Dynamic Documentation Generation and Crowdsourcing in SasView

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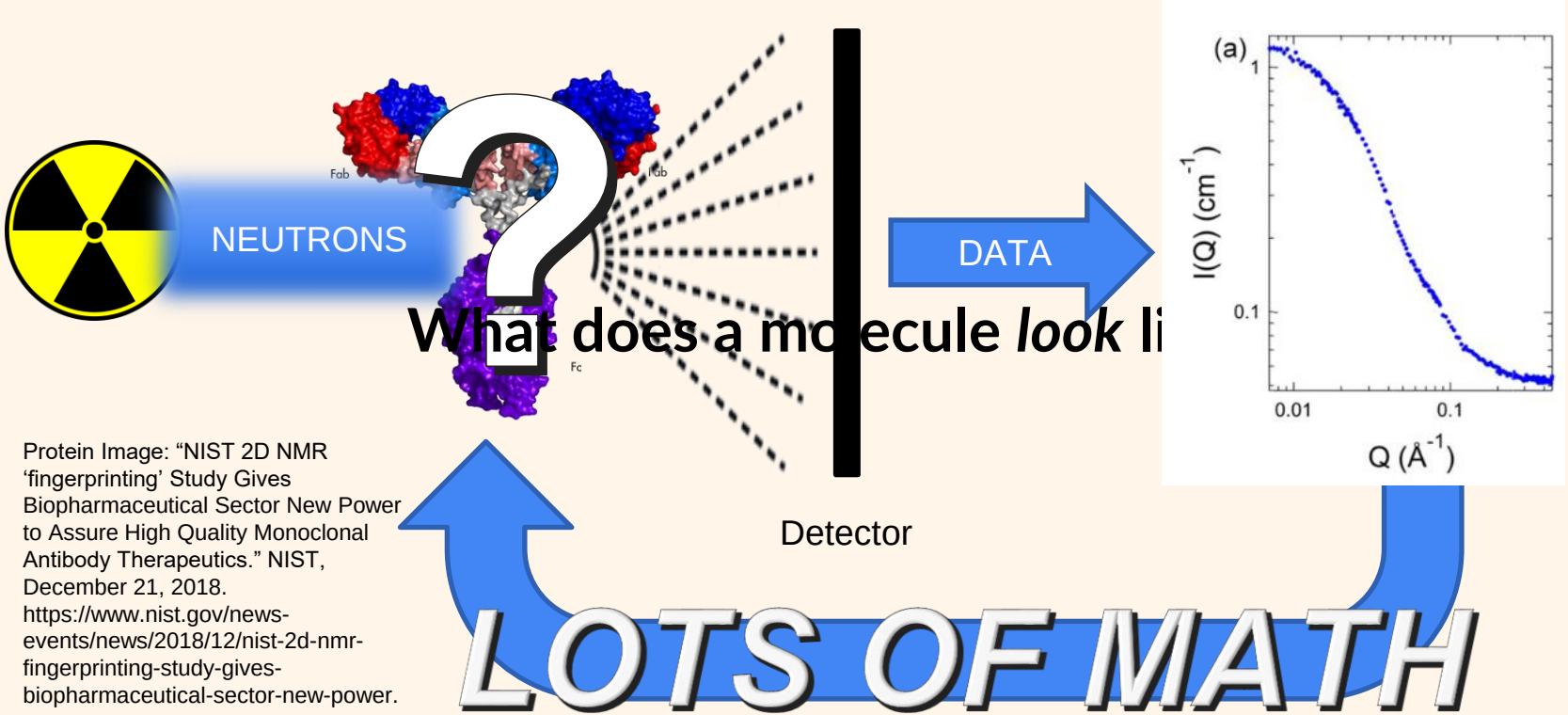
Our Facility

A nuclear reactor

A variety of instruments

"NCNR East Guide Hall." *NIST*, April 17, 2017. https://www.nist.gov/image/20170417016guidehalljpg.

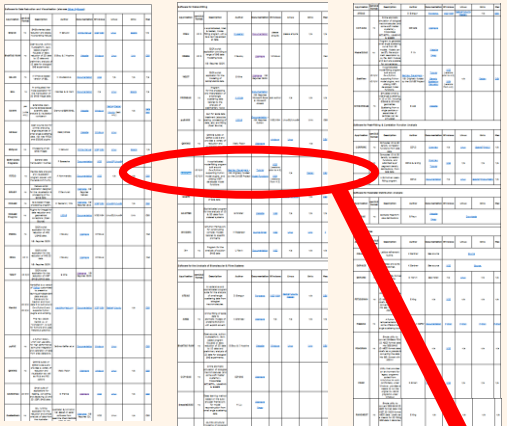
Background: What is SANS?



Protein Image: "NIST 2D NMR 'fingerprinting' Study Gives Biopharmaceutical Sector New Power to Assure High Quality Monoclonal Antibody Therapeutics." NIST, December 21, 2018. https://www.nist.gov/news-events/news/2018/12/nist-2d-nmr-fingerprinting-study-gives-biopharmaceutical-sector-new-power.

Yearley, Eric J., Isidro E. Zarraga, Steven J. Shire, Thomas M. Scherer, Yatin Gokarn, Norman J. Wagner, and Yun Liu. "Small-Angle Neutron Scattering Characterization of Monoclonal Antibody Conformations and Interactions at High Concentrations." *Biophysical Journal* 105, no. 3 (August 6, 2013): 720–31. https://doi.org/10.1016/j.bpj.2013.06.043.

Analysis software—It does the math for us!



What makes SasView unique?

- Capable of a wide variety of analysis operations
- **Extensive documentation *~140 Pages, some ~6,000 words***
- Maintained by community

SasView

Abo

Ar

Pro

BU

NIST

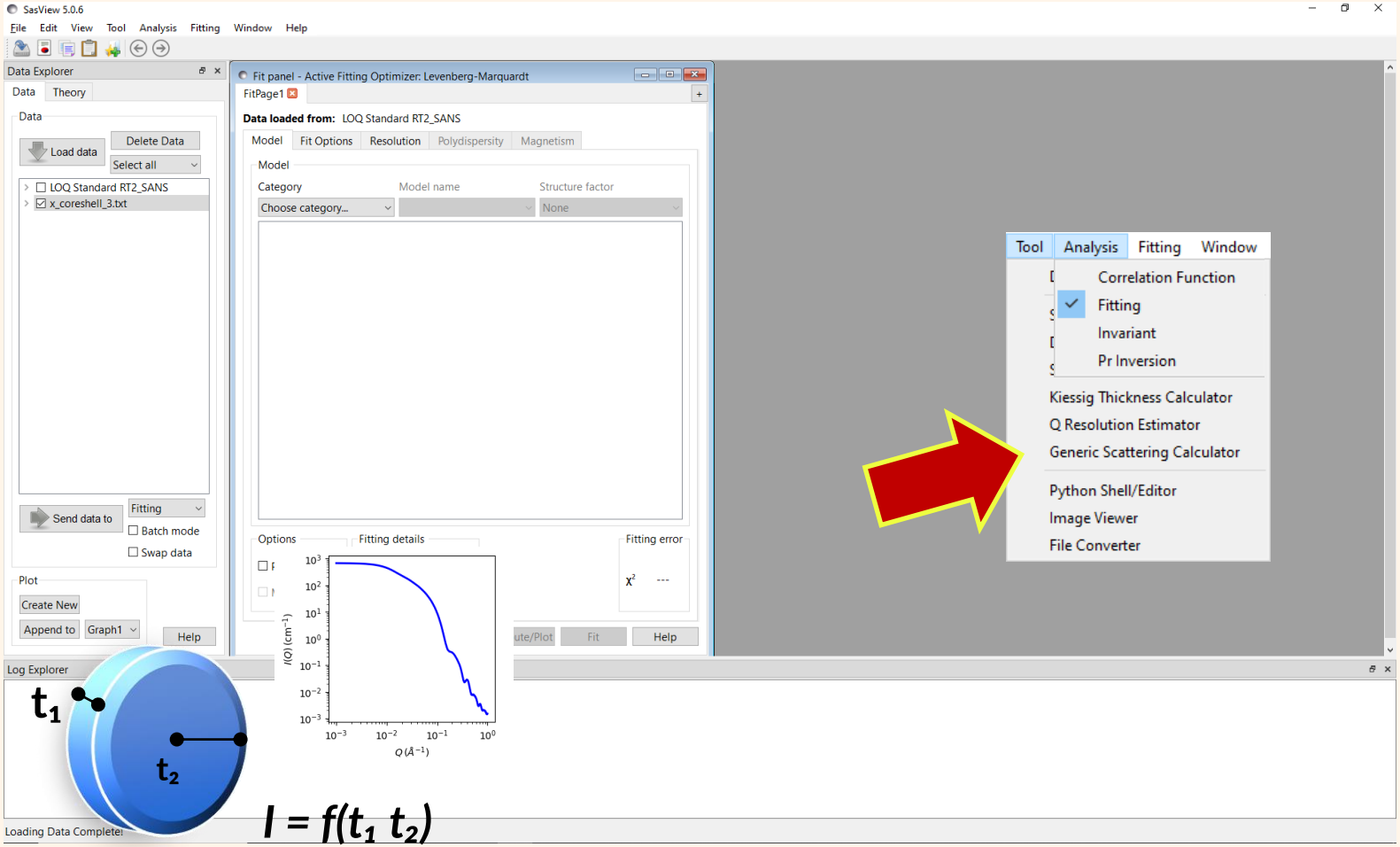
Bundesanstalt für Materialforschung und -prüfung

ISIS

CHRNS NSF CENTER FOR HIGH RESOLUTION NEUTRON SCATTERING NIST

Ahmed, Adnan. “The Bus Factor.” *Tajawal* (blog), May 4, 2018. https://medium.com/tech-tajawal/the-bus-factor-6ea1a3ede6bd.

UT TUDelft OAK RIDGE National Laboratory


SasView 5.0.6
File Edit View Tool Analysis Fitting Window Help
Data Explorer
Data Theory
Load data
Delete Data
Select all
LOQ Standard RT2_SANS
x_coreshell_3.txt
Send data to
Fitting
Batch mode
Swap data
Plot
Create New
Append to
Graph1
Help
Fit panel - Active Fitting Optimizer: Levenberg-Marquardt
FitPage1
Data loaded from: LOQ Standard RT2_SANS
Model
Fit Options
Resolution
Polydispersity
Magnetism
Category
Model name
Structure factor
Choose category...
None
Options
Fitting details
Fitting error
Fit
Help
Tool
Analysis
Fitting
Window
Correlation Function
Fitting
Invariant
Pr Inversion
Kiessig Thickness Calculator
Q Resolution Estimator
Generic Scattering Calculator
Python Shell/Editor
Image Viewer
File Converter
Log Explorer
Loading Data Complete!
t1
t2
I = f(t1 t2)

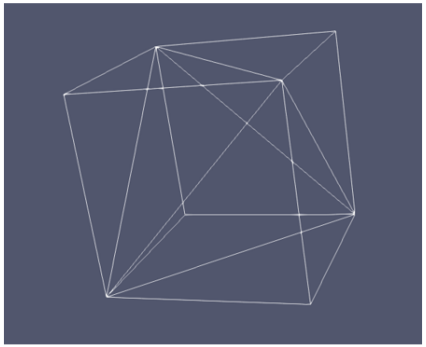
What does documentation look like?

```
Element Type Data
^^^^^^^^^^^^^^^^^

The simulation box can be described as collection of finite elements forming a mesh.
For example this cube is formed of five finite elements:

.. figure:: vtk_mesh_example.png
   :align: center

Each element has an associated scattering length
density ($\beta_j$) for the occupied space $V_j$ and the elastic scattering
intensity is calculated as

.. math::
    I(\mathbf{Q}) = \frac{1}{V}\left\lvert\sum_j^N\beta_j\iiint\limits_{V_j}\exp(i\mathb


Note that the Fourier transform is calculated over each element - allowing
regions of space with little variation in $\beta$ to have larger finite
elements, and regions of interest to have much smaller finite elements, and
hence more detail.

In Sasview an algorithm is implemented to calculate the Fourier transform over
polygons utilizing the divergence theorem as described in Maranville
[#MARANVILLE1]_
```

What we write

Element Type Data

The simulation box can be described as collection of finite elements forming a mesh. For example this cube is formed of five finite elements:



Each element has an associated scattering length density (β_j) for the occupied space V_j and the elastic scattering intensity is calculated as

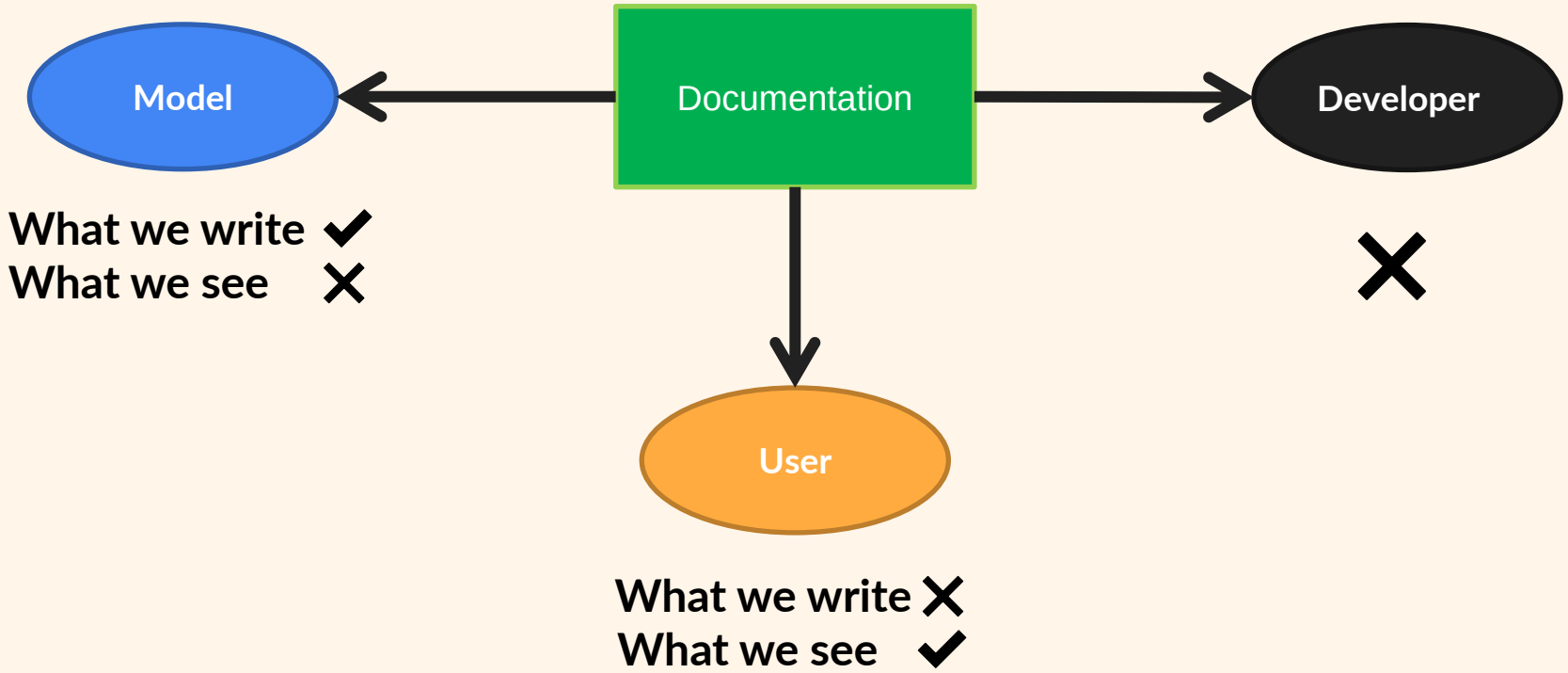
$$I(\mathbf{Q}) = \frac{1}{V}\left|\sum_j^N \beta_j \iiint_{V_j} \exp(i\mathbf{Q}\cdot\mathbf{r_j})\mathrm{d}V\right|^2$$

Note that the Fourier transform is calculated over each element - allowing regions of space with little variation in β to have larger finite elements, and regions of interest to have much smaller finite elements, and hence more detail.

In Sasview an algorithm is implemented to calculate the Fourier transform over polygons utilizing the divergence theorem as described in Maranville [1]

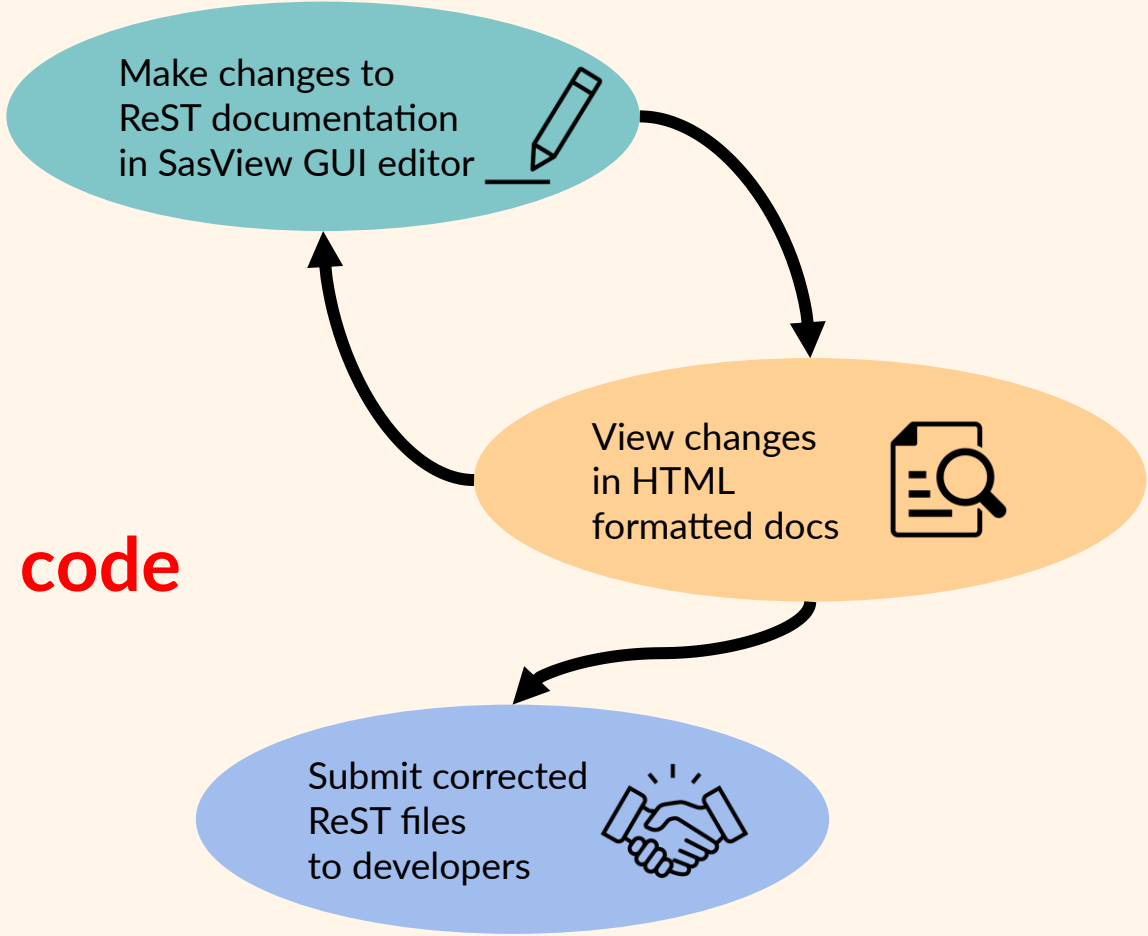
What we see

Documentation Problems:



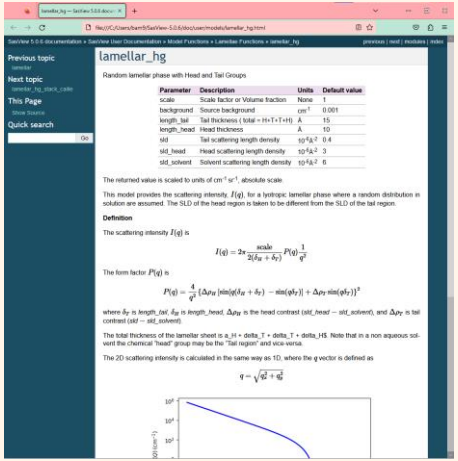
Objective

Functional
Easy to use
Minimal changes to code structure

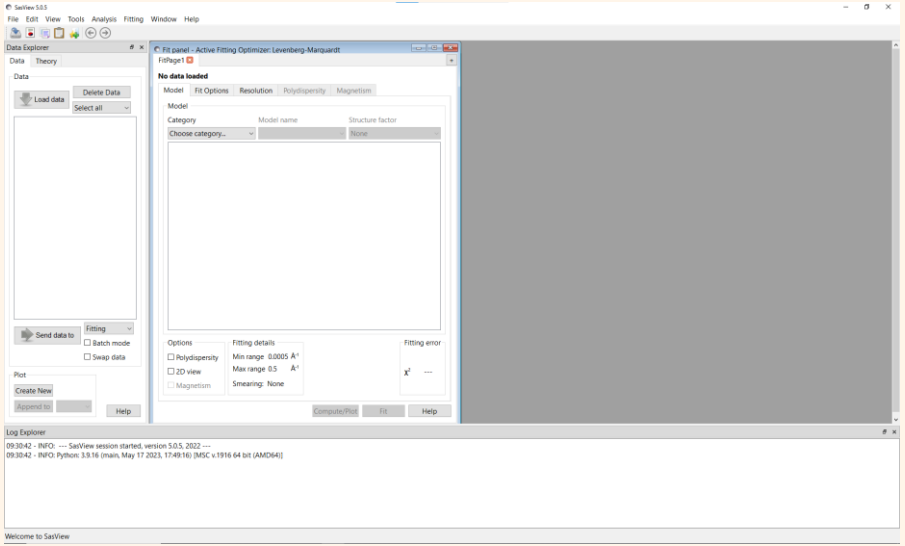


Restructuring changes

Web Browser

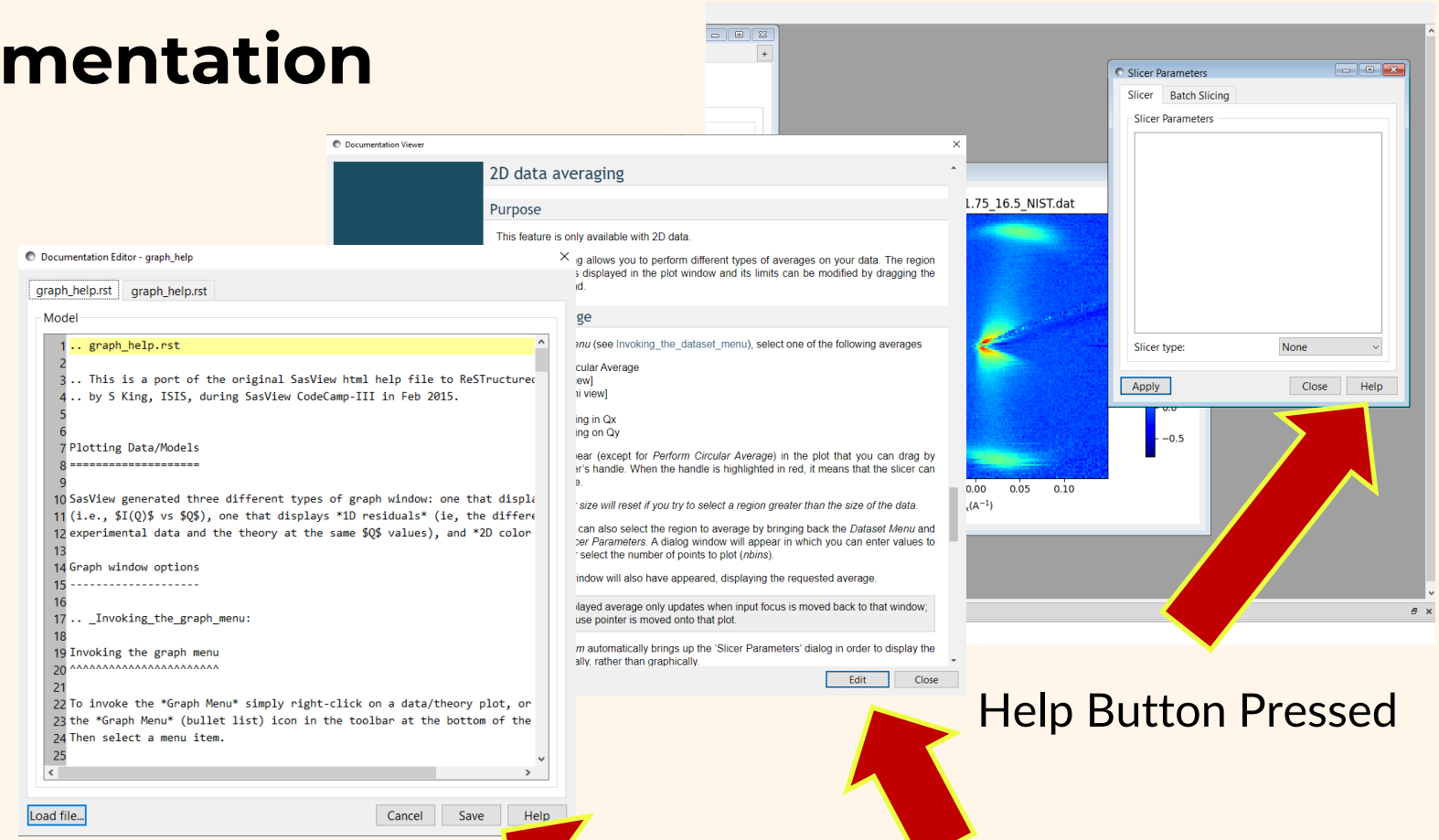


SasView

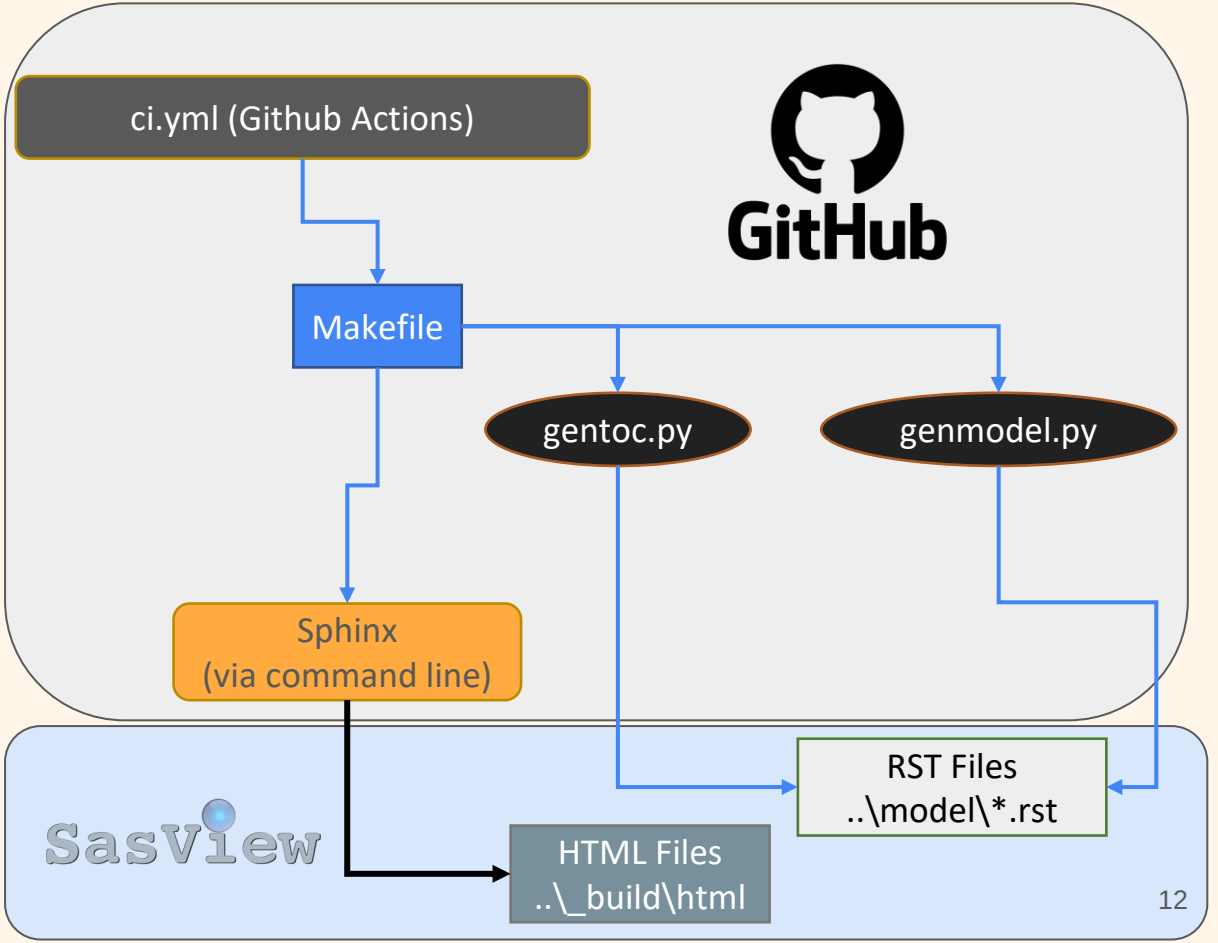


Old approach

Implementation

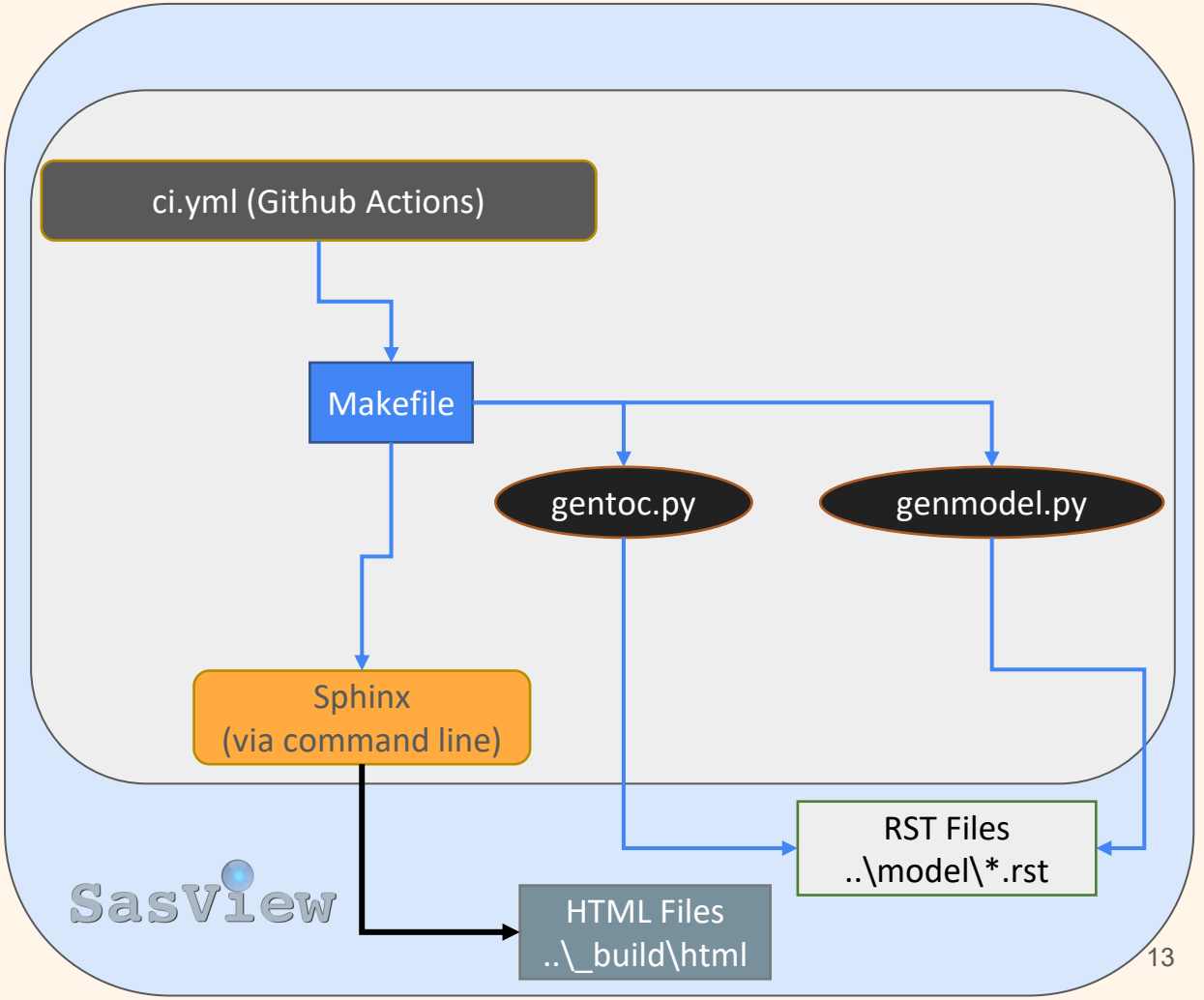


Working locally



Working locally

- Replaced functionality of current GitHub actions to compile
- Reduced runtime of GitHub processes
- Avoided using new dependencies



Summary

Accomplishments:

- Allow users to edit documentation locally
- Create opportunities for crowdsourcing SasView
- Documentation for community models is now visible

Bonus:

- Math will display regardless of browser settings

Future work:

- Automatic submission of edits to documentation
- Documentation regeneration scripts can be optimized
- Math still needs internet connection to display correctly

Special Thanks

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And other SHIP Students