



Solution scattering from biological macromolecules

19 – 26 November 2018 | Hamburg, Germany

ORGANIZERS

Dmitri Svergun
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CO-ORGANIZERS

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EMBL Hamburg, DE

REGISTRATION

Registration deadline
31 August 2018

Student/Postdoc 50 EUR
Academic 100 EUR
Industry..... 1000 EUR

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University of Milan, IT

meetings.embo.org/event/18-sas

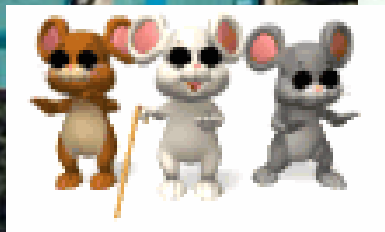
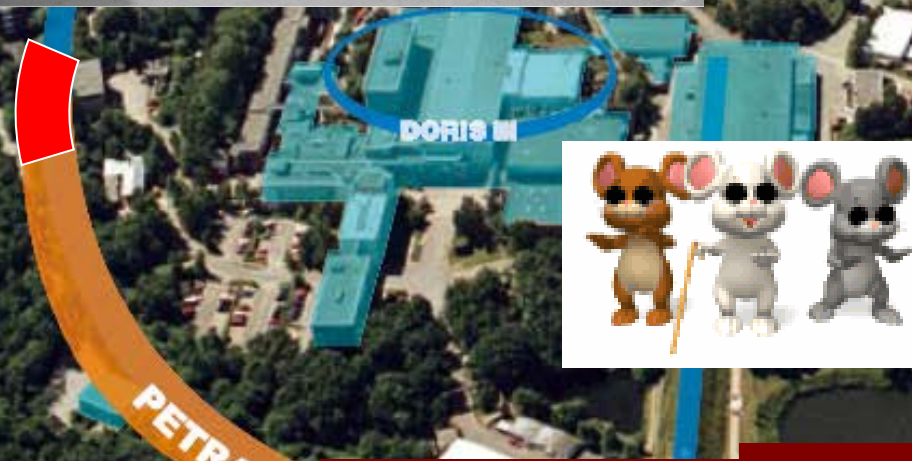
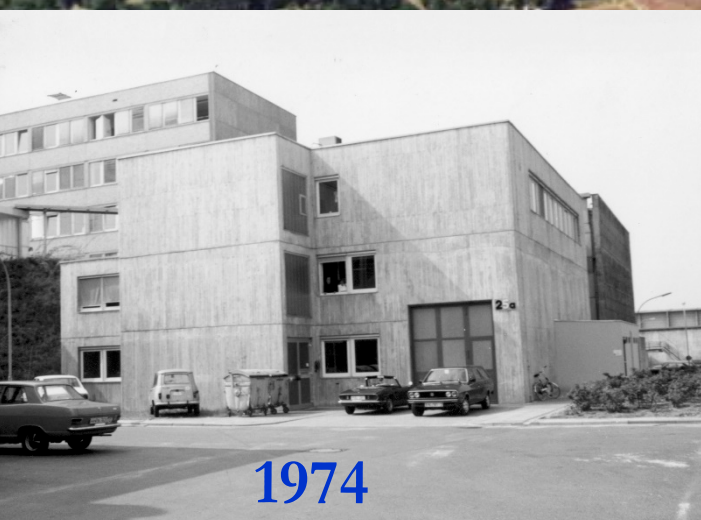
Welcome!

26 course participants
(19 nationalities
representing institutes
from 17 countries)

1 local attendant

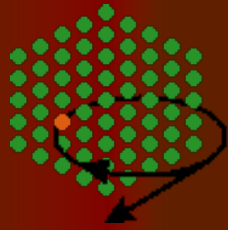
9 external lecturers and
9 tutors/lecturers from
EMBL-Hamburg

EMBL Outstation at DESY, Hamburg



EMBL synchrotron facilities at the upgraded Petra-3 ring
Sample preparation and characterization facility (SPC)

2 MX beamlines (P13, P14)
1 BioSAXS beamline (P12)



Biological SAXS @ EMBL-HH

Group leader: D. Svergun

**Staff : C.Jeffries,
C.Blanchet, D.Franke,
A.Kikhney, H.Mertens,
M.Graewert, C.Borges**

**Postdocs: M.Schroer,
A.Gruzinov, S. da Vela,
D. Molodenskiy,
N.Hajizadeh**

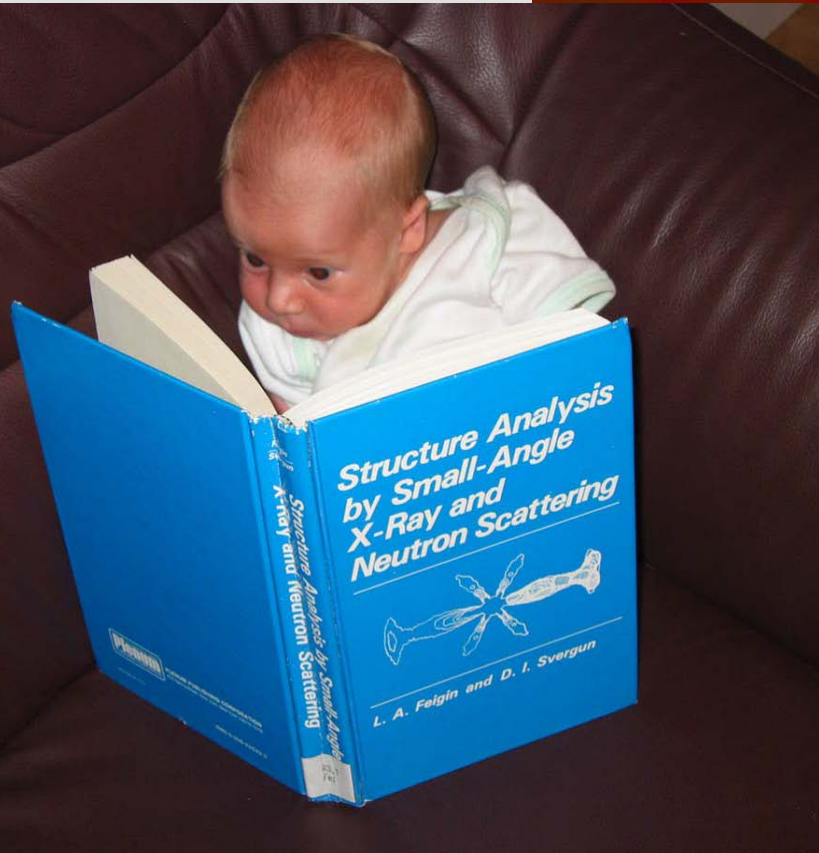
**Predocs: K.Malanastas,
T.Cheremnykh**



Major tasks:

- ❑ Development of data analysis methods
- ❑ Running and developing SAXS beamlines
- ❑ User support and collaborative projects
- ❑ Interactions, education and training

Small-angle scattering in structural biology



In preparation for an EMBO Course ...
(courtesy of F.Gabel, IBS, Grenoble)

Bioinformatics

Biochemistry

AUC

FRET

EPR

tion, nm:

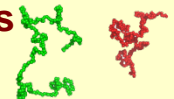
1 1.6 1.0 0.8

Scattering

The new SAS book is not yet available for everyone (courtesy of M.Graewert, EMBL-HH)



flexible systems



All new is well forgotten old

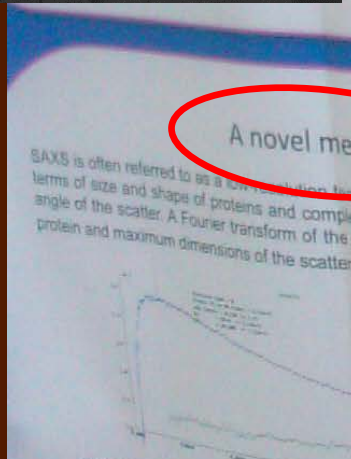


On finishing my university studies, in 1936, I obtained a post as assistant, which gave me the opportunity to work towards my thesis...

My "boss", who looked after my dissertation, ... was a crystallographer who kept an eye on my work rather distantly, but he did pass on a very good idea on me: to study, in addition to Bragg diffractions, diffuse scattering.

<He> asked me to make a camera with monochromatic primary radiation and with minimum parasitic radiation... That is why I studied especially small-angle scattering. I observed that ... the scattering is strong when the sample contains fine grains (10 to 100 nm).

I produced next the means of determining the grain size from the scattering curve. It was the beginning of X-rays small-angle scattering...



Guinier, A. (1939). "La diffraction des rayons X aux tres petits angles; application a l'etude de phenomenes ultramicroscopiques." Ann. Phys. (Paris) 12: 161-237.

When biologists go for SAS



This is just a trivial case:
You will learn that
SAXSMAN (© A.Kikhney)
yields much more

Care for a shape?

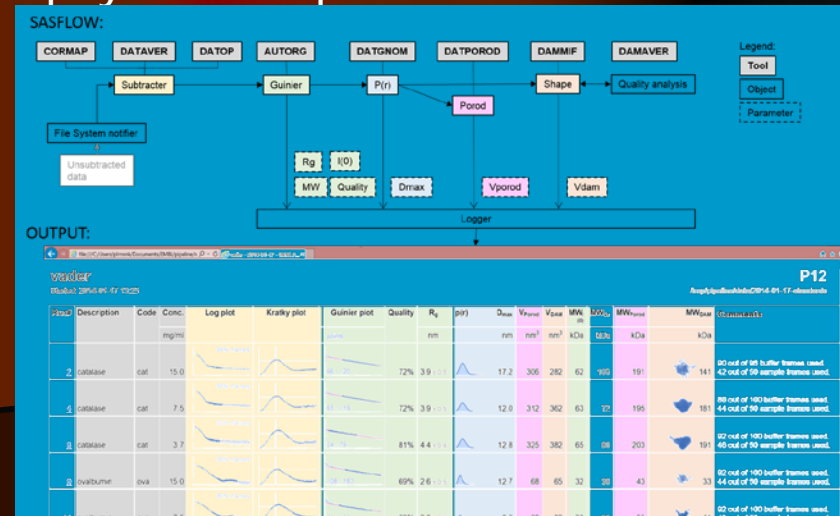


High brilliance EMBL SAXS beamline P12



- Robotic EMBL/ESRF sample changer
- Automated FPLC/HPLC in parallel with biophysical sample characterisation

- About 10^{13} ph/sec in 200×120 mm²
- Energy between 4 and 20 keV (3.0 to 0.6 Å)
- Divergence below 0.05×0.05 mrad²
- Multilayer monochromator mode: over 5×10^{14} ph/sec
- SASFLOW pipeline for on-line data processing and analysis
- Full automation, remote and mail-in access



ATSAS (All That SAS) roadmap



- World most comprehensive program suite for small-angle scattering data analysis from biomacromolecular solutions
- Consists of more than 80 programs developed at EMBL-HH since 1991
- Available for download since 1999, accessible on-line since 2006
- Presently, ATSAS has over 16,000 users from over 50 countries; on-line usage: over 4,000 users/~35,000 jobs per year

Polydispersity

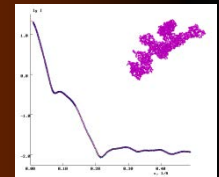
Volume
Unfold



Databases of computed

analysis

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head modelling
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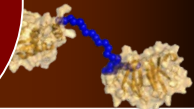


Data



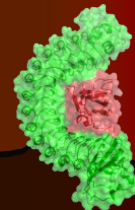
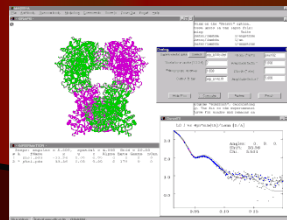
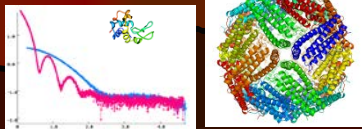
Raw data

ing fragments
solution models

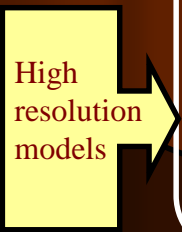
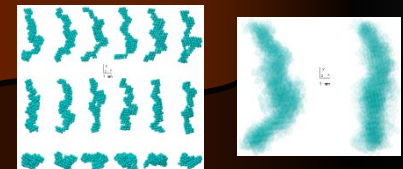


multisubunit complexes modelling
Multidomain proteins modelling
against multiple data sets

Computational solution
scattering from atomic models
(X-rays and neutrons)



Models superposition,
averaging and clustering



High
resolution
models

Schedule of the Course



- Day 1 : Basics of small-angle scattering (Mon 19 Nov)
- Day 2 : From sample to data (Tue 20 Nov)
- Day 3 : From data to shape (Wed 21 Nov)
- Day 4 : Rigid body (hybrid) modelling (Thu 22 Nov)
- Day 5 : Mixtures and interacting systems (Fri 23 Nov)
- Day 6 : SAXS and complementary methods I (Sat 24 Nov)
- Day 7 : SAXS and complementary methods II (Sun 25 Nov)
- Day 8 : General discussion (Mon 26 Nov)

Lectures and Practicals

- **Theory Lectures** (48e Seminar Room, 2nd floor)
- **Software Demonstrations/Tutorials** (48e Seminar Room, PC, LCD projector)
- **Structural Biology Seminars** (48e Seminar Room, 2nd floor)
- **Practicals:** (P12 beamline and user room, 48e, ground floor).
- **Data Analysis and SAXS Quest** (48e Seminar Room , 2nd floor)

SAXS Play Station VI (anti-sleeping pills)

- SAXS Quest



Practical measurements at P12

➤ **Own samples**

- Those who brought their own samples, shall measure them, analyse the data, and report the results at the end of the Course.

➤ **No own samples**

- Those who brought no samples, shall measure the alien proteins provided by us, analyse the data, and report the results at the end of the Course.

➤ **Measurements on Mon 19.11 and Tue 20.11**

- Sample changer+SEC-SAXS setup

➤ **Measurements on Fri 23.11**

- Sample changer

Whom to ask

- **General questions:**
 - Dmitri Svergun (internal 125, mobile *127), Alexey Kikhney (170, mobile *150)
- **Organizational questions:**
 - Margret Fischer (internal 110, mobile *108)
 - Sarah Marshall (111)
- **Computer hardware:** Felipe Goncalves (133)
- **Computer software:**
 - Daniel Franke (244), Nelly Hajizadeh (217), Peter Konarev (129), Maxim Petoukhov (179)
- **SAXS practicals:** Clement Blanchet (192), Martin Schroer (241), Melissa Graewert (115), Cy Jeffries (177)
- **Beamline P12 phone:**
 - 040 89902 312 (internal 312)



Miscellaneous

- **Course photos:** 20.11 and 24.11, first coffee breaks
- **Free afternoon:** Thursday, 22 November
- **Course dinner:**
 - Sunday November 25, as of 20:00
- **Pairing for the Quest:**
 - The list is given in the Course materials
 - Quest winners will get very SAXSy prizes
 - Quest run starts tomorrow
- **Own laptops:** network 'EMBL_GUEST' (password available in the seminar room)
- **Your presentations:**
 - 26 participants (with or without PPT, as you wish)
 - Will be on the 1st and 3rd days (19.11 + 21.11)
 - 8 minutes per participant (SHARP: 6 min talk + 2 min questions)