

DANSE / SANS

canSAS-V
October 2007

<http://danse.chem.utk.edu>

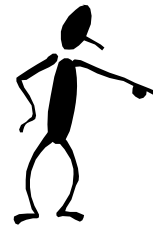
DANSE: A five-year project to develop analysis software for materials science, with the UT group dedicated to SANS

- Overview of the functionality we will be providing
- Structure of the code
- Release plan
- Released prototypes
- Software development process



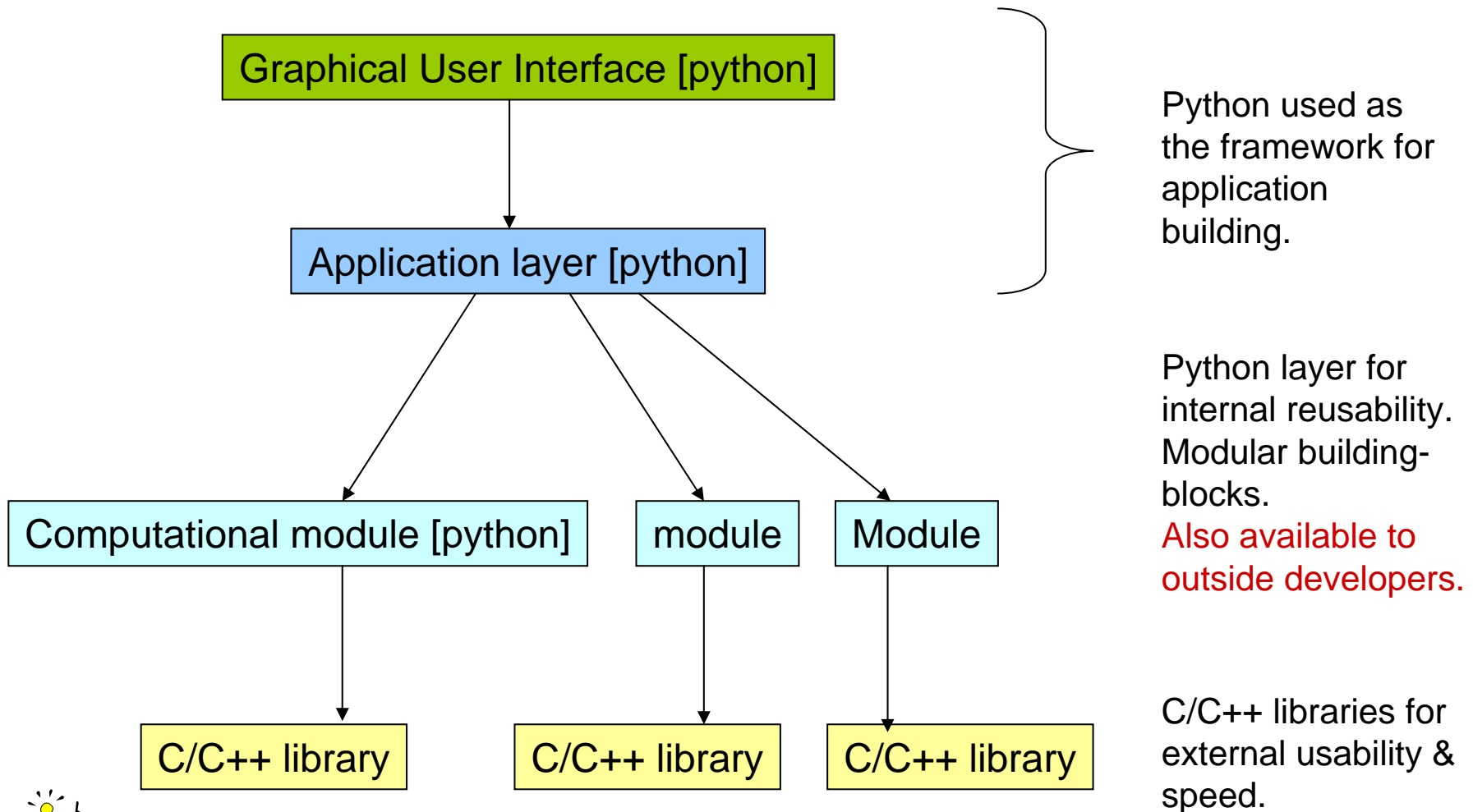
Functionality

1. **Basic modeling:** $I(q)$ [1D], $I(q_x, q_y)$ [2D or “oriented”], non-shape models, magnetic modeling...
2. **Scattering intensity simulation of real-space systems:** $I(q)$ and $I(q_x, q_y)$.
3. **Interface with community software (IGOR):** limited to modeling so-far, but in principle could be anything.
4. **Inversion of $P(r)$.**
5. **Ab initio modeling.**
6. **Experiment planning tools.**
7. **Constrained fitting.**
8. **Series analysis and simultaneous fitting.**
9. **MC simulation.**



Functionality provided as independent modules, used as building blocks for our applications.

Structure of the code



- **C libraries used as a way to give functionality to other groups of developers before the applications are ready.**
- **Currently used by NIST IGOR developers.**

Release Plan

“Give me six hours to chop down a tree and I will spend the first four sharpening the axe.”

- Abraham Lincoln

Prototypes for requirements gathering (selected functionality):

- **Real-space simulation** [completed]
- **Shape-based model analysis** [currently open]
- **Shape-independent analysis** [starts 1/08]
- **Experimental planning tools** [starts 1/09]

Roll-out of applications (full functionality):

- **Shape-based model fitting analysis** [starts 6/08]
- **Shape-independent analysis** [starts 4/09]
- **Experimental planning tools** [starts 3/10]

Our philosophy for maximizing scientific impact:

- Involve the community early with prototypes
- Work with external users with analysis needs for their publications
- Listen to the feedback to design a better final product

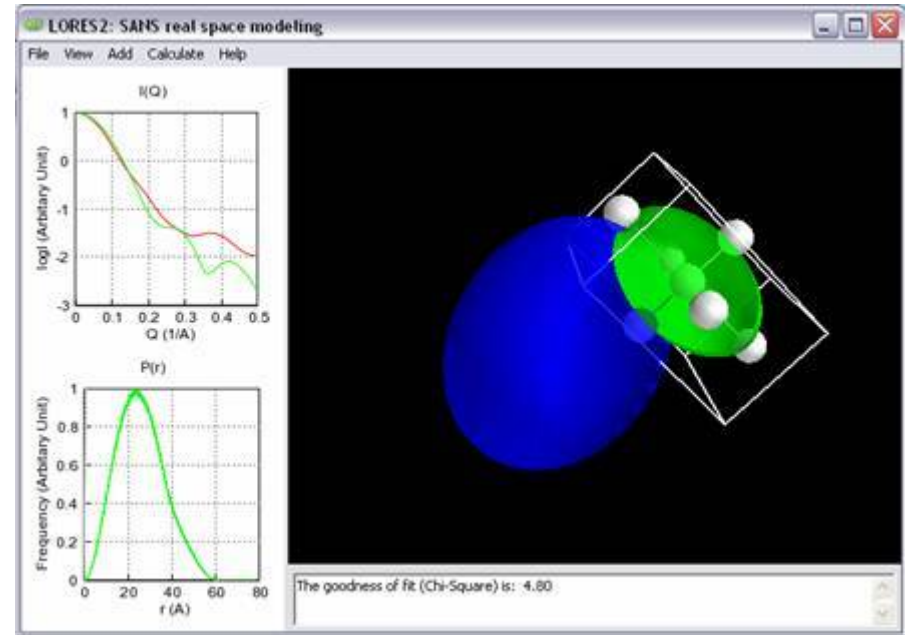
Real-space simulation

The purpose of the prototype:

1. Let the users give us feedback, requirements.
2. Explore the risks and explore design and technology issues for the GUI.

Functionality:

1. Let the user arrange shapes in 3D space.
2. Compute $I(q)$ for an arrangement of shapes in space.
3. **Oriented system (2D) simulation is now available as a C++ library or python module.**

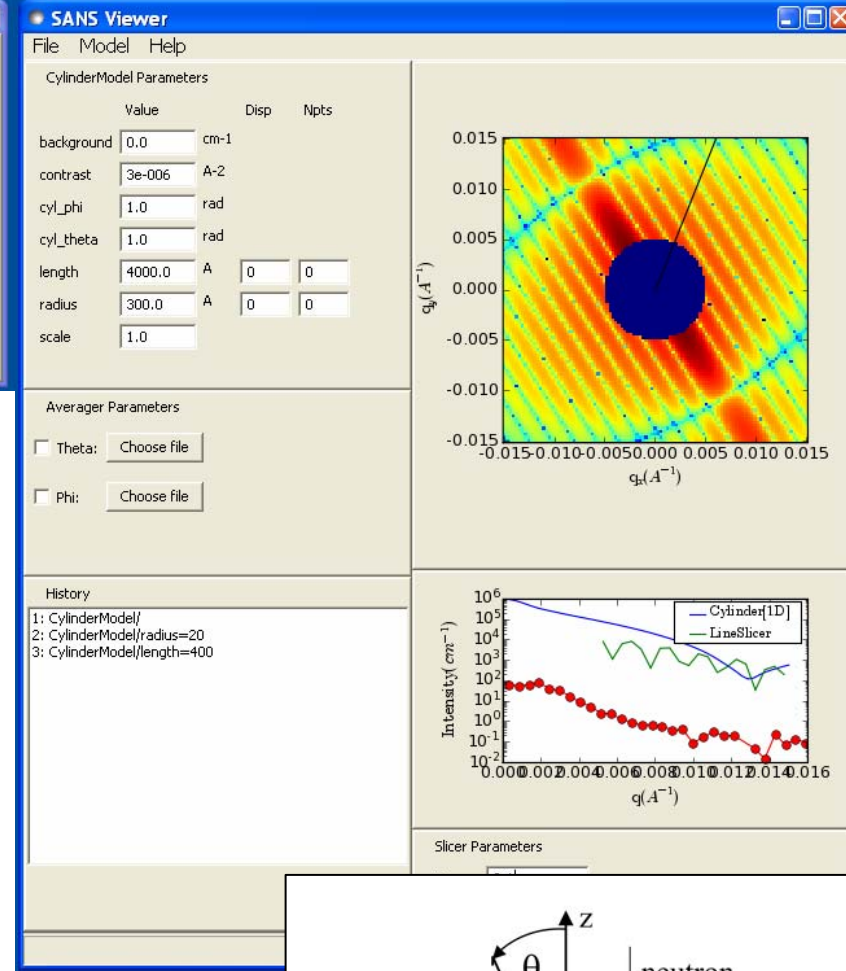
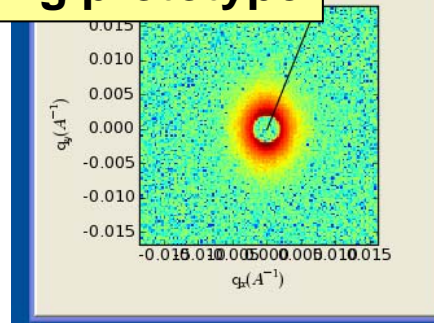


Status:

- This prototype has served its purpose and is no longer supported.
- The functionality is currently available through python modules or C++ libraries.
- The GUI will be available with our final application.

Shape-based 2D modeling prototype

An application to view shape-based oriented systems and compare their properties to data.



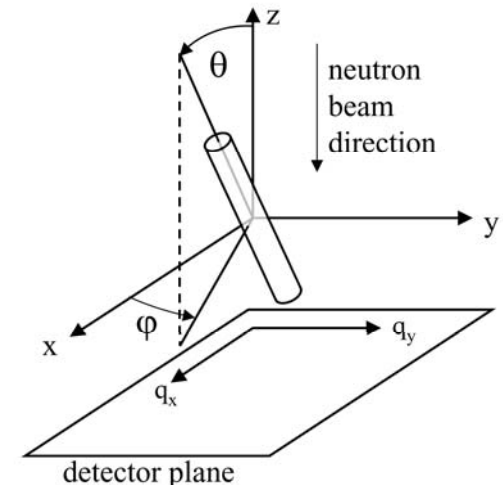
The purpose of the prototype:

- Let the users give us feedback, requirements.
- Explore the risks and explore design issues.

What it does:

- Use all the SANS 1D and 2D models coded so far.
- Polydispersity and averaging over angular distributions.
- Data comparison for slices/cuts of the 2D image.

<http://danse.chem.utk.edu/sliceview.html>



Software Development Process



- We want users and other developers to trust our software.
- We want to trust the software of other developers in the community.

- Developing good software implies having a good process.
- Each piece of functionality is treated like an independent mini-project, with a complete documented software engineering life-cycle.
- Community involvement is emphasized throughout development:
 - requirements,
 - user feedback through prototyping, ...
- **Quality Assurance** is also emphasized:
 - unit-testing, automated testing [minimize bugs]
 - validation [making sure that the outputs are correct]

Conclusion

- DANSE will be around until mid-2011.
- During that period we will progressively make our computational functionality available to the community, first with prototypes, then with real applications.
- Functionality will continue to be available in C libraries.
- Systematic approach with emphasis on testing.
- Status and prototypes are available on our public web page:

<http://danse.chem.utk.edu>