GSC Refactoring

Generic Scattering Calculator

SLD Data File

Nuclear Data | No File Loaded | Load

Magnetic Data | No File Loaded | Load

Shape | Rectangular | Draw

Input Parameters

Polarisation Settings

In Polarisation (fraction up) 1.0

Out Polarisation (fraction up) 1.0

Up Polarisation Direction, θ 0.0 °

Up Polarisation Direction, φ 0.0 °

SLD/Geometry Settings

Background 0.0 cm⁻¹

Scale 1.0

Solvent SLD 0.0 Å⁻²

Total volume 216000.0 Å³

Q Range

No. of Qx (Qy) bins 30

Qx (Qy) Max 0.3 Å⁻¹

Qx (Qy) Min -0.3 Å⁻¹

Log Spacing

Radius of Gyration

Rg - Mass No Data

RG - SLD No Data

Plugin Models

Export Model

Fixed orientation

Compute | Reset | Close | Help

SLD Pixel Info

No. of Pixels 1000

Mean SLD

Mx 0.0 Å⁻²

My 0.0 Å⁻²

Mz 0.0 Å⁻²

Nucl. 6.97e-06 Å⁻²

Draw Points | Save SLD Data

Nodes

x 10

y 10

z 10

Step Size

x 6 Å

y 6 Å

z 6 Å

Coordinate System Info

Environment Coordinates (uvw)

Yaw 0.0 °

Pitch 0.0 °

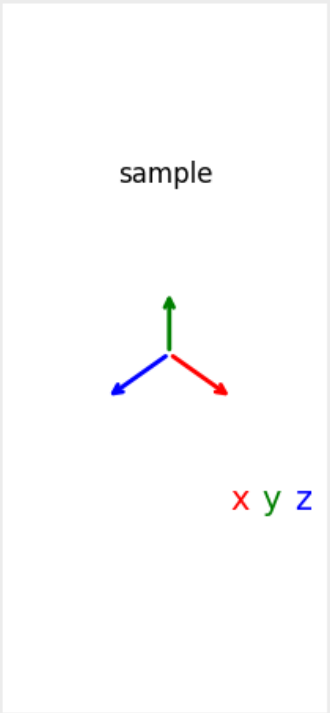
Roll 0.0 °

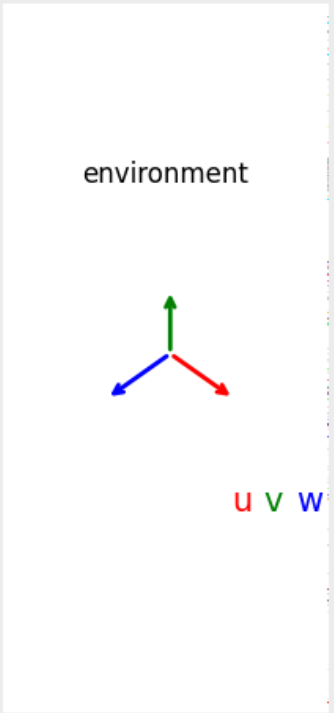
Sample Coordinates (xyz)

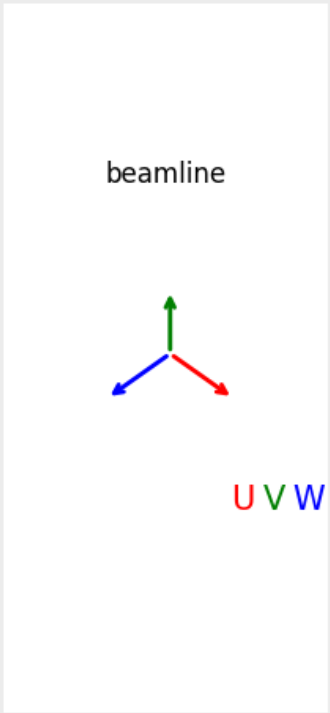
Yaw 0.0 °

Pitch 0.0 °

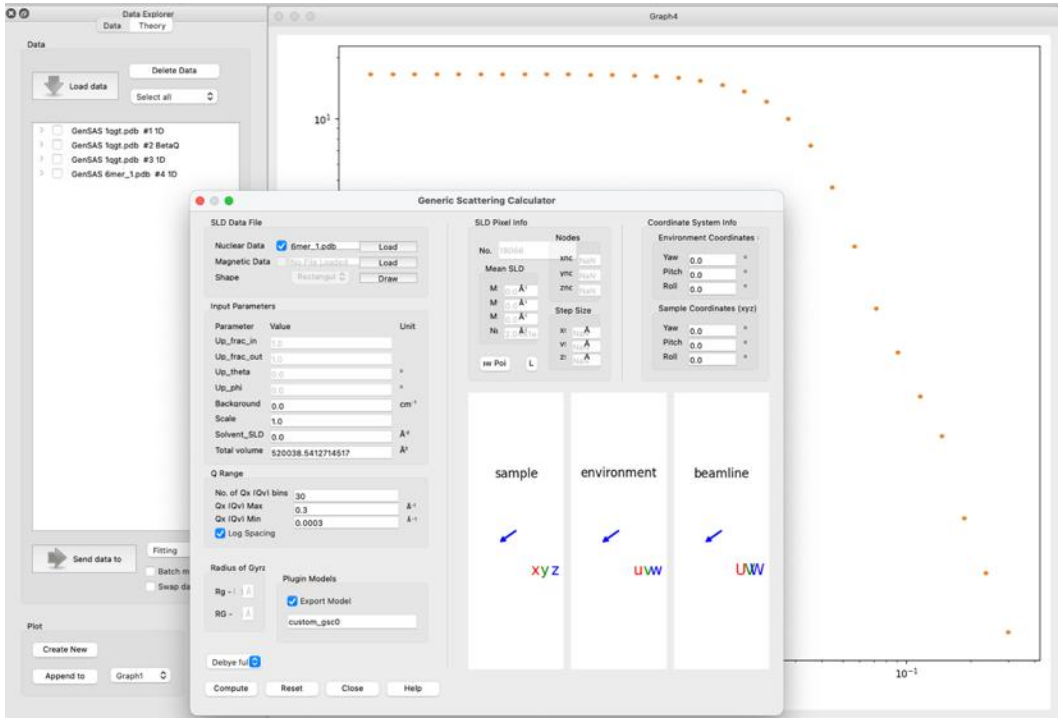
Roll 0.0 °

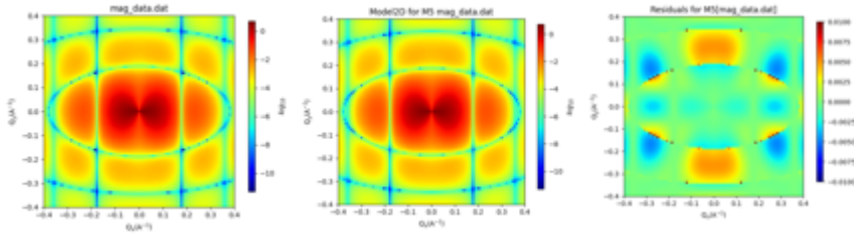






Generic Scattering Calculator





Magnetic/polarized SANS

- Generic Scattering Calculator supports magnetic/polarized SANS
- Coordinate data in VTK formats supported

Interacting bio-molecules

- Generate scattering profile from PDB file
- Save as a custom/plugin model
- Use for fitting with structure factors (including beta approximation)
- PDB reader and engine refactored

Validation of electron-microscopy maps using solution small-angle X-ray scattering
Kristian Lytje and Jan Skov Pedersen, Volume 80| Part 7| July 2024| Pages 493-505

Workflow Summary Table

#	Workflow Name	Data Input	Mode	Output
1	**Fixed-Nuclear**	Nuclear only Grid/Elem	Mode 0	2D I(qx, qy)
2	**Fixed-Magnetic**	Magnetic only Grid/Elem	Mode 0	2D I(qx, qy) + Magnetic
3	**Fixed-Both**	Nuclear + Magnetic Grid/Elem	Mode 0	2D I(qx, qy) + Both contrib
4	**Fixed-Default**	No files Grid only	Mode 0	2D I(qx, qy)
5	**Debye-Average**	Nuclear only Grid only	Mode 1	1D I(Q) + Plugin*
6	**Debye-Beta**	Nuclear only Grid only	Mode 2	1D I(Q) + β(Q) + Plugin*

Calculation engines

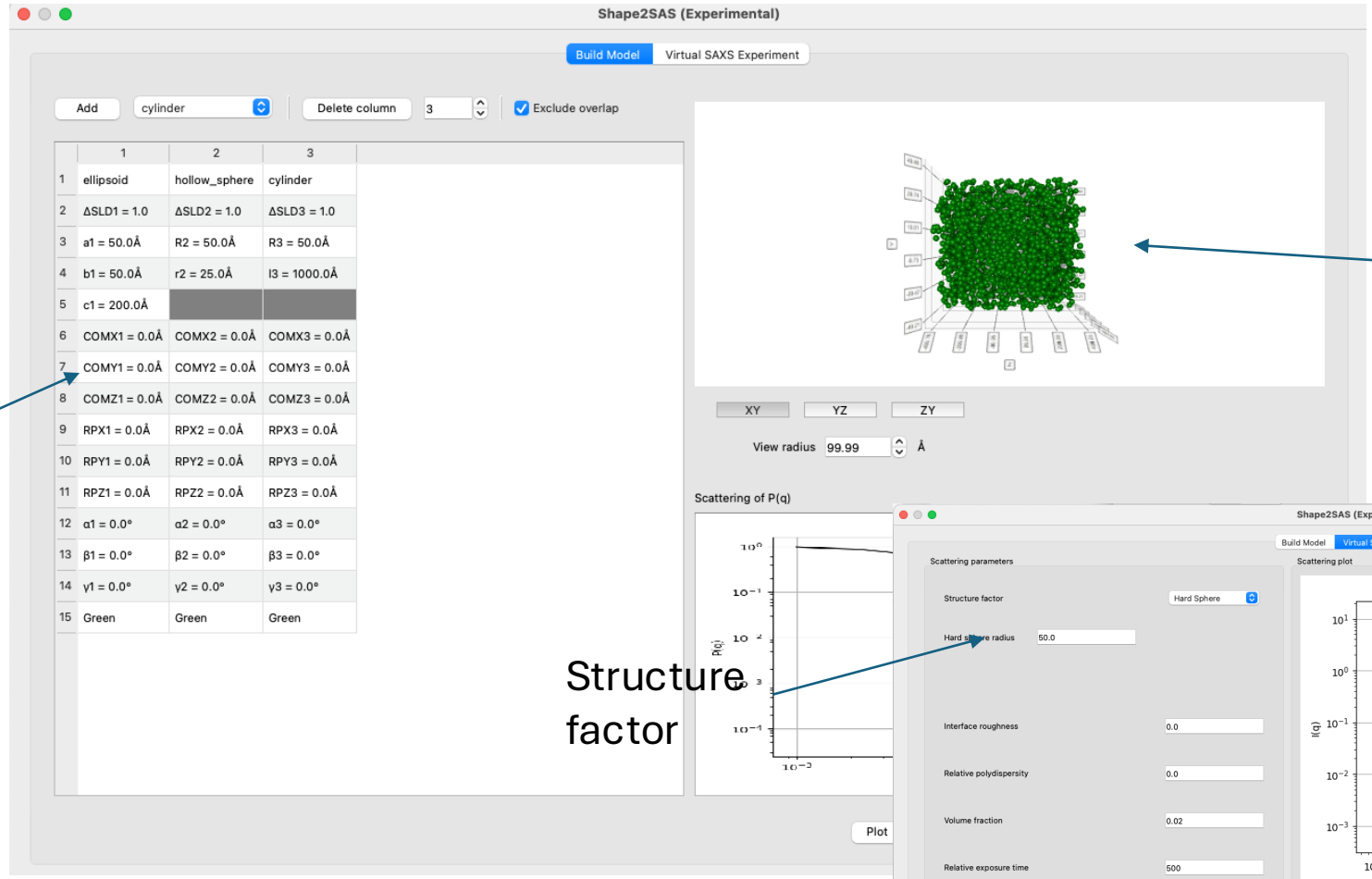
Calculation modes (cbOptionsCalc)

Mode	Index	is_avg	is_beta	Output	Available For
Fixed Orientation	0	False	False	2D I(qx, qy)	All data types
Debye Full Average	1	True	False	1D I(Q)	Nuclear only, grid type
Debye + β(Q)	2	True	True	1D I(Q) + β(Q)	Nuclear only, grid type

Constraint matrix

Data Input	Fixed Orientation	Debye Average	Debye + β(Q)
Nuclear Only	✅	✅*	✅*
Magnetic Only	✅	❌	❌
Nuclear + Magnetic	✅	❌	❌
Default Grid	✅	✅	✅

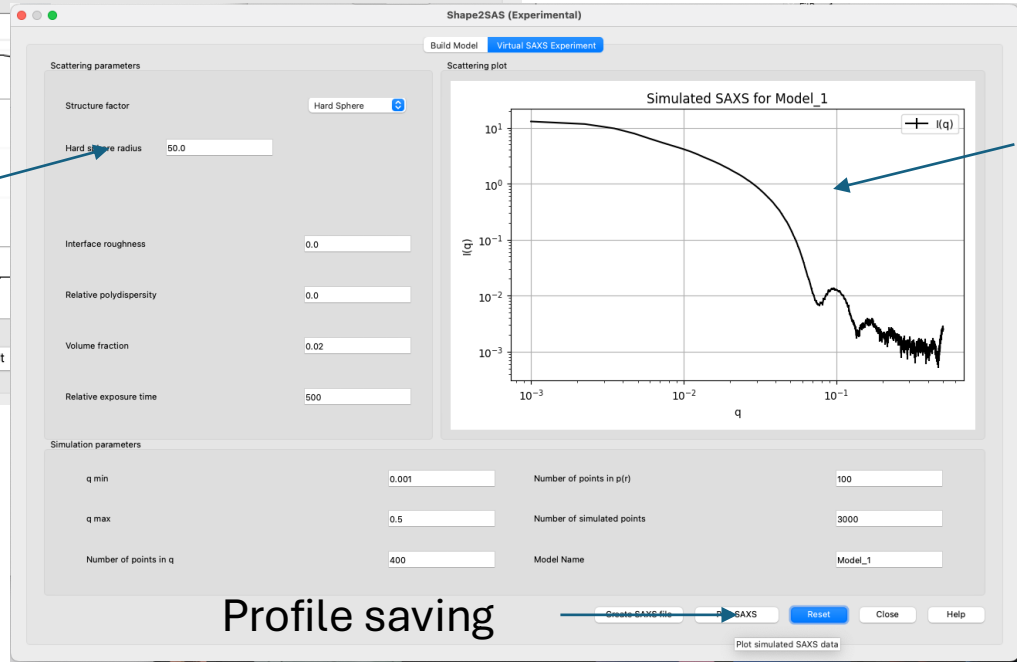
Shape2SAS



Shape definition

Shape visualization

Structure factor



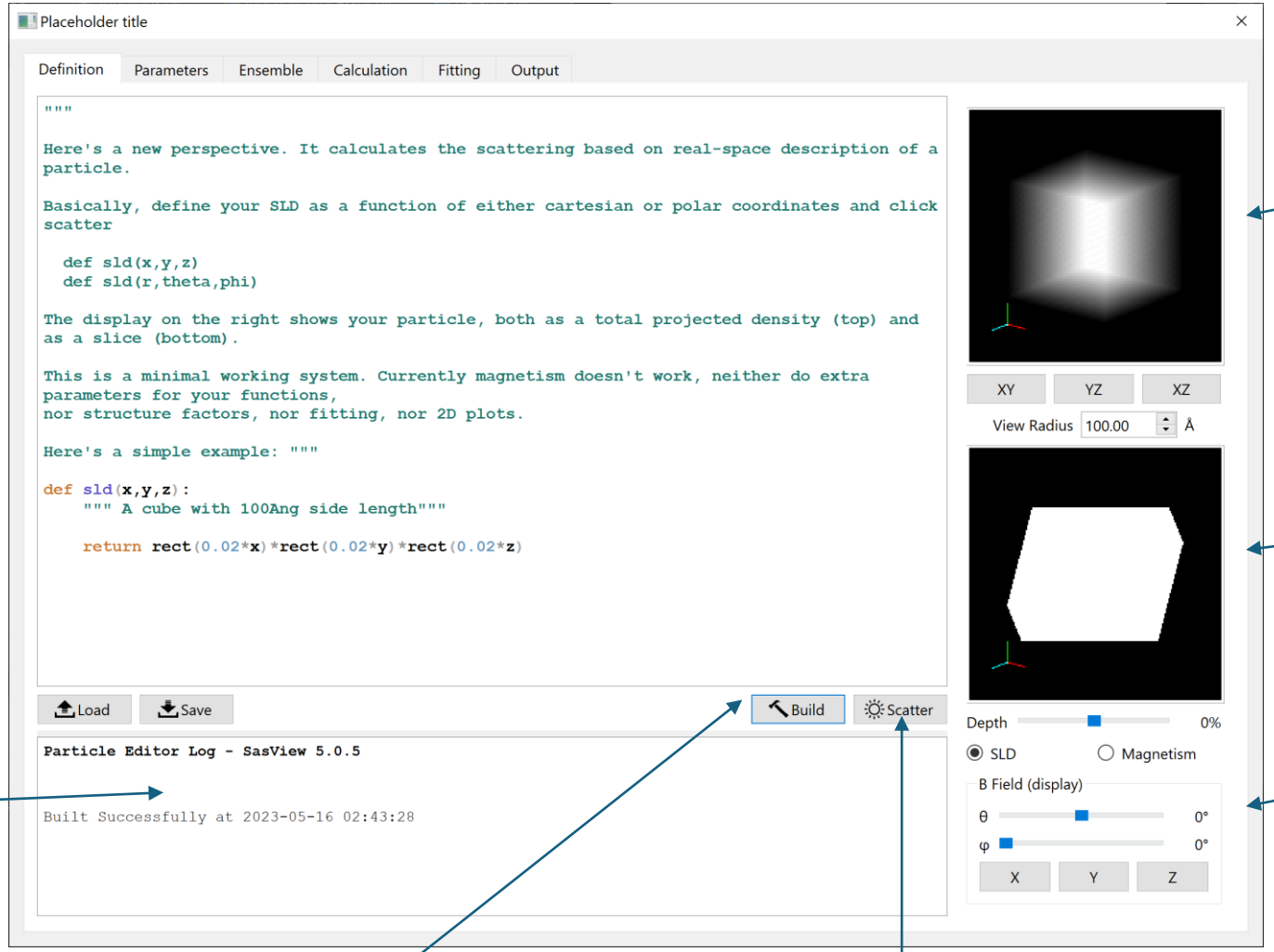
Scattering profile

Profile saving

Shape2SAS: a web application to simulate small-angle scattering data and pair distance distributions from user-defined shapes.

Andreas Haahr Larsen,[a*] Emre Brookes,[b] Martin Cramer Pedersen[c] and Jacob Judas Kain Kirkensgaard[c,d]

Features beyond 6.0.0 - particle editor



Define functions sld and (optionally) magnetism

sld / magnetism "x-ray" projection

sld / magnetism cross section

Feedback on code and calculations

Magnetic field controls for display

"Recompile" and update display

Compute scattering

GSC on GitHub

- #3676 — Resolve weakness in the Generic SANS Calculator tool
- Discussion #2351 — Weakness in the Generic SANS Calculator tool
- #1847 — Weakness in the Generic SANS Calculator tool
- #1400 — Generic scattering calculation is incorrect for orientation-averaged asymmetric particles
- #596 — Generic Scattering Calculator Enhancements: make a theory curve
- #597 — Generic Scattering Calculator Enhancements: integrate into fitting
- #598 — Generic Scattering Calculator Enhancements: accept MD trajectory files
- #2011 — Extend generic scattering calculator with tabs for other simulators
- #2552 — Generic Scattering Calculator GUI needs redesign
- #2734 — GSC not drawing the structure
- #2798 — Saving Project with the general scattering calculator throws an error
- #2537 — Log spacing for Generic Scattering Calculator
- #1886 — “Save SLD Data” saves rows/columns the wrong way around

A few options moving forward

- Refactor the current interface
- Move out from Tool to Perspective
- Send any data to any Tool or Perspective

Potential next step

- Identify the working group
- Develop strategy/roadmap moving forward
- Engage Users for early feedback
- Implementation loop (including users’ feedback)

GSC Refactoring

Part II

Generic Scattering Calculator

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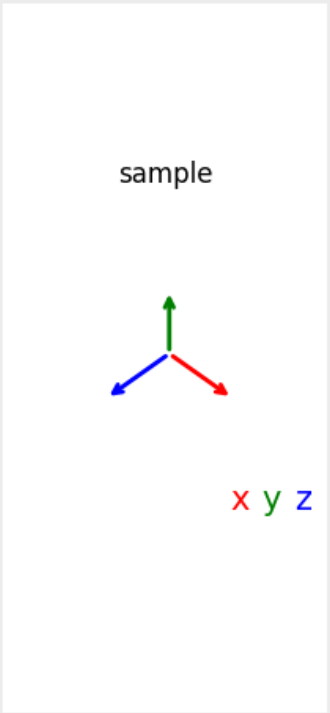
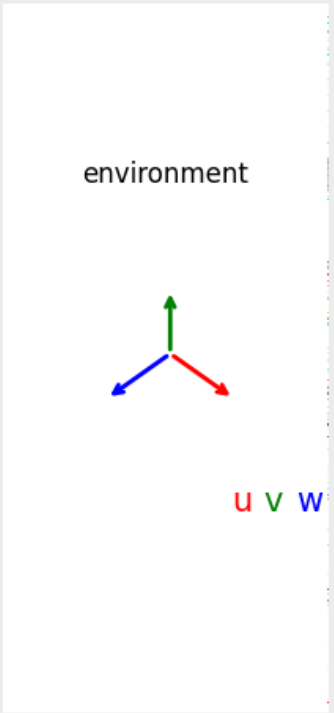
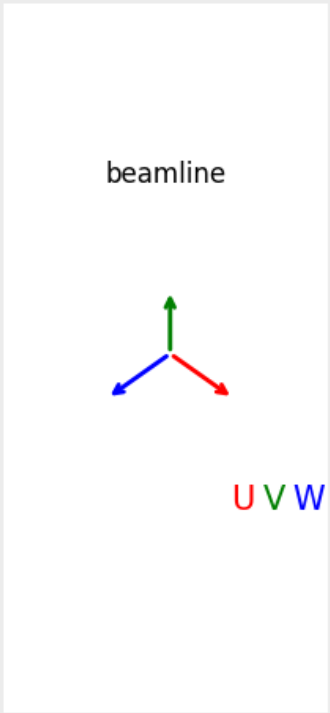






Conclusion from the previous meeting

We will try to look at:

1. Entry layer (molecule type, magnetic data, volume/normalization)
2. Modality (magnetic soft matter, bioSAS, etc.)
3. Calculation engines (pluggable backends)

What is the target group?	**What information/functionality are they looking for?**
Why do they want to find this information?	How do we know it?

What is the target group?

PhD Students, Postdocs, PIs

Instrument (Data) Scientists

Industrial Users?

What information/functionality are they looking for?

How the scattering pattern of my system look like?

Why do they want to find this information?

To explain their data

To better plan the experiment

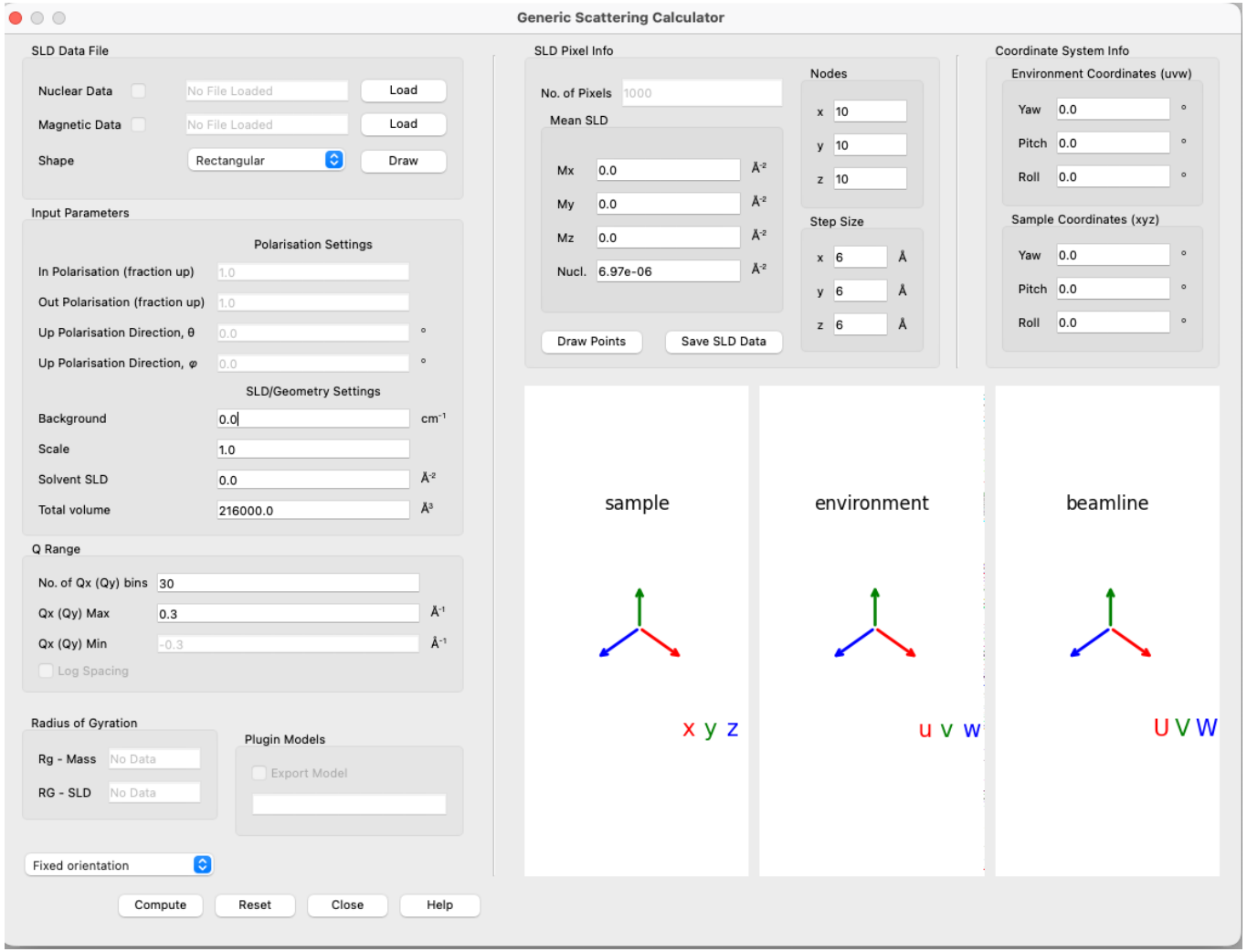
How do we know it?

Because we used it this way

Because we heard from the users

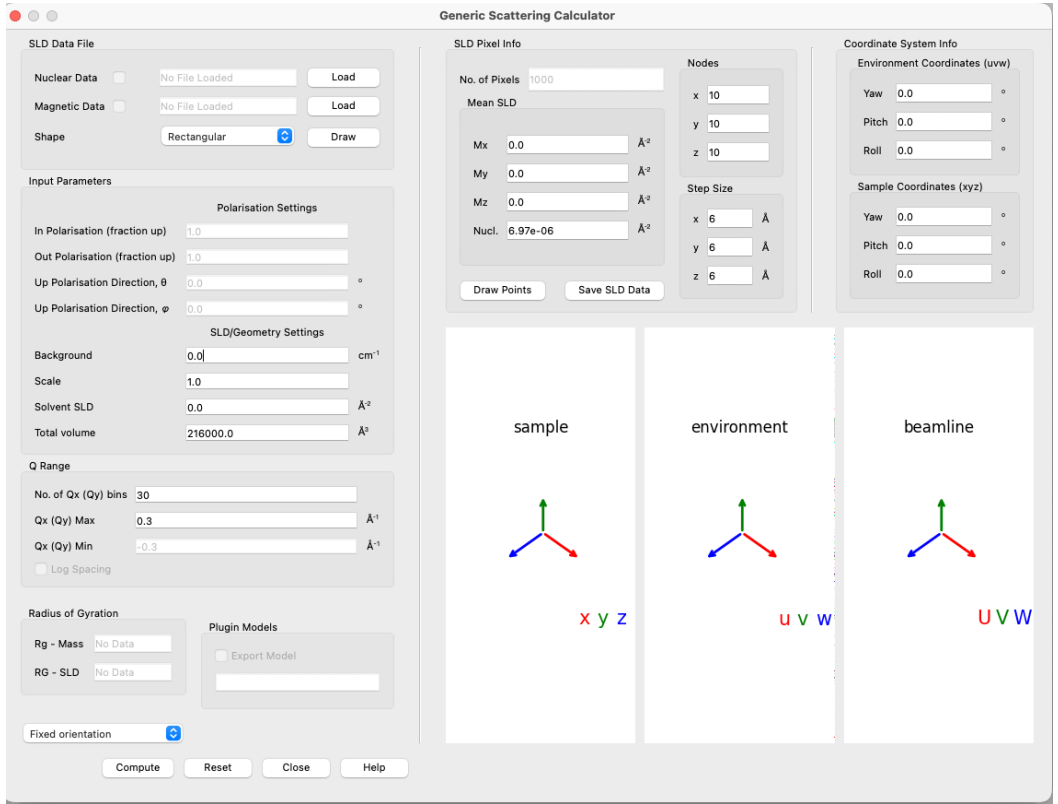
Map the current UI to layers

1.Entry layer (molecule type, magnetic data, volume/normalization)
2.Modality (magnetic soft matter, bioSAS, etc.)
3.Calculation engines (pluggable backends)



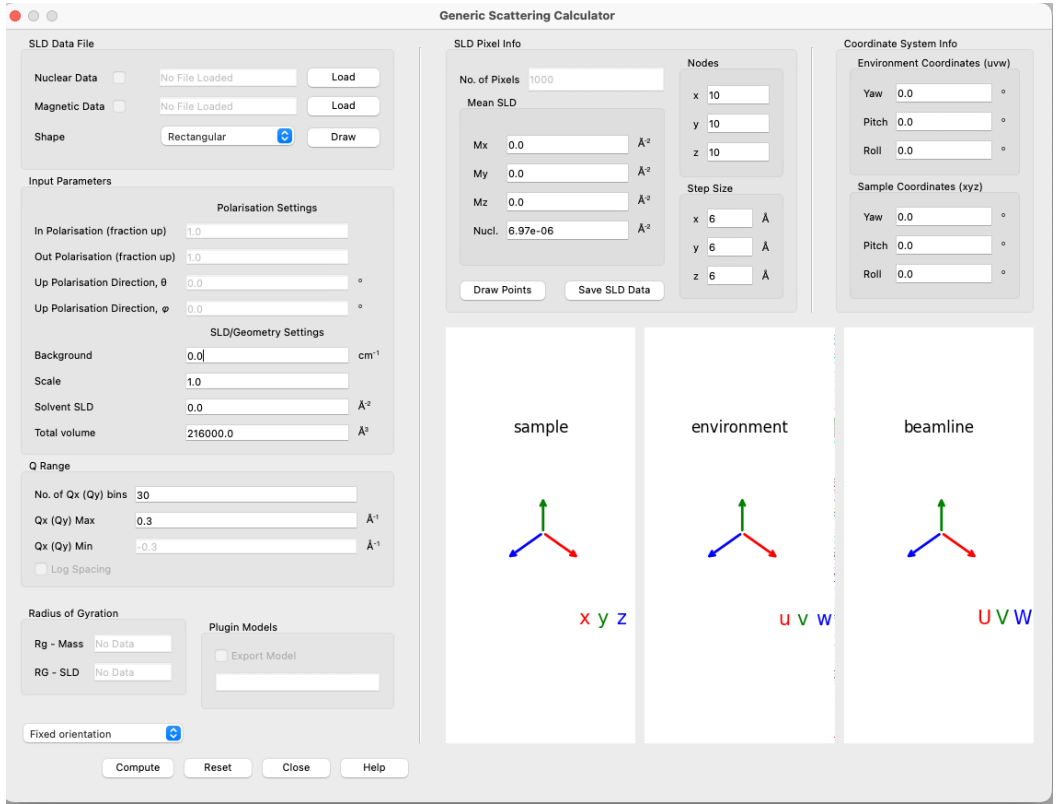
Entry Layer

- What are the mandatory fields to compute anything?
- What fields are optional but should be strongly recommended?
- What should be inferred from files vs explicitly set by user?



Modality

- What outputs does each modality need (I(q), I(qx,qy), 2D/1D)?
- Which controls are common across all modalities (q-range, scale/background?) and which are modality-only (polarization, spin channels)?



Calculation Engines

- What is the smallest common denominator engine interface?
- Which options belong to the engine vs modality vs entry?
- How do we represent engine capabilities so UI can enable/disable controls?