

Dynamic Documentation Generation and Crowdsourcing in SasView



Dr. Paul Butler, Mentor

Brayden Miller
Albert Einstein High School



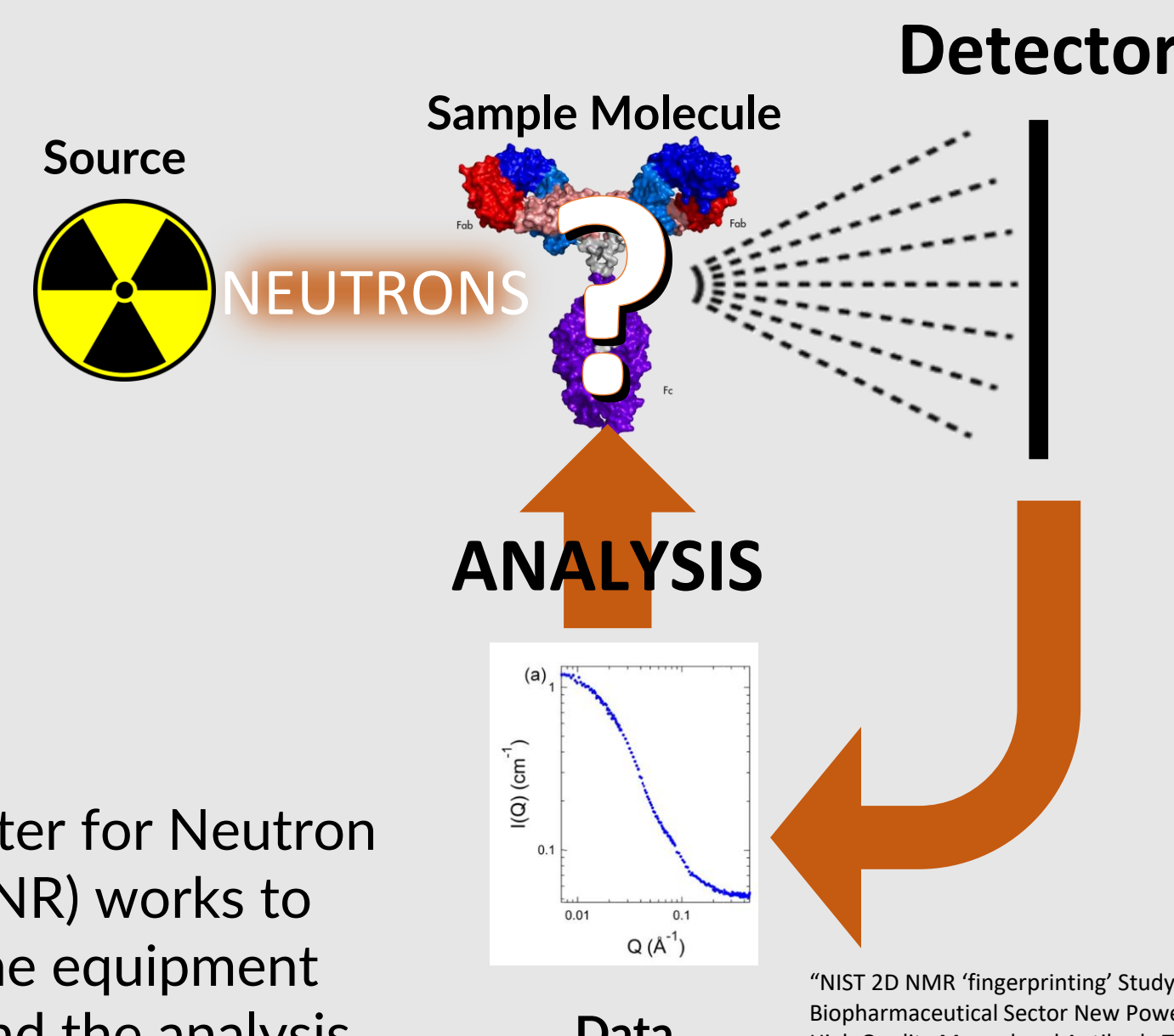
Background

Small angle scattering (SAS): What is it?

Scientists ask a question:

WHAT ARE CHARACTERISTICS OF THIS MOLECULE?

SAS is used to determine these characteristics, giving us data that must be analyzed. This can be done manually but is greatly enhanced using analysis software.



The NIST Center for Neutron Research (NCNR) works to supply both the equipment (shown left) and the analysis software necessary for modern SAS techniques.

"NCNR East Guide Hall." NIST, April 17, 2017. <https://www.nist.gov/image/20170417016guidehall.jpg>

SasView

SasView is a SAS software analysis suite.

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

SasView is an open-source, collaborative, and international project

Open source - **READABLE AND CONTRIBUTABLE BY ALL**

Collaborative - **PROTECTED FROM THE "BUS FACTOR"**

This means SasView is developed sustainably, with the goal that it can continue to be developed in the future. Unlike many alternative tools for SAS analysis, it has a consistent release cycle.

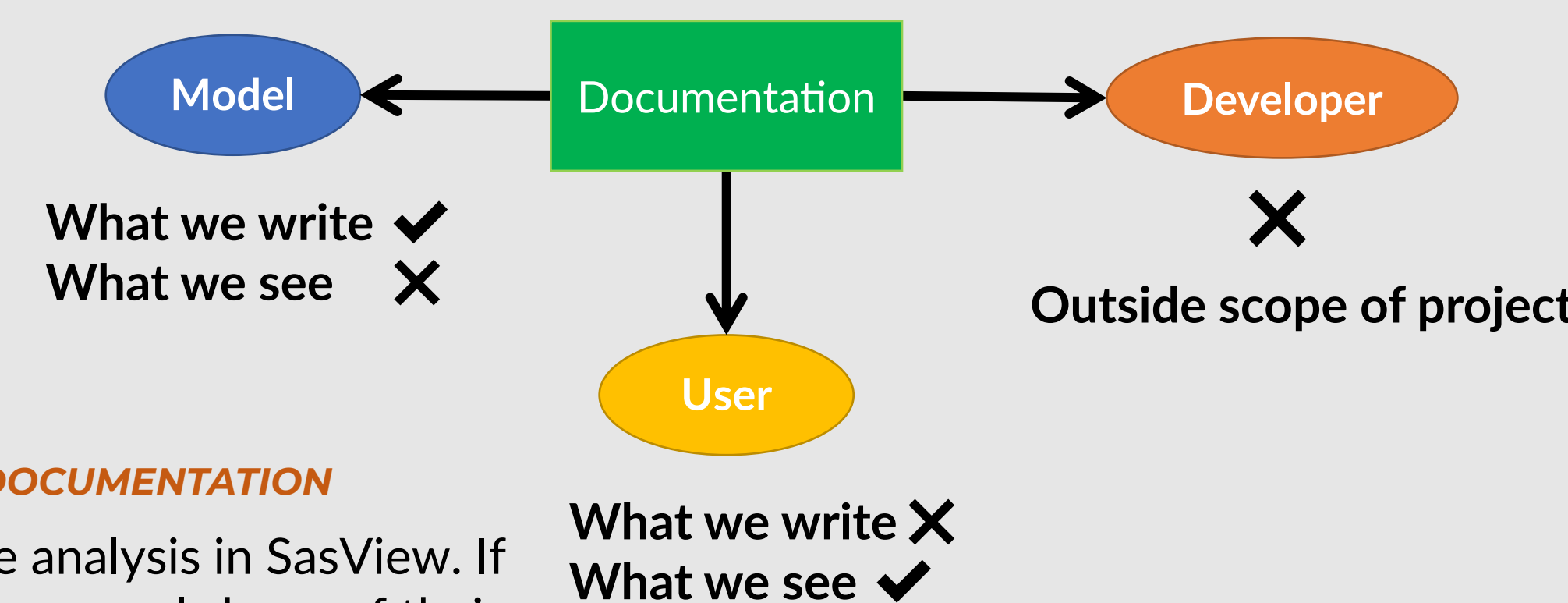
If a bus were to hit members of the developer team (or if they were to retire), the project will live on!



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

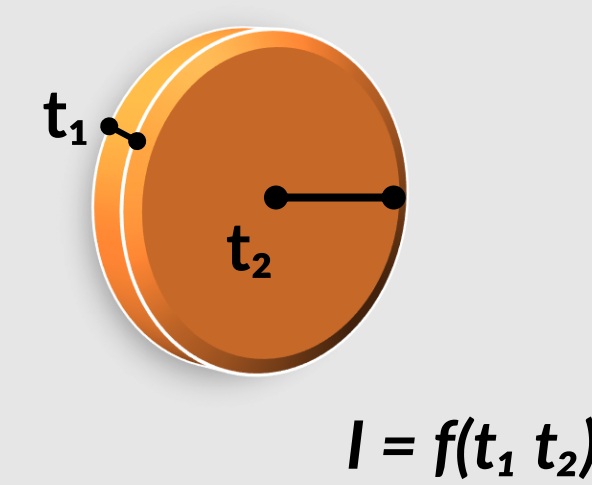
The Documentation Problem (cont'd)

SasView has three types of documentation, each with its own problems:



MODEL DOCUMENTATION

Fitting is a core analysis in SasView. If users know the general shape of their molecule, they can write an equation, called a model, to represent its shape. Variables in this model represent unknown parameters, like radius and length below.



Researchers frequently write their own models and share them with the community. Writing documentation is possible, but it is not visible to users when 'Help' is pressed for their models.

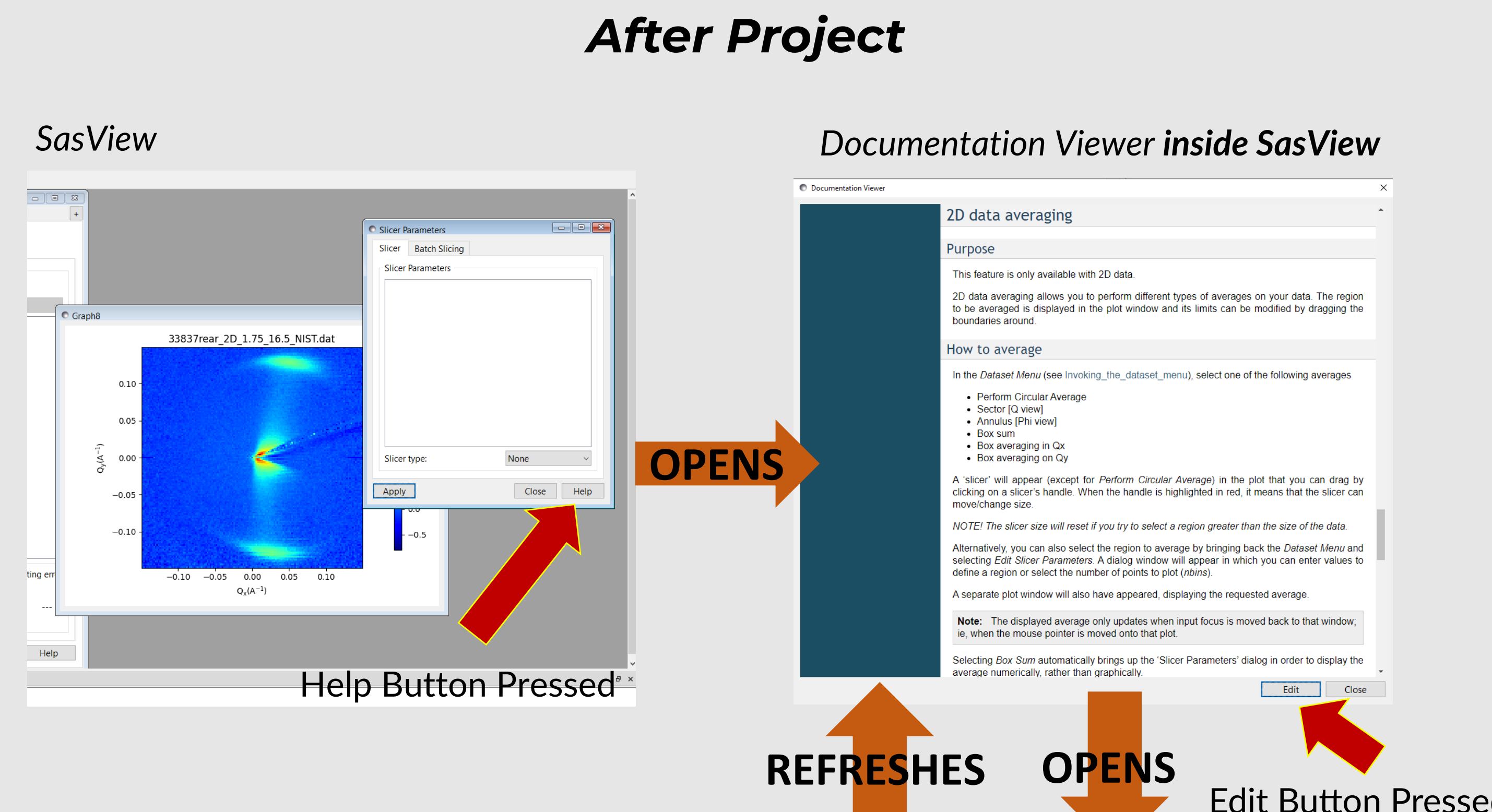
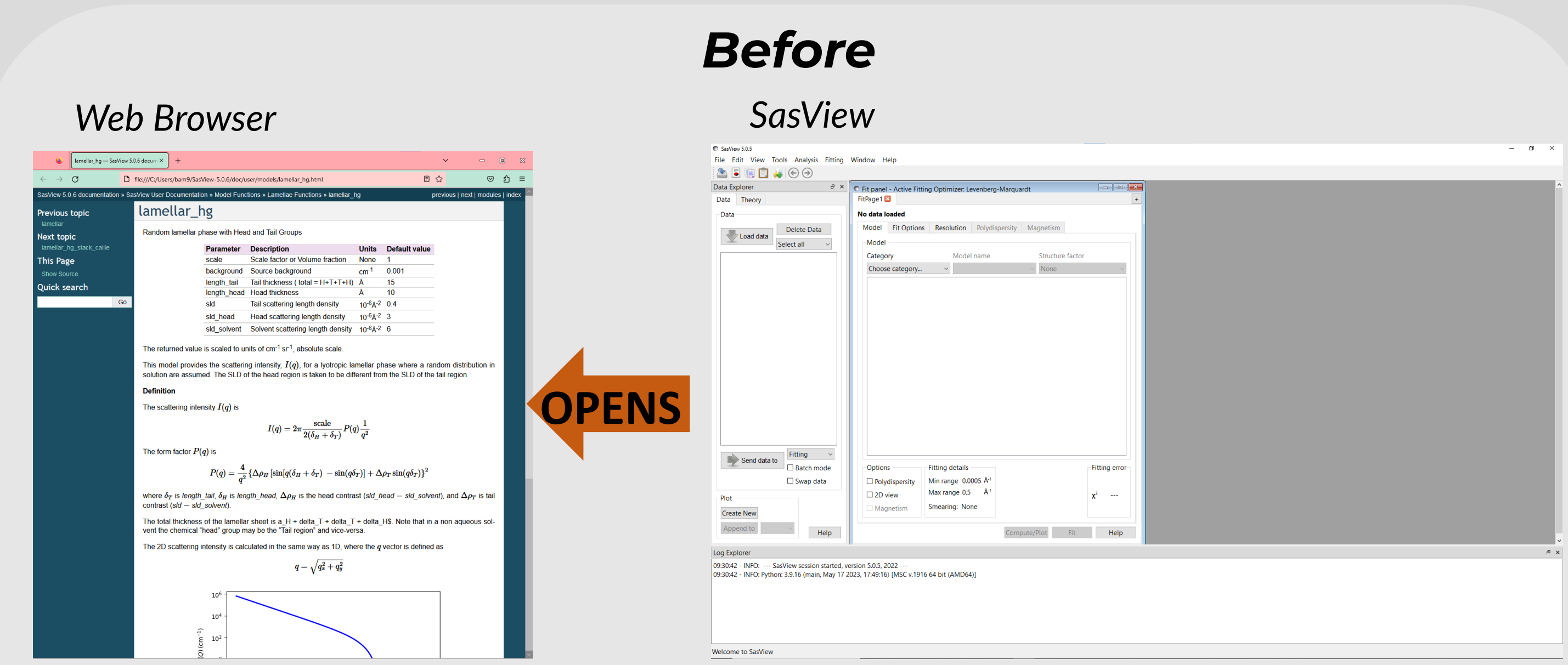
SASVIEW IS COLLABORATIVE **DOCUMENTATION MUST BE CONSTANTLY EVOLVING**

We need to have an easy solution for letting the community edit documentation!

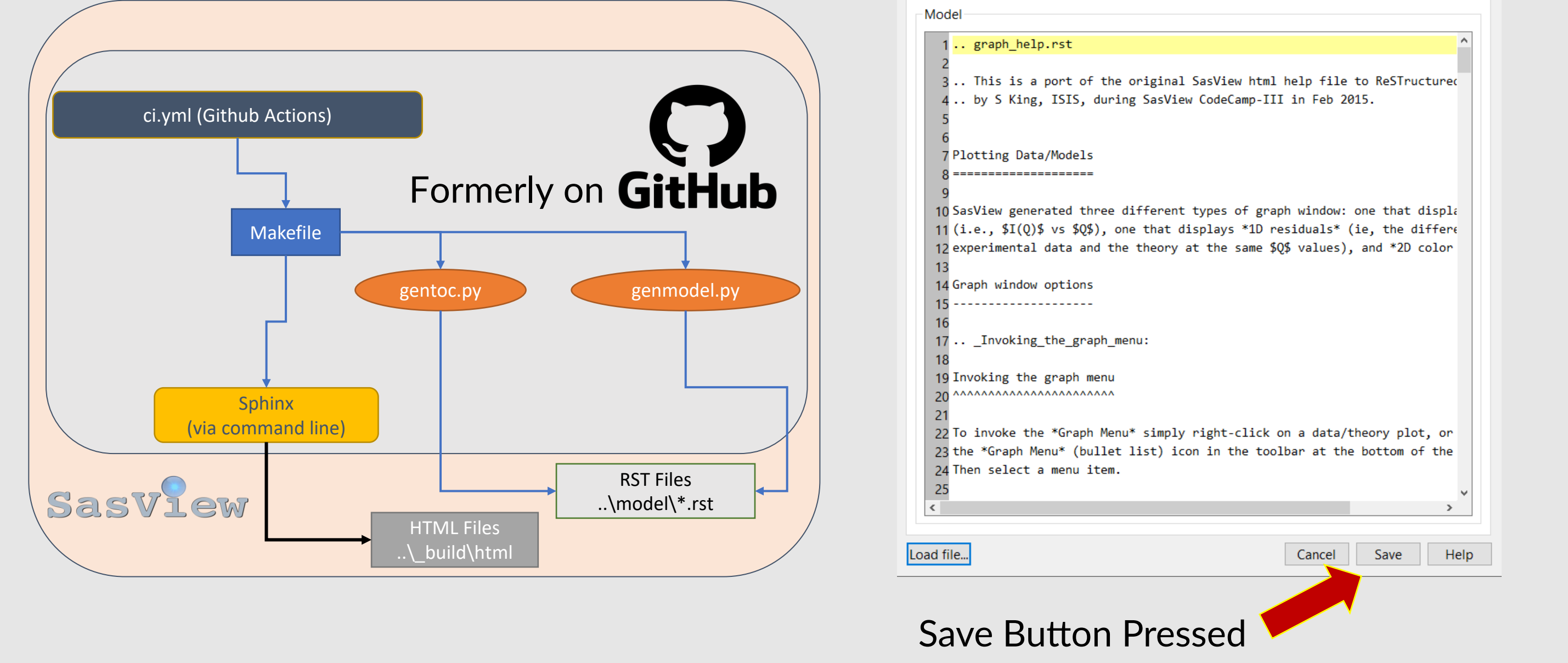
Users may see errors in documentation or be knowledgeable in an area of documentation and want to contribute. The current process involves:

- Using a GitHub account
- Cloning a repository
- Installing dependencies
- Running setup and config files via command line
- Edit raw RST documentation files by navigating source tree
- Running Makefile via command line to view HTML version

THIS IS TOO DIFFICULT OR TIME CONSUMING FOR A LARGE SET OF USERS!



Functionality Included



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

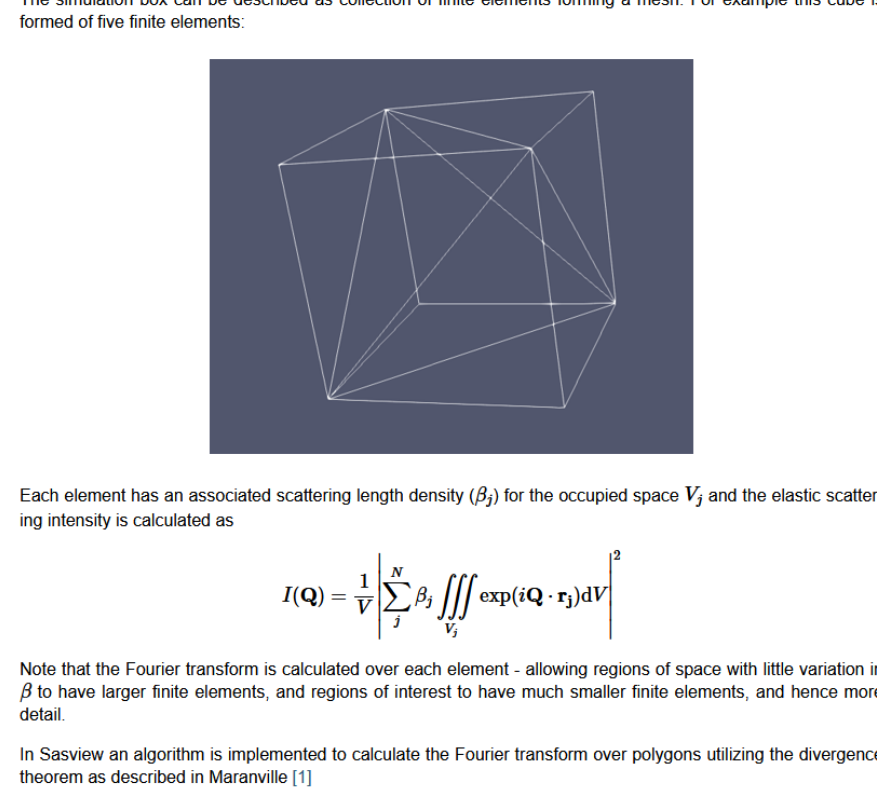
The Documentation Problem

WHAT DOES DOCUMENTATION LOOK LIKE?

```

92 Element Type Data
93 =====
94 The simulation box can be described as a collection of finite elements forming a mesh.
95 For example this code is formed of five finite elements:
96
97 .. figure:: vts_mesh_example.png
98 .. align: center
99
100 Each element has an associated scattering length
101 density (rho_e, S) for the occupied space rho_e and the elastic scattering
102 intensity is calculated as
103
104 .. math::
105 I(\mathbf{Q}) = \sum_{i=1}^N \rho_{e,i} \exp(i\mathbf{Q} \cdot \mathbf{r}_i)
106
107 Note that the Fourier transform is calculated over each element - allowing
108 regions of space with little variation in S to be treated as a single finite
109 element, and regions of interest to have much smaller finite elements, and hence more detail.
110
111 In SasView an algorithm is implemented to calculate the Fourier transform over
112 multiple, utilizing the divergence theorem as described in Mariani [1].
113 [MURIANVILLE1]
    
```

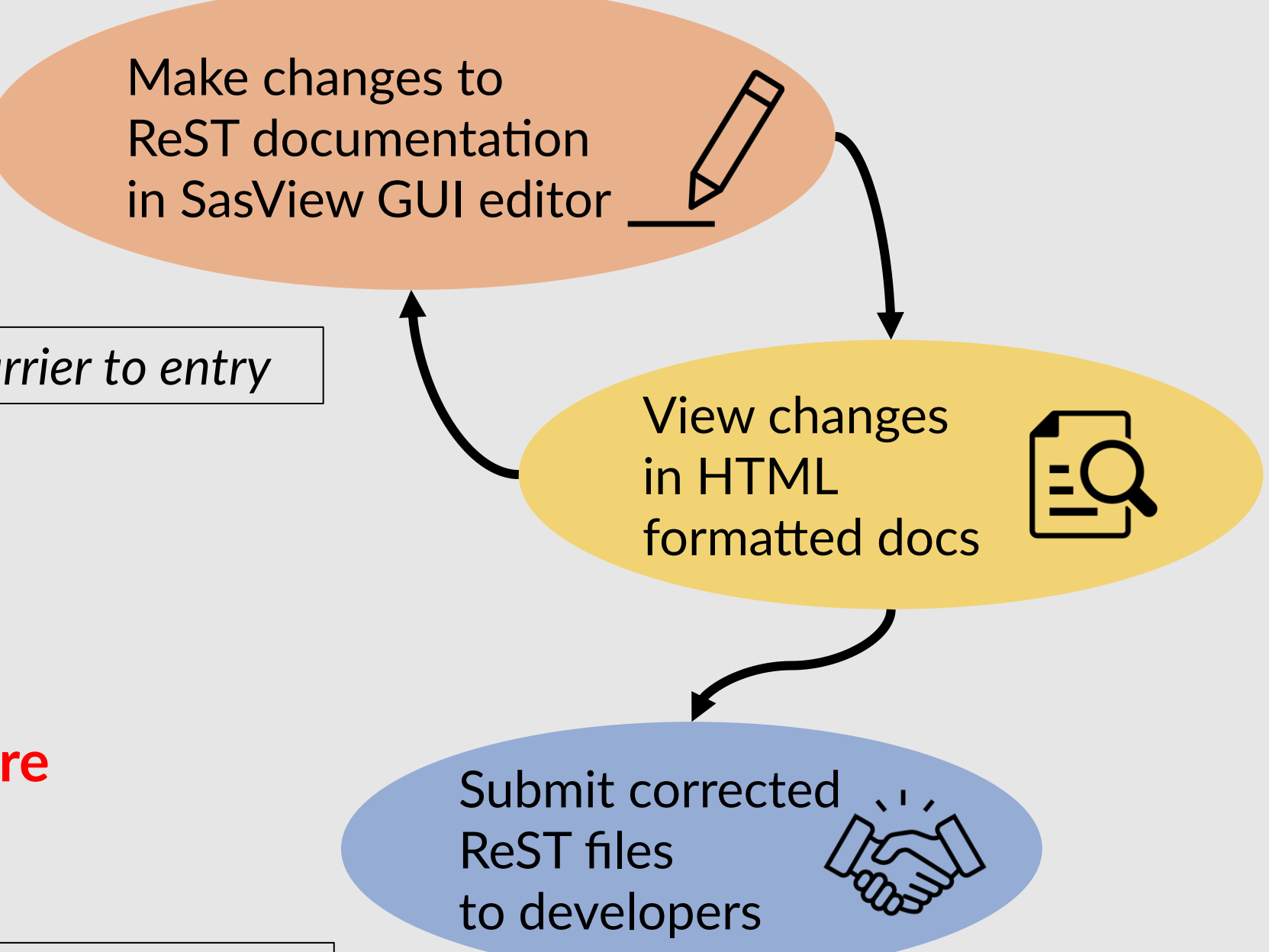
Compiling + Formatting



What we see (user-friendly)

Files are written in a mix of Restructured Text (ReST) and LaTeX for embedded mathematics. The viewable files are structured using HTML.

Objective:



Design Considerations:

- Purpose is to lower barrier to entry
- Functional
- Easy to use
- Minimal changes to code structure
- SasView is a large codebase, we need to develop sustainably