Welcome to SasView

(Pre)hackthon introduction to coding in SasView

Wojtek Potrzebowski (ESS)

Paul Butler (NIST)

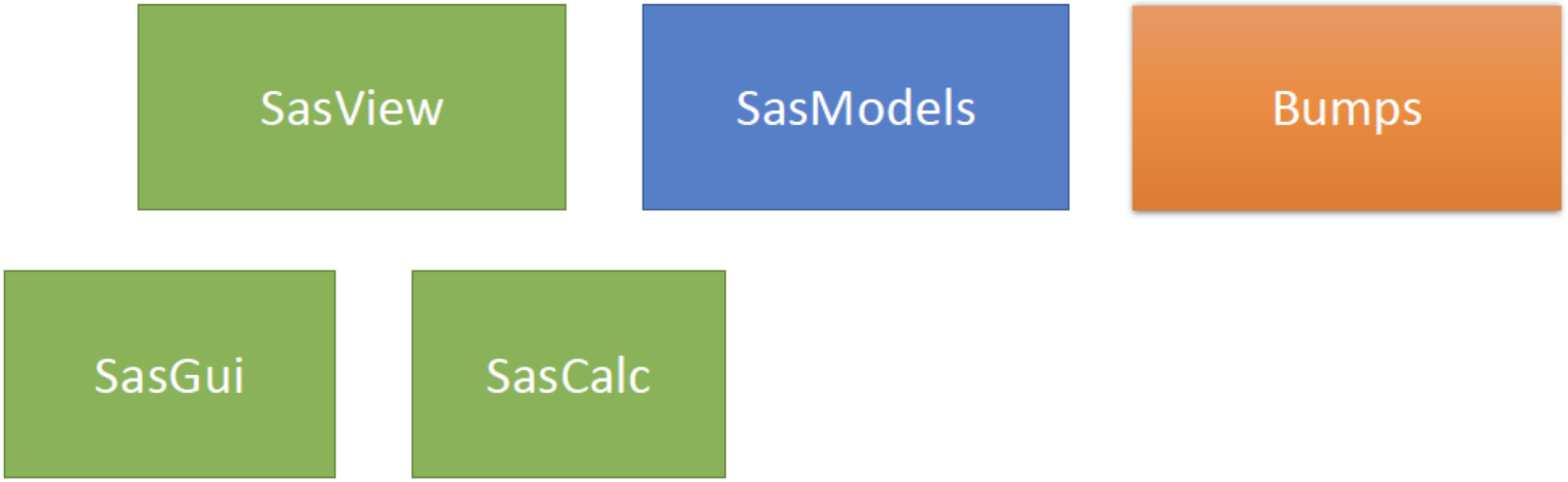
Outline

- Hacktahon Goals
- Build system
- Code overview
- Writing tests
- Build system
- Model Marketplace

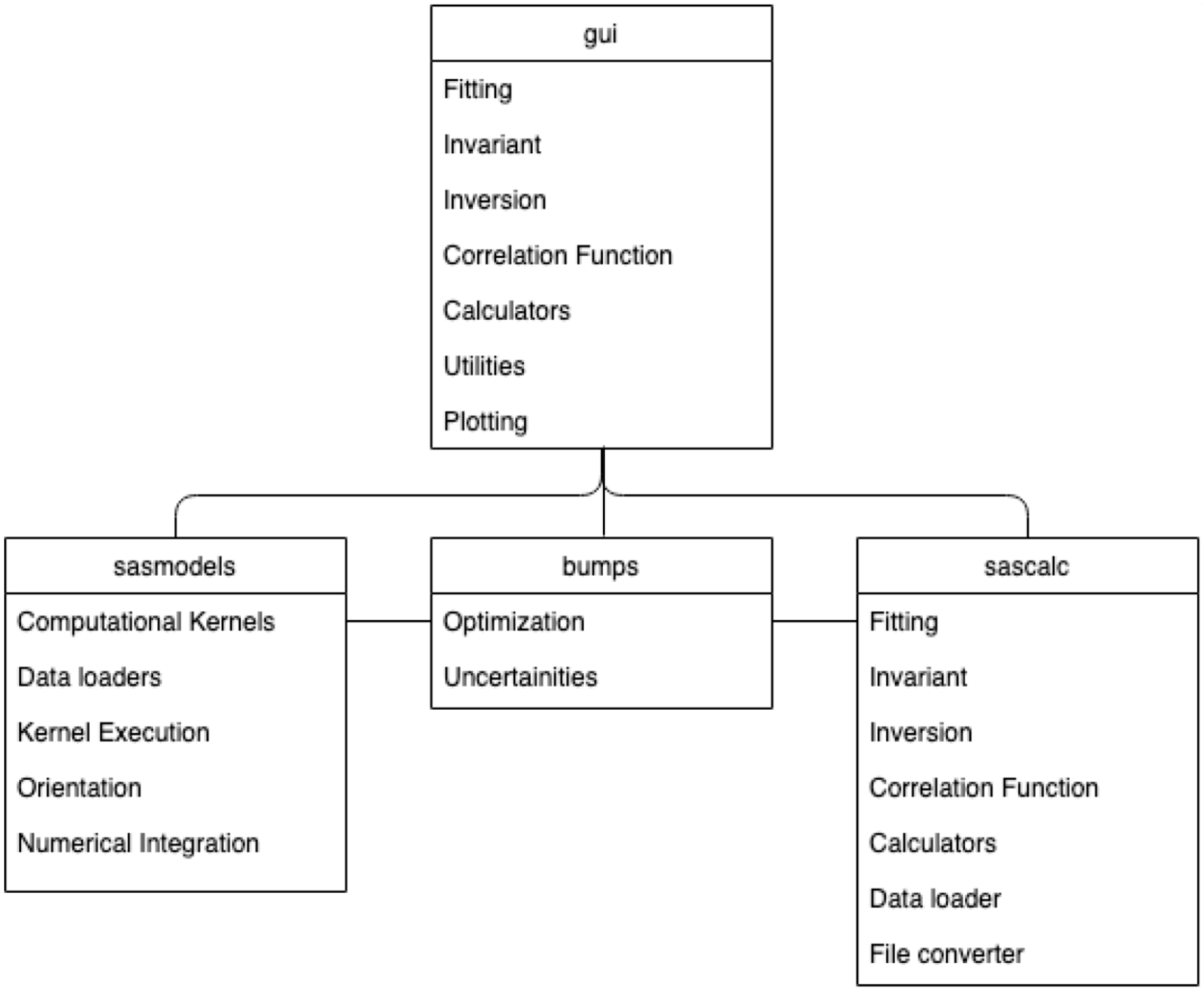
Goals for hackathon

- Jan 13-15
- Improving SasView5 functionality and user experience
- Making SasView5 ready for NCNR ”summer” school
- ”Non-functional” tasks
  - Continuous integration
  - Model Marketplace
  - Calculation engine separation
- Have some fun

SasView Architecture

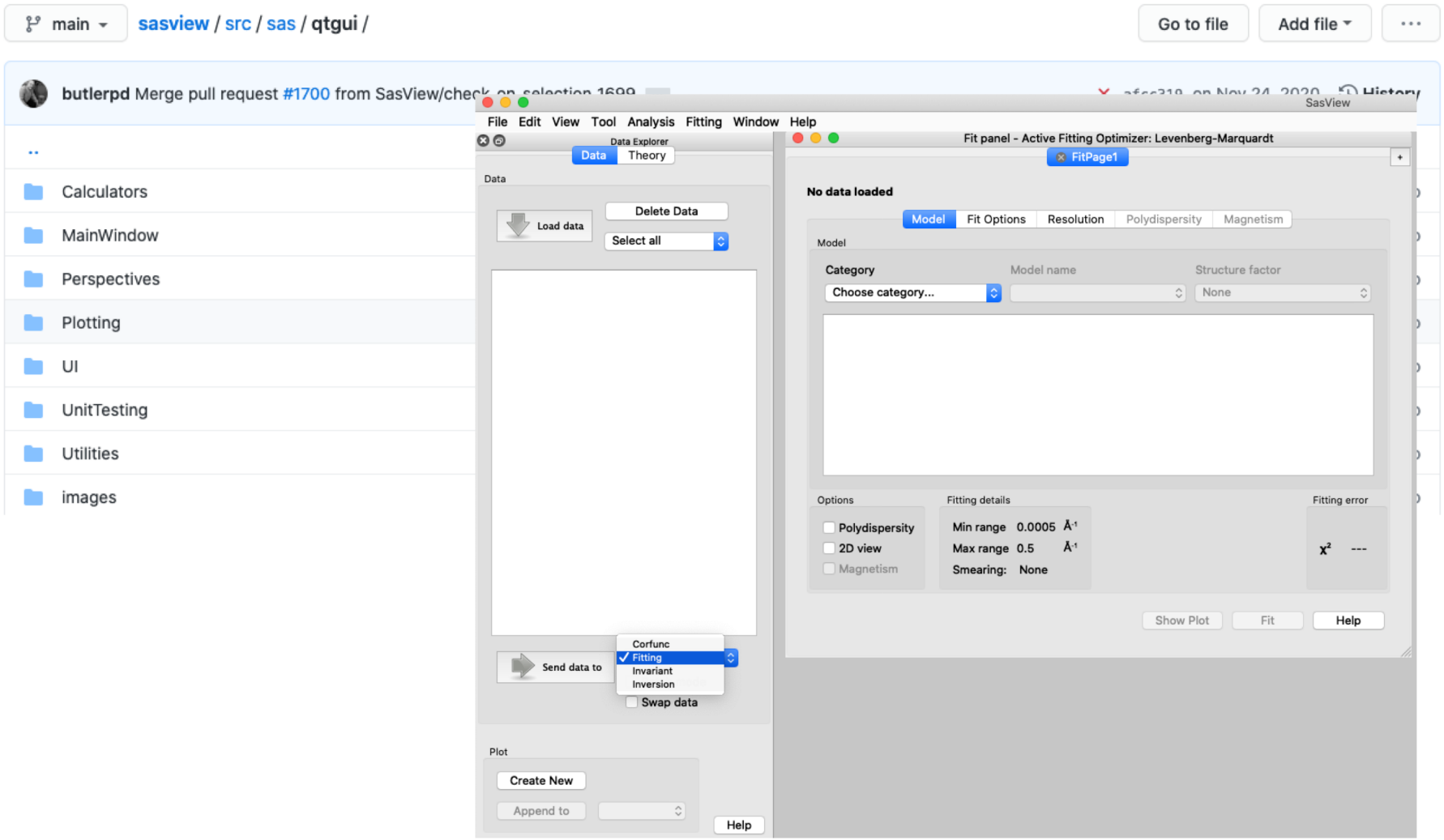


SasView Arhcitecture



SasGUI (qtgui)

Note: we are using **main** branch not **master**!



SasGUI Invariant Perspective

main ▾ **sasview** / src / sas / qtgui / Perspectives / **Invariant** /

krzywon Plot any corfunc and invariant plots when loading projects. Enable co... ...

..	
UI ← Qt UI definitions	Addressing review findings on PR #1590 (plus new problems found)
UnitTesting ← Unit tests	Fix failing unit tests
media ← Images Doc files	Tweaks and cleanups in 5.x invariant_help
InvariantDetails.py	Addressing review findings on PR #1590 (plus new problems found)
InvariantPerspective.py	Plot any corfunc and invariant plots when loading projects. Enable co...
InvariantUtils.py	Replace all(?) references to filename when display name is more appro...
__init__.py	Initial commit of the main window prototype

Slicer code

main ▾ sasview / src / sas / qtgui / Plotting / Go to file Add file ▾ ···

murphyryanp Merge pull request #1567 from SasView/ESS_GUI_1554_slicer 80bcf85 on Jun 2, 2020 History

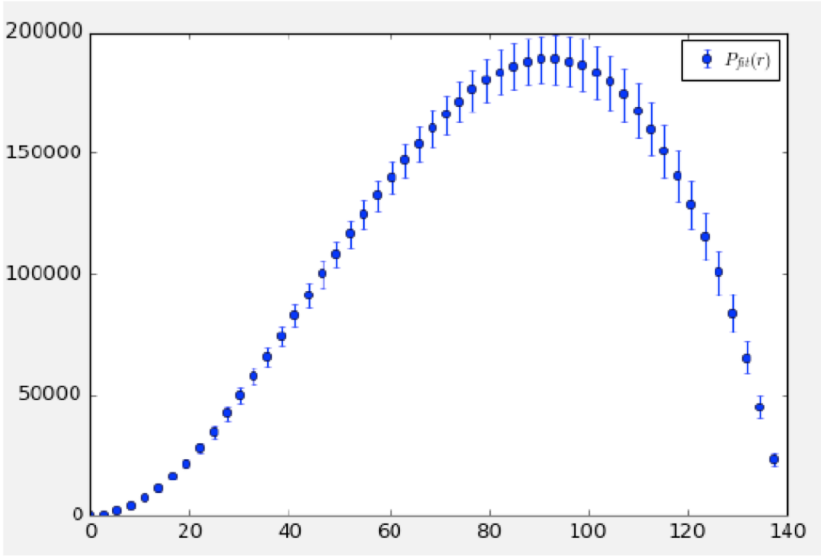
..		
Masks	Fix for 2D masking - SASVIEW-1361	14 months ago
Slicers	Updated AnnulusSlicer to improve slicer min limits (low-q 2D data) an...	8 months ago
UI		
UnitTe		
AddTe		
Arrow		
Binder		
BoxSu		
MaskEditor.py	Replace Apply button menu driven functionality with additional button.	2 years ago
PlotHelper.py	cherry picking sascalc changes from master SASVIEW-996	2 years ago
PlotProperties.py	Replace Apply button menu driven functionality with additional button.	2 years ago
PlotUtilities.py	Improved line colour handling for 1D data charts.	2 years ago
Plottables.py	Fixed erroneous error bars. SASVIEW-994	2 years ago
Plotter.py	Added context menu item for legend toggle, for quick and regular 1D	8 months ago
Plotter2D.py ←	Merge pull request #1567 from SasView/ESS_GUI_1554_slicer	7 months ago
PlotterBase.py	Added/modified unit tests	8 months ago
PlotterData.py	Added plot roles to Data1D/Data2D structures to allow for smoother pl...	2 years ago
ScaleProperties.py	Replace Apply button menu driven functionality with additional button.	2 years ago
SetGraphRange.py	Replace Apply button menu driven functionality with additional button.	2 years ago
SlicerModel.py ←	Updating annulus slicer, batch slicing, and slicer parameters	8 months ago
SlicerParameters.py ←	Removed the batch slicing tab and associated widgets	8 months ago
WindowTitle.py	Replace Apply button menu driven functionality with additional button.	2 years ago
__init__.py	cherry picking sascalc changes from master SASVIEW-996	2 years ago
rangeSlider.py	Remove copyright header from docstring	13 months ago

SasCalc

- Back-end calculations for sasgui perspective
- Data fitting:
  - src/sas/sascalc/fit/
- Pr inversion
  - src/sas/sascalc/pr/
- Data loader: src/sas/sascalc/dataloader/loader.py

SasCalc

```
from sas.sascalc.dataloader.loader import Loader
from sas.sascalc.pr.invertor import Invertor

loader = Loader()
test_data = loader.load("sphere_80.txt")

pr = Invertor()

# Set data
pr.x   = test_data.x
pr.y   = test_data.y

# Perform inversion and show graph
x, y = pr.invert()

import matplotlib.pyplot as plt
plt.plot(x, y)
plt.show()
```



And more at: https://github.com/SasView/documents/blob/master/Meetings/User_Meeting_2018/SasView%2BCLI%2Boverview.html

SasModels

- Models located in: sasmodels/models
- Three different types of models:
  - Python only: broad_peak.py
  - Python with embedded C: stickyhardsphere.py
  - Python and separate C: barbell.py and barbell.c

SasModels essential components

- Model Description: Docstring
- Name, title, short description
- Parameters table
- C files to be included during compilation
- Unit tests

SasModels functions

- Iq - 1D scattering intensity functions for the case where the scattereris randomly oriented
- Iqxy - the 2D scattering intensity functions provide I(Q,ϕ) for an oriented system as a function of a Q
- Form_volume - calculates the volume of particle V, which is used tonormalize form factor.
- ER – calculates effective radius
- VR - calculate particle volume/total volume for shape models
- INVALID(v) returns False if v.parameter is invalid for some parameter or other (e.g., v.bell_radius < v.radius).

SasModels core modules

- Model computation:
  - sasmodels/sasview_model.py – interface to sasview
  - sasmodels/kernel.py -interface to all kernel models
  - sasmodels/kerneldll.py –dll driver for c kernels
  - sasmodels/kernelpy.py – python driver
  - sasmodels/kernelcl.py – opencl driver
  - sasmodels/core.py - prepares the model for the execution
  - sasmodels/generate.py – generates model file based on the template

Running bumps with sasmodels

- Sasmodels example contains data set for oriented rod-like shape
- sasmodels/examples/fit.py (sasmodels interface to bumps)
- Running
  - bumps fit.py cylinder –preview
  - Fit.py accepts two arguments: type of model and view (radial and tnagential)

Custom settings

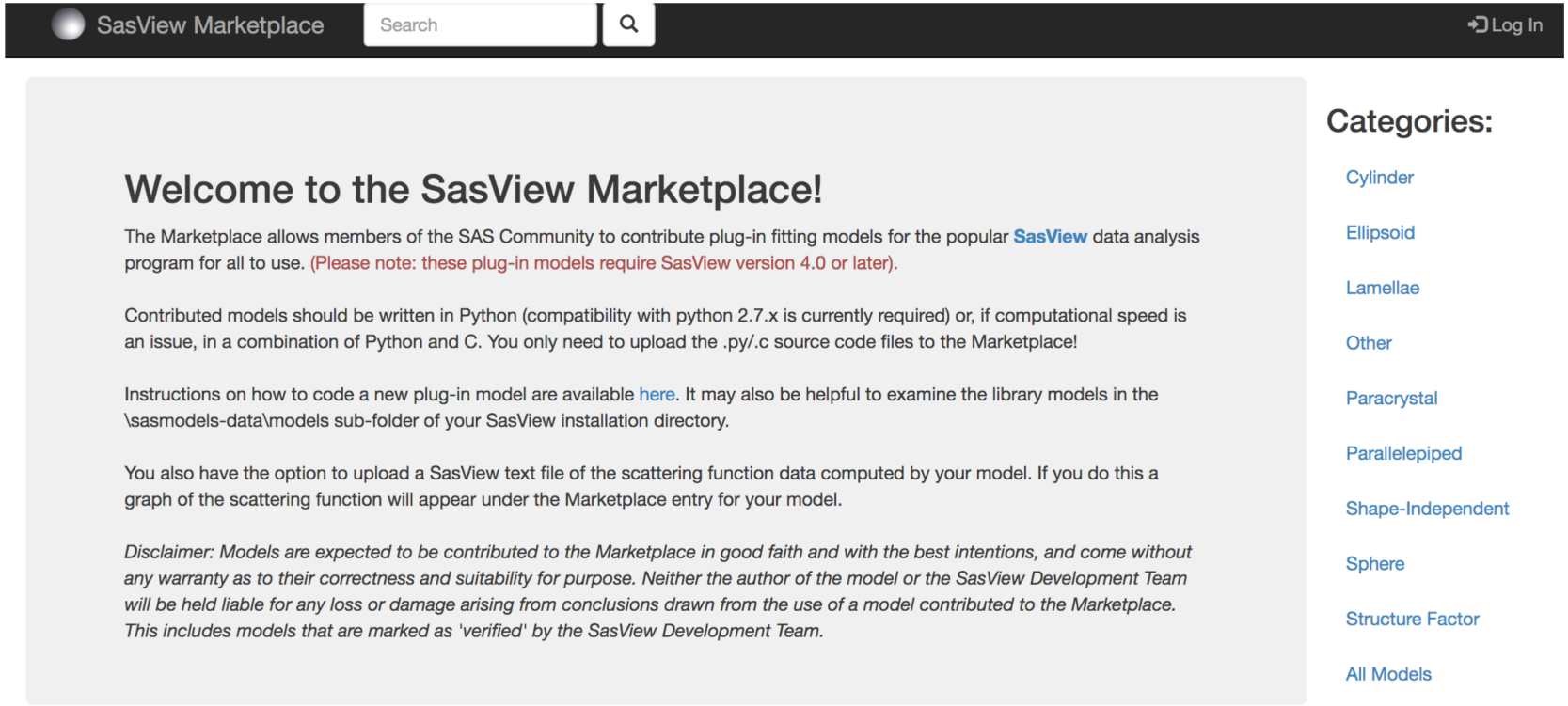
- Local configuration
  - ~/.sasview/config/custom_config.py
- Compiled sasmodels
  - ~/.sasview/compiled_models/
- Plugin models:
  - ~/.sasview/plugin_models/
- Model categories:
  - ~/.sasview/categories.json

Unit, GUI, sasmodels tests

- For sasview core, tests are located in sasview/test.
  - Tests are stored in subdirectories of the test directory, as *package/test/utest_*.py*.
  - Other files in the test subdirectory are data, expected output and other support files.
  - Before running any tests you must first run *setup.py build* in the root.
  - Tests are run against the current source directory with run magic to find the compiled code, so you only need to rebuild between tests if you are modifying the C code.
- For GUI, tests are located in respective folders e.g for Fitting sasview/src/sas/qtgui/Perspectives/Fitting/UnitTesting/.
  - For this part we use unit test with MagickMock (for general introduction please refer to https://www.thedigitalcatonline.com/blog/2016/03/06/python-mocks-a-gentle-introduction-part-1/ and https://aaronlelevier.github.io/python-unit-testing-with-magicmock/)
- For sasmodels tests are part of model definition (see https://github.com/SasView/sasmodels/blob/master/doc/guide/plugin.rst#test-your-new-model)

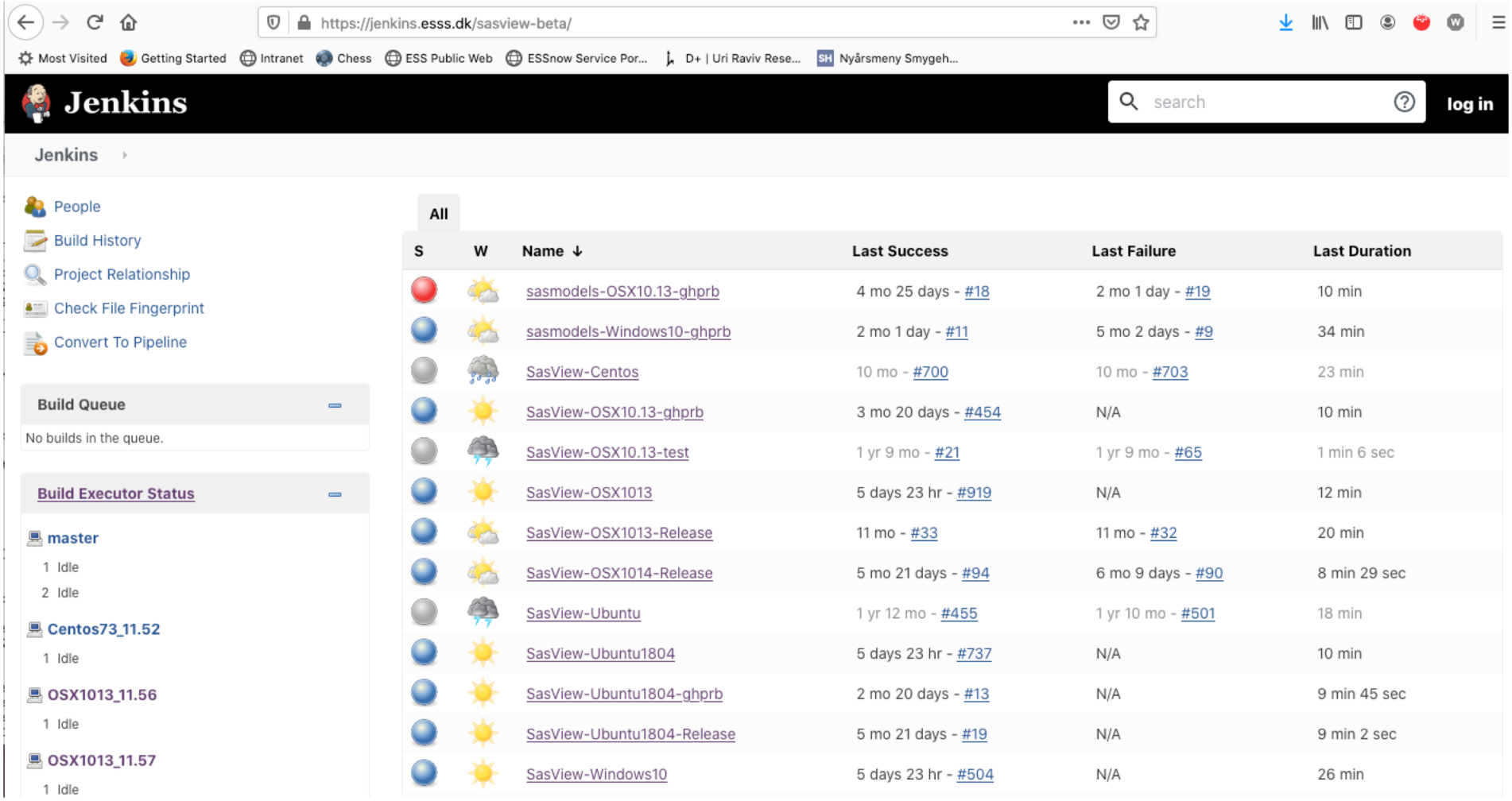
More about tests: https://github.com/SasView/sasview/wiki/DevNotes_DevGuide_CodeTesting

Model marketplace



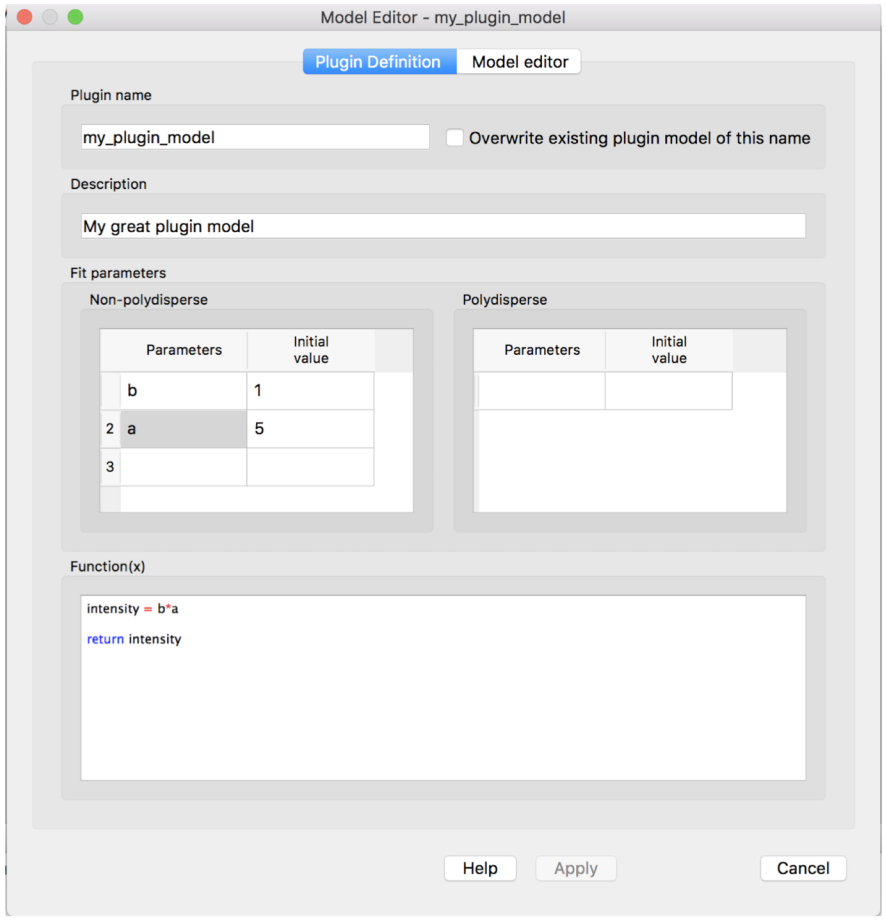
It is **python 2.7**…

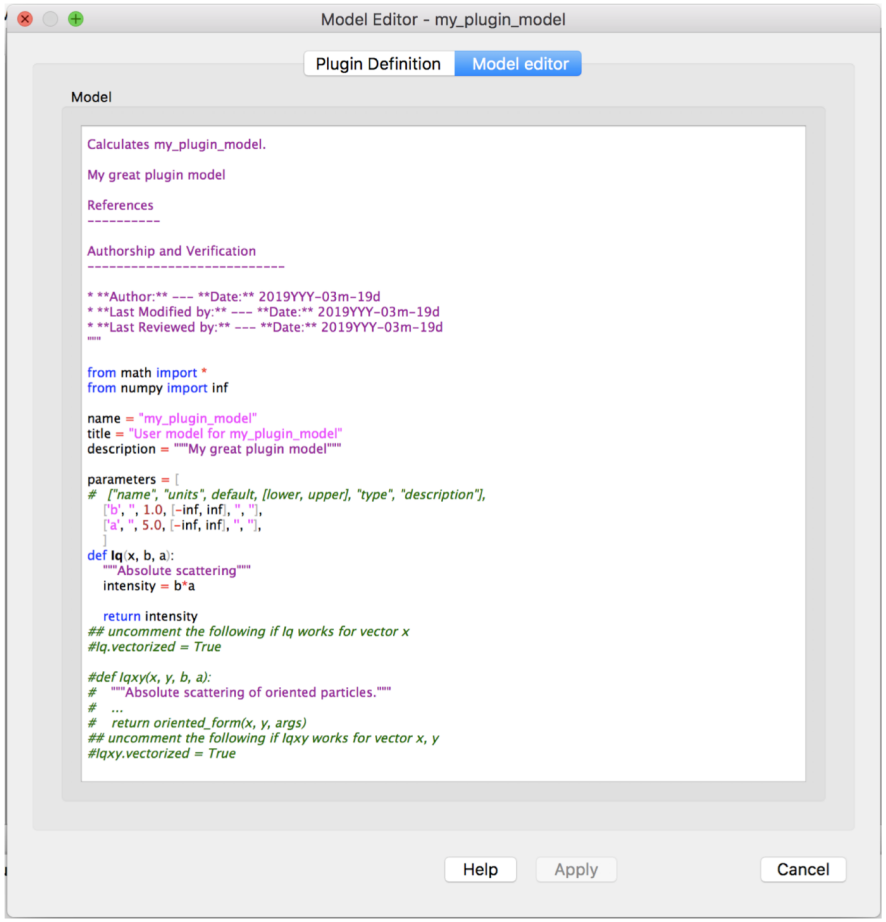
Build system



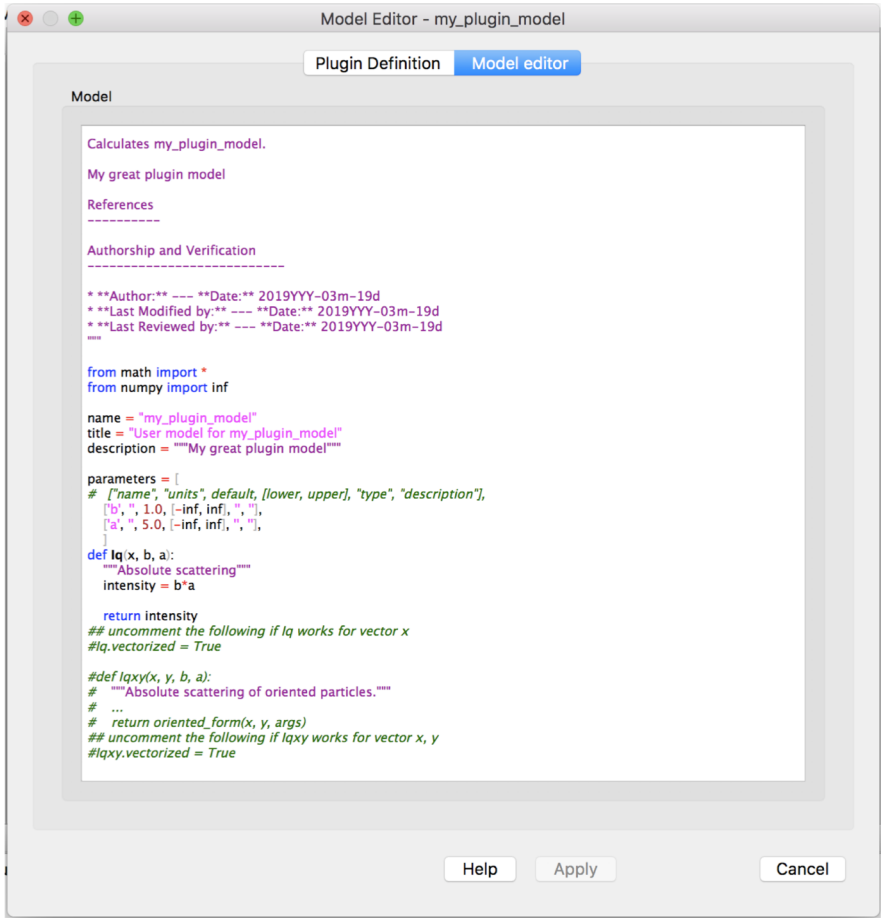
Becoming more and more difficult to maintain -> Github actions!

Plugin model editor (Fitting->Add Custom Model)





Python and C files



cylinder.c

```c
#define INVALID(v) (v.radius<0 || v.length<0)

static double
form_volume(double radius, double length)
{
    return M_PI*radius*radius*length;
}

static double
fq(double qab, double qc, double radius, double length)
{
    return sas_2J1x_x(qab*radius) * sas_sinx_x(qc*0.5*length);
}

static double
orient_avg_1D(double q, double radius, double length)
{
    // translate a point in [-1,1] to a point in [0, pi/2]
    const double zm = M_PI_4;
    const double zb = M_PI_4;

    double total = 0.0;
    for (int i=0; i<GAUSS_N ;i++) {
        const double theta = GAUSS_Z[i]*zm + zb;
        double sin_theta, cos_theta; // slots to hold sincos function output
        // theta (theta,phi) the projection of the cylinder on the detector plane
        SINCOS(theta , sin_theta, cos_theta);
        const double form = fq(q*sin_theta, q*cos_theta, radius, length);
        total += GAUSS_W[i] * form * form * sin_theta;
    }
    // translate dx in [-1,1] to dx in [lower,upper]
    return total*zm;
}

static double
Iq(double q,
    double sld,
    double solvent_sld,
    double radius,
    double length)
{
    const double s = (sld - solvent_sld) * form_volume(radius, length);
    return 1.0e-4 * s * s * orient_avg_1D(q, radius, length);
}
```

Category manager (View->Category Manager)