

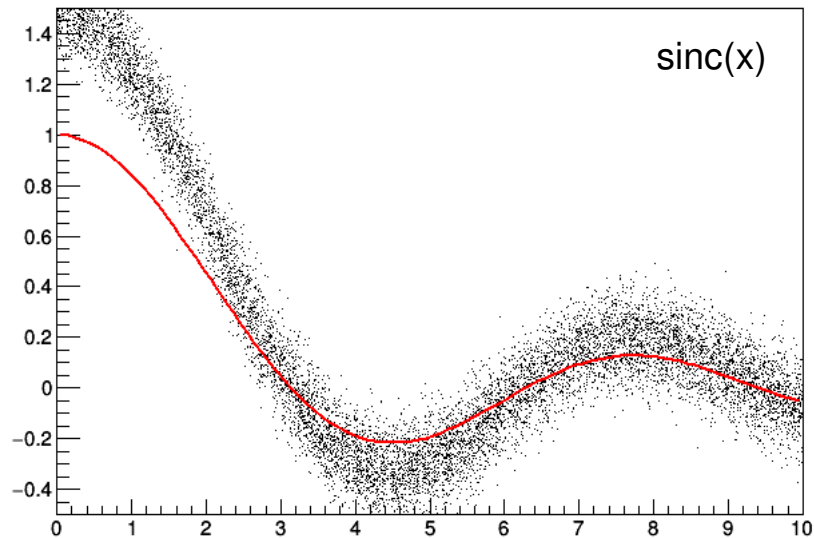
Fitting from BornAgain GUI

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GISAXS2019, BornAgain training session
Hamburg, November 2019

Basic concept

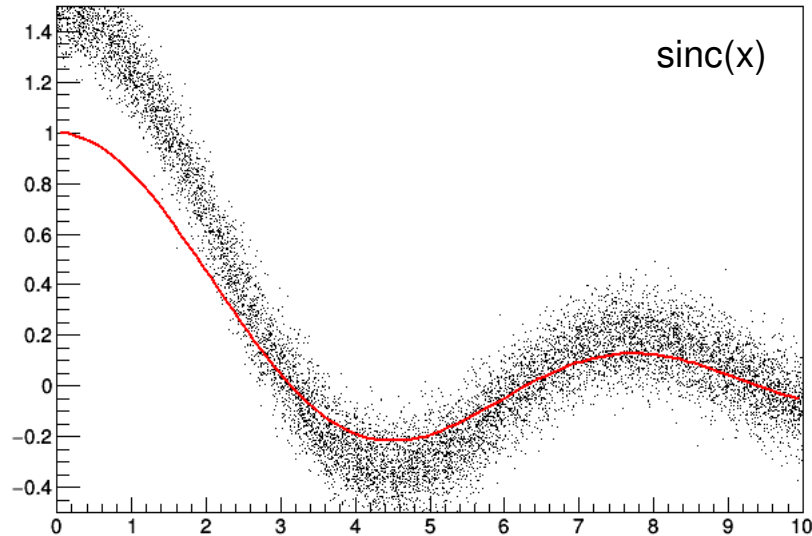
Finding the best set of parameter values for a model function to represent the data according to some criteria



Data	Set of (x,y) points
Model	$p_1 * \text{sinc}(p_2 * x)$
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



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Model	$p_1 * \text{sinc}(p_2 * x)$
Fit criteria	minimum of χ^2

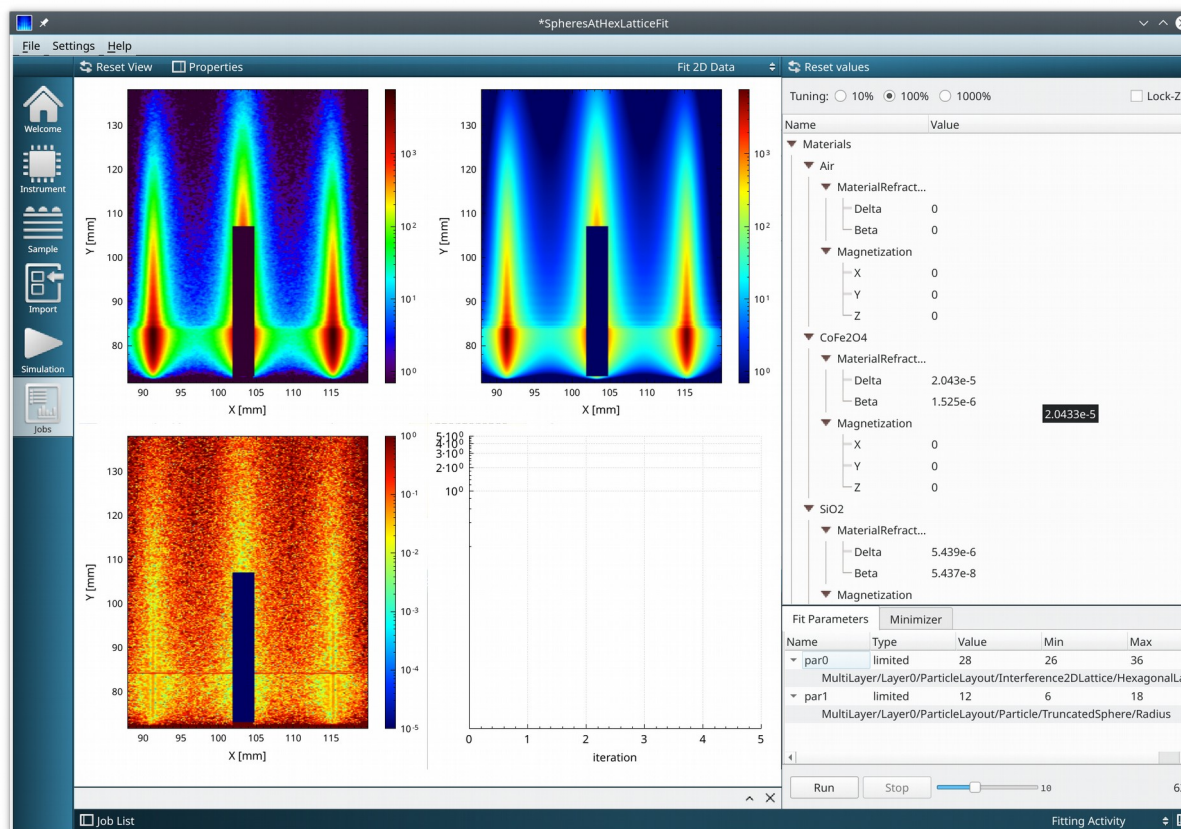
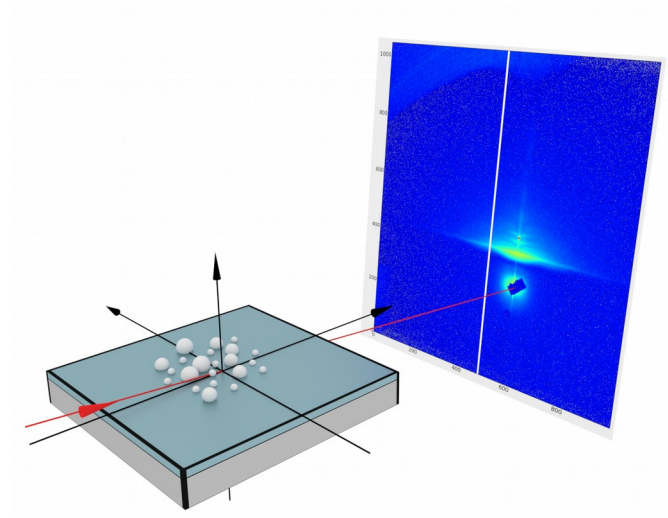
```
float objective_function(p1, p2):  
    foreach (x,y)  
        chi2 += (y - p1*sinc(p2*x))**2  
    return chi2
```



Minimizer

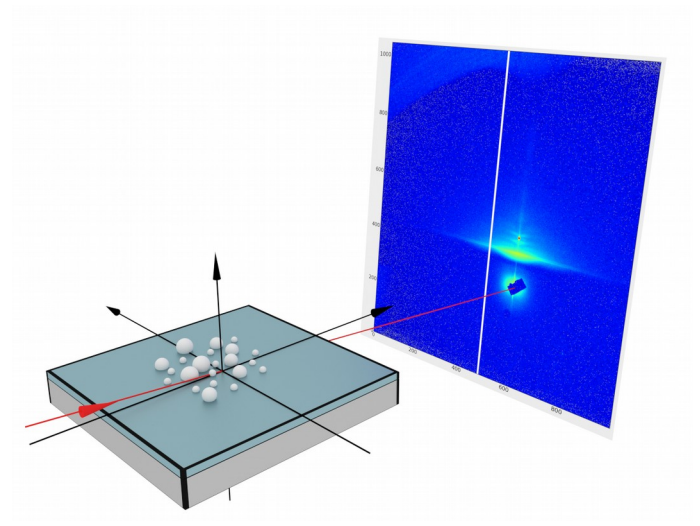
Fitting in BornAgain

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



Fitting in BornAgain

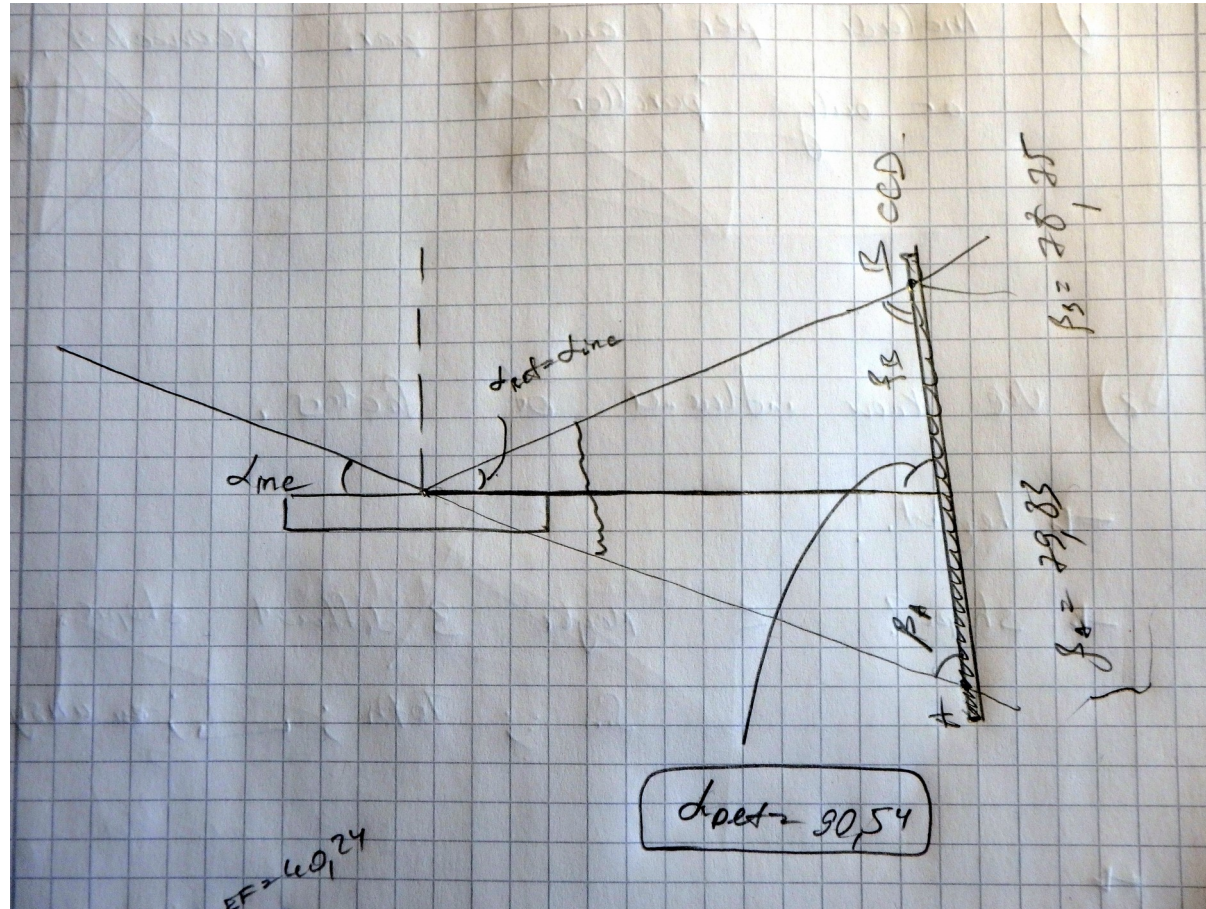
Finding the values of sample parameters that best represent the data obtained in scattering experiment



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 \mathbf{n} to the detector plane in sample coordinate system
- (u_0, v_0) of intersection of \mathbf{n} and the detector plane in local detector coordinates

Example: detector is perpendicular to direct beam

$n_{x\text{bins}} = 100$

width = 200 mm

$n_{y\text{bins}} = 100$

height = 180 mm

$\alpha_i = 0.2$ degree

distance = 2000 mm

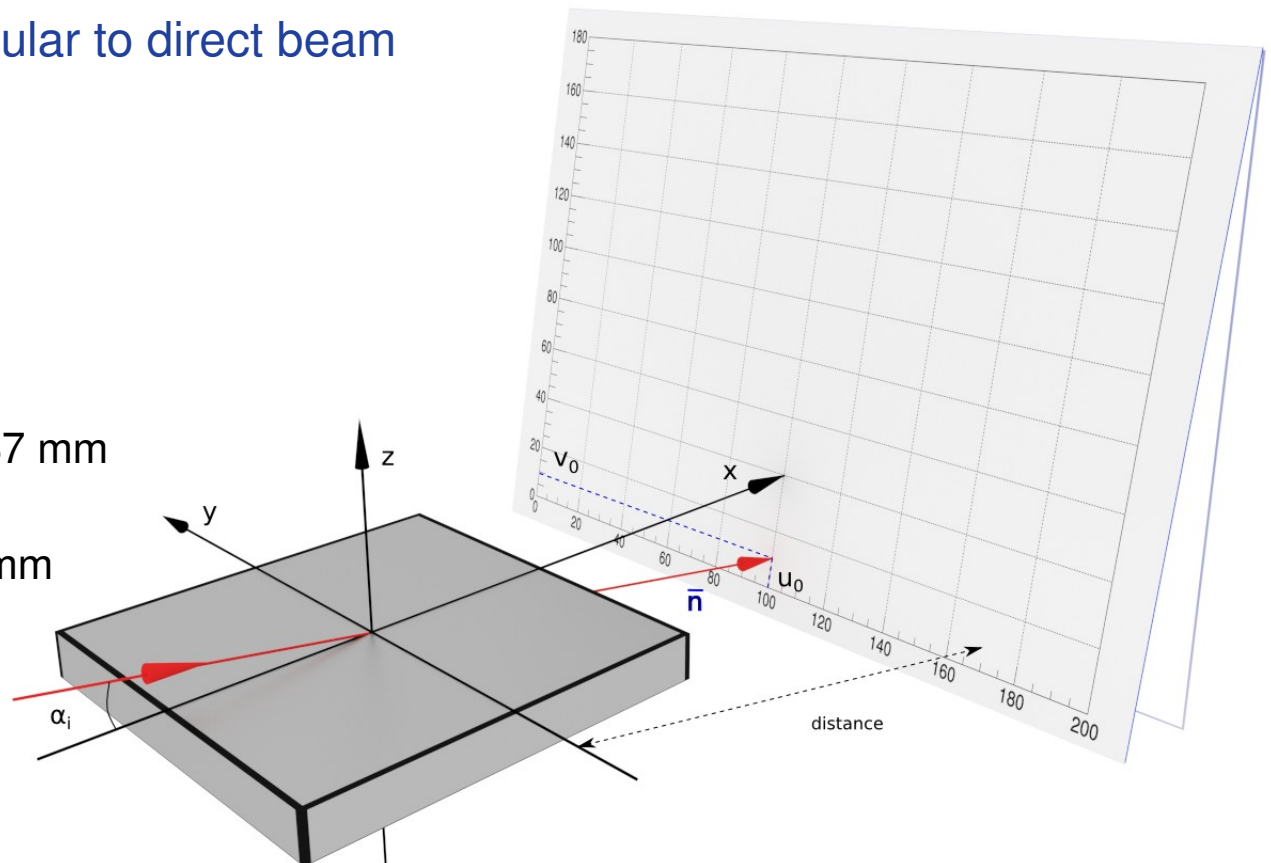
$n_x = \text{distance} \cdot \cos(\alpha_i) = 1999.987$ mm

$n_y = 0$

$n_z = -\text{distance} \cdot \sin(\alpha_i) = -6.981$ mm

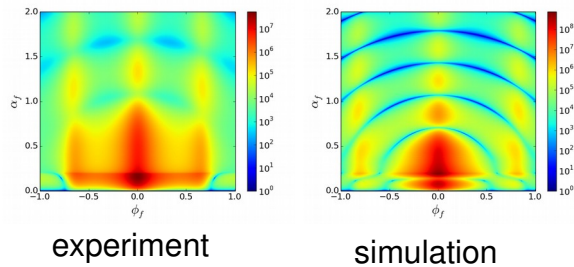
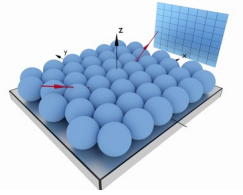
$u_0 = 100$ mm

$v_0 = 10$ mm



Objective function

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



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

*Sum over all unmasked
detector channels*

- Three options for intensity functions

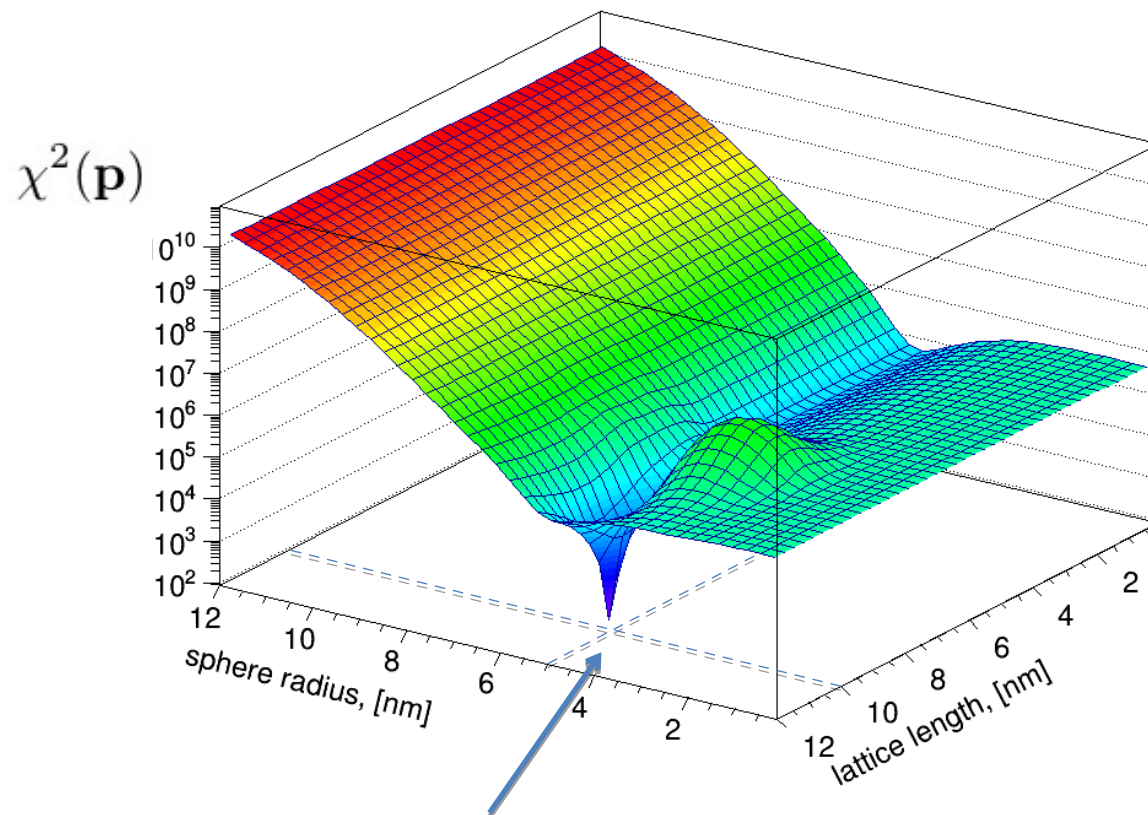
$$f(I) = I, \quad f(I) = \sqrt{I}, \quad f(I) = \log(I)$$

- Two options for residual error

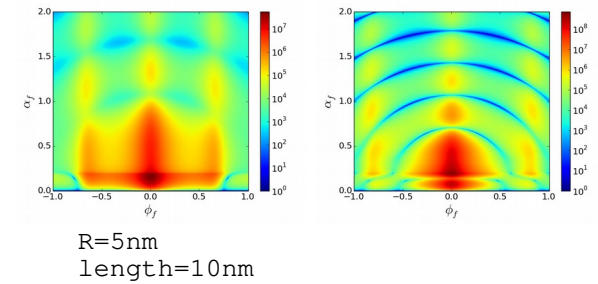
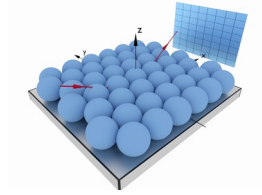
$$\sigma = 1, \quad \sigma = \sqrt{\max(\epsilon, f(I))}$$

Fit Parameters		Minimizer	
Name	Value		
Minimizer	Minuit2		
Algorithms	Migrad		
Strategy	1		
ErrorDef	1.000		
Tolerance	0.010		
Precision	-1.000		
MaxFunct...	0		
Intensity fun...	None		
Variance	Simulation value based		
epsilon	1.000		

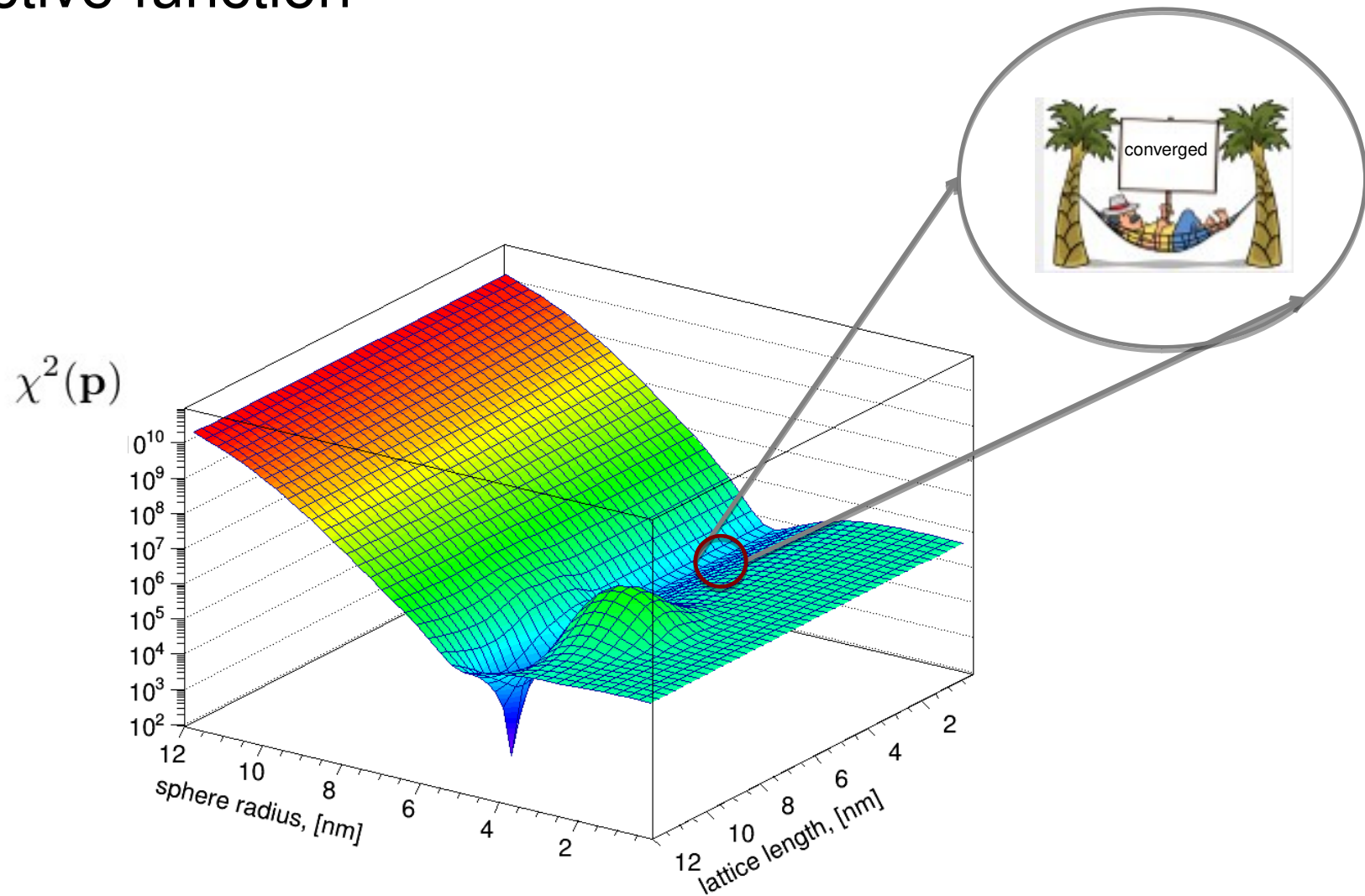
Objective function



- 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

Fit Parameters		Minimizer	
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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.
GSLLMMA		Levenberg-Marquardt Algorithm
GSLSimAn		Simulated Annealing Algorithm
Genetic		Genetic Algorithm

Task

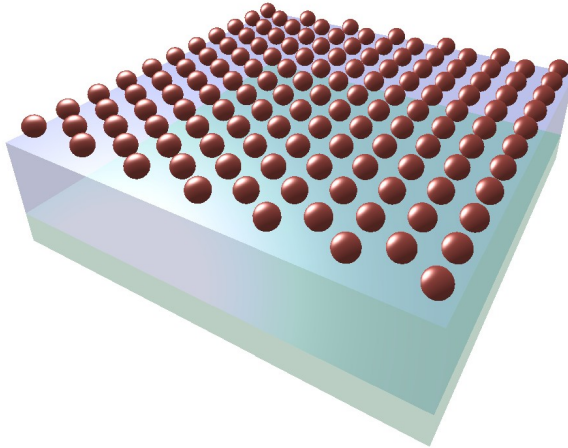
Fitting spheres at hexagonal lattice

`SpheresAtHexLattice_task`
`experimental_data.txt.gz`

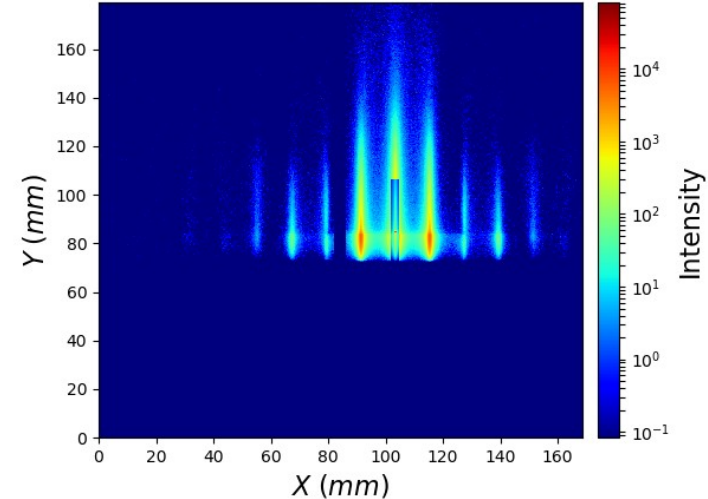
Spheres at hexagonal lattice

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