Multiprobe and Multimodal Analysis

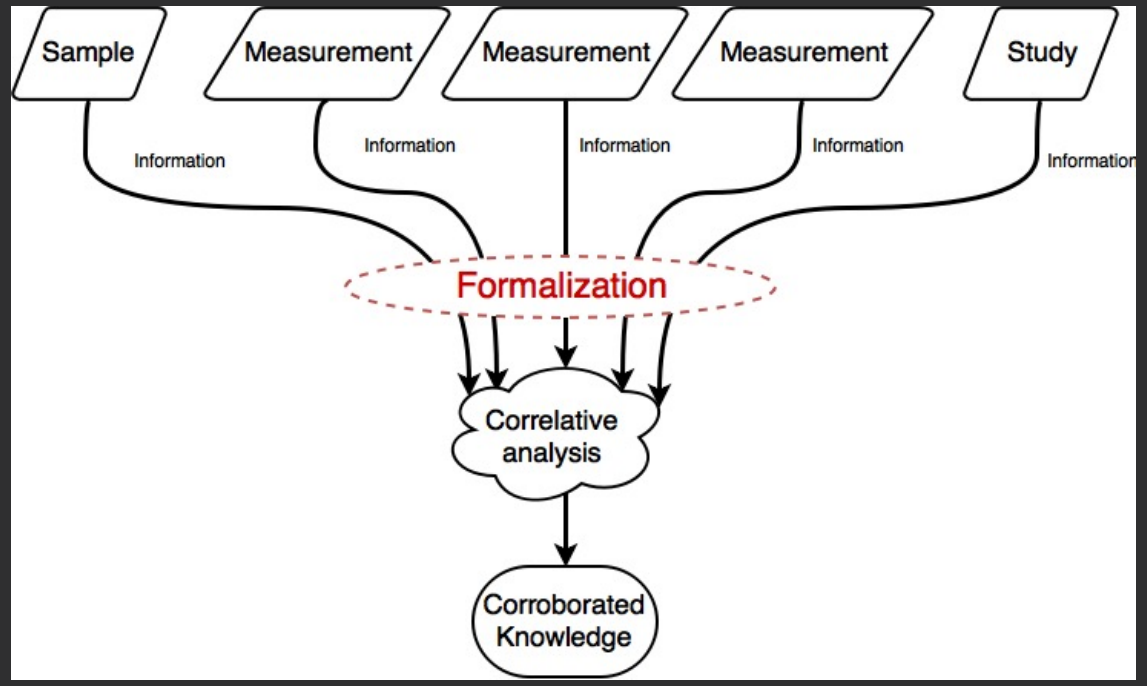
Tim Snow – September 2022

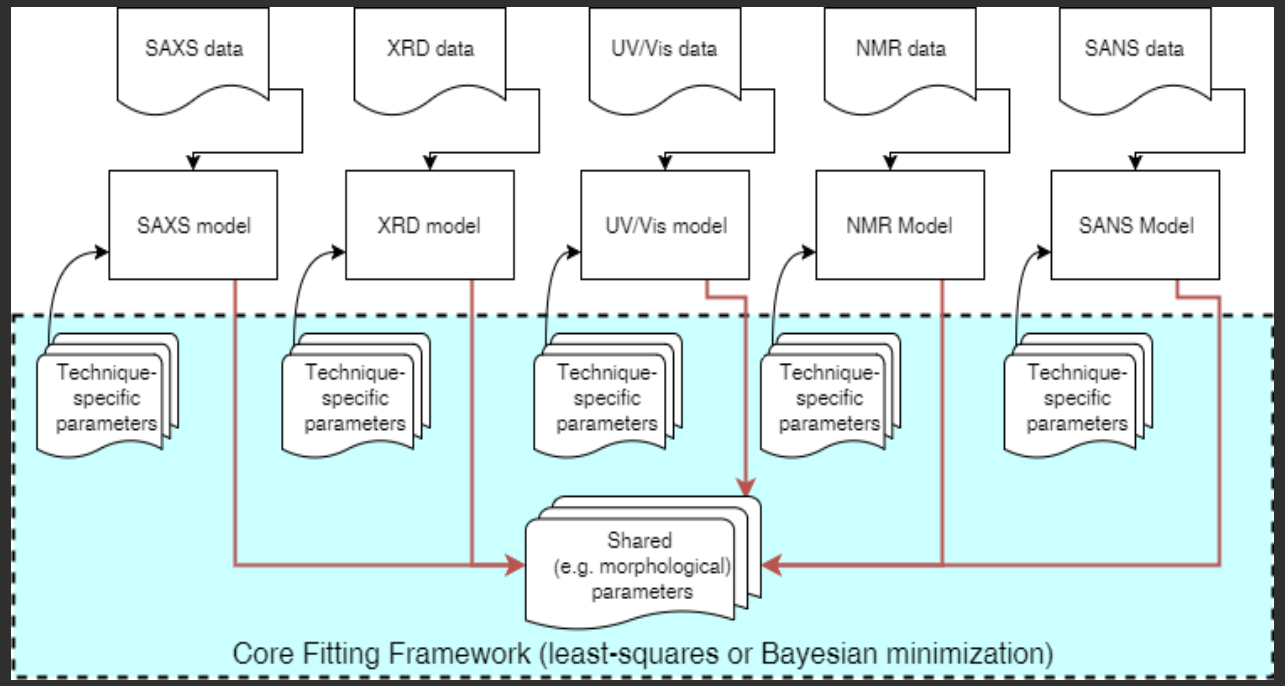
Discussion Topics

- Co-refinable dataset analysis
- Same sample: multiple detector locations
- Visualisation and fusion of correlated datasets

Combining Everything: Developing Rigorous Pan-Metrological Correlative Analyses

- COST Action proposal, Pan-CORAL, in 2018 – led by Brian Pauw
- 15 European supporters, 1 US supporter
- Did not receive funding





Co-refinable Dataset Analysis

Start Smaller – SAXS & SANS

- Pan-CORAL is a big idea but canSAS should be able to help the community with the co-refinement of SAXS and SANS data
- Software exists to co-refine data, *e.g.* SasView
- Establishing a viable methodology would be useful
- Uncertainties in both I and *q* are essential:
  - How to transition the SAXS community to always providing uncertainties in I and *q*?
  - Always assume a baseline of uncertainty unless values specifically given?
- Weighting of χ^2 values in a co-refined fit
  - How to determine weights?

Same Sample:
Multiple Detector Locations

Multi-detector Beamlines

- Beamlines with detectors at different sample-to-detector distances are common now
  - How best to deal with co-refining / merging of datasets
  - Multiple NeXus entries for different detector plates?
- Beamlines with multiple types of detector are also becoming more common (*e.g.* SAXS & XRF)
  - Currently independent result interpretation
  - In future co-refinement of different types of data?
  - How to weight datasets?
  - Elucidation of new information possible?

Visualisation and Fusion of Correlated Datasets

Visualisation and Fusion of Datasets

- Overlaying of different datasets is the current ‘state of the art’
  - Can this be improved?
- Visualisation of high dimensionality datasets
  - What can we do with displaying correlated overlays
  - Volume rendering?
  - Visualisation of uncertainties in volumes?
- Fusion of datasets
  - NXcanSAS datasets alongside NXfluro inside the same NeXus file for example
  - How to best show correlated results
  - Timestamping and frame alignment

Discussion

Discussion Principles

- ☑ Define what we're looking for in fuzzy principles
  - ⚠ Steer clear from drilling down into the details: high level principles please
- ☑ Review the current 'state of the art' – if there is one
  - ⚠ Try to think if these could be built upon / repurposed
- ☑ Identify people to lead working groups for areas where progress could be made
  - 🔥 Avoid overcommitting
    - 🧨 If in doubt volunteer Andrew Jackson