

SAXS breakout session summary

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Call-in: Quan Hao (Cornell/CHESS), Joanna Krueger (UNCC), Pat Loll (Drexel)

Overall Assessment

- The group recognize the need for multiple beamlines to cover different aspect of life science, but agree that the white paper should be focused on solution scattering.
 - Rapidly increasing demand
 - Lack of representation at NSLS
- Two beamlines
 - High throughput: 10^{12} ph/s desired, 3PW + ML mono
 - High brightness: shared ID beamline w/ PX or soft matter???
 - Time to change-over vs. staff support: depends on what samples will be studied
 - Slower dynamics (ms - s) is important (e.g. enzyme activity)

Technical development

- Simultaneous SAXS/WAXS
 - Users get additional information from the same samples; facility save effort and time in change-over
 - BioCAT and X9 are both working on this
- Software
 - Alternative to Svergun's black boxes: CCP4-like open source software suite
 - How to deal with mixtures
 - Cooperative data analysis with other experimental data (e.g. NMR)
 - Structure depository
- Should revisit contrast variation / anomalous SAXS now that high-quality data is easy to get (small differences?)
 - Membrane protein (detergent)
 - Inter-atomic vectors for PX

Supporting infrastructure

- Common LOB with protein production capability
- Non-X-ray protein characterization at the beamline
- High throughput sample handling
 - High throughput sample handling also require high throughput data processing and analysis
 - Beamline staff must be knowledgeable: staff have their own research
 - Should learn from protein crystallization about sample handling
 - Sample format: micro well-plates are standard, PCR tubes on the same pattern

Transition

- Whitepaper should emphasize community development
 - Encourage use of solution scattering
 - Regional aspect is important
 - Support, support, support
 - New users may not want go through the learning process, but rather want it as a service
- Build new beamline as soon as possible
 - One workhorse solution scattering sufficient?
 - Big (capacity) users? Structural genomics?

Synergy

- Footprinting
 - Good complementary information
 - Not necessary/possible to get the information from the same sample
- XAS
 - Good to have as for PX?
 - May be not. SAXS too global, XAS too local.
- PX
 - Low resolution envelope to help phasing (Quan Hao, CHESS)
 - SAXS studies of crystallization
 - Quality control for membrane protein purification? (Mark Dumont, Rochester)