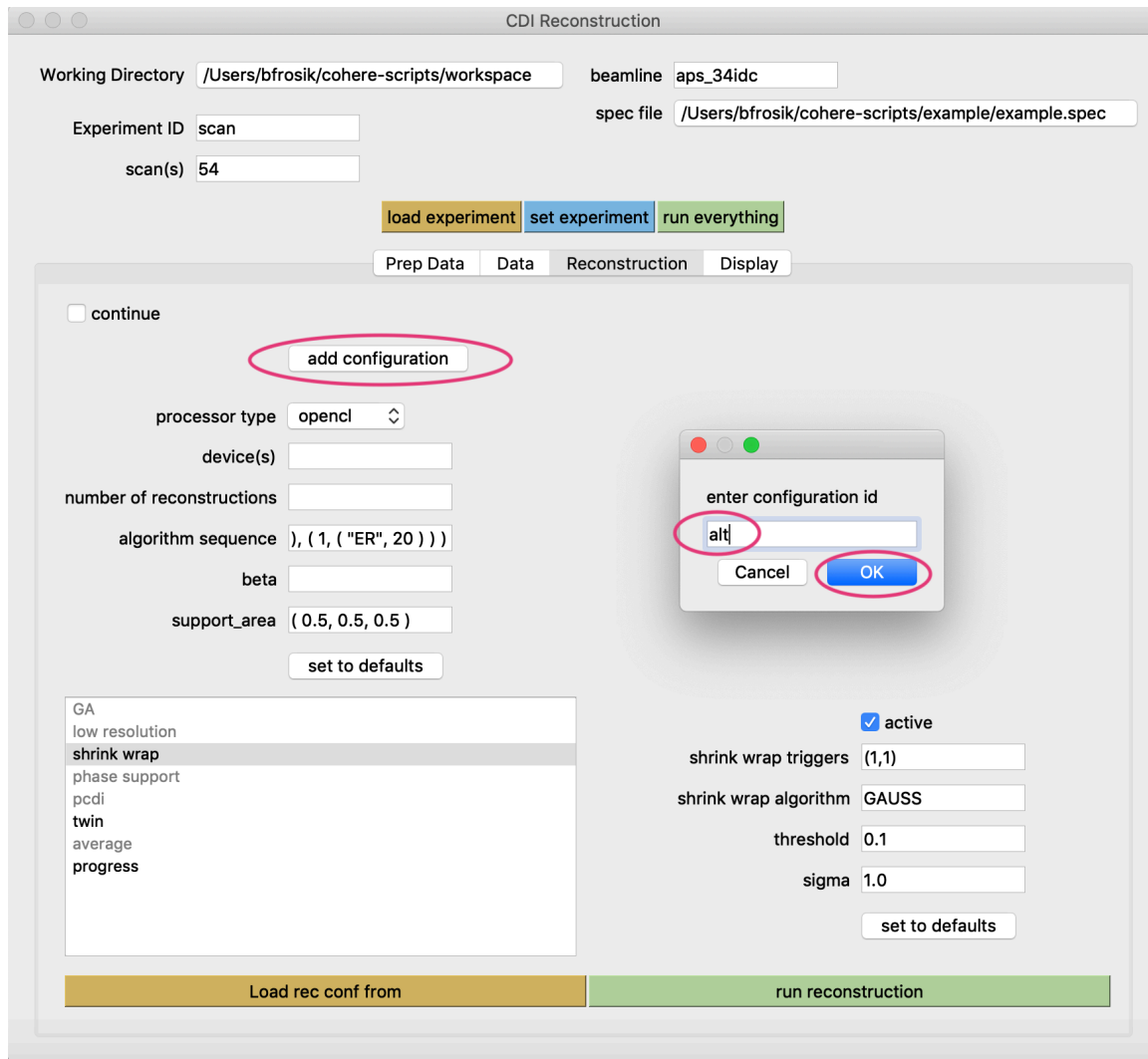
Select Working Directory
from dialog box
Enter beamline
Enter Experiment ID
Select spec file from dialog
box
Enter scan(s) to be
processed
Press “set experiment”

After filling entries in the main window press the “set experiment” button. This will create a new experiment space but only the main config file is created. In this example an experiment directory /temp/Analysis/created_54 will be created.

8. Reconstruction with alternate configurations

User may wish to run reconstruction with the same data but with different parameters. The “add configuration” button allows for alternate multiple configurations to be included in the experiment work space.

After pressing the “add configuration” button a pop-up dialog shows up. Enter any literal that will identify the configuration. The process is shown below.



In the dialog box type the configuration id and press “ok” button. At this moment a new configuration file is created in experiment space: /local/workspace/example/conf/alt_config_rec. Under the “add configuration” button a new field shows up that displays currently active configuration.

CDI Reconstruction

Working Directory beamline

Experiment ID spec file

scan(s)

☐ continue

processor type

device(s)

number of reconstructions

algorithm sequence

beta

support_area

☐ active

GA
low resolution
shrink wrap
phase support
pcdi
twin
average
progress

This field allows user to choose the active configuration that will be used in reconstruction. You can modify the parameters, activate/deactivate features in the alternate configuration. Start the reconstruction processing by pressing the “run reconstruction” button. After the process is completed a new results directory, that includes the configuration id, is created: /local/workspace/example/alt_results. The reconstructed files will be saved there.