SasView

Update and Roadmap Discussion
2019-03-29

A little history …

2006 2011 2012 2013 2014 2015 2016 2017 2018 2019

Heritage: NIST IGOR macros
SansView is DANSE project output
~ 8.5% of funds were for SANS

NIST Supported initial transition from NSF funding

Transition to Community project.

Move to GitHub
Rename to SasView

v3.0 released
v3.1 released

v4.0 released

v4.1 released

v4.2 released
v5.0b1 released
v4.2.1 released
v5.0b2 released

1st Code Camp at NIST April 2013

2nd Code Camp at ISIS April 2014

3rd Code Camp at ESS Feb 2015

4th Code Camp at TU Delft March 2016

5th Code Camp at ORNL Oct 2016

6th Code Camp at ILL/ESRF April 2017

7th Code Camp at DMSC October 2017

8th Code Camp at ESS Sept 2018

1st SasView User Meeting at SAS2018

9th Code Camp at ILL/ESRF March 2019

How We Work

Open, Collaborative, Community Development

Code is open source and publicly hosted at Github

Released under BSD 3-clause license

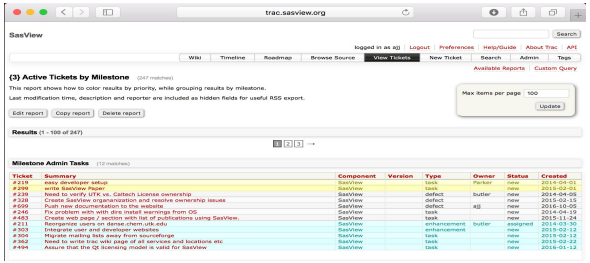
Bug and Enhancement Ticket System (Trac)

Bi-weekly developer calls **Code Camps** **5 Year Roadmap**

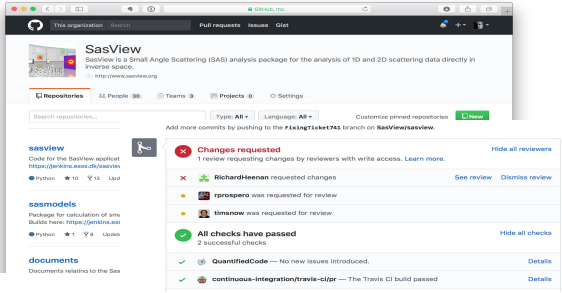
Model Marketplace

Task and bug tracking. Developer wiki

trac.sasview.org

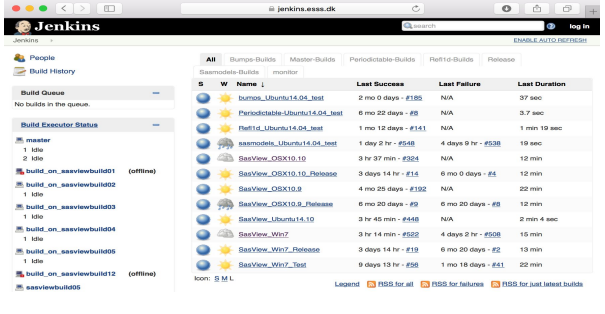


Code Hosting and some CI/testing of PRs



Automated Builds

build.sasview.org



http://www.sasview.org

http://github.com/SasView

Open, Collaborative, Community Development

Collaborative:

- (S)he who brings the resources (time and effort or funds to buy time and effort) chooses what to work on
  - You are not allowed to break what is already there for others.

Community Development:

Ask not what the community is going to do for you,
ask what you can do for the community

The RoadMap

SasView 5 Year Roadmap

The purpose of building and operating large scattering facilities is to provide unique tools to answer new scientific questions with the final presentation of results (usually in the form of a paper) as the output. The biggest obstacle to that output is often the analysis of the acquired data. Data analysis software has been variously viewed as being in the domain of the scientist using the facility, a service to be provided by scattering facilities, or as the individual responsibility of the scientists running the facility beamlines. The result has been a proliferation of packages and libraries, many written and supported by one key person, often not as their primary responsibility [1].

Over the past decade several trends have contributed to exacerbate the analysis bottleneck: 1) As the techniques have matured the user pool has broadened. This combined with an apparent decrease in the overall level of programming taught to scientists, means that fewer users are capable of building their own analysis tools. 2) With the increasing maturity of the field, a large amount of basic modeling is well understood and developed. Even those capable of coding their own should not be wasting their time re-inventing the wheel but focus on new science and perhaps new analysis developments to enable that new science. 3) The quantity of data being produced by instruments and the complexity of the experiments being performed have increased. 4) Finally, as the general software landscape has moved towards increased quality of usability a
expectatio
data.

Late 2018 to mid 2019 (from code camp VIII - ESS) - Release 4.2, Release 5.0

The focus in this period will be on development and release of version 5.0 of SasView. In parallel version 4.2 and possibly 4.3 will be released providing a maintained, stable, release for current users of SasView. This managed transition from the 4.x series to the 5.x series will allow for extensive user testing of the 5.0 version prior to release. We expect to continue maintenance of the final 4.x release beyond the release of 5.0, with an eventual end-of-life for 4.x occurring with the 5.2 release.

Full integration of the beta approximation work into 5.0 will be completed, with some limited beta approximation functionality being made available in 4.x.

The first SasView community meeting will be held at the SAS 2018 meeting in October 2018 providing SasView users and contributors with an introduction to the new functionality being made available in 5.0 and training on how to get involved in contributing to the SasView project. Building on this meeting a plan for expanding community interactions will be developed.

Release 4.2 and 5.0 will support separate plotting of the P(Q) and S(Q) components in a P*S

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deployment, including bringing the backend up to recent versions.

Living document

Directs work for developers and helps find candidate projects for funding.

Discussed and updated at each Code Camp - NOW!

https://github.com/SasView/documents

Roadmap Late 2018 to mid 2019

- Move focus of all GUI efforts to the new Qt GUI Done. Major bug fixes only to 4.x GUI
- Parallel development and release tracks (5.x + 4.x) Working, but needs streamlining from 5.0 release
- Complete beta approximation work In testing
- New, more flexible interaction volumes/radii Underway?
- Community meeting at SAS 2018 Done
- Complete SasView paper Started
- Consolidate and extend training material - both written tutorials and hands-on training material. Ongoing
- Update model marketplace Needs developer
- Create plan for developing community interactions. Started
- Fixes to custom model editor to support polydispersity Done
- Incorporation of models from:
  a. SASFit[^7] Work done, but not shipping by default. https://github.com/SasView/sasfit-models
  b. Scatter[^8] (Förster - crystalline materials models primarily) In discussions with BornAgain team
- Project infrastructure cleanup:
  a. ticket review/cull given 5.0 release Ongoing
  b. possible move to GitHub issues. Underway
- Release
  a. 5.0 alpha (late 2018) Done
  b. 5.0 beta (early 2019) Done
  c. 5.0 (mid 2019) On track
  d. 4.2 Done

Not in roadmap for this period …

- Complete separation of sascalc package / headless usage

https://github.com/SasView/documents

Current Status of Future Roadmap Activities

- Status of 5.0 and transition from SINE2020 to community - *Wojciech*
- Developing community interactions
  - Welcoming new contributors - *Butler for Jackson*
  - New website and cleanup of twitter feed - *Butler for Jackson*
  - e-learning - *King*
  - Future code camps vs boot camps - *Wojciech*
- SasView paper, DOIs and publication tracking - *Butler for Jackson*
  - Paper on Overleaf with assignments
  - DOI for EVERY release for traceability in emerging publication standards
    - https://zenodo.org/communities/sasview-analysis/?page=1&size=20
  - Publication tracking - Sneak peak at www.sasview.org/publications
- Headless operation - *Wojciech*
- Infrastructure work - moving fully to github - *Ricardo*

Roadmap Late 2019 to mid 2020

- Begin model fitting refactoring work to allow custom re-parameterization of models, allow reading in an array representing either PQ or SQ for P*S fits, fitting oriented model to 1D cuts including revisiting orientation definitions etc. Discussed at this code camp
- Complete architecture manual
- Begin work on refactoring constrained/simultaneous fits.
- Begin work on adding custom workflows identified as highest priority
- Work to update tutorials to support 5.x
- Begin work on advanced model fitting tutorial
- Usual bug fixes and other minor improvements as time and interest permit
- Integration of McSAS
- Begin work on generic O-Z solver
- Inclusion of PRISM^9 functionality
- Begin work to refactor/improve generic scattering calculator
- Improvements to custom model editors including features from compare.py
- Support for multi-GPU, multi-CPU and CPU/GPU computation

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Roadmap mid 2020 to mid 2024

- Refactor Simultaneous/Constrained fitting - significant changes in 5.0
- New Workflows
- Web UI (and Phone App)
- Headless - essentially done in 5.1?
- Intelligent limits/help ⇒ “AI” ?
- Add support for ASAXS
- Enable transparently running computational code remotely from within local GUI - dependent on headless

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Discussions this week

- Reparameterisation of models
- Including more complex structure factors
- Include material from Scatter
- 1D oriented data … How to fit a slice from a 2D dataset
- Project to do benchmarking of optimisers
- Computation speed and integration options and approaches

Aiming to move to 9-monthly cadence for code camps
Camp X - Jan/Feb 2020 (likely in US)
Camp XI - Oct/Nov 2020 (likely in Europe)

Discussion ...

What do you want to see in SasView?

How can you help?