Fitting in BornAgain
using graphical user interface

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BornAgain school and user meeting
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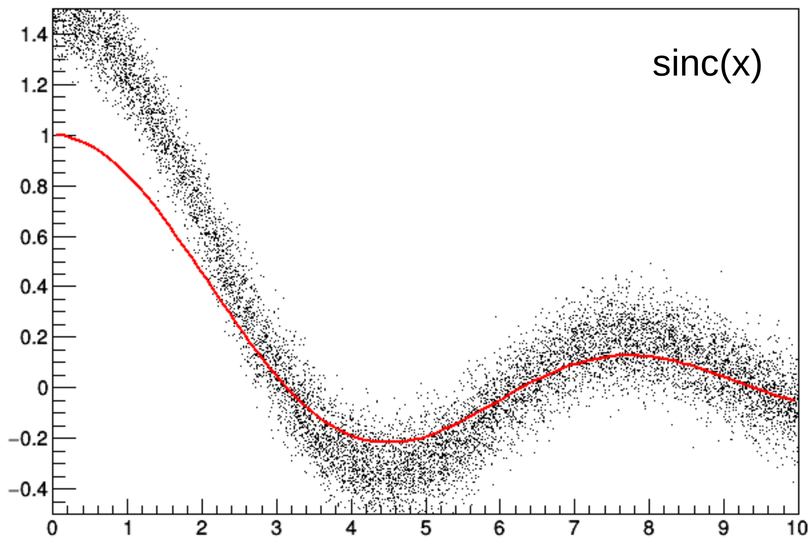
day_1

Basic concept

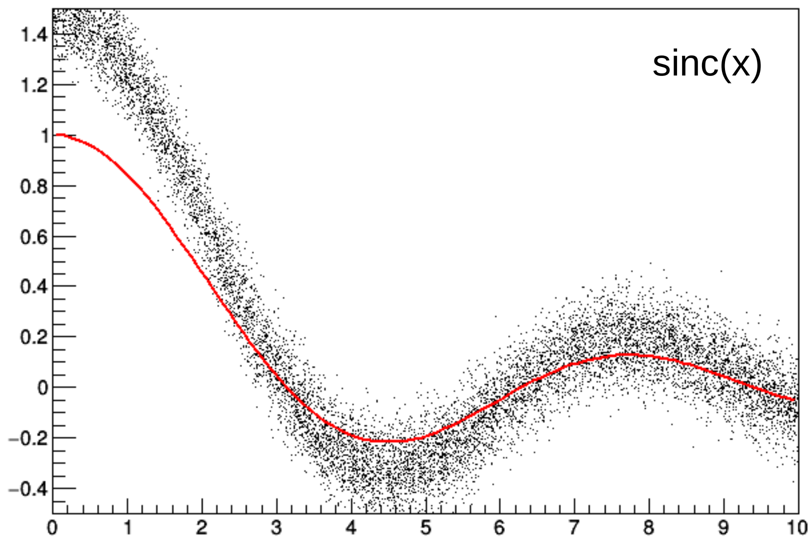
Finding the best set of parameter values for a model function to represent the data according to some criteria



Data	Set of (x,y) points
Model	`p`$_1$`*sinc(p`$_2$`*x)`
Fit criteria	minimum of χ^2

Basic concept

Finding the best set of parameter values for a model function to represent the data according to some criteria



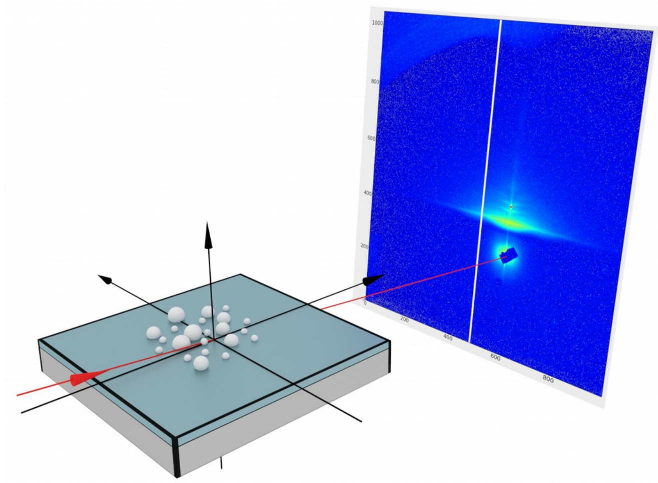
Data	Set of (x,y) points
Model	p_1*sinc(p_2*x)
Fit criteria	minimum of χ^2

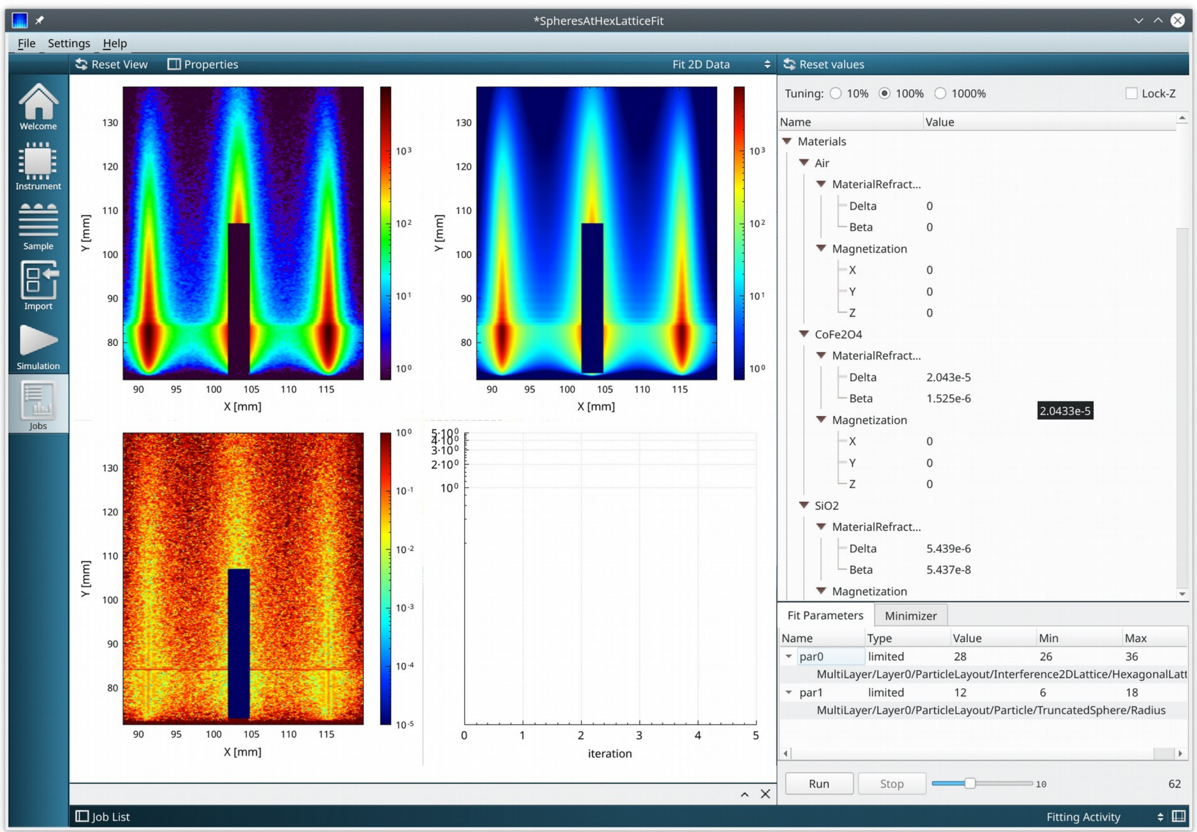
```
float objective_function(p1, p2):
    foreach (x,y)
      chi2 += (y - p1*sinc(p2*x))**2
    return chi2
```

Minimizer

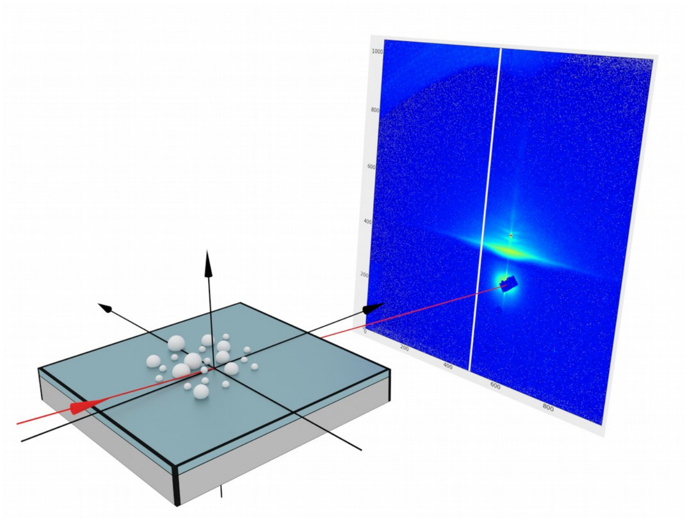
Fitting in BornAgain

Finding the values of sample parameters that best represent the data obtained in scattering experiment





Fitting in BornAgain

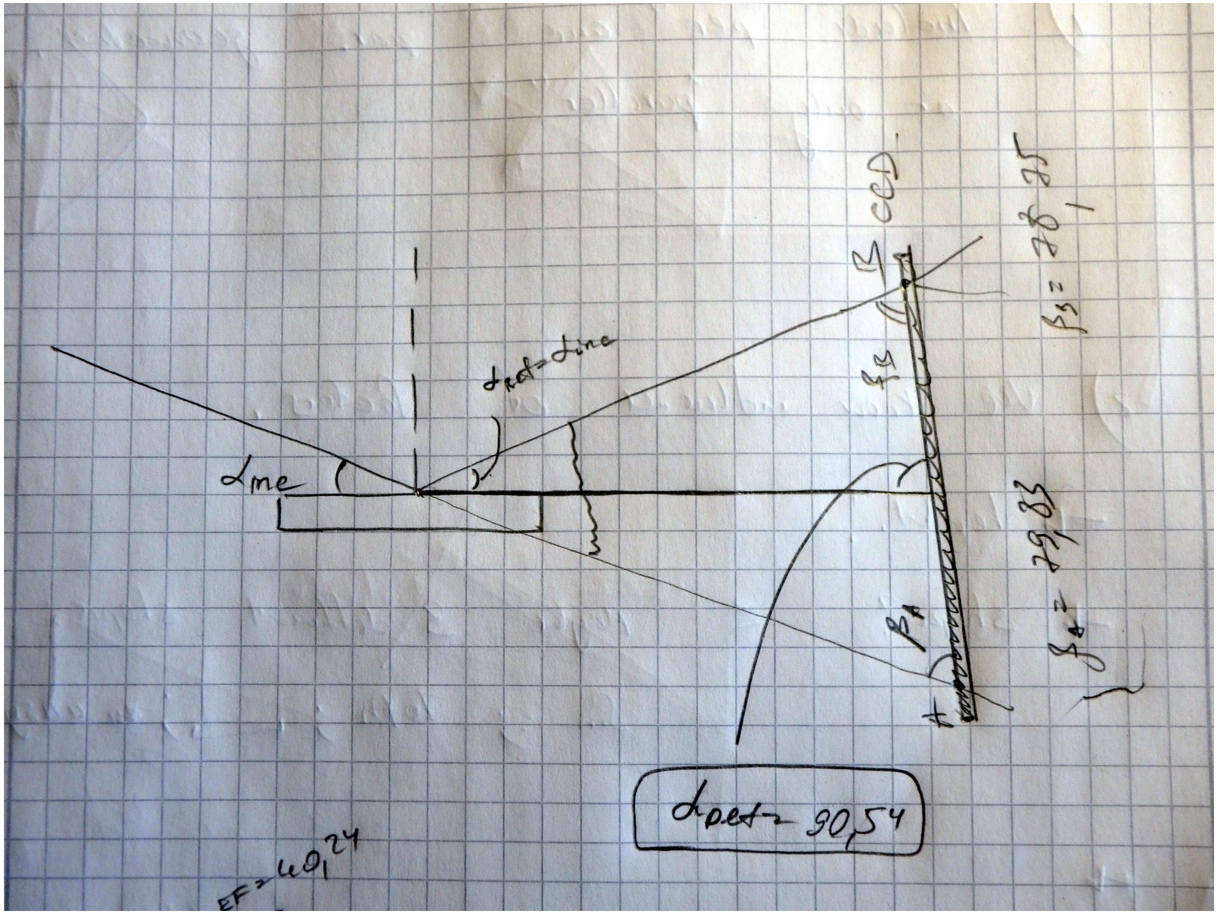


Finding the values of sample parameters that best represent the data obtained in scattering experiment

Necessary components

- Experimental data
  - File with intensities measured in detector channels
- Numerical model
  - Working GISAS simulation with instrument and sample defined
  - Good knowledge of experimental setup
  - Idea about sample structure and expected values of sample parameters
  - Good guess what to fit
- Objective function
- Minimizer

Knowledge of experimental setup



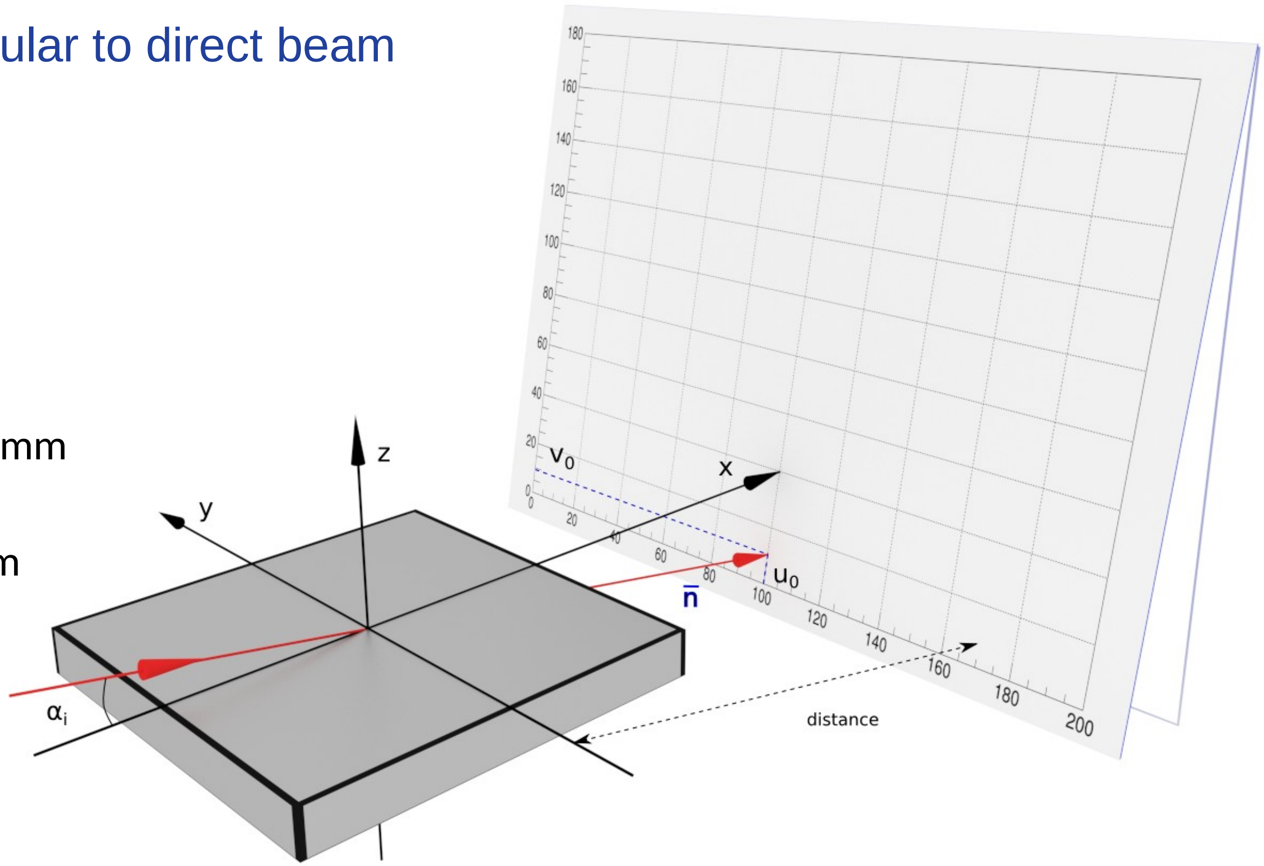
Knowledge of experimental setup

Detector orientation

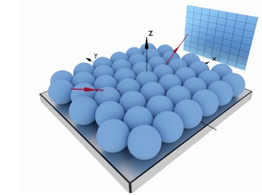
- Normal **n** to the detector plane in sample coordinate system
- (u_0, v_0) of intersection of **n** and the detector plane in local detector coordinates

Example: detector is perpendicular to direct beam

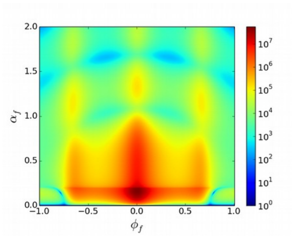
nxbins = 100
width = 200 mm
nybins = 100
height = 180 mm
α_i = 0.2 degree
distance = 2000 mm
n_x = distance*cos(alpha_i) = 1999.987 mm
n_y = 0
n_z = -distance*sin(alpha_i) = -6.981 mm
u_0 = 100 mm
v_0 = 10 mm



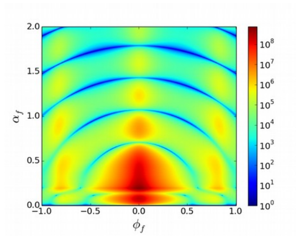
Objective function



- Provides similarity metric for experimental/simulated images
- GUI uses simple chi2



experiment



simulation

$$\chi^2 = \frac{1}{d} \cdot \sum \frac{(f(I_{exp}) - f(I_{sim}))^2}{\sigma^2}$$

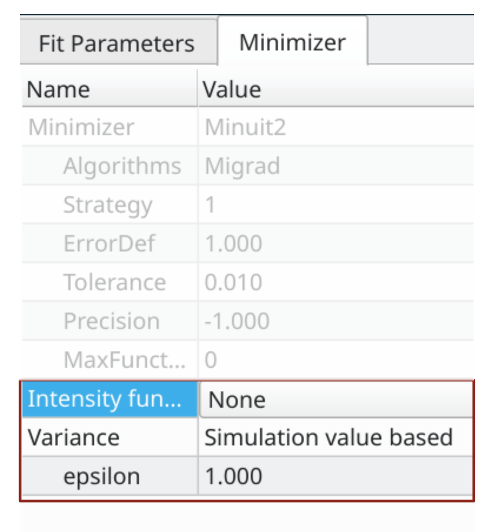
Sum over all unmasked detector channels

- Three options for intensity functions

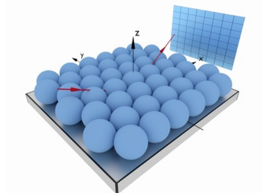
$$f(I) = I, \quad f(I) = \sqrt{I}, \quad f(I) = log(I)$$

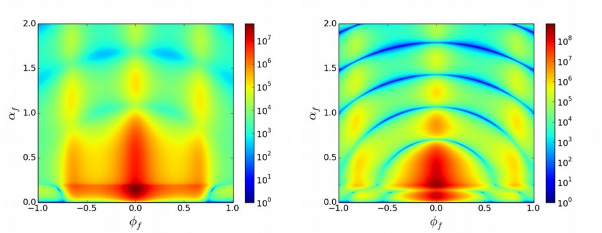
- Two options for residual error

$$\sigma = 1, \quad \sigma = \sqrt{max(\epsilon, f(I))}$$

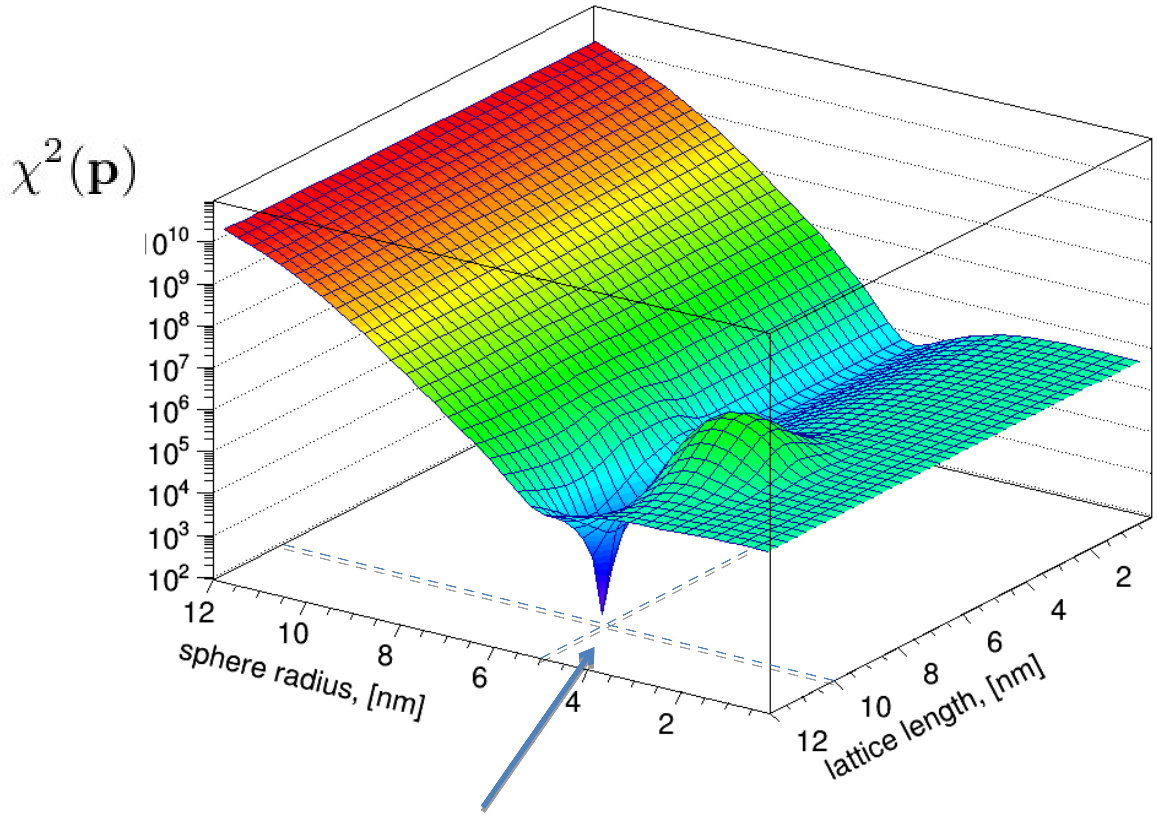


Objective function



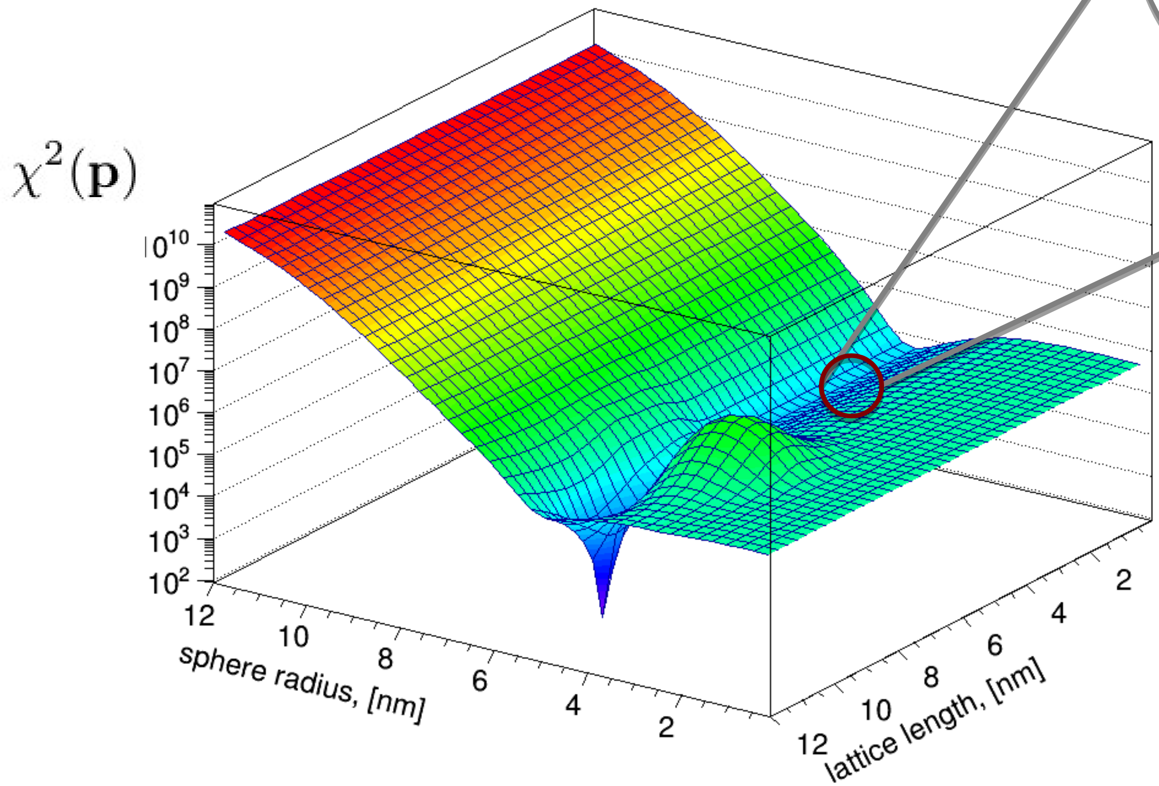


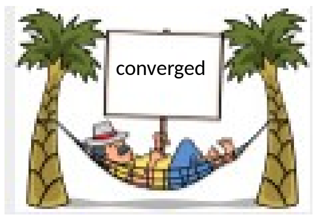
R=5nm
length=10nm



- Minimum of the function corresponds to optimal sample parameters

Objective function





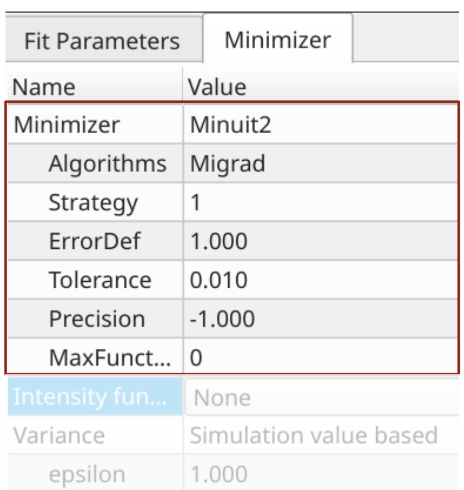
- Minimum of the function corresponds to optimal sample parameters

Available minimizers

GUI contains collection of minimizers from ROOT and GSL libraries

Two most useful

- Minuit2
- Genetic



Minimizer name	Algorithm	Description
Minuit2	Migrad	According to the tutorial, best minimizer for nearly all functions, variable-metric method with inexact line search, a stable metric updating scheme, and checks for positive-definiteness.
	Simplex	Simplex method of Nelder and Mead usually, slower than `Migrad`, rather robust with respect to gross fluctuations in the function value, gives no reliable information about parameter errors.
	Combined	Minimizes with `Migrad`, but switches to `Simplex` if `Migrad` fails to converge.
	Scan	Not intended to minimize, just scans the function, one parameter at a time, retains the best value after each scan.
	Fumili	Optimized method for least square and log likelihood minimizations.
GSLMultiMin	ConjugateFR	Fletcher-Reeves conjugate gradient algorithm.
	ConjugatePR	Polak-Ribiere conjugate gradient algorithm.
	BFGS	Broyden-Fletcher-Goldfarb-Shanno algorithm
	BFGS2	Improved version of `BFGS`.
	SteepestDescent	Follows the downhill gradient of the function at each step.
GSLLMA		Levenberg-Marquardt Algorithm
GSLSimAn		Simulated Annealing Algorithm
Genetic		Genetic Algorithm

Task

Fitting spheres at hexagonal lattice

~/talks/day_1/gui_basics_3_G

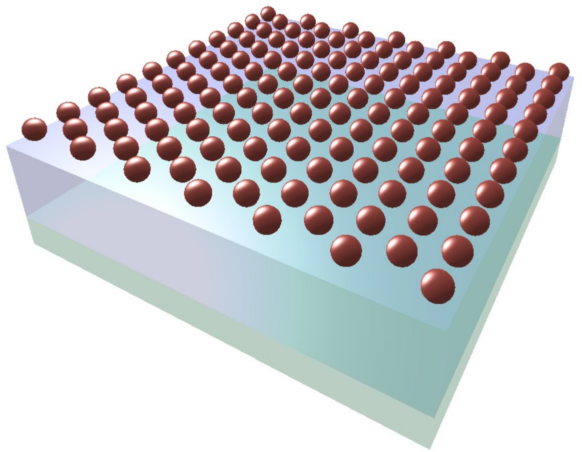
`SpheresAtHexLattice_task`

`experimental_data.txt.gz`

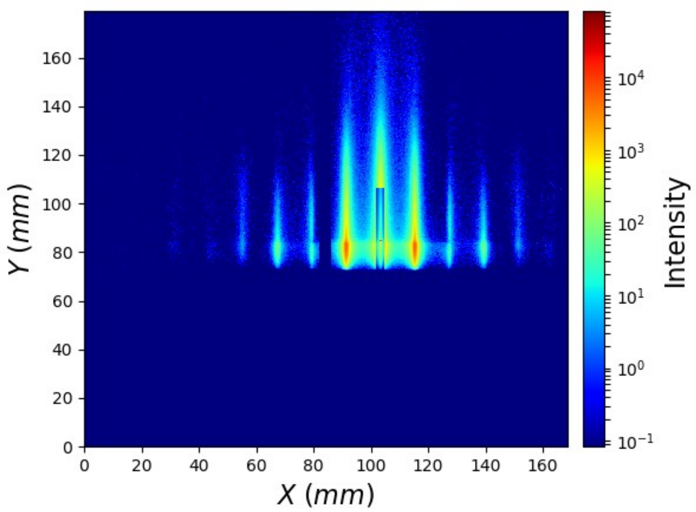
Spheres at hexagonal lattice

SpheresAtHexLattice_task
experimental_data.txt.gz

- 3 layers system, known materials
- Perfectly defined instrument
- Unknown lattice length and sphere radius, may be something else?



Expected sample structure



Experimental image

Task: simulate and fit experimental image

Start from opening GUI project and loading experimental file