# Meeting Reports

## CanSAS III, 17th-19th May 2001, Grenoble

The third annual 'Collective Action for Nomadic Small-Angle Scatterers' meeting was held at the ILL in the picturesque surroundings of Grenoble between May 17th to 19th. The meeting was convened in order for small-angle scatterers to share and extend data analysis tools and was composed of short talks as well as software demonstrations and group discussions.

Following lunch on the Thursday Wim Bras (DUBBLE) welcomed the delegates with an introduction to small-angle scattering. John Barnes (NIST) then presented a review of previous canSAS meetings before Ron Ghosh (ILL) briefly introduced use of simple XML in SAS data examples prepared for the meeting.

Elena Pourmal (NCSA) discussed the Hierarchical Data Format, listing the features of hdf5, such as the advances since hdf4 and the conversion technology that exists. She pointed out the limitations of hdf4 , such as its 2GB file limit, maximum object number, and multiple data models and explained how hdf5 was designed to rectify these and other shortcomings (including thread safety). Uwe Filges (PSI) then gave a brief account of porting NeXus to hdf5.

Following afternoon coffee, Trevor Forsyth (ILL & Keele University) spoke about using complementary X-ray and neutron techniques to observe both reversible and irreversible transitions between A,B,C,D and Z-type DNA. The day was drawn to a close by Dmitri Svergun (EMBL) who discussed solution scattering from mono-disperse and poly-disperse systems. He demonstrated a computational method of simulating the scattering from biological macromolecules using arrays of fixed-radius close-packed spheres.

Friday morning began with Marc Malfois (EMBL & ESRF) describing structured one-dimensional SAS data storage using sasCIF and continued with Peter Boesecke (ESRF) detailing requirements for processing synchrotron SAS experiments.

A major theme of the meeting was the dissemination of details of the myriad software packages available for small-angle scatterers. To this aim SANS data analysis was discussed by Elena Litvinenko (JINR, Dubna), who spoke about Visual Numerics' PV-Wave package and Charles Dewhurst (ILL) who demonstrated his Matlab-based 'Grasp' programme.

After lunch Steve King (ISIS) addressed the diverse fields of fibre diffraction, potholing and caving. He discussed his fibre-diffraction results concerning detergent-treated commercial nylon ropes. Steve explained that his interest stemmed from a wish to guard his own gear from any harm they may encounter during cleaning between excursions. Andy Hammersley (ESRF) then described the present status of FIT2D, and Rex Hjelm (LANL) explained the recombination of data within certain quality criteria neede to analyse TOF-SANS experiments. A poster and software demonstration session followed which touched on some enlightening code developments detailed by Els Homan (EMBL), Charles Dewhurst, John Barnes and Alan Munter (NIST).

The final day of the meeting began with Adrian Rennie (King's College,London) explaining the challenges in analysing soft matter small-angle scattering. The rest of the morning was devoted to a group discussion led by Ron Ghosh on the disparities in approach to data format in the community in general. A proposal was made to promote an XML-based solution to unifying *reduced* 1D and 2D small-angle scattering data files with the current push in the larger X-ray/neutron community towards the NeXus (HDF compatible) format. At the close of the meeting there was agreement on collaboration on a number of joint projects, including evaluation of XML and HDF tools on example small-angle scattering HDF datasets and developing a NeXus file definition for small-angle scattering. Progress will be

reported at SAS-2002 in Venice.

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# Contributed Articles

## Analysis of the disordered myosin lattice in muscle

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### Introduction

Vertebrate muscle is made up of many parallel, long, thin strands known as microfibrils [1]. The repeating unit of the microfibrils is called the muscle sarcomere, and is the basic contractile unit of muscle. The sarcomere is made up of alternating ordered arrays of myosin and actin filaments, which are helical assemblies of myosin and actin molecules, together with various regulatory proteins [2]. The sarcomere exhibits a banded structure, the bands corresponding to different ordered arrays of myosin and/or actin filaments. One of these bands, the A-band, is spanned by the myosin filaments which are arranged on a hexagonal array, and also contains myosin cross-linking proteins and part of the actin filaments. The actin filaments extend partially into the ends of the A-band where they fit into the trigonal positions of the hexagonal myosin filament array. Mechanical force is believed to be developed by specific interactions between the myosin and actin molecules. The myosin molecules are a two-chain, coiled-coil, $\alpha$-helical rod, and many rods form a roughly cylindrical filament that has three-fold helical symmetry.

The packing of myosin filaments within the lattices has been studied by X-ray diffraction, and also imaged directly by electron microscopy of thin transverse sections. The packing of the myosin filaments is most clearly seen in electron micrographs of transverse sections through the so-called “bare region” of the A-band [3]. This region is devoid of actin filaments and cross-linking proteins,