Documenting

SasView

UT NIST ISIS diamond OAK RIDGE National Laboratory ILL NEUTRONS FOR SCIENCE ess Ansto TU Delft

SasView
‘documentation’
comes in many
forms…

SasView 5.0.5

File Edit View Tool Analysis Fitting Window Help

Documentation
Tutorial
Model Marketplace
Acknowledge
About
Welcome to SasView
Check for update

Data Explorer

Data Theory

Data

Load data | Delete Data | Select all

Ludox 1mm M4 TRANS_SANS

Send data to | Fitting | Batch mode | Swap data

Plot

Create New | Append to | Graph1 | Help

timizer: DREAM

n M4 TRANS_SANS

olution | Polydispersity | Magnetism

Model name: sphere | Structure factor: hayter_msa

Parameter	Value	Error	Min	Max	Units
scale	1		0.0	∞	
background	0.86891	0.0042623	-∞	∞	cm^{-1}
structure_factor_mode	P*S				
radius_effective_mode	radius				
sphere					
sld	3		-∞	∞	$10^{-6}/Å^2$
sld_solvent	6.3		-∞	∞	$10^{-6}/Å^2$
radius	158.27	0.11678	0.0	∞	Å
Polydispersity					
Distribution	0.10374	0.00043217			lognormal
hayter_msa					
radius_effective	159.12		0.0	∞	Å
volfraction	0.46723	0.00067104	0.0	0.74	None
charge	3.6438	0.23768	1e-06	200.0	e
temperature	298		0.0	450.0	K
concentration_salt	0.0		0.0	∞	M
dielectconst	78		-∞	∞	None

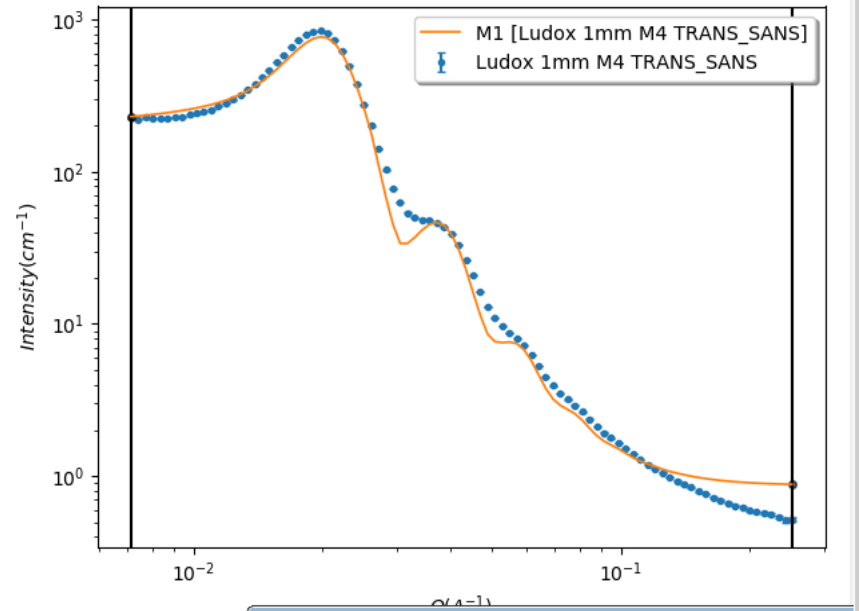
Options: Polydispersity, Magnetism

Fitting details: Min range 0.00714 $Å^{-1}$, Max range 0.25169 $Å^{-1}$, Smearing: Use dQ Data

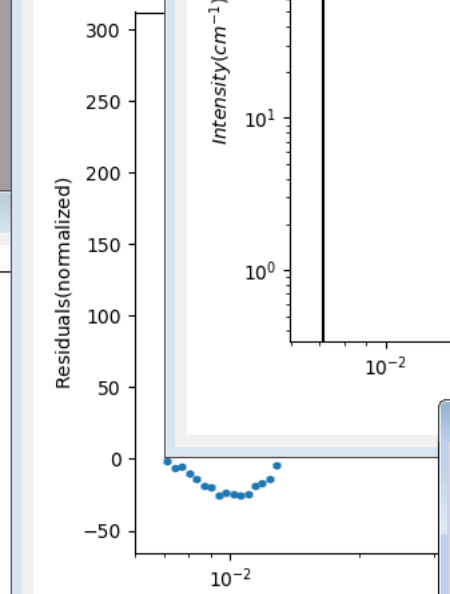
Fitting error: χ^2 6657.1

Compute/Plot | Fit | Help

Graph1



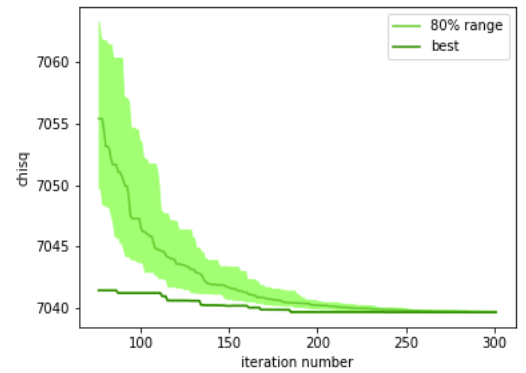
Graph2



Graph3

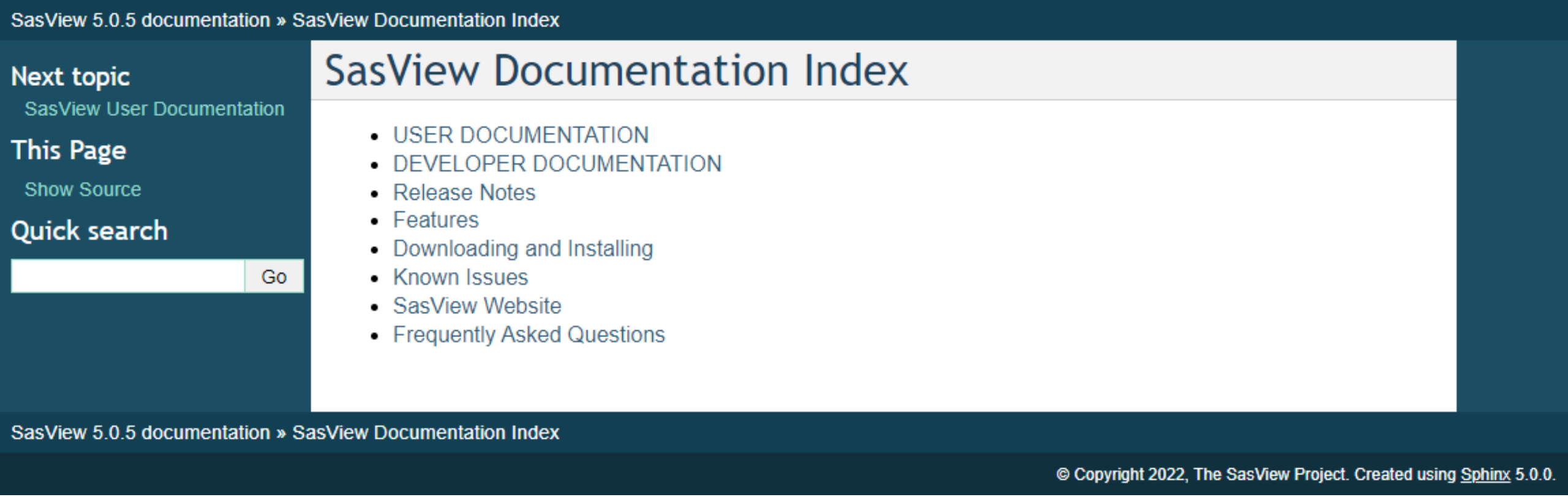
Result panel - Ludox_silica.xml - DREAM

Convergence | Correlation | Uncertainty | Parameter Trace



Log Explorer

M1.background: 0.869 | M1.charge: 3.64 | M1.radius: 158
M1.radius.width: 0.104 | M1.volfraction: 0.467 |
22:15:07 - INFO: 2022-06-09 22:15:07 === Steps: 301 of 300 chisq: 7.04e+03 ETA: 0s
M1.background: 0.869 | M1.charge: 3.64 | M1.radius: 158
M1.radius.width: 0.104 | M1.volfraction: 0.467 |



USER DOCUMENTATION:

- ★★ Fitting model descriptions ★★
- How to use SasView
- 'Encyclopedia content'

DEVELOPER DOCUMENTATION:

- Is mostly auto-generated
- Lists of program modules/classes
- Overview of Sasmodels

Available in-program and online – but single-source

C:/SasView-5.0.5/doc/index.html & https://www.sasview.org/docs/index.html

USER DOCUMENTATION:

- Is written in ReSTructured text (.rst)
- Lightweight, portable, human-readable, but also software-processable
- Supports LaTeX-like math

```
Invariant
^^^^^^^^^
SasView implements the invariant calculation for a two-phase (or pseudo
two-phase) system, which represents the most commonly encountered situation.
The invariant for this is

.. math::

    Q^* = {2 \pi^2 (\Delta\rho)^2 \phi_1 \phi_2}

where $\Delta\rho = (\rho_1 - \rho_2)$ is the SLD contrast and $\phi_1$ and
$\phi_2$ are the volume fractions of the two phases ($\phi_1 + \phi_2 = 1$).
Thus from the invariant one can either calculate the volume fractions of the
two phases given the contrast or, calculate the contrast given the volume
fraction. However, the current implementation in SasView only allows for the
former: extracting the volume fraction given a known contrast factor.
```

invariant_help.rst

Keep lines to ≤80 characters

Do not end lines with whitespace! It upsets 'linters'

We then use SPHINX PYTHON DOCUMENTATION GENERATOR to autoconvert the .rst to the desired output (.html, .pdf, …)

```
r"""
For information about polarised and magnetic scattering, see
the :ref:`magnetism` documentation.

Definition
----------

The 1D scattering intensity is calculated in the following way (Guinier, 1955)

.. math::

    I(q) = \frac{\text{scale}}{V} \cdot \left[
        3V(\Delta\rho) \cdot \frac{\sin(qr) - qr\cos(qr)}{(qr)^3}
        \right]^2 + \text{background}

where *scale* is a volume fraction, $V$ is the volume of the scatterer,
$r$ is the radius of the sphere and *background* is the background level.
*sld* and *sld_solvent* are the scattering length densities (SLDs) of the
scatterer and the solvent respectively, whose difference is $\Delta\rho$.

Note that if your data is in absolute scale, the *scale* should represent
the volume fraction (which is unitless) if you have a good fit. If not,
it should represent the volume fraction times a factor (by which your data
might need to be rescaled).

The 2D scattering intensity is the same as above, regardless of the
orientation of $\vec q$.

Validation
----------

Validation of our code was done by comparing the output of the 1D model
to the output of the software provided by the NIST (Kline, 2006).


References
----------

#. A Guinier and G. Fournet, *Small-Angle Scattering of X-Rays*,
   John Wiley and Sons, New York (1955)

Authorship and Verification
---------------------------

* **Author:**
* **Last Modified by:**
* **Last Reviewed by:** S King and P Parker **Date:** 2013/09/09 and 2014/01/06
"""

import numpy as np
from numpy import inf

name = "sphere"
title = "Spheres with uniform scattering length density"
description = """\
P(q)=(scale/V)*[3V(sld-sld_solvent)*(sin(qr)-qr cos(qr))
                /(qr)^3]^2 + background
    r: radius of sphere
    V: The volume of the scatter
    sld: the SLD of the sphere
    sld_solvent: the SLD of the solvent
"""
category = "shape:sphere"

#             ["name", "units", default, [lower, upper], "type","description"],
parameters = [["sld", "1e-6/Ang^2", 1, [-inf, inf], "sld",
               "Layer scattering length density"],
              ["sld_solvent", "1e-6/Ang^2", 6, [-inf, inf], "sld",
               "Solvent scattering length density"],
              ["radius", "Ang", 50, [0, inf], "volume",
               "Sphere radius"],
             ]

source = ["lib/sas_3j1x_x.c", "sphere.c"]
have_Fq = True
radius_effective_modes = ["radius"]
#single = False
```

sphere.py

Previous topic
raspberry
Next topic
spherical_sld
This Page
Show Source
Quick search
Go

sphere

Spheres with uniform scattering length density

Parameter	Description	Units	Default value
scale	Scale factor or Volume fraction	None	1
background	Source background	cm^{-1}	0.001
sld	Layer scattering length density	$10^{-6}Å^{-2}$	1
sld_solvent	Solvent scattering length density	$10^{-6}Å^{-2}$	6
radius	Sphere radius	Å	50

The returned value is scaled to units of cm^{-1} sr^{-1}, absolute scale.

For information about polarised and magnetic scattering, see the Polarisation/Magnetic Scattering documentation.

Definition

The 1D scattering intensity is calculated in the following way (Guinier, 1955)

$$I(q) = \frac{\text{scale}}{V} \cdot \left[3V(\Delta\rho) \cdot \frac{\sin(qr) - qr\cos(qr))}{(qr)^3}\right]^2 + \text{background}$$

where *scale* is a volume fraction, V is the volume of the scatterer, r is the radius of the sphere and *background* is the background level. *sld* and *sld_solvent* are the scattering length densities (SLDs) of the scatterer and the solvent respectively, whose difference is $\Delta\rho$.

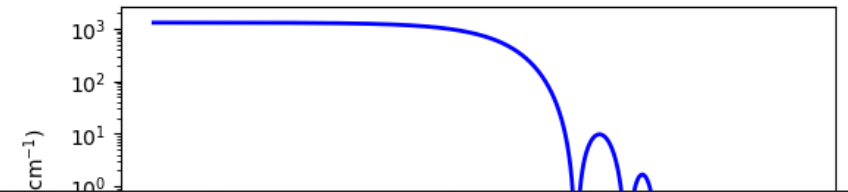
Note that if your data is in absolute scale, the *scale* should represent the volume fraction (which is unitless) if you have a good fit. If not, it should represent the volume fraction times a factor (by which your data might need to be rescaled).

The 2D scattering intensity is the same as above, regardless of the orientation of $\vec{q}$.

Validation

Validation of our code was done by comparing the output of the 1D model to the output of the software provided by the NIST (Kline, 2006).

Figure autogenerated from the default model parameters



BUILDING THE DOCUMENTATION:

- The *full* documentation comprises that from *Sasmodels* plus that from *SasView*, so **if you want the model descriptions you must build the *Sasmodels* documentation first!**

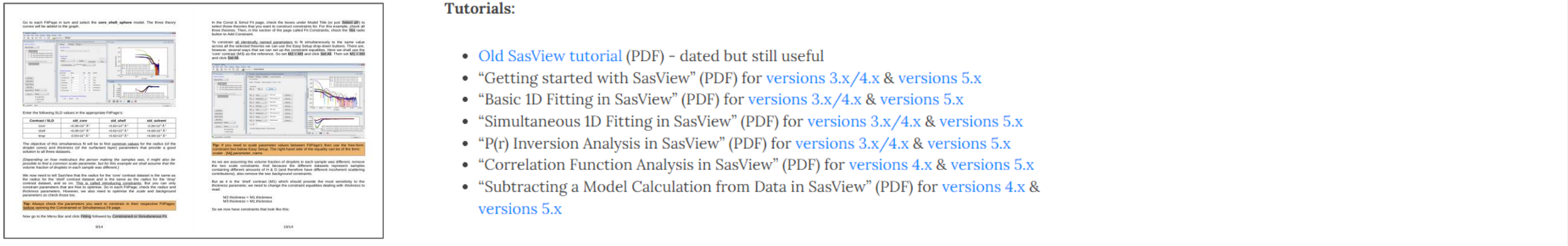
```
> cd <sasmodels_installation_folder>\doc
> make clean html
```

then

```
> cd <sasview_installation_folder>\doc
> python setup.py build install          (only if you have not already built SasView)
> python setup.py build docs
```

WRITTEN TUTORIALS:

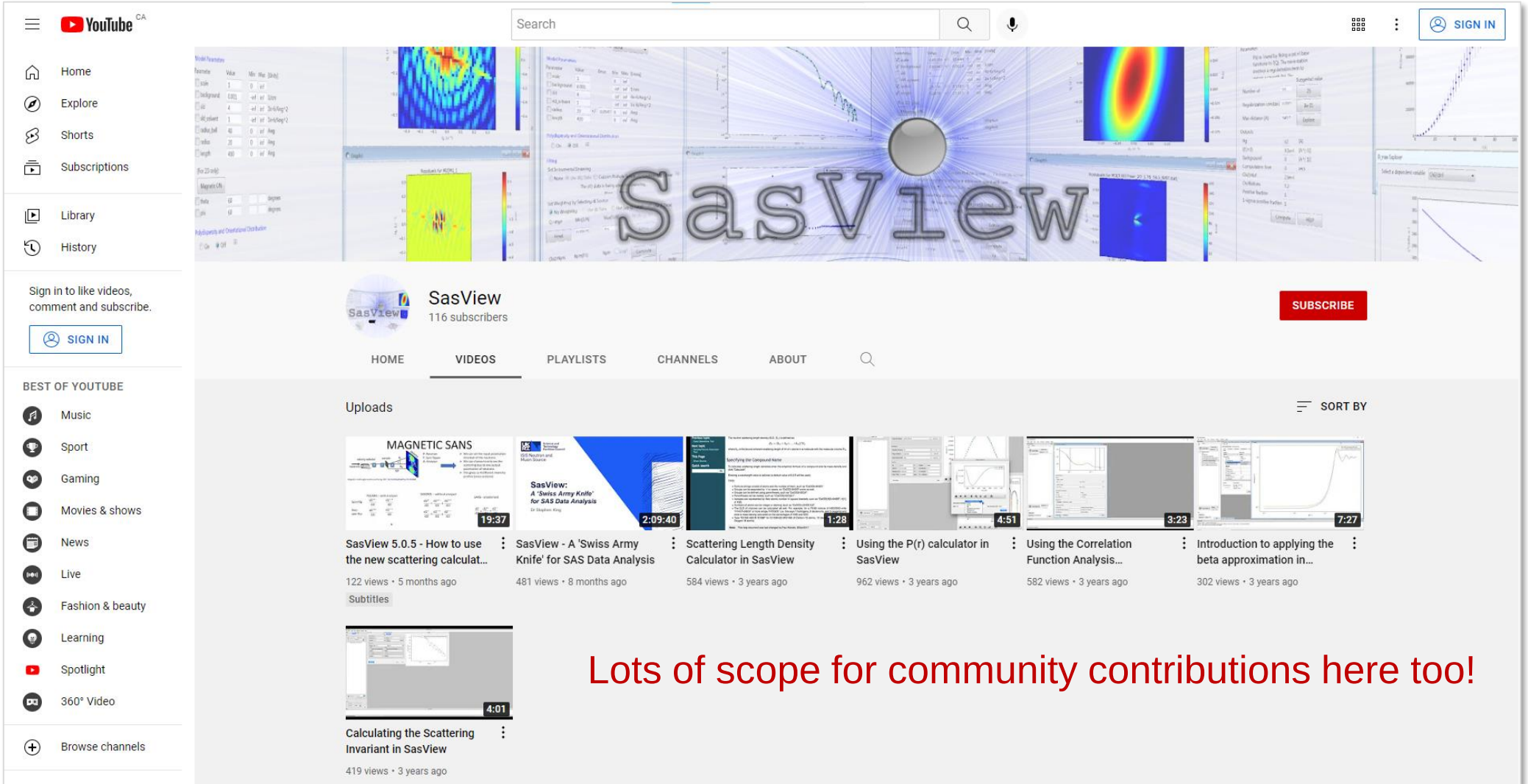
- See https://github.com/SasView/sasview/wiki/TutorialsTNGForAuthors
- Are written in LibreOffice The Document Foundation Writer (download from https://www.libreoffice.org/)
- Are saved in OpenDocument Text Format (.fodt)
- The .fodt can be processed by SPHINX PYTHON DOCUMENTATION GENERATOR *(but is not being at present)*



Lots of scope for community contributions here!

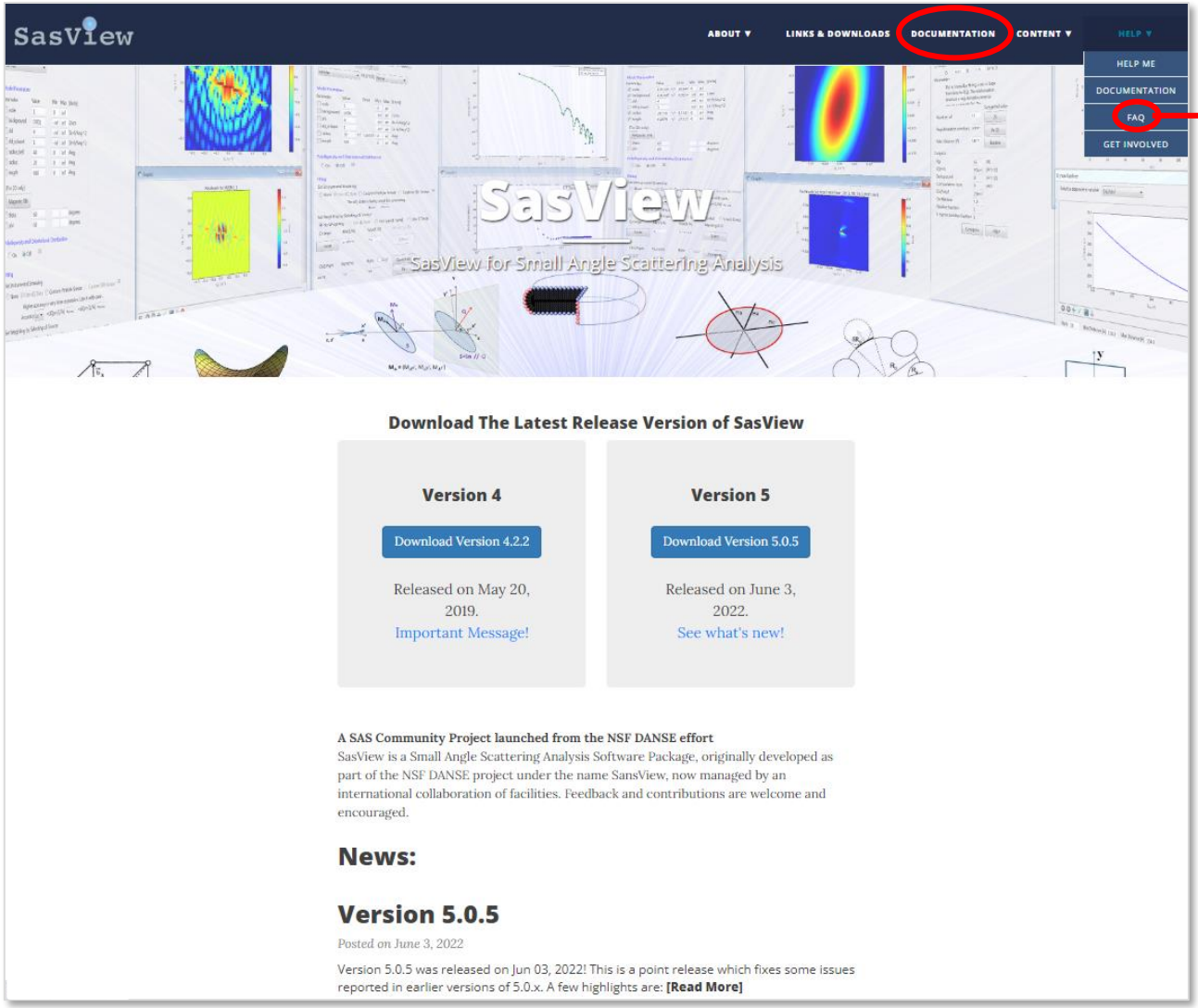
VIDEO TUTORIALS:

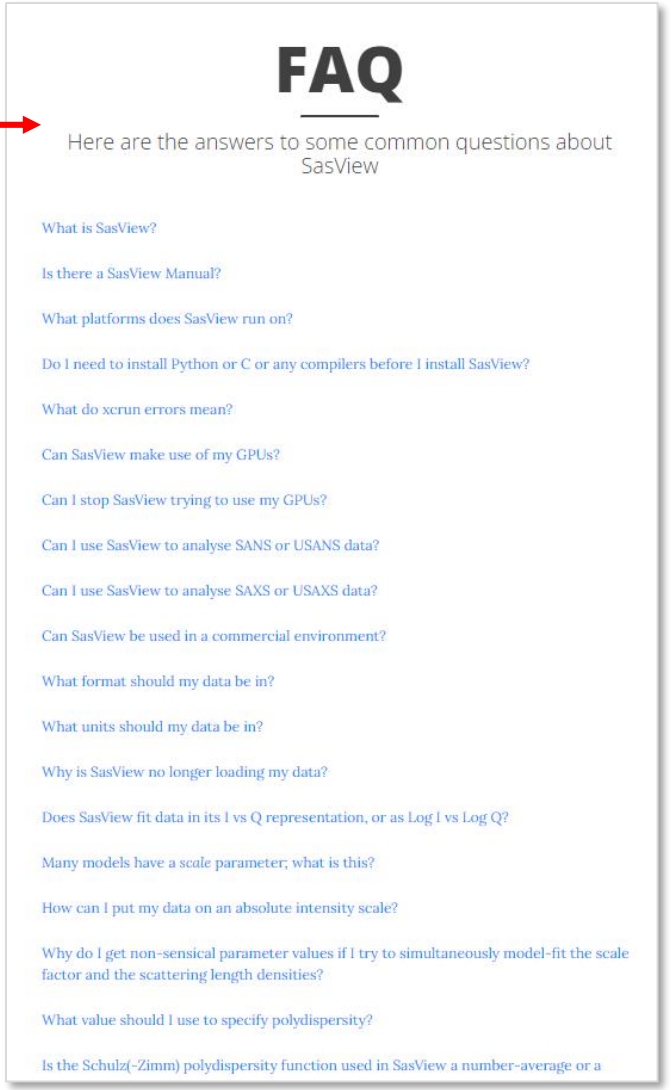
- See https://www.youtube.com/channel/UCxvD3ysXJ05l6MgY7YKjEFQ
  or https://www.sasview.org/documentation/



WEBSITE:

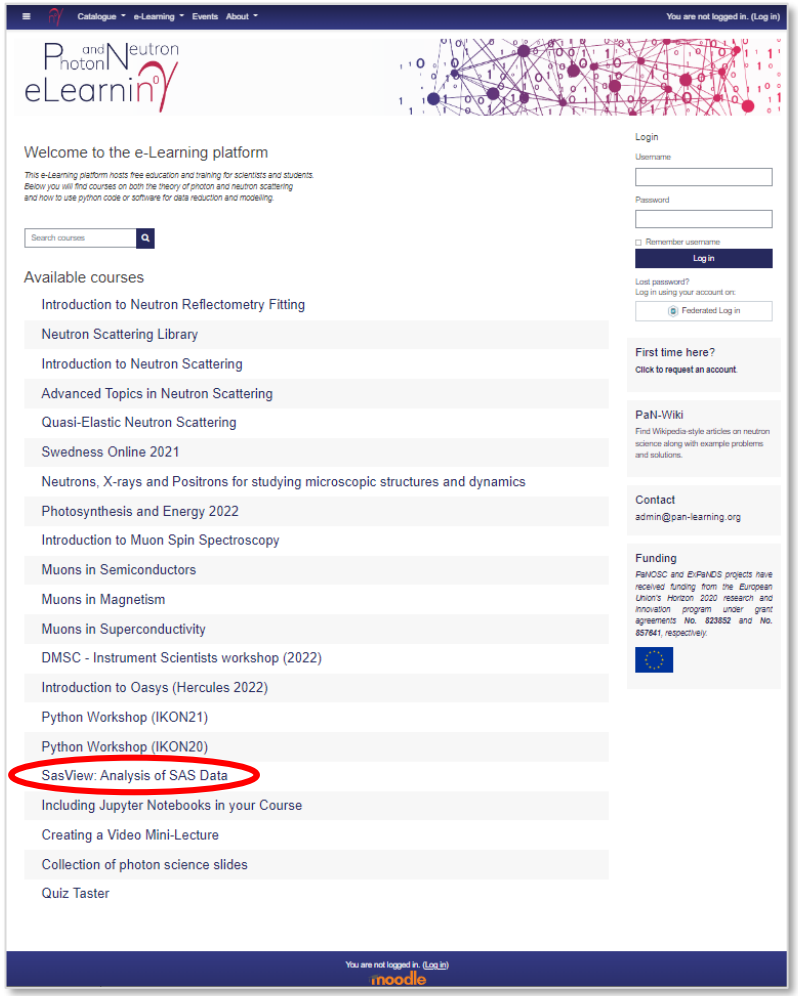
- See https://www.sasview.org/ < https://github.com/SasView/sasview.github.io





OTHER ONLINE RESOURCES:

- See https://pan-learning.org/
- Contains a ‘SasView Analysis’ module
- Written in Moodle

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