Welcome

AUSTRALASIAN SOFT MATTER SCATTERING WORKSHOP 6-9 February 2017

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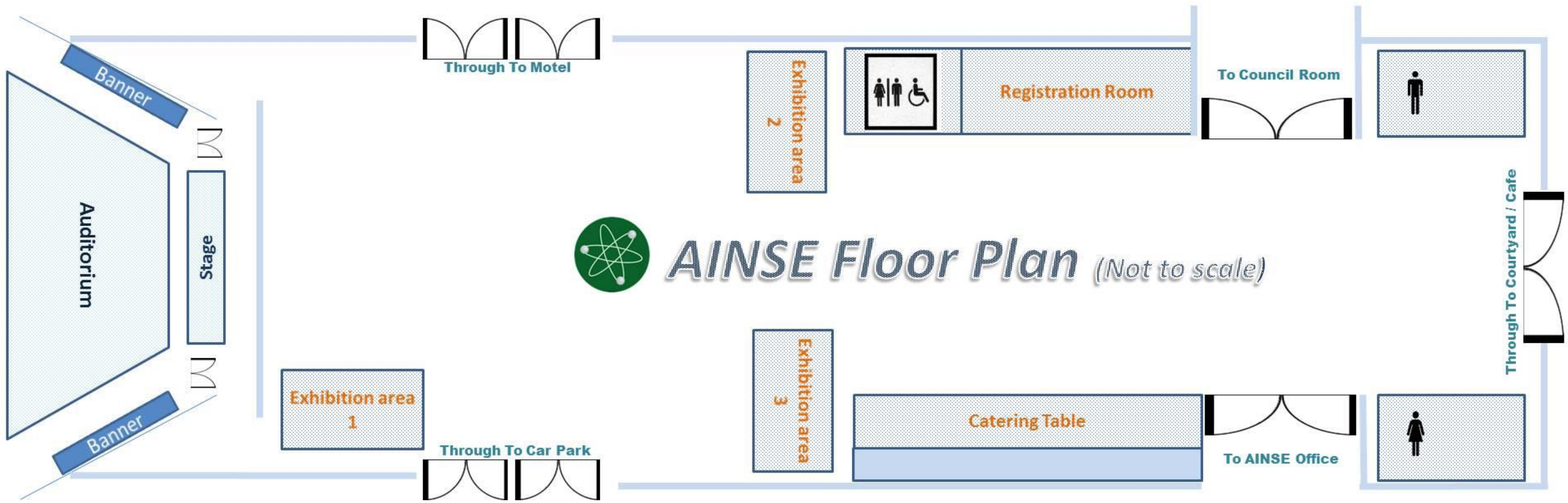
Plan



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Sponsors

ATA SCIENTIFIC instruments

MEP instruments
The right chemistry.

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Also thanks to

Organisations

- AINSE
- ANSTO
- Xenocs

Team

- Kelly Cubbin
- Rachel Caldwell
- Stuart Prescott
- Cherylie Thorn

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And you the participants

5pm special session for those taking the instrument workshop

Saving time, inherently statistical measurements of structure!

Chris Garvey
(ANSTO, cjg@ansto.gov.au)

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People here

- I have a scientific problem:
  - What could I learn from a scattering experiment?
  - What are the typical issues which can be resolved by the scattering experiment?
- Have scattering data – what to do with it now?
- Scattering really helped me resolve my problem.
- Experienced practitioners.

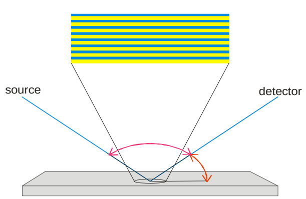
What is scattering?

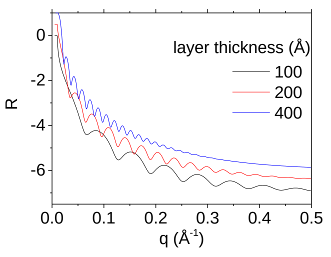
- Measured intensity of radiation after interaction with a sample at some well defined position.
- We consider of small subset of the experiments generally characterized by an elastic interaction of light, x-rays or neutrons with matter
- A knowledge of the probability of the interaction (scattering cross-section) allows reconstruction structural details of the samples

Scattering (x-rays and neutrons)

One-dimensional

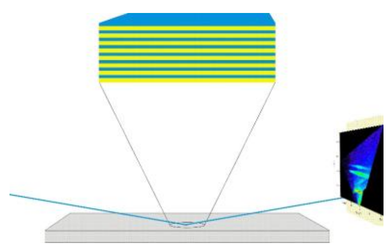
- Specular reflectivity.
- Thickness of thin layers.





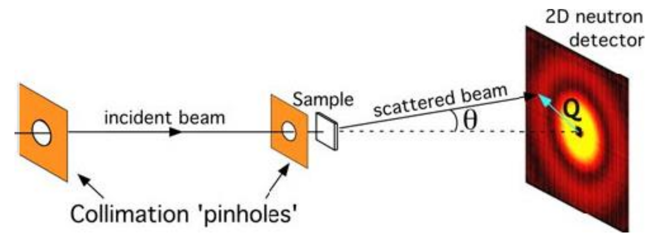
Two-dimensional

- Grazing incidence/off-specular intensity.
- In-plane organisation.
  - Correlated density fluctuations.



Three-dimensional

- Transmission small angle scattering



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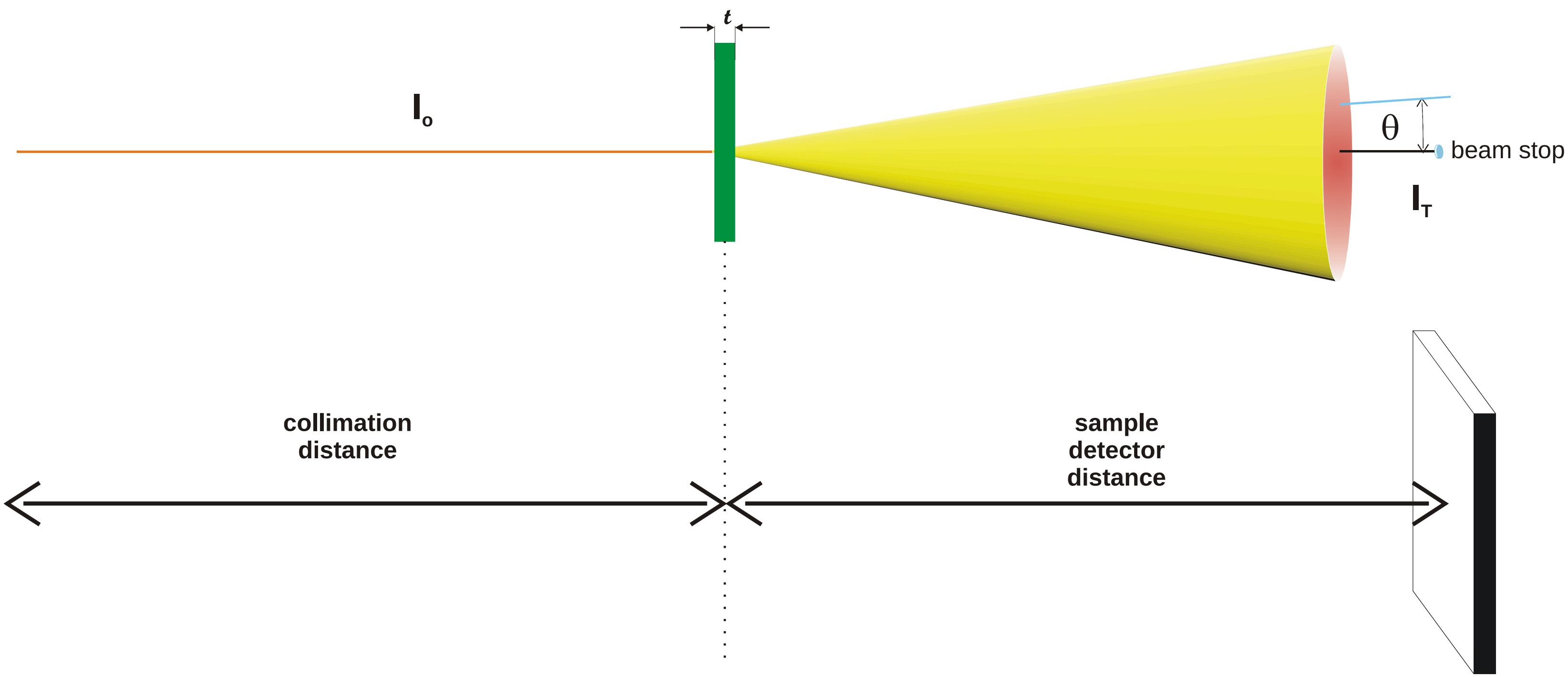
Why does scattering happen and what it does tell us?

- Due to heterogeneities in sample:
  - Light, changes in refractive index (measured).
  - X-rays, changes in electron density (calculated).
  - Neutrons, variations in a nuclear property (calculated).
- From the scattering pattern we work in reverse to determine spatial/length-scales distribution of heterogeneities in the sample (structure).

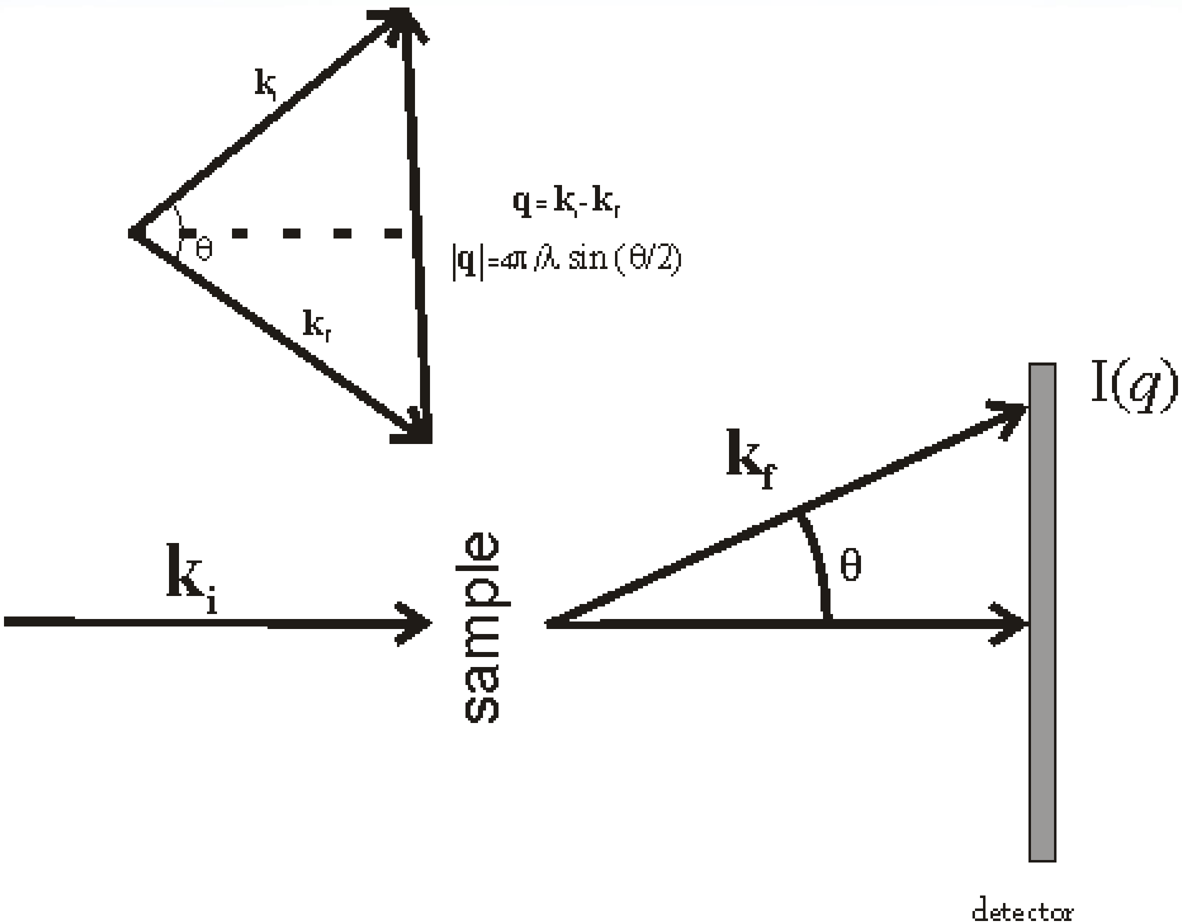
Aims

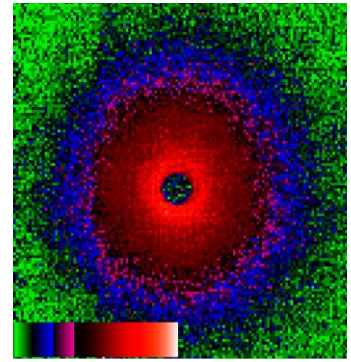
- To provide a framework to determine the internal structure of a sample from a scattering measurement:
  1. Separating that scattering which is produced by the sample from that which is an artefact of the measurement.
  2. Careful definition of the scattering problem and a physically meaningful reconstruction of the scattered intensity into a real space model.

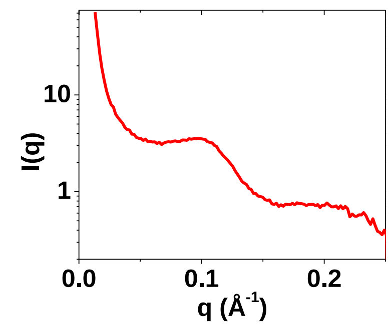
Small Angle Scattering – transmission geometry
3 dimensional structure



Small Angle Scattering







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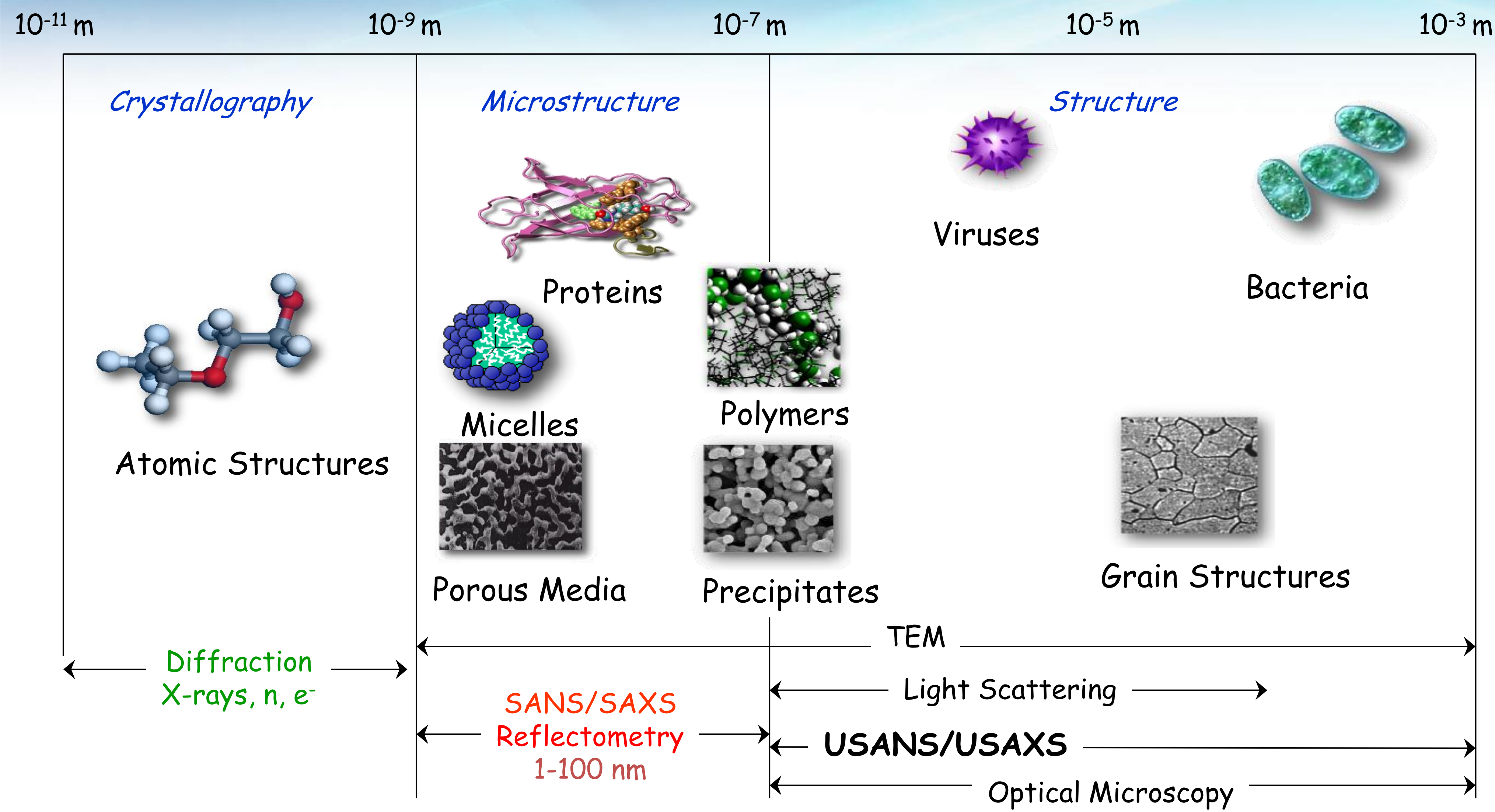
Size Scales Probed by Scattering Techniques



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Small Angle Scattering as a Black Box or a Mathematical Transformation

- Structural information is spatial variation of scattering length density.

$$I(\boldsymbol{q}) = \frac{1}{V}\left|\int_V \rho(\boldsymbol{r})\, e^{i\boldsymbol{q}.\boldsymbol{r}} dr\right|^2$$

i.e. Fourier transform of the density correlation function

Why use scattering?

- It provides an average structure (statistical sampling) in the region sampled by the incident beam over several orders of magnitude in length-scale.
- Can probe the internal structure (ideally) non-destructively.
- Evolution of structure and characterization *in situ:*
  - *external field (electric, strain, magnetic, shear).*
  - *solution, solid and gas phases.*
  - model and real membranes.
  - Cells.

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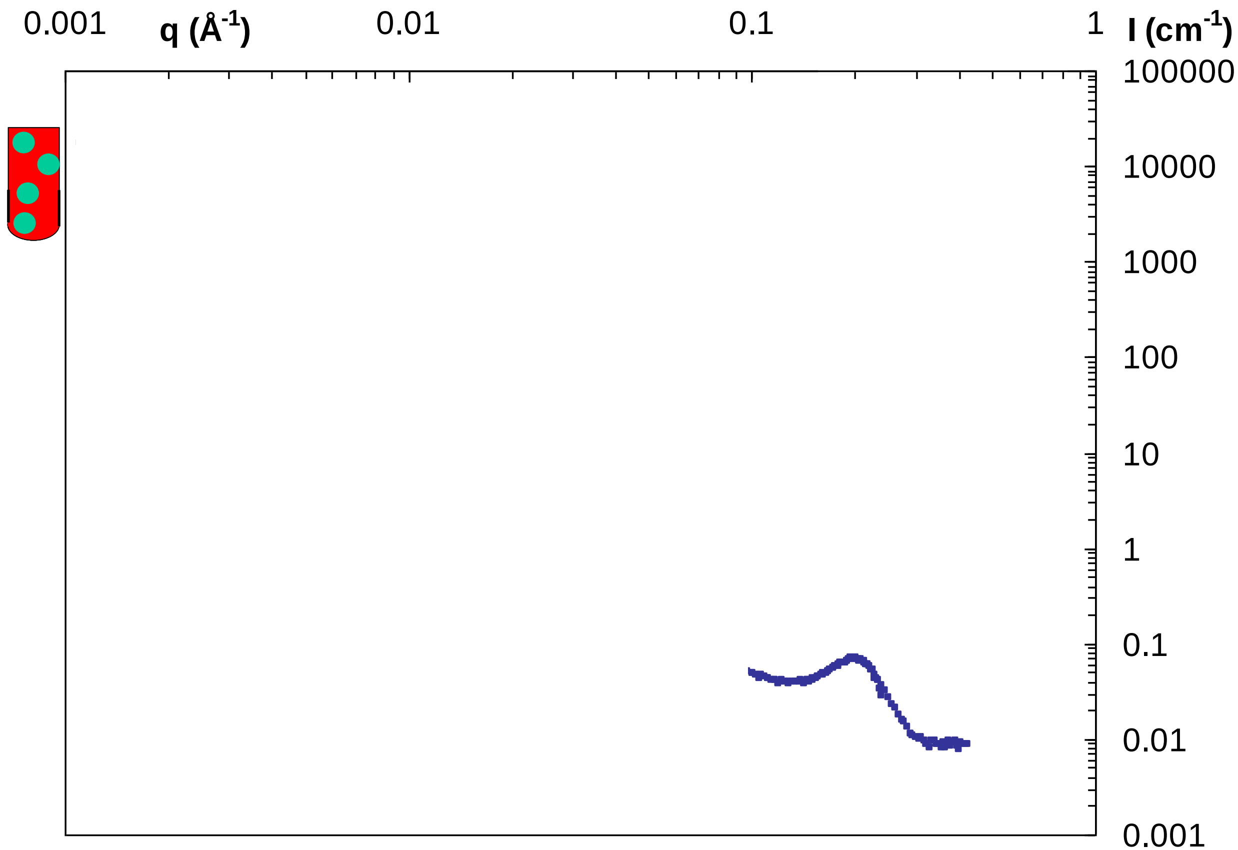
Analysis of (radially averaged) SAS Curves

- ***Isotropic scattering***, radially symmetric, scattering objects
- Ideal scattering curve is an absolutely scaled from flat background (high-q) to I(0) with scattering due to sample environment (container) subtracted, real measurements usually contain a small angular range (need to assume how it behaves at low-q).
- Real measurements consist of a finite range which ideally include low-q and high-q behavior:
  - Lab-based/synchrotron SAXS single configuration.
  - SANS multiple wavelengths and/or sample to detector distances.

*Strunz, P.; Šaroun, J.; Keiderling, U.; Wiedenmann, A.; Przenioslo, R. General formula for determination of cross-section from measured SANS intensities. *Journal of Applied Crystallography* **2000**, *33*, 829-833.

Example
protein / polystyrene sulfonate solutions
F. Boue

Liquid turbid: lysozyme signal



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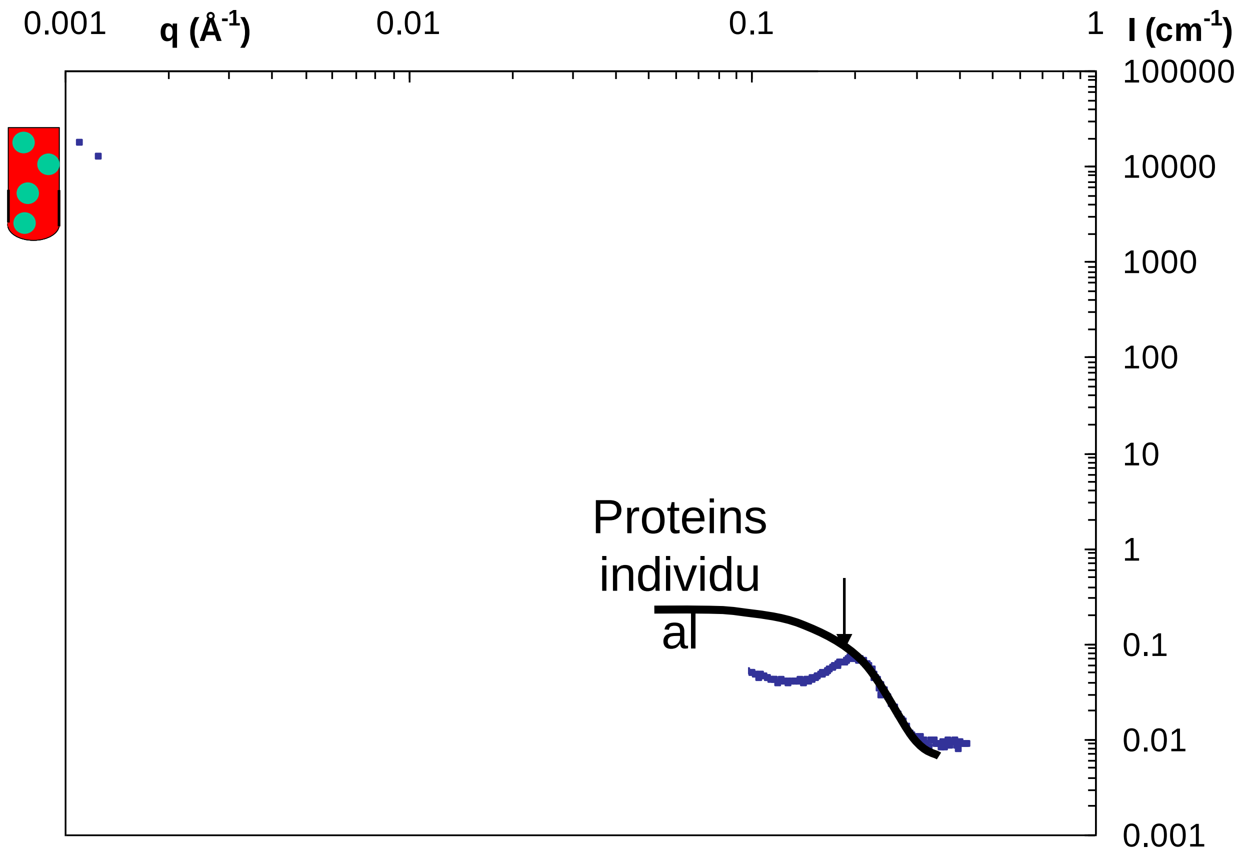
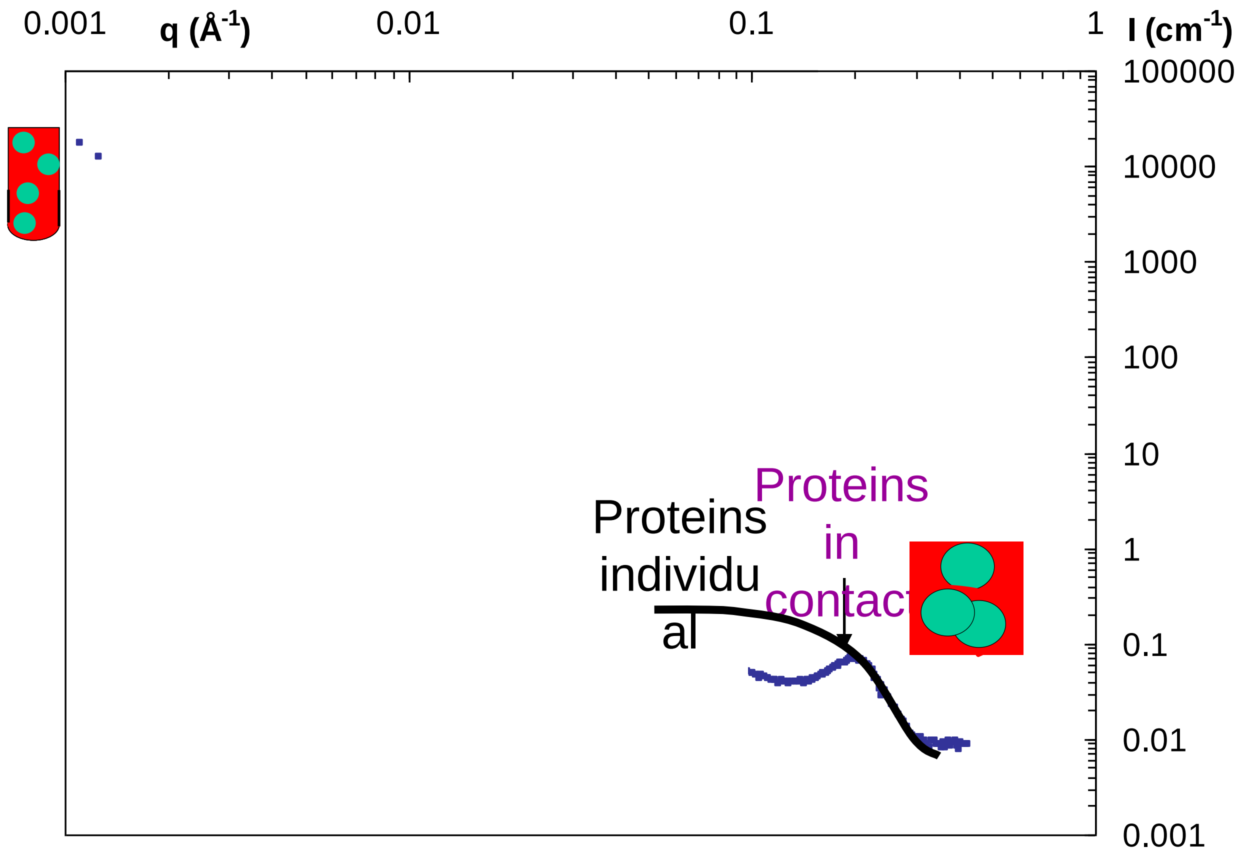
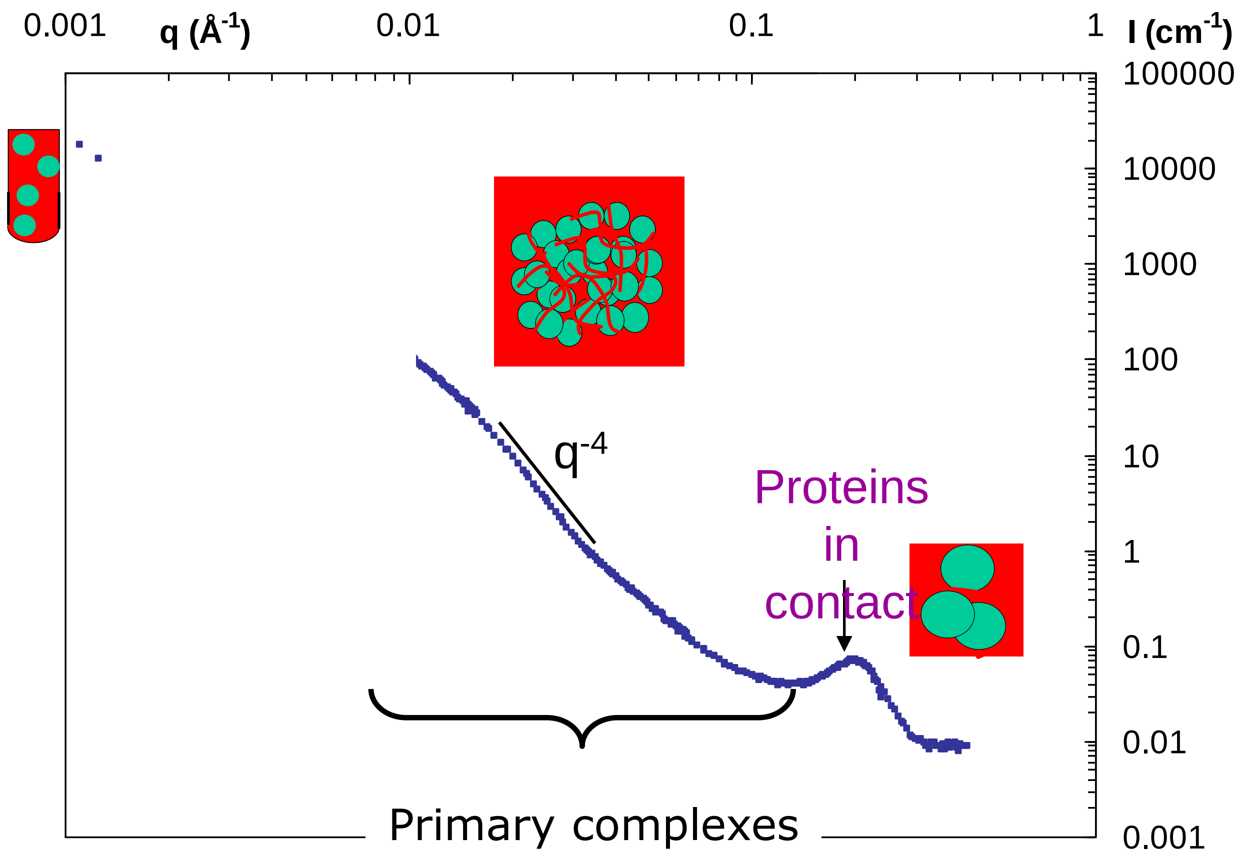
Liquid turbid: lysozyme signal



Liquid turbid: lysozyme signal



Liquid samples: structure (lysozyme signal)



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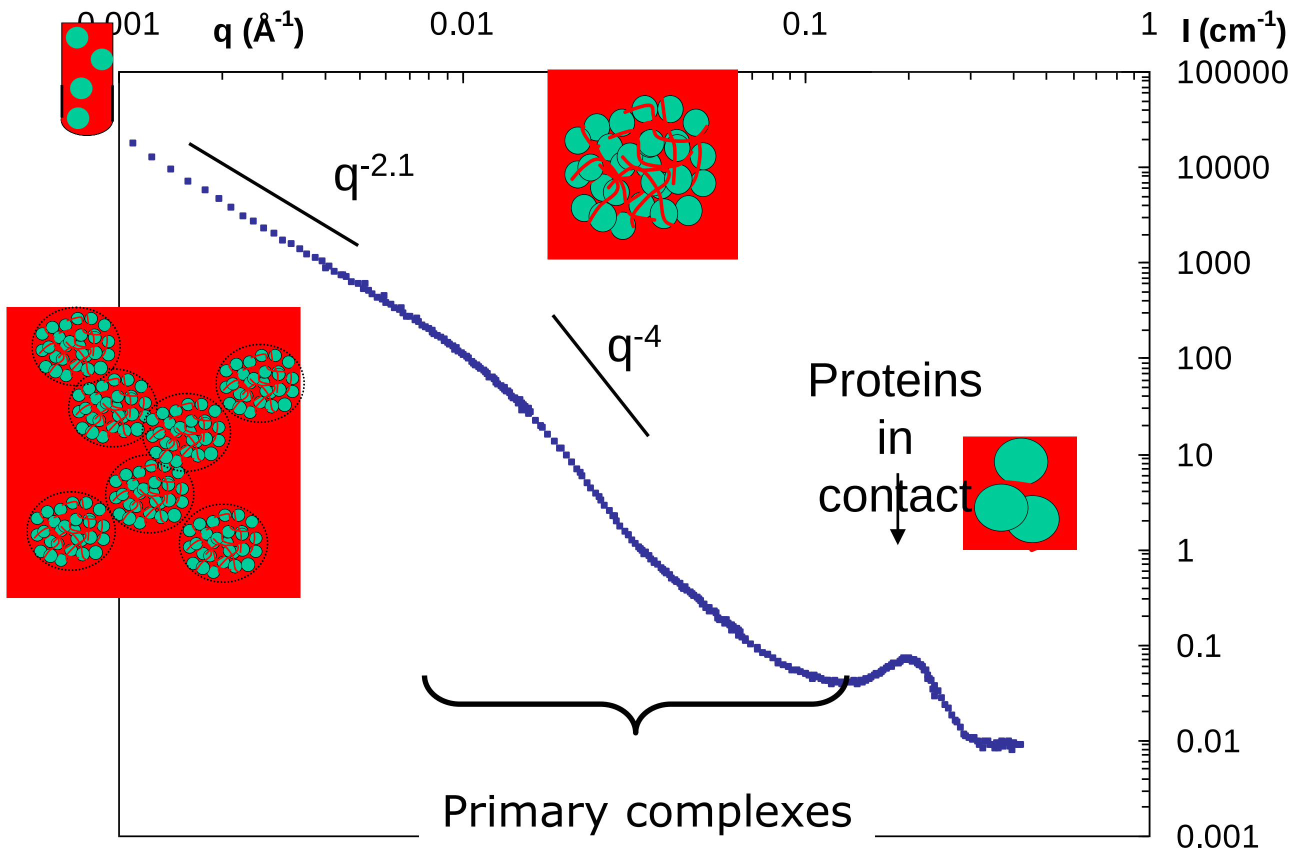


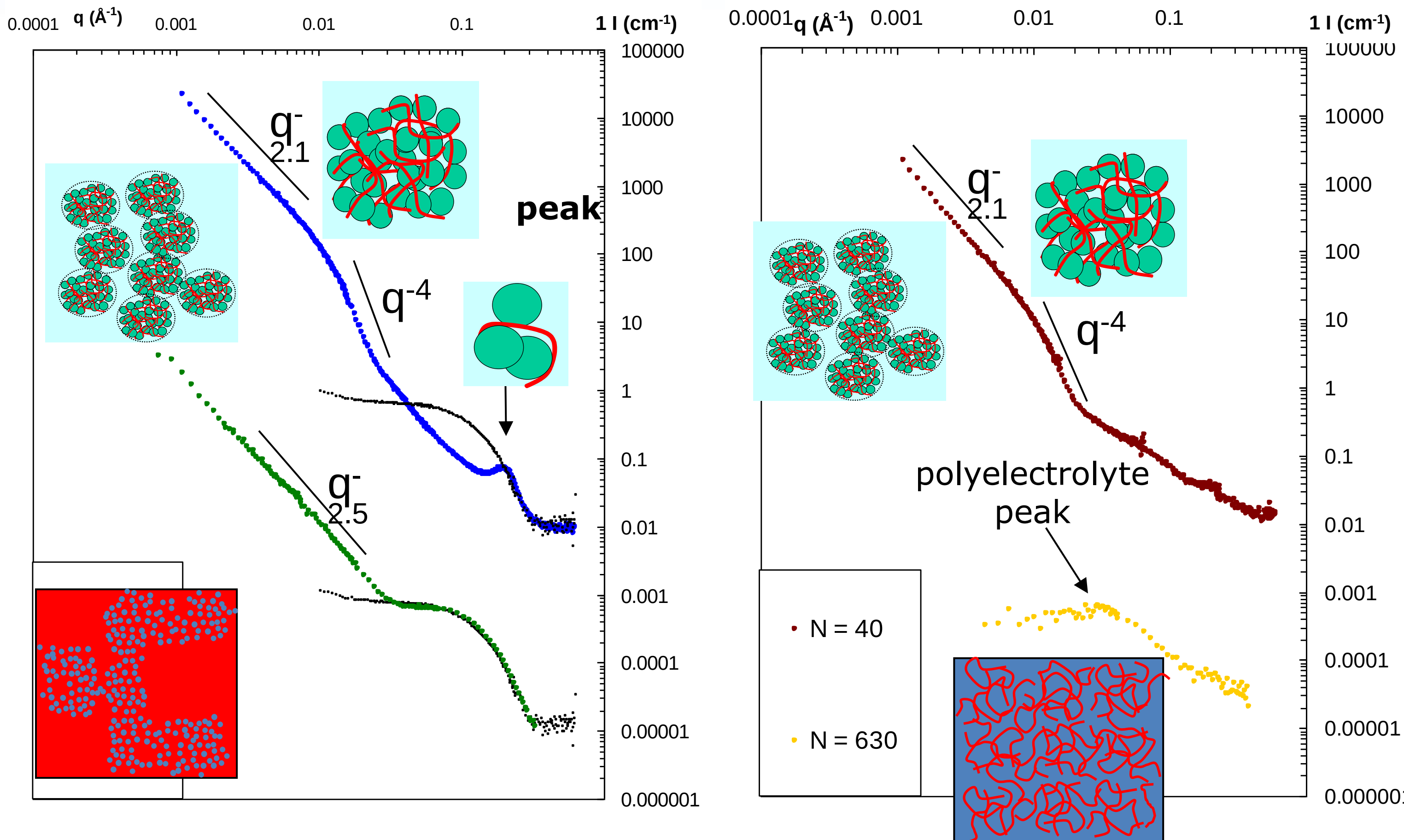
Power Laws – describe a characteristic dimension

- Rigid Rod 1
- Linear Gaussian Chain 2.
- Chain with excluded volume 5/3.
- Gaussian Chain randomly branched 16/7.
- Swollen branched chain 2
- Smooth 2-d object.
- Smooth 3-d object 4.
- Etc…..

Beaucage, G. (1995) Approximations leading to a unified exponential power-law approach to small-angle scattering, *Journal of Applied Crystallography*, **28**, 717-728.
Teixeira, J. (1988) Small-angle scattering by fractal systems, *Journal of applied crystallography*, **21**, 781-785

SANS signals vs PSS chains length

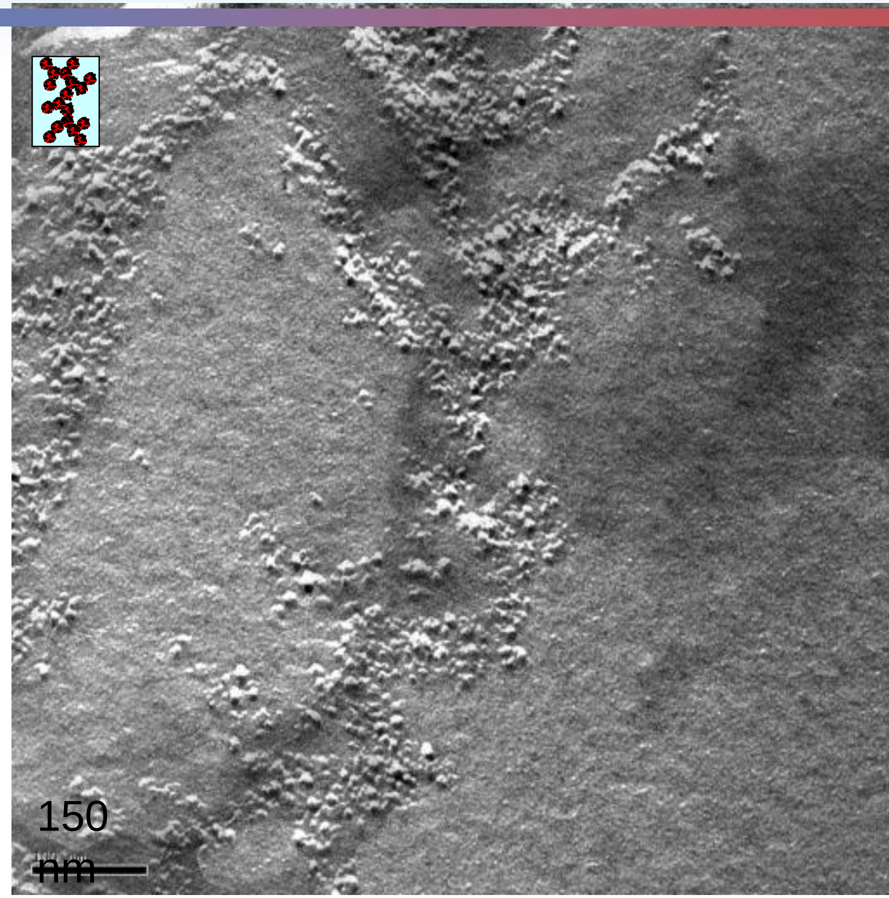
François Boué



Cousin, Gummel, Ung et Boué, ***Langmuir***, 2005, 21, 9675-9688

Organization at higher scale

Fractal aggregation at higher scale



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Scattering versus real Space

Real Space

+

- Recognizable – excellent information content.

-

- Sampling statistics generally poor.
- Limited resolution.
- Special sample preparation.

Scattering (inverse space)

-

- Poorly recognizable – poor information content.

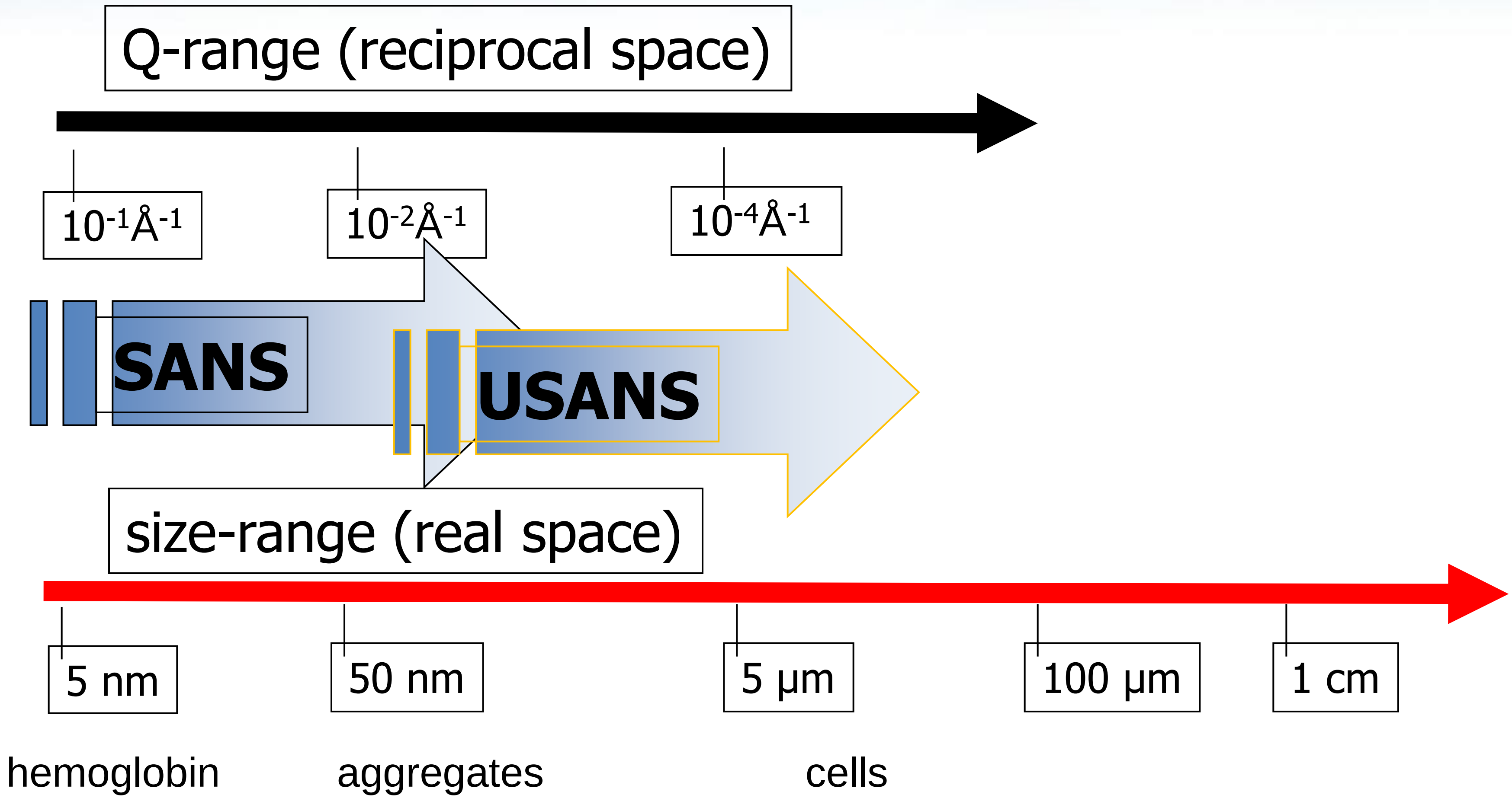
+

- Excellent sampling statics.
- Large range of length-scales.
- No special sample preparation.

Methods

- Transmission small angle scattering.
- Reflectivity.
- Grazing Incidence Scattering.
- Light scattering.
- PFGSE NMR (Is this scattering)?

Imaging- Real Vs q-space



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