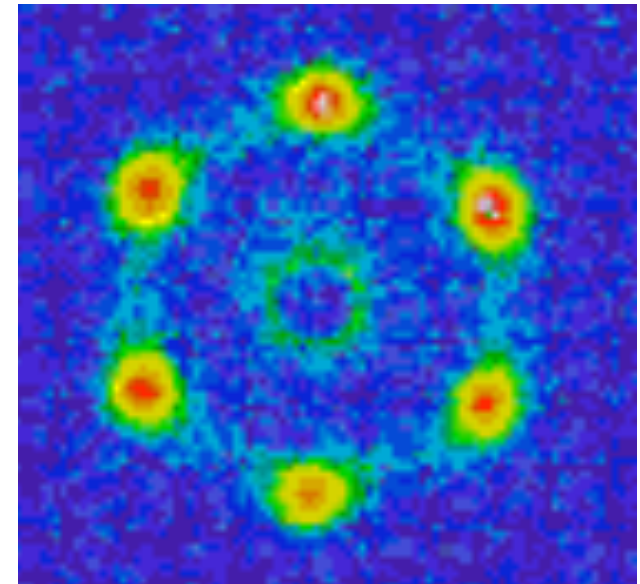
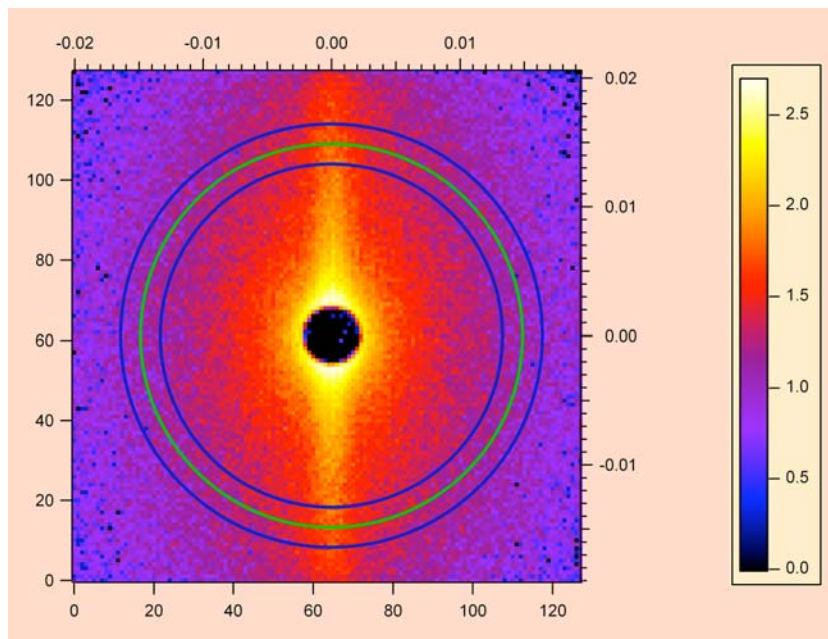


# Small Angle Neutron Scattering (SANS)

## A DANSE Subproject

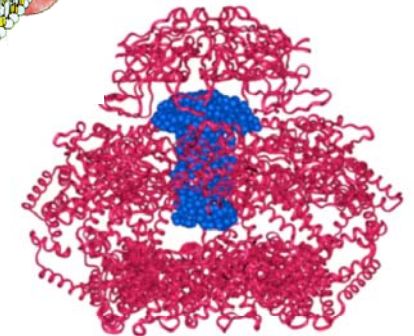
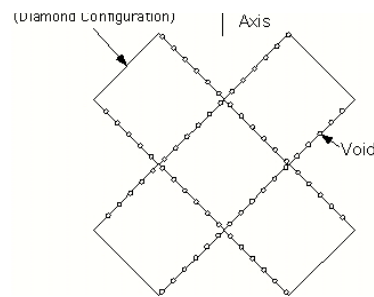
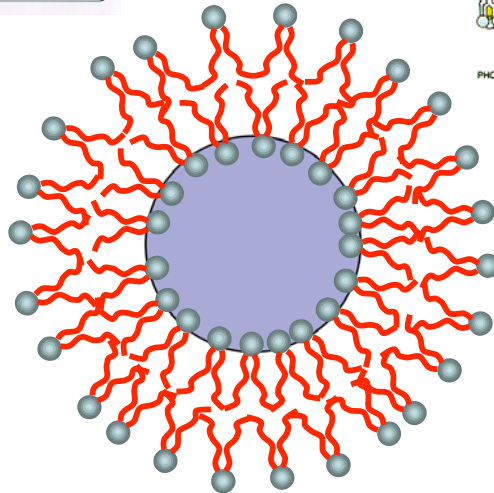
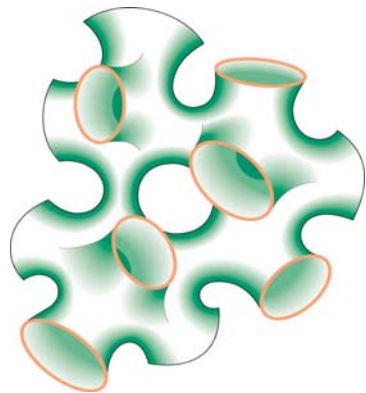
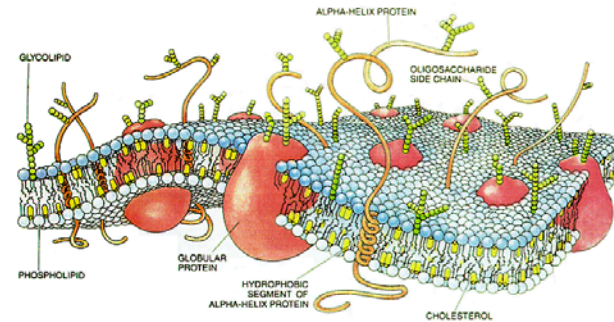
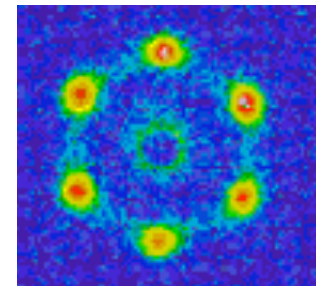
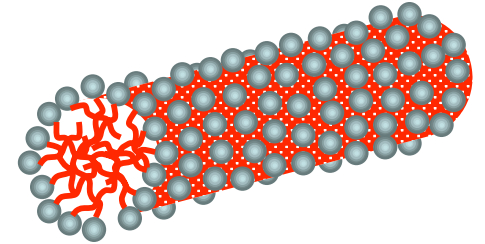
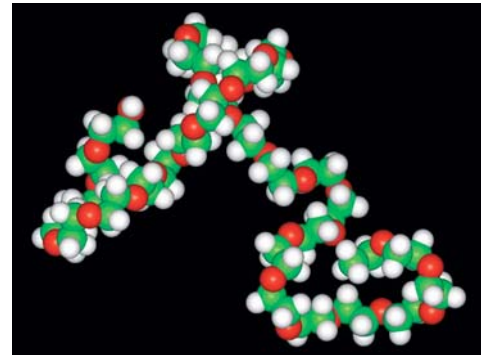
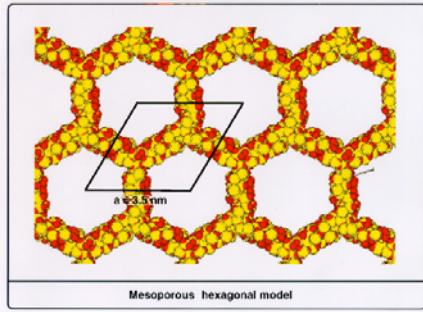


May 31, 2007 Manassas VA

A University of Tennessee  
Subproject report

# SANS measures time averaged structure of 1 - 300 nm or more

- Mesoporous structures
- Biological structures (membranes, vesicles, proteins in solution)
- Polymers
- Colloids and surfactants
- Magnetic films and nanoparticles
- Voids and Precipitates



# Challenge and Opportunity

## What are the obstacles to optimal/novel use of beam time:

- Need time to think → weak source ... or powerful and fast tools.
- Poorly planned experiment (use neutrons to do the thinking).  
Will it work? how long to count? what configurations to use? Etc?
- Lack of ability to extract information from the data

## Applications:

1. Model-Independent Analysis
2. Model Fitting Analysis
3. Experimental Planning Tools

# WBS items

1. Analytical modeling in 1D
2. Analytical modeling in 2D
3. Real space modeling 1D
4. Real space modeling in 2D
5. Non shape driven analysis
6. Series analysis and simultaneous fitting
7. Ab-Initio modeling
8. Inversion to  $P(r)$
9. Constrained fitting
10. Experimental planning and optimization tools
11. MC instrument simulations
12. Integration of MC and MD simulations
13. UI requirements gathering
14. Interface to reduction and community Software
15. Applications 1, 2 and 3 including UI
16. Documentation

# Approach

Need to balance providing new functionality early with the ability to make that functionality accessible to the end user early.

## A unique opportunity for SANS

NIST IGOR macros have had ~8 years of formal releases, complete with certification and documentation. Current release in August 2006

Vers 5.0

SANS Reduction

Vers 3.0

Analysis

Vers 2.0

USANS Reduction

\* Nearly 350 unique IP downloads/year for Analysis (most popular – followed by nearly 300 for SANS reduction)

(IGOR framework also used at Argonne SAXS, SANS, USAXS)

→ Partner with NCNR and ORNL to enable a platform for rapidly distributing DANSE functionality and reaching a large existing user base whenever feasible.

# IGOR based reduction and analysis (a digression - facility info)

## **Facilities**

2 video conferences between NCNR and ORNL

agreement in principle on both Reduction and Analysis col.

Next major release will require IGOR 6 or higher

ANSTO has expressed interest in using once HFIR data can be read

in

HANARO has expressed interest and may join actively.

## **Code**

n x m detector

restructured so that all facility/instr. specific items are in two files

waiting for ORNL to validate above

Restructuring analysis for XOP (c code) up to 10x faster

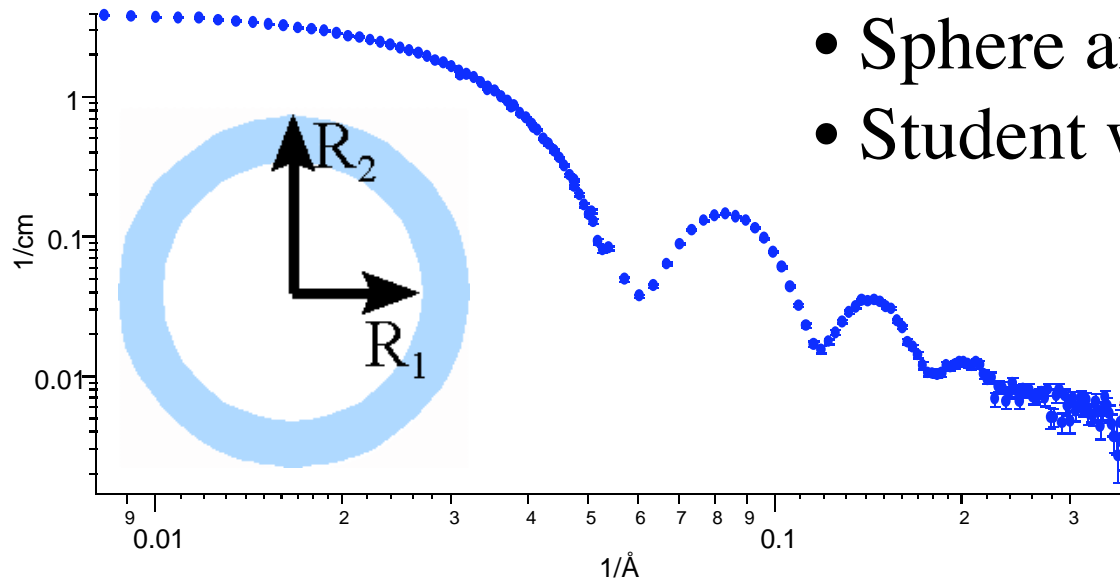
## **Plans**

document subtle details of reduction better

work closely with DANSE team on analysis and interfaces needs

# 1D Analytical tasks

- Architecture and design complete
- Sphere and rod complete
- Student will plug-in rest of models

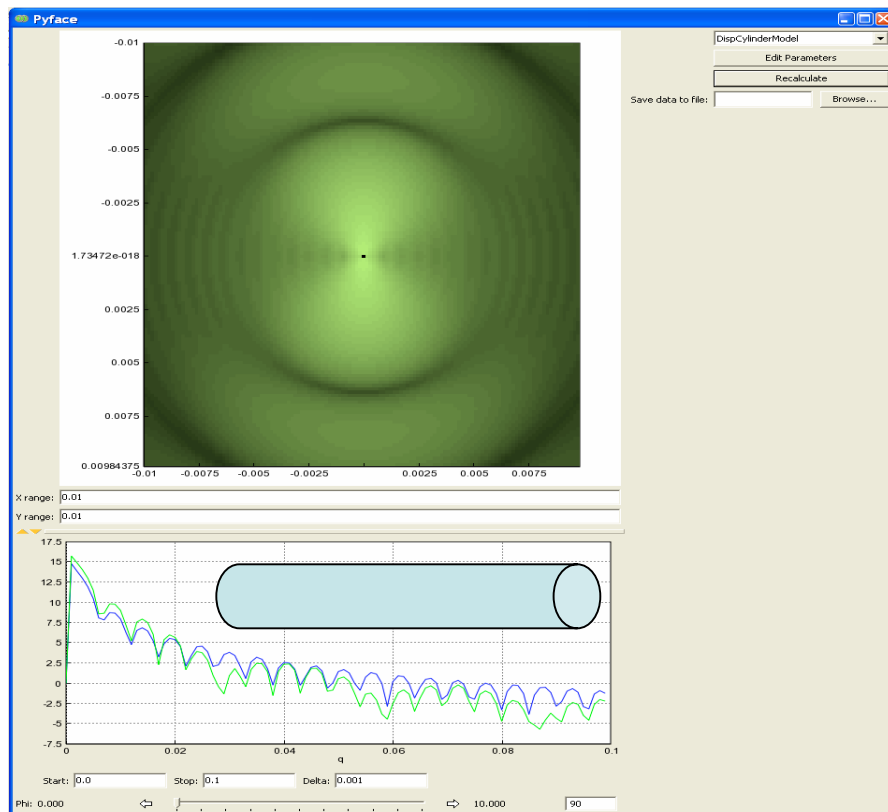


- SANS macros turned into C libraries by NCNR.
- Script written by DANSE team to help wrap them into python components.

→ 1D will be mostly “free”

# 2D Analytical tasks

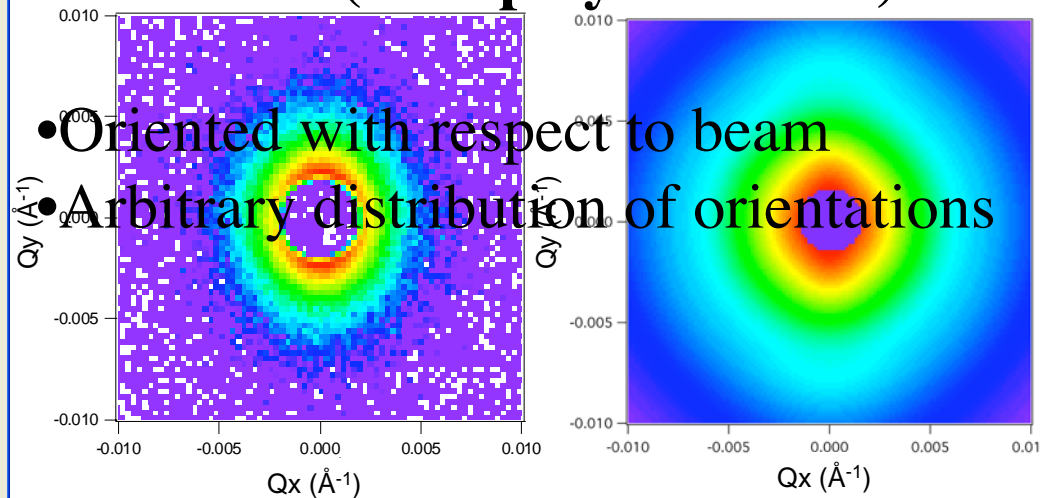
DANSE code wrapped into IGOR XOP by NCNR team. Left is Data for rodlike objects under flow visualized within IGOR environment. Bottom figure is DANSE code used from IGOR macros = First contribution from DANSE incorporated for “free” into facility code



Fibrin data (blood clot)  
courtesy D. Pozzo, L.

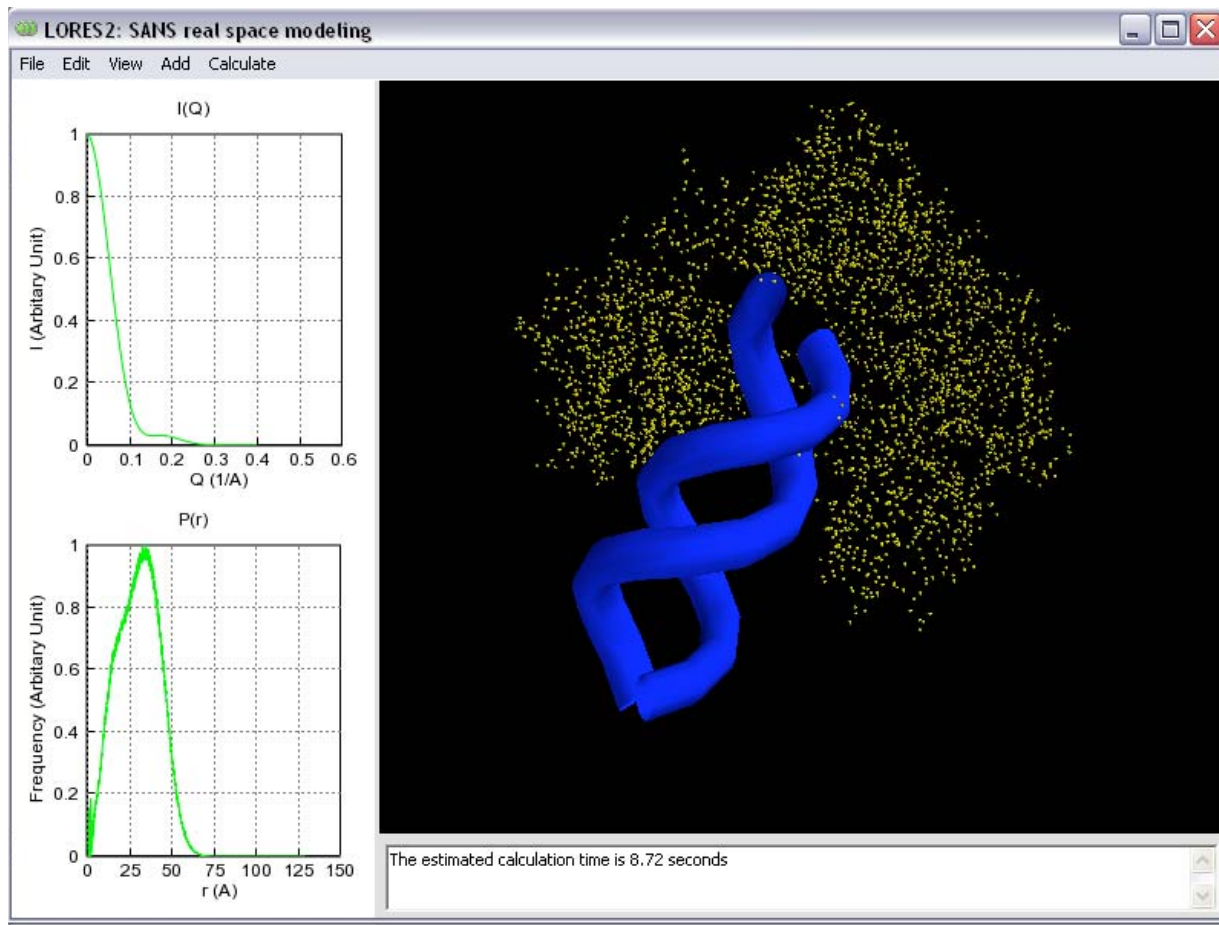
## 2D for rod (with poly diameter)

- Oriented with respect to beam
- Arbitrary distribution of orientations



Simulation  
Courtesy A.  
Jackson

# Real Space Simulation



- 4 available shapes:
  - Sphere
  - Cylinder
  - Ellipsoid
  - Helix
- 3D graphical placement
- text box placement
- compare to real data
- PDB reader/writer
- Calculate with mixed PDB and shape

Prototype release on track for June 24 Colloid symposium

- Windows install
- distribute on CD at poster (also available on website)
- feedback button

# Documentation availability

The screenshot shows a Windows Internet Explorer browser window displaying the Trac documentation page for the DANSE SANS group. The browser's address bar shows the URL <http://danse.us/trac/sans/>. The page features the Trac logo (a red paw print) and the text "trac Integrated SCM & Project Management". A navigation menu includes links for "Wiki", "Timeline", "Roadmap", "Browse Source", "View Tickets", "New Ticket", and "Search". Below the menu, there are links for "Start Page", "Title Index", "Recent Changes", and "Page History". The main content area is titled "Welcome to DANSE SANS group" and contains several sections: "News Items" with a link to "List of all new items"; "Current Tasks" with a list of tasks including "8.2.2: Basic 1D Modeling", "8.2.3: Basic 2D Modeling", "8.3.1: Real Space Models", and "8.4.1.4: Model Fitting Analysis UI"; "Meetings" with a link to "Weekly Meetings"; "Monthly Project Highlights" with a list of months from "April 2007" to "January 2007"; and "Templates" with a list of templates including "Requirements Document", "Use Cases", and "Architecture". A search box is located in the top right corner, and a "Search" button is next to it. The browser's status bar at the bottom shows "Internet" and "100%" zoom.

sans - Trac - Windows Internet Explorer

<http://danse.us/trac/sans/> Live Search

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sans - Trac

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Integrated SCM & Project Management

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## Welcome to DANSE SANS group

### News Items

- [List of all new items](#)

### Current Tasks

- [8.2.2: Basic 1D Modeling](#)
- [8.2.3: Basic 2D Modeling](#)
- [8.3.1: Real Space Models](#)
- [8.4.1.4: Model Fitting Analysis UI](#)

### Meetings

- [Weekly Meetings](#)

### Monthly Project Highlights

- [April 2007](#)
- [March 2007](#)
- [February 2007](#)
- [January 2007](#)

### Templates

- \* [Requirements Document](#)
- \* [Use Cases](#)
- \* [Architecture](#)

News Items  
Current Tasks  
Meetings  
Monthly Project Highlights  
Templates  
Useful links

Internet 100%

NCNR SANS Software

Welcome to the Trac site for NCNR SANS Software

This wiki and subversion repository browser are for software developed and managed by the SANS group at the NIST Center for Neutron Scattering.

The NCNR has a long history of providing easy to use data reduction and analysis tools to its users. In the case of the SANS and USANS instruments, this is through a set of macros and functions implemented using the IGOR Pro™ package from Wavemetrics Inc, which is a general purpose plotting and data analysis package with a rich in-built programming language.

With the advent of the NSF funded DANSE Project, which aims to build a complete suite of neutron scattering data analysis tools, and the opening of new neutron scattering user facilities at the Oak Ridge National Lab (HIFR cold source), ANSTO in Australia (OPAL reactor) and KAERI in South Korea (HANARO cold source) we are taking the opportunity to evaluate the packages we provide.

This has led to two initiatives. The first of these is collaboration with the above mentioned facilities to produce a shared code base of IGOR procedures for the reduction and analysis of small angle scattering data. This will provide to users a familiar environment whichever facility they use and make co-analysis of data from different facilities simpler.

The second initiative is to convert as much of the IGOR procedure code – which is written in an IGOR specific language and compiled within the IGOR program – to a generic library written in C. This separation of the graphical components from the analysis routines (scattering form factor and structure factor calculation, resolution smearing of models to match instrument geometry) provides both speed of calculation benefits and collaborative benefits. The former is important for co-fitting of multiple datasets (varying contrast, concentration, temperature etc) with complex models and initial testing suggests we can gain up to a 10-fold increase in computation speed. The latter is important because by abstracting out the actual computation code we can more easily make use of code from other sources – in particular we are working with the DANSE SANS subproject to define common interfaces to our libraries so that we can utilize each others work.

These initiatives are aimed at enhancing the tools available to our users in order to permit faster, more complex analyses of their scattering data than are currently possible.

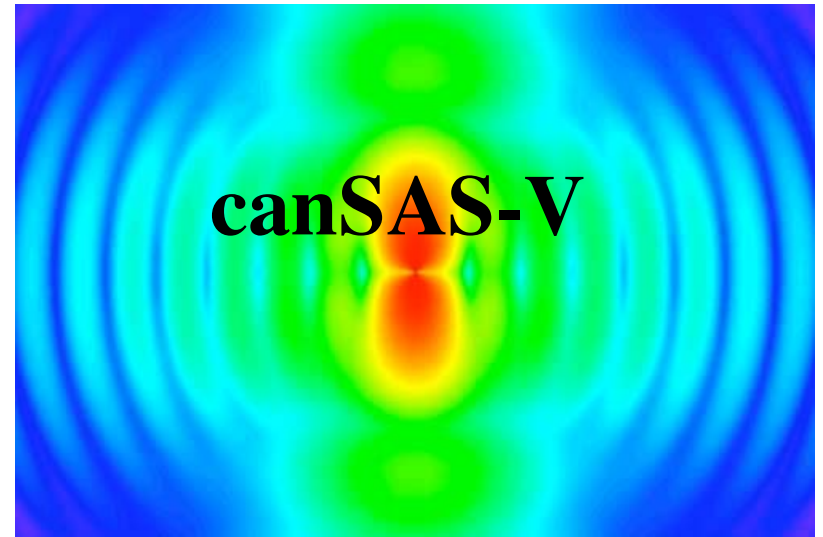
Contained here currently are links to release versions of:

- [SANS and USANS Data Reduction macros for IGOR Pro](#)
- [USANS Data Reduction macros for IGOR Pro](#)
- [SANS and USANS Data Analysis macros for IGOR Pro](#)

- NCNR has also recently adopted TRAC and SVN for managing its IGOR development.
- The SANS DANSE group has agreed to host the server at UTK as they migrate from a totally NCNR project to a joint development project with ORNL and others.

# Staffing and future

- 2 primary full time developers
  - Jing Zhou
  - Mathieu Doucet
- Summer grads and undergrads planned



June 24, 2007

Prototype release of real space modeling

October 28-31

CANSAS meeting

Jan 2008

Prototype release of model fitting

Coming year

IGOR interface defined for distribution of libraries

Finish 1&2D real space and analytical

Constrained fitting

$P(r)$