How to use Refl1d and Bumps

User guide (including usage on IDAaaS)

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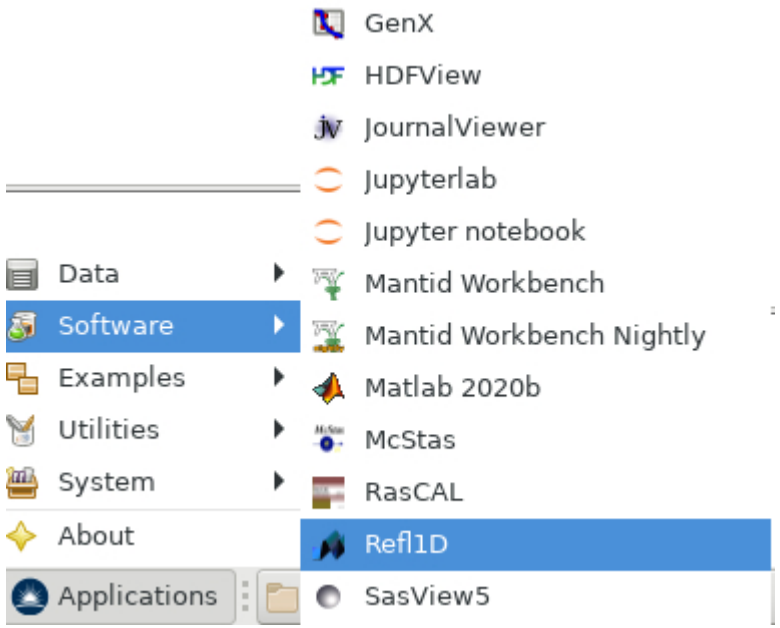
IDAaaS: Loading refl1d GUI

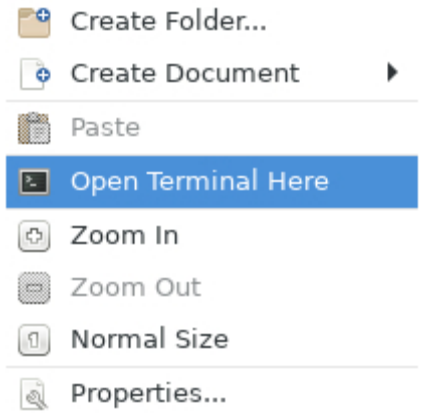
- Click on applications:
  - Software/Refl1d



- This will bring up the GUI only.
- If you want to use refl1d in command line format – or you want to open the GUI up in a specific folder – then you need to launch the GUI from the terminal

IDAaaS: Loading refl1d in a specific folder

- Right click in the folder you are working in – e.g. “Practical 8”
- Click on “Open Terminal Here”:



- In the terminal you should see:

[username@host-ip-address folder_name]$

- If it is anything else just ask
- Next, type the following command:

source /opt/refl1d/bin/activate

- This activates the refl1d virtual environment.
- From here you should just be able to launch refl1d using the command:

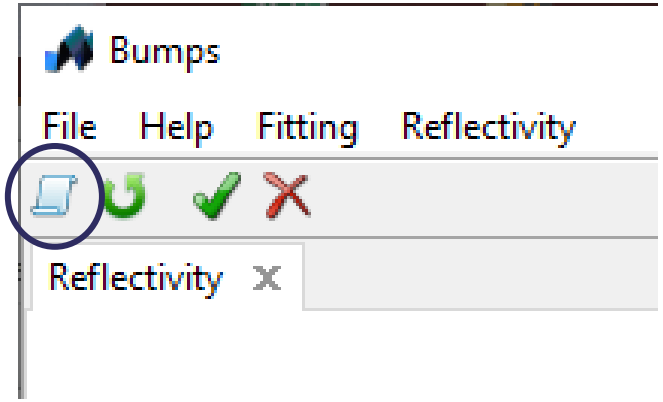
refl1d --edit

Installing Refl1d (if using away from IDAaaS)

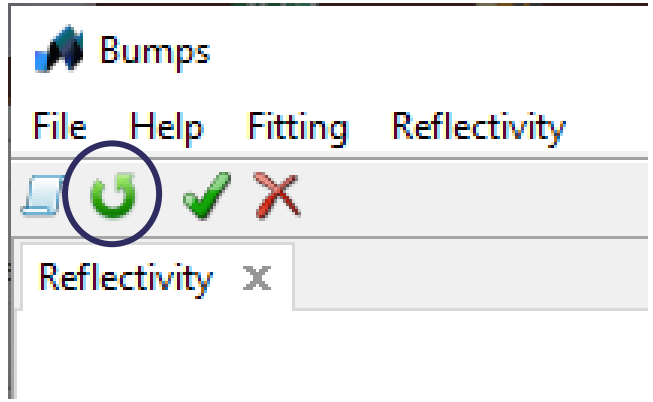
- There are a couple of different options for installing refl1d:
- Python install via pip: if you have an existing python install then refl1d can be easily installed by running the command:
  - pip install refl1d wxpython
- Download and use the standalone Windows refl1d release from: https://github.com/reflectometry/refl1d/releases/
  - Here you just extract into a folder of choice and run refl1d_gui.bat
- For now, command line operation of refl1d is easier from using a python install.

Loading a model file into refl1d

- To load a model click the scroll button in the top left corner of the GUI :

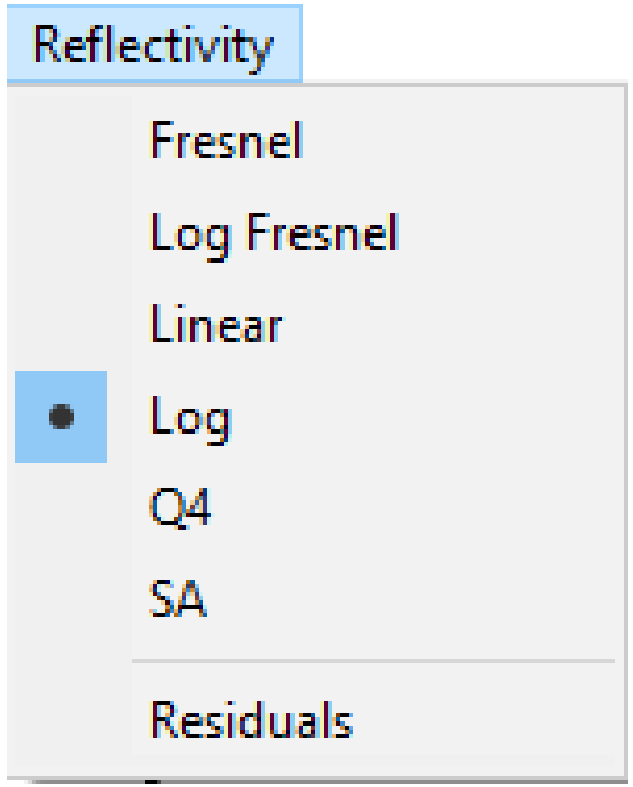


- To reload an already loaded model click the circular arrow (note, this will only work if your model initially loaded without errors):



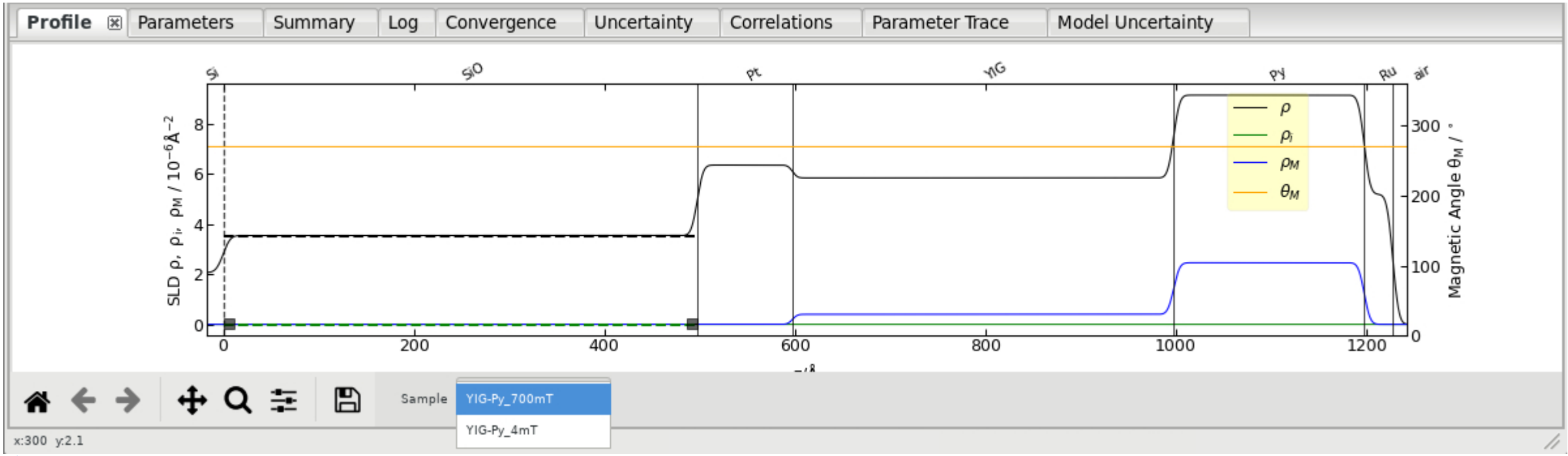
Reflectivity Views:

- In the GUI, you can view the reflectivity in a few different ways:
  - Log y-scale
  - Q^4 y-scale
  - Fresnel reflectivity (reflectivity/substrate reflectivity)
  - Log Fresnel reflectivity
  - Spin Asymmetry (SA) for PNR/PA
  - Residuals



Profile View – Shows SLDs

- Here you can view all of the profiles present in the model
- You can manipulate the SLD and iSLD profiles directly in the profile to get a feel for how this affects the reflectivity profile
- If multiple profiles/datasets are included in the model a dropdown menu will appear



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Parameter View

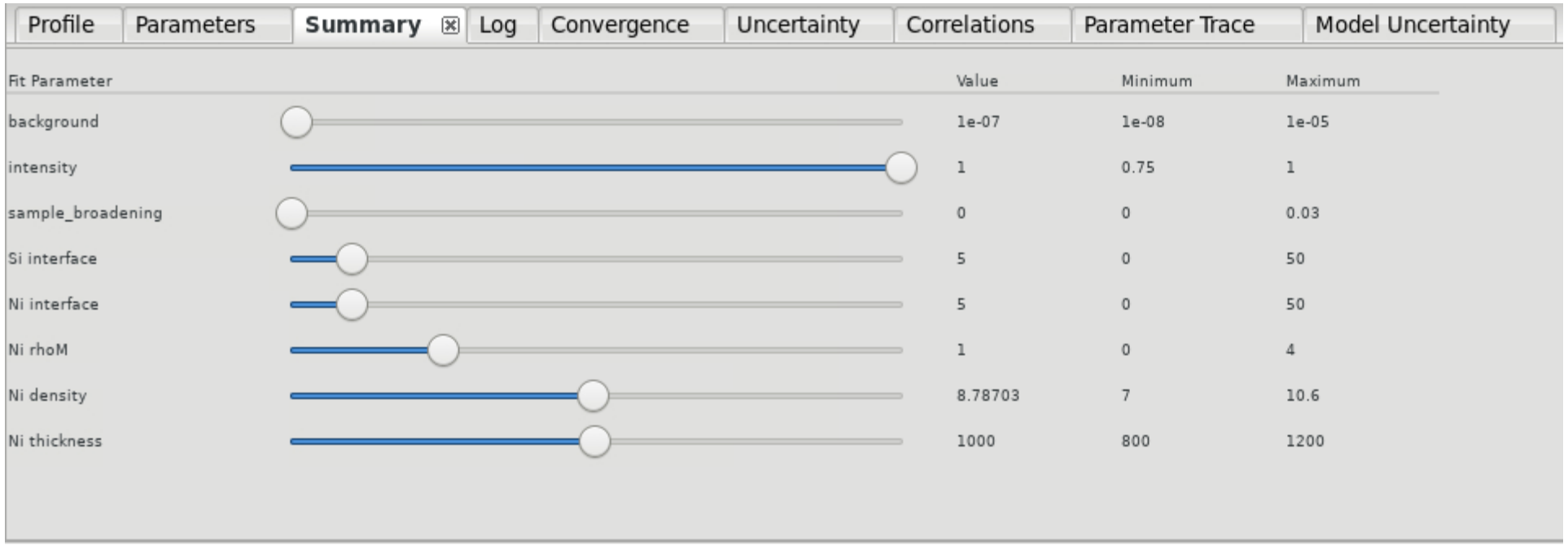
- Here you can view the full list of parameters included in the model
- You can choose to fit or not fit parameters by clicking the tickboxes
- You can alter the fit ranges and parameter values in the table
- Note: these new ranges and fittable parameters will not be passed back to the model file: If you reload the model file it will reset this.

Profile | **Parameters** | Summary | Log | Convergence | Uncertainty | Correlations | Parameter Trace | Model Uncertainty

Fit?	Parameter	Value	Minimum	Maximum	Path	Link
☑	SiO rho	3.545	2	4.1	M.models[1].sample.layers[1].material.rho	M.models[0].sample.layers[1].material.rho
☑	SiO thickness	497.5	300	600	M.models[1].sample.layers[1].thickness	M.models[0].sample.layers[1].thickness
☑	Pt interface	4.0	1	40	M.models[1].sample.layers[2].interface	M.models[0].sample.layers[2].interface
☐	Pt irho	0			M.models[1].sample.layers[2].material.irho	M.models[0].sample.layers[2].material.irho
☑	Pt rho	6.357	6.03	6.68	M.models[1].sample.layers[2].material.rho	M.models[0].sample.layers[2].material.rho
☑	Pt thickness	100.0	75	125	M.models[1].sample.layers[2].thickness	M.models[0].sample.layers[2].thickness
☑	YIG interface	5.0	1	30	M.models[1].sample.layers[3].interface	M.models[0].sample.layers[3].interface
☑	YIG deadM above	0	0	40	M.models[1].sample.layers[3].magnetism.dead_above	

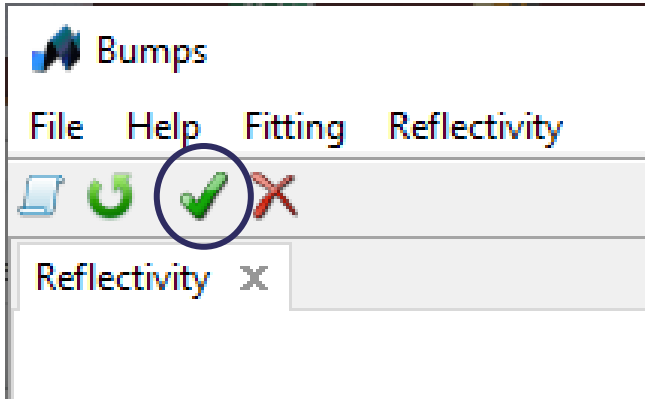
Summary View

- In this view, all of the parameters that are being fitted are present
- The current value, min and max ranges and parameter name are displayed
- Finally each parameter can be adjusted using a slider

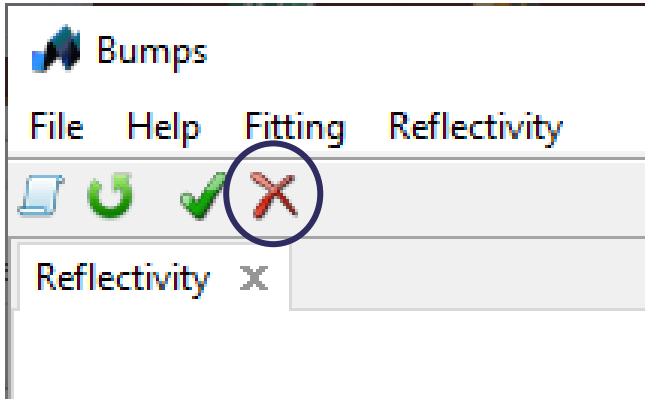


Running a fit:

- To start a fit click the tick in the top left corner of the GUI:



- To stop a fit click the cross:



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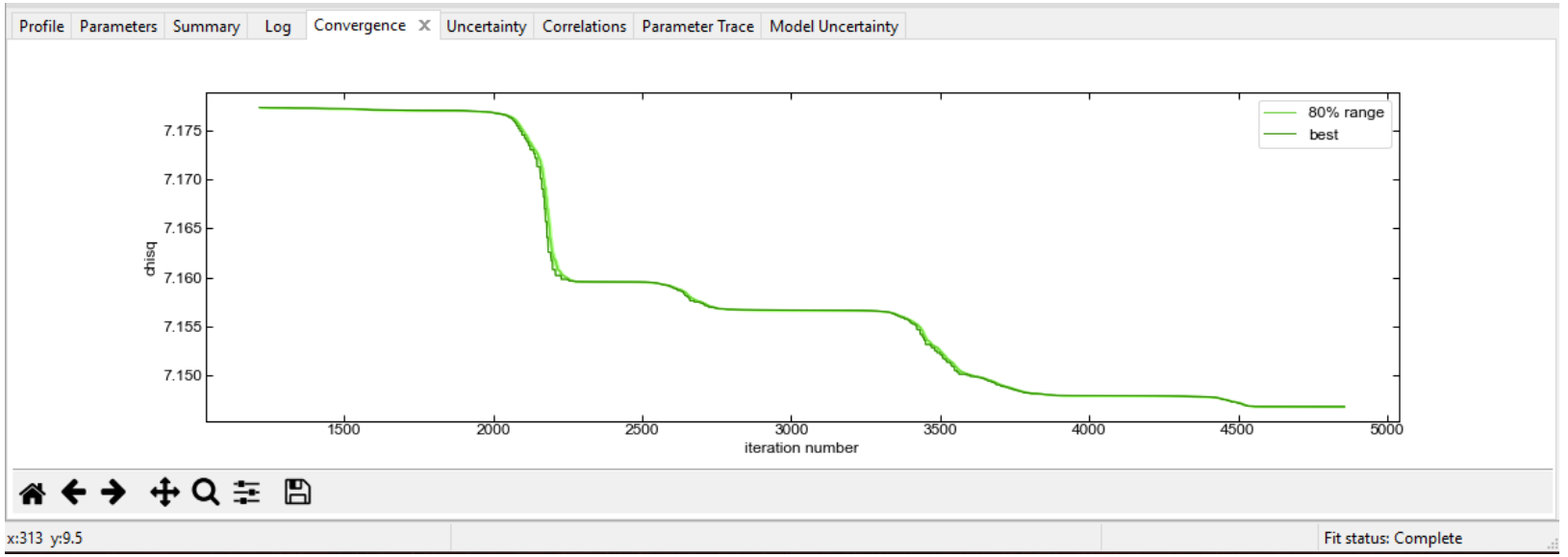
In the bottom right corner is the fit status:

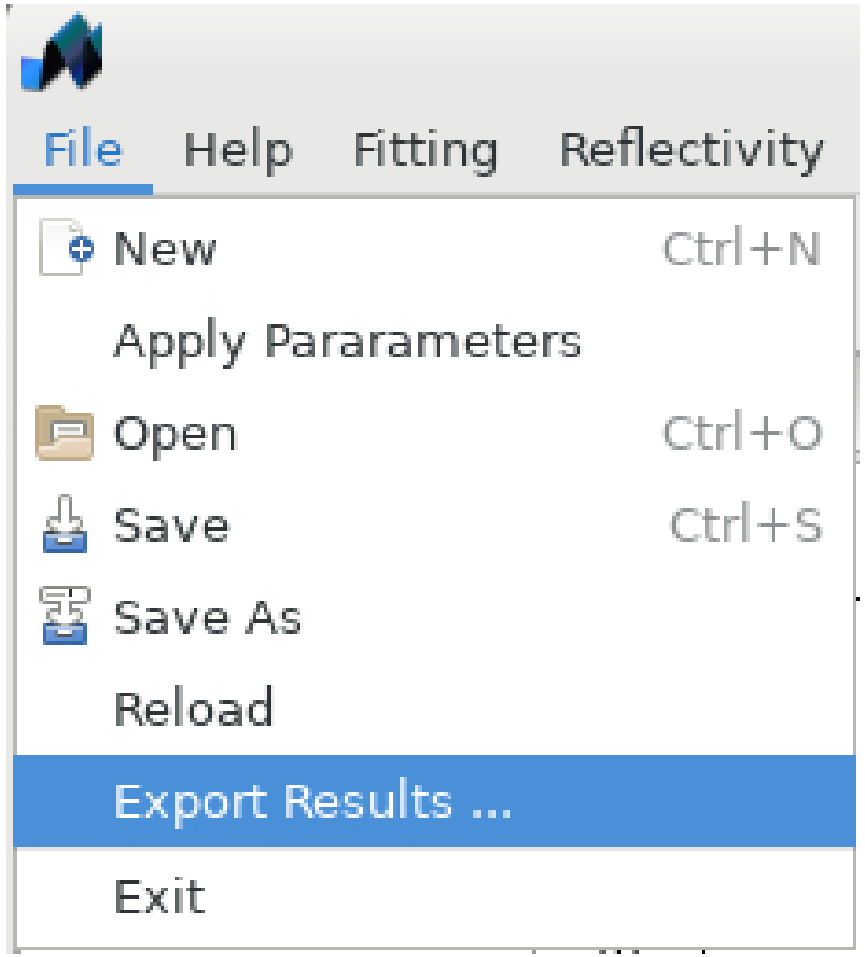
Convergence View

- You can check the progress of a fit using the convergence tab:



Exporting Results

- To export fit results click on the File → Export Results
- Due to the number of files that are exported it is strongly suggested that you create a new folder to export the results into
- The output depends on the fitter used: DREAM exports a large number of files including the data used to work out the parameter and fit statistics (some of these files can be large)



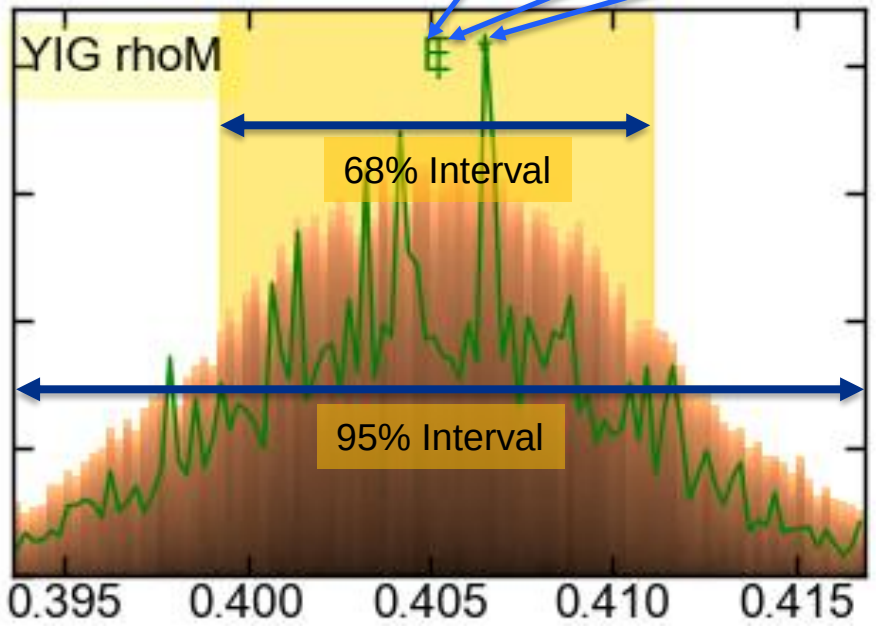
“Export Results” output:

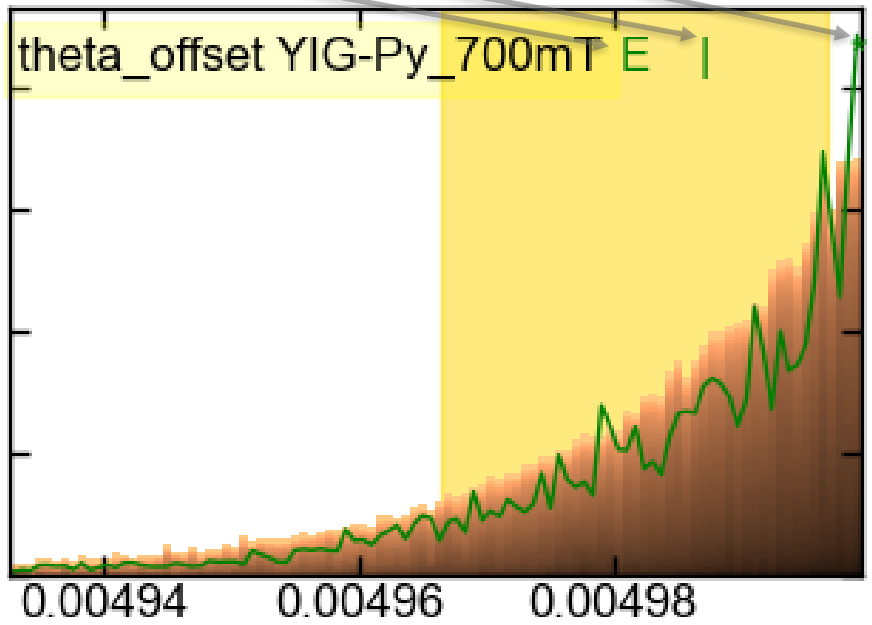
Below is detailed the list of files saved out by refl1d when clicking the export results option (the GUI output is slightly different to the CLI):

- General output:
  - .par – free (fitted) parameters and their values – this is used to reload a model state – say after fitting
  - .out – Hierarchical structure of the model parameters and values (includes non-fitted parameters in addition to fitted parameters) – Chisq is found in this file including total chisq if multi-fit
  - .err – values and uncertainties output from the fit – if DREAM is used this will include the 1 and 2 sigma uncertainty ranges found
  - -err.json – JSON store of the .err file above – allows for pulling in of these values to a python script with relative ease
  - NR: -refl.dat – reflectivity curve output including data and theory and Fresnel reflectivity.
  - PNR/PA:
    - refl.datA = mm = -- = DD
    - refl.datB = mp = -+ = DU
    - refl.datC = pm = +- = UD
    - refl.datD = pp = ++ = UU
  - .pickle: GUI model state will load in the state of the model and parameters at the point the model was exported
  - -slabs.dat – includes profile information based on the slabs used to construct the model
  - -steps.dat – lists regions of constant SLD and there start and stop position in Z
  - -profile.dat – provides SLD profiles (including iSLD and mSLD – if polarised) which can be passed to a plotter of choice
  - -expt.json – JSON store of model parameters – everything that was used to create the model
- DREAM output:
  - DREAM MCMC metric figures:
    - -logp.png – log likelihood history for the uncertainty analysis (effectively chisq vs model generation) – use this to check if model is converged
    - -corr.png – parameter correlation corner plot – shows correlations between pairs of parameters (this plot will only be produced for small-moderate numbers of parameters – for very large numbers of parameters this will need to be generated afterwards
    - -trace.png – parameter traces of the MCMC chains – look at these to check for good mixing in the chains
    - -vars.png – posterior distributions – these should always be checked – are they a smooth function or are they spikey (need more samples if it is the latter)
  - DREAM MCMC output files – these files store all of the MCMC output and can be reloaded back into relf1d using scripts to generate uncertainty contour plots and correlation plots:
    - -stats.mc.gz
    - -chain.mc.gz
    - -point.mc.gz

Error file explanation:

```
Parameter          mean  median    best [   68% interval] [   95% interval]
theta_offset YIG-Py_700mT 0.004982(18) 0.0049872 0.0049991 [0.004967 0.004997] [0.004933 0.004999]
          YIG rhoM 0.4052(59)  0.4052  0.4064 [  0.399    0.411] [  0.394    0.417]
```





Key:
E = Mean
| = Median
* = Best
— = best likelihood for that bin

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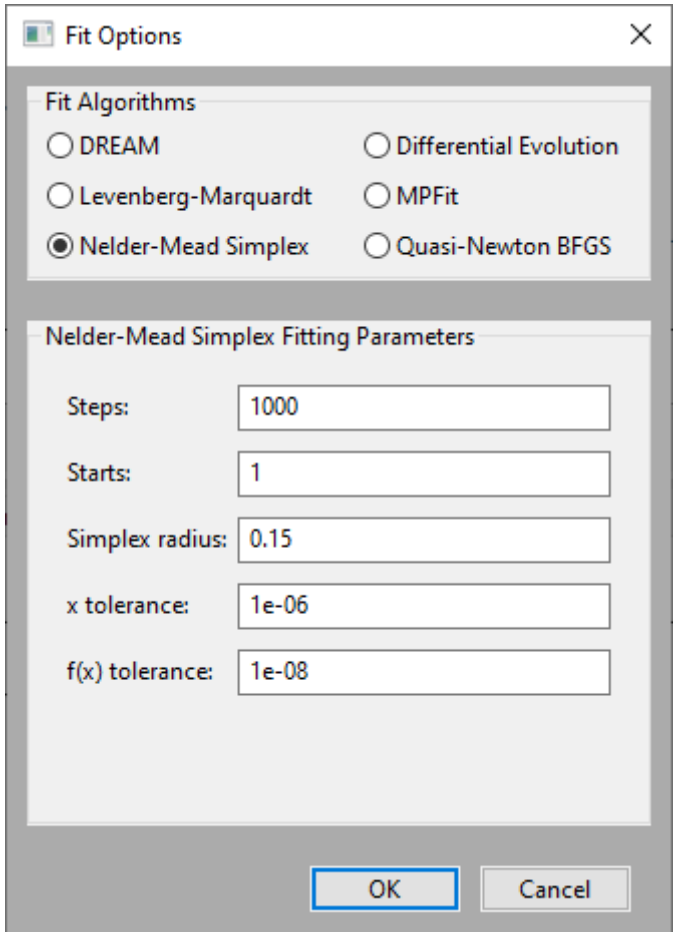
For more info read: https://bumps.readthedocs.io/en/latest/guide/optimizer.html#fit-dream

Bumps fitters: Simplex

- The simplex fitter in bumps (the underlying fit engine to refl1d), is very effective at quickly doing a local search – for very simple models it will also be able to find the global minima quite effectively.
- As models become more complex, with many parameters, the simplex fitter will not perform as well as other more robust global optimisers (DE and DREAM).
- We advise using the simplex for very quick initial fits, to make sure the model is behaving as you would expect, before using a more robust global optimiser.

Using Nelder-Mead Simplex

- Options in Nelder-Mead Simplex:
- Steps – Number of fit iterations
- Starts – how many times to restart the fit
- For more detailed information see: https://bumps.readthedocs.io/en/latest/guide/optimizer.html#fit-amoeba



Using DREAM – MCMC Uncertainty analysis

- Options in DREAM:
- Samples – no. of samples to take in analysis
- Burn-in steps – how many steps to run before taking samples
- Population – relative (total pop = pop * free params)
- Initializer: Global (LHS) or local (EPS)
- Thinning = what factor of sample to remove after sampling
- Convergence – 1 = don't check, 1> check if converged and start sampling early < 0
- Outliers – IQR, Grubbs, Mahal – every no of samples if chains lie outside of some range, remove these and place them back in the "main bunch"
- For more detailed information see: https://bumps.readthedocs.io/en/latest/guide/optimizer.html#fit-dream