Simple Instructions to Install & Use REFL/PARK package

Version 0.3.5

1. Download the Windows binary file **park-0.3.5.zip**
   Web site: http://chemnuc-20.umd.edu/~DANSE/download/index.html

2. Unzip **park-0.3.5.zip**

3. Run the program **parkWin.exe**

4. Prepare the data source for the fitting

5. Prepare the model for the fitting

6. Submit the job for the fitting

7. View the fitting results

The following is the details about how to prepare the data source and prepare the model.

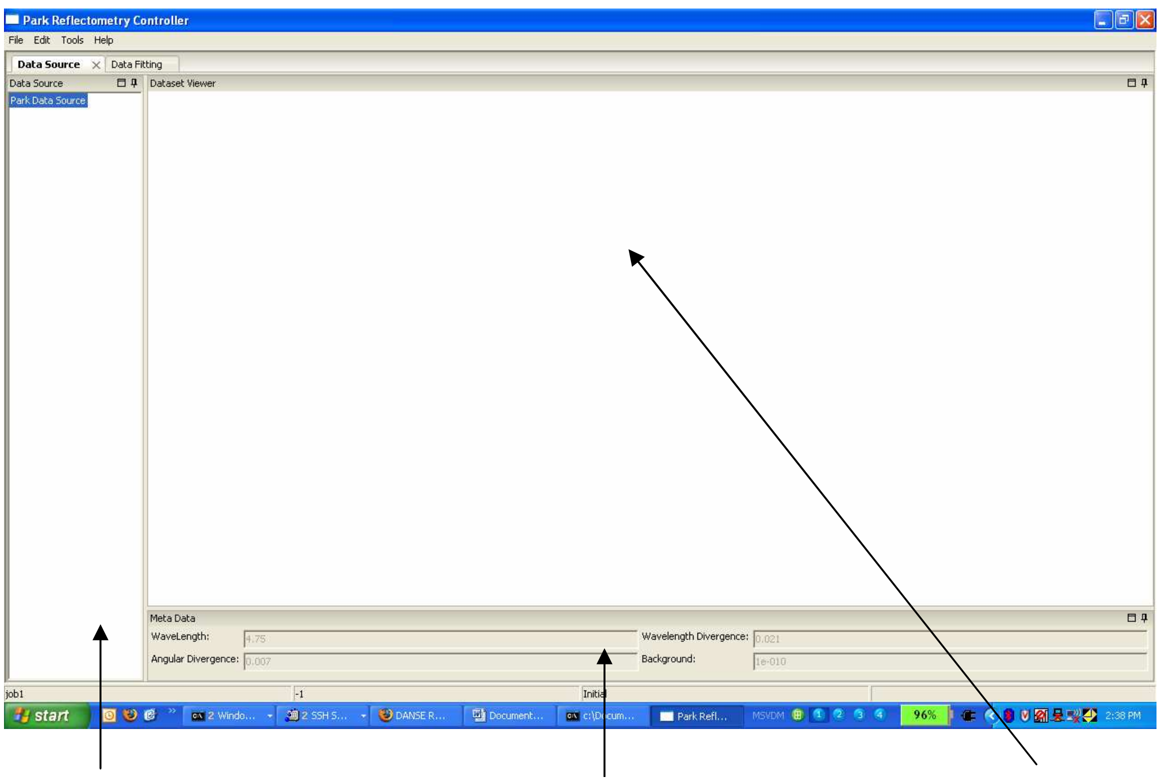
1. Prepare the data source for the fitting

When the program **parkWin.exe** is running, the data source window will appear, as shown in Fig. 1. This window can also be shown by clicking the Data Source. This window is used to do the preprocessing of the data source that can be used for the fitting. Currently only the column-based text data files can be processed.

There are three main sub-windows under this window:

a. DataSource control panel: load/save/clear the data source
b. DataSource view panel: add/remove/clear/view the individual dataset within the data source
c. Metadata panel: edit the meta data for the individual data within the data set.

Logically, one data source has one or more datasets, while one dataset can have one or more data, while one data corresponds to one file in the disk.



DataSoure control panel Metadata panel Data View panel

Fig . 1

Both the DataSource control panel and Data view panel has the corresponding context menu. The context menu can be shown by right-mouse clicking. The context menu on the Data view panel is visible only when a valid dataset is selected on the DataSource control panel.

1. Create a new dataset
    a. Go to the DataSource control panel
    b. Right click the mouse to show the context menu
    c. Click the "New dataset" menu item to create a new dataset
    d. Select one dataset
2. Add data to the selected dataset
    a. If the dataset has some data, the combined data will be shown on Data view panel, otherwise an empty panel is shown on Data view panel,
    b. Got to the DataViewer window
    c. Right click the mouse to show the context menu
    d. Select 'Add' menu item to add a new data to the dataset.

    The context menu has the following items:
    Add: Add a new data file
    Remove: Remove the current data

    Original Viewer: the scales are set to 1.0
    Match with Res: Auto-match with the resolution
    Match without Res: Auto-match without the resolution

    Normal: Normal mode
    Drag: Drag mode, the user can drag the plotting
    Zoom: Zoom mode, the user can zoom the plotting

    Log scale: show R in log scale
    Show Legend: show the legends
    Show Lines: show the connection lines
    Show Marker: show the markers

    Print Setup: Setup the printer
    Print Preview: Preview the results to be printed
    Print: Print the results

    Save as: Save the results in Text format:
    Property: Not used right now. Will be used later to change the properties of the plotting, such as the title, x-axis label, y-axis label, …

3. Change the meta data for each data
    a. Go to the Data source control panel, select one data under a dataset
    b. Go to the Metadata panel and edit the individual meta data
    c. The metadata panel is enabled only when a valid data under a dataset is selected.

4. Save the data source (Optional)
    a. Go to the Datasource control panel

b. Select the ‘Save’ or ‘Save as’ menu item to save the data source in an xml file.
c. The saved data source can be reloaded by clicking the “Load” menu item.

5. The data source can be cleared by clicking the ‘Clear’ menu item

2. Prepare the model for the fitting

In order to build the model for the fitting, the data fitting window must be shown by clicking the Data Fitting tab -> Refl Model Builder, which is shown in Fig. 2:

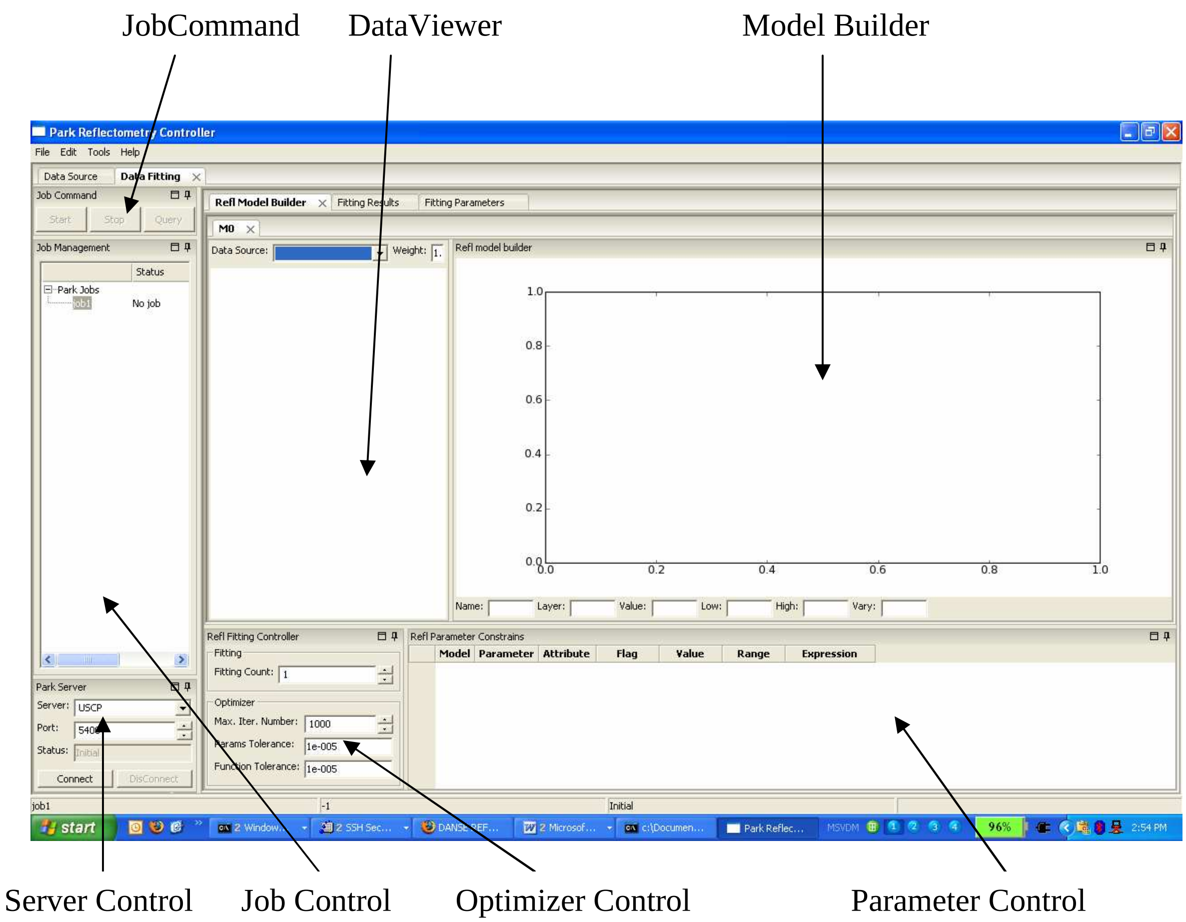


Fig. 2

1. Go to Job control panel, show the context menu, click ‘Load’ to select job or ‘New’ item to create a new job
2. Go to Data View panel to select the dataset by clicking Data Source choices
3. Go to Model Builder panel to build a model. If the job is not loaded from the file, you need to use ‘Init Model’ to initialize a model or ‘Load Model’ from the previous created model. See Fig. 3
4. Once the model is shown, you can use the ‘Add layer’ / ‘Remove layer’ context menu item to add or remove a layer, and drag the profile lines to change the value. The corresponding theoretical results will be shown on Data Viewer panel.
5. Change the control parameters on optimizer control panel.
6. Connect to the server by pressing the ‘Connect’ button on ‘Server Control’ panel.

7. Once the server is successfully connected, the buttons on JobCommand panel will be enabled. Press ‘Start’ button to start the fitting. (The fitting can be stopped by pressing ‘Stop’ button)
8. Once the fitting starts, the ‘status’ column in “Server Control’ will indicate the number of tasks (N) that will be done for this job and the number of tasks (N) that have been done by tag of ‘n / N’. The lowest chi square value is also shown in ‘Chisq’ column. N is the number indicated by the ‘Fitting count’ field on the “Optimizer Control” panel.
9. Once one task was finished, you can go to the “Fitting Results” page to view the fitting results and the “Fitting Parameters” page to view the final fitting parameters. See Fig. 4
10. Once the job is done, it can be saved as an xml file (Go to job control panel -> select ‘Save as’ context menu item), and loaded later. When it is loaded, the fitting results will the initial value for the model parameters.

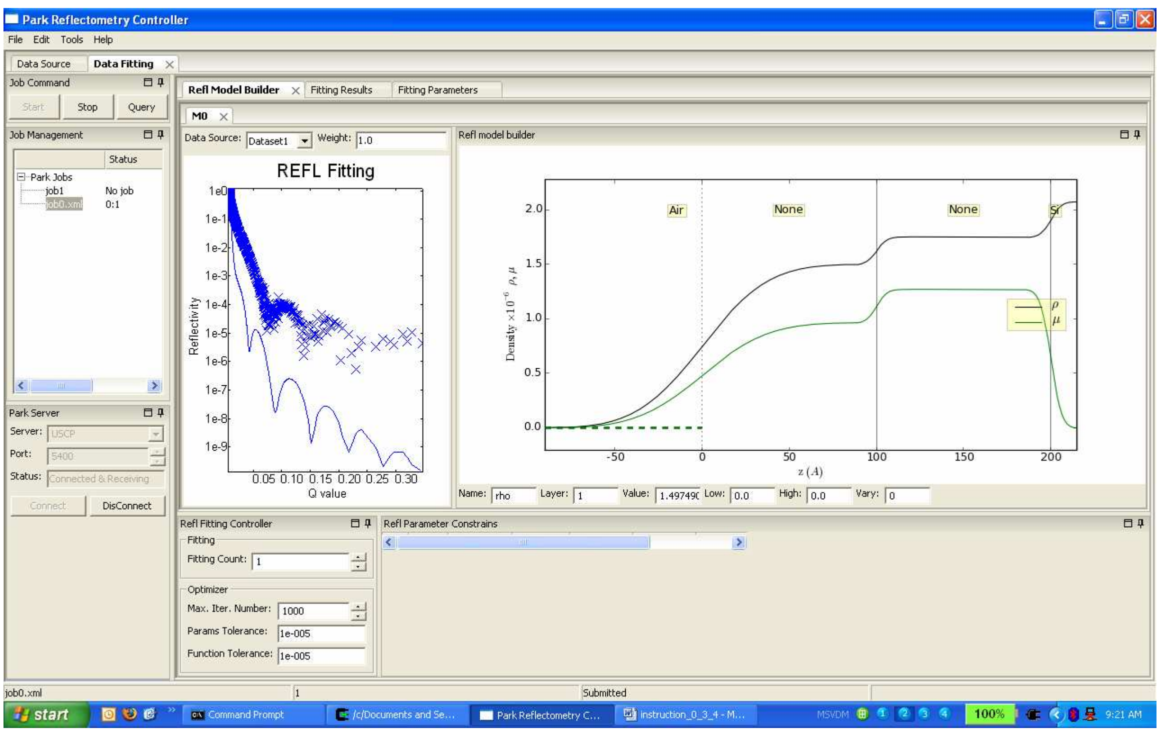


Fig. 3

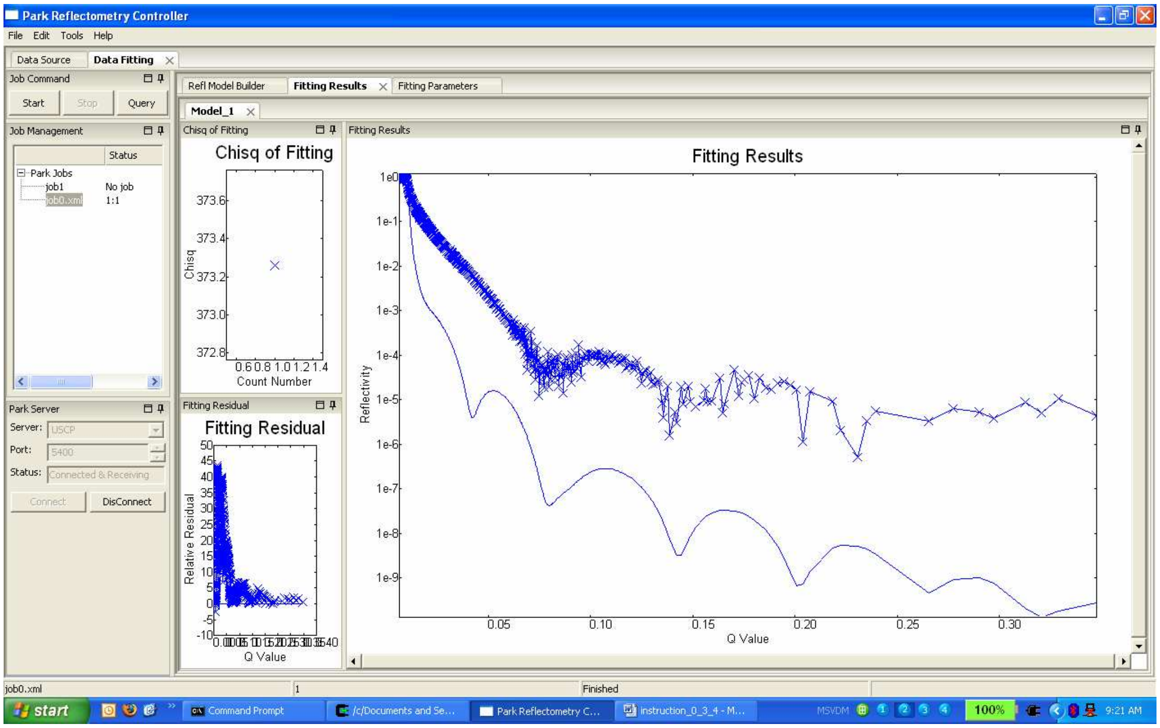

Park Reflectometry Controller
File Edit Tools Help
Data Source
Data Fitting
Job Command
Start
Stop
Query
Job Management
Status
Park Jobs
job1
No job
job0.xml
1:1
Park Server
Server:
Port:
Status:
Connect
DisConnect
Refl Model Builder
Fitting Results
Fitting Parameters
Model_1
Chisq of Fitting
Chisq
Count Number
Fitting Residual
Relative Residual
Q Value
Fitting Results
Reflectivity
Q Value
Finished

Fig. 4