Imaging and Modeling in Electron Microscopy - Recent Advances
May 18-23, 2014

MEALS

*Breakfast (Buffet): 7:00–8:45 am, Sally Borden Building, Monday–Friday
*Lunch (Buffet): 11:30 am–1:30 pm, Sally Borden Building, Monday–Friday
*Dinner (Buffet): 5:30–7:30 pm, Sally Borden Building, Sunday–Thursday
Coffee Breaks: As per daily schedule, in the foyer of the TransCanada Pipeline Pavilion (TCPL)
***Please remember to scan your meal card at the host/hostess station in the dining room for each meal.**

MEETING ROOMS

All lectures will be held in the lecture theater in the TransCanada Pipelines Pavilion (TCPL). An LCD projector, a laptop, a document camera, and blackboards are available for presentations.

SCHEDULE

Sunday

16:00	Check-in begins (Front Desk - Professional Development Centre - open 24 hours)
17:30–19:30	Buffet Dinner, Sally Borden Building
20:00	Informal gathering in 2nd floor lounge, Corbett Hall Beverages and a small assortment of snacks are available on a cash honor system.

Monday

7:00–8:45	Breakfast
8:45–9:00	Introduction and Welcome by BIRS Station Manager, TCPL
9:00–9:40	Thomas Vogt, *From Picture to Data - the iconoclastic struggle in materials science*
9:40–10:10	Christian Dwyer, *Simulating core-loss scattering in the STEM*
10:10–10:35	Coffee Break, TCPL
10:35–11:30	Chandrajit Bajaj, *Macro-molecular Map and Model Refinement Techniques for Electron Microscopy*
11:30–13:00	Lunch
13:00–14:00	Guided Tour of The Banff Centre; meet in the 2nd floor lounge, Corbett Hall
14:00–14:10	Group Photo; meet in foyer of TCPL (photograph will be taken outdoors so a jacket might be required).
14:10–14:40	Otmar Scherzer, *Optical Flow Decomposition on Evolving Surfaces*
14:40–15:10	Deanna Needell, *Greedy algorithms in super-resolution*
15:10–15:30	Coffee Break, TCPL
15:30–16:00	Rachel Ward, *Linear dimension reduction in the L_1 norm: When and how is it possible?*
16:00–16:30	Zineb Saghi, *Compressed sensing approaches for novel 3D imaging modes in the TEM*
16:30–17:00	Andrew Stevens, *Machine Learning and Compressive Sensing for Electron Microscopy*
17:00–17:30	Mark Davenport, *Adaptive sensing for compressive imaging*
17:30–19:30	Dinner
19:30–20:30	Discussion Browning/Binev, *How can Mathematics help Electron Microscopy?*

Tuesday

7:00–8:45	Breakfast
8:45–9:40	Yoel Shkolnisky, *Viewing Direction Estimation in cryo-EM Using Synchronization*
9:40–10:10	James Evans, *Data analysis challenges for observing protein dynamics with fast electrons and x-rays*
10:10–10:35	Coffee Break, TCPL
10:35–11:30	Amit Singer, *Covariance Matrix Estimation for the Cryo-EM Heterogeneity Problem*
11:30–13:30	Lunch
13:30–14:00	Sarah Haigh, *Exploring the limitations of energy dispersive X-ray mapping of nanomaterials with the Titan ChemiSTEM*
14:00–14:30	Scott Findlay, *Quantitative interpretation of atomic resolution scanning transmission electron microscopy images in the presence of multiple scattering: progress and challenges*
14:30–15:00	Jerzy Sadowski, *Spectro-microscopy of 2D materials: challenges and perspectives*
15:00–15:20	Coffee Break, TCPL
15:20–16:10	Joachim Mayer, *PICO - Chromatic Aberration Correction in TEM and its impact on new experiments and signals*
16:10–17:00	Discussion Haigh/Saghi, *Elemental quantification using energy dispersive x-ray spectrometry in the STEM*
17:00–17:30	Bryan Reed, *Movie Mode DTEM*
17:30–19:30	Dinner
19:30–	Informal Discussions

Wednesday

7:00–8:45	Breakfast
8:45–9:40	Felix Krahmer, *A partial derandomization of phase retrieval via PhaseLift*
9:40–10:10	Philipp Lamby, *Solving the Regularized Reconstruction Problems Arising in Limited-Angle Tomography*
10:10–10:35	Coffee Break, TCPL
10:35–11:30	Dirk Van Dyck, *Addressing Feynman's Challenge - The 3D Shape of NanoCrystals from Single Projections at Atomic Resolution*
11:30–13:30	Lunch
13:30–17:30	Free Afternoon
17:30–19:30	Dinner
19:30–	Informal Discussions

Thursday

7:00–8:45	Breakfast
8:45–9:40	Benjamin Berkels, *Image registration techniques for electron microscopy*
9:40–10:10	Andrew Yankovich, *Applications of NR registration for enhanced signal to noise ratio, spatial precision, and standardless atom counting in STEM images*
10:10–10:35	Coffee Break, TCPL
10:35–11:30	Gitta Kutyniok, *A Compressed Sensing Approach to Component Separation in Imaging*
11:30–13:30	Lunch
13:30–14:30	Discussion Voyles/Dahmen, *Improving Precision and Signal to Noise Ratio in Electron Micrographs*
14:30–15:00	Zuowei Shen, *Image Restoration: Wavelet Frame Approach, Total Variation and Beyond*
15:00–15:30	Coffee Break, TCPL
15:30–16:00	Toby Sanders, *Practical 3-D Reconstruction Techniques for Electron Tomography*
16:00–16:30	Ilke Arslan, *Advanced reconstruction algorithms for electron tomography in the physical sciences*
16:30–17:00	Niklas Mevenkamp, *Non-local Means based Denoising and Reconstruction of STEM Images*
17:00–17:30	Teng Zhang, *A Semidefinite Programming Approach to 3D Reconstruction of Macromolecules*
17:30–19:30	Dinner
19:30–	Informal Discussions

Friday

7:00–8:45	Breakfast
8:45–9:40	Kevin Kelly, *Multidimensional Compressive Imaging with a Two-Dimensional Modulator*
9:40–10:10	Ivan Lobato, *On accurate modeling of electron scattering factors for TEM, STEM and diffraction*
10:10–10:45	Coffee Break, TCPL
10:45–11:30	Bin Han, *Image denoising using directional separable complex tight framelets*
11:30–13:30	Lunch

Checkout by 12 noon.

** 5-day workshop participants are welcome to use BIRS facilities (BIRS Coffee Lounge, TCPL and Reading Room) until 3 pm on Friday, although participants are still required to checkout of the guest rooms by 12 noon. **

Imaging and Modeling in Electron Microscopy - Recent Advances
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ABSTRACTS
(in alphabetic order by speaker surname)

Advanced reconstruction algorithms for electron tomography in the physical sciences

Ilke Arslan[1], *Toby Sanders*[1,2], *Peter Binev*[2], *John D. Roehling*[3], *Sanchita Dey*[3], *K. Joost Batenburg*[4], *Burtron H. Davis*[5], *Bruce C. Gates*[3], *Alexander Katz*[6]

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Advancements in nanotechnology have necessitated the construction of complex structures with nanosized building blocks. In order to understand the functionality (or lack thereof) of a material system, it must be characterized on the nanoscale. Electron microscopy is the ideal tool for such analysis, but only provides a 2-D projection of a very intricate, 3-D object. Electron tomography in the scanning transmission electron microscope (STEM) has provided valuable information in the physical sciences for over a decade. However, the "standard" 3-D reconstruction techniques of weighted back projection and simultaneous iterative reconstruction technique (SIRT) applied to the small number of projections available for beam sensitive materials typically leave elongation artifacts due to the missing wedge and no longer provide the necessary resolution. The new methods of total variation (TV) minimization within compressed sensing (CS) and discrete algebraic reconstruction technique (DART) allow us to obtain unprecedented understanding of many complicated materials systems. Some examples will include layered materials and small metal particles in supports. Looking forward, the possibilities of in-situ/ex-situ 3-D imaging will be discussed.

Thursday, 16:00 – 16:30

Macro-molecular Map and Model Refinement Techniques for Electron Microscopy

Chandrajit Bajaj

University of Texas at Austin

Molecular shape and conformation elucidation is the problem of recovering the three-dimensional structure of an individual molecule, a protein or a macromolecular assembly at the finest possible resolution and in its natural environment. Despite the advances in X-ray imaging and Electron Microscopy (EM), it has been difficult to simultaneously achieve the goals of recovering shape and conformation at finer resolution, and the larger scale of protein/nucleic acid assemblies. In this talk, I shall highlight current progress on several co-mingled computational mathematics algorithms for refinement of 3D EM map and models of macromolecular assemblies. The algorithms are based on new improved solutions to low discrepancy sampling of rotational product spaces $SO(3)^n$, and non-equispaced SO(3) Fourier transforms for fast multi-dimensional rotational correlations.

Monday, 10:35 – 11:30

Image registration techniques for electron microscopy

Benjamin Berkels

RWTH - Aachen

This talk consists of two parts. In the first part, we discuss image registration, i. e. the task of transforming two or more images into a common coordinate system, from the perspective of electron microscopy. The classical registration approach for image pairs is extended to handle the registration of hundreds of consecutive images to a single image with a special emphasis on input data with a low signal-to-noise ratio and periodic structures.

The proposed approach allows us to average a series of noisy scanning transmission electron microscopy (STEM) images producing an improved image that surpasses the quality attainable by single shot STEM images. One of the key ingredients is the use of a non-rigid transformation model that is able to cope with the frame-to-frame distortions resulting from the serial pixel-wise acquisition of STEM images.

In the second part, we discuss how to find global minimizers of a class of variational models that have a convex regularization term like total variation. This is achieved by constructing a convex minimization problem with a pointwise constraint in a higher dimension whose minimizers fulfill a thresholding theorem: The 0.5-level set of a minimizer of the convex problem is the subgraph of a minimizer of the original problem. Unlike the functional in the existing convexification models, the target functional in our proposed reformulation is strongly convex. Two immediate advantages of the strong convexity are that the reformulation has a unique solution and that more efficient minimization algorithms can be used.

A typical usage example for this kind of convexification model is stereo reconstruction, a special type of image registration: Here, the x-shift, called disparity, is estimated from a stereo image pair. The horizontal distortion inherent to STEM images is also an x-shift, so the convexification model paves the way for recovering and correcting these distortions.

The registration approach is joint work with Peter Binev, Douglas A. Blom, Wolfgang Dahmen, Robert Sharpley, Paul Voyles, Thomas Vogt and Andy Yankovich. The convexification model is joint work with Alexander Effland and Martin Rumpf.

Thursday, 8:45 – 9:40

Adaptive sensing for compressive imaging

Mark A. Davenport

Georgia Institute of Technology

In this talk I will focus on the problem of recovering a sparse image from a small number of noisy measurements. To begin, I will consider the case where the measurements are acquired in a nonadaptive fashion as in the standard compressive sensing framework. I will describe lower bounds on the minimax mean-squared error of the recovered vector which very nearly matches the performance of ℓ_1-minimization techniques, and hence shows that in certain regimes these techniques are essentially optimal. I will then consider the case where the measurements are acquired sequentially in an adaptive manner. I will describe a lower bound that shows that, surprisingly, in certain worst-case regimes, adaptivity does not allow for substantial improvement over standard nonadaptive techniques in terms of the minimax MSE. Nonetheless, I will also show that there are important regimes where the benefits of adaptive sensing are clear and overwhelming, and can be achieved via relatively simple algorithms. The talk will focus primarily on theoretical performance bounds and practical algorithms for the specific setting of imaging, but will also have implications for the broader context of generic compressive sensing.

Monday, 17:00 – 17:30

Simulating core-loss scattering in the STEM

Christian Dwyer

Forschungszentrum Juelich

One of the major challenges in simulating inelastic scattering in the TEM/STEM is the large number of inelastic channels that must be included, even for a specific energy loss. This arises because a typical TEM specimen has many excited states at the same energy. Core-loss scattering, whereby the incident electrons excite atomic-core states, is a case in point. On the one hand, core-loss scattering underlies a class of extremely useful analytical techniques, which nowadays can even be performed at atomic spatial resolution, making it ideal for studying interfaces and other types of defects in materials. On the other hand, the simulation of core-loss scattering, as required for the quantitative interpretation of such experiments, is generally very time-consuming owing to the large number of atoms in a typical specimen. In this talk, I will consider this problem from a formal perspective, combining ideas from symmetry (group) theory and information theory. These ideas enable a formal analysis, and thereby optimization, of the efficiency of inelastic scattering simulations (and quantum mechanical calculations in general). Applied to simulations of core-loss scattering in the TEM/STEM, these ideas provide up to a 10-fold improvement in efficiency compared to current methods.

Monday, 9:40 – 10:10

Data analysis challenges for observing protein dynamics with fast electrons and x-rays

James Evans

Pacific Northwest National Laboratory

Time-resolved imaging of biological or nanomaterial structural dynamics is a highly data intensive task. Not only do we attempt to collect enough data to solve the three-dimensional structure of an object, we also try to collect that same data at multiple time points during a reaction cycle to see how the object changes over time. Handling the data, which for a single dataset can be on the order of terabytes in size, is a barrier unto itself but analyzing the data and identifying slight changes from one image to the next can be even more daunting - especially when the timing offset or magnitude of changes is unknown a priori. In this talk I will describe some of the challenges identified from current ultrafast x-ray diffraction experiments and simulated Dynamic TEM datasets to highlight areas where the development of automated algorithms could dramatically improve throughput and reliability of interpretation.

Tuesday, 9:40 – 10:10

Quantitative interpretation of atomic resolution scanning transmission electron microscopy images in the presence of multiple scattering: progress and challenges

Scott D. Findlay[1], *Leslie J. Allen*[2]

[1]Monash University, [2]University of Melbourne

To use scanning transmission electron microscopy (STEM) efficiently as a tool for discovery, real time imaging modes that are directly and reliably interpretable are necessary. The long-standing high-angle annular dark-field (HAADF) mode, steady improvements in resolution and recent developments such as annular bright field imaging have been very successful in this regard. Nevertheless, visual inspection is insufficient to obtain quantitative information – such as inter-column spacing, chemical composition, the depth of and structure surrounding dopants, local bonding information and the detailed electric field distribution. Increased stability and robust image processing have greatly improved image quality. But even with "perfect-quality" images, analysis is limited by the scattering physics that connects the structure qualities sought to the signal(s) measured. The chief limitation is multiple elastic and thermal scattering, which enhances the spread of probe. Consequently, the recorded signal comprises an admixture of information about the full interaction volume and not simply the column nominally under the probe.

This talk will review some limitations of "naïve" interpretation of STEM images, in particular that an image with atomic scale features cannot automatically be interpreted as allowing perfect column-by-column analysis. Select recent advances in analysis which account for the detailed scattering of the probe will be presented. One is the ability to put experimental HAADF images on an absolute scale, which through comparison with simulations allows the number of atoms in a column to be counted, and in some cases the depth of individual dopant atoms to be determined. Another is an approach for removing the effects of elastic and thermal probe scattering from a spectrum image, disentangling the fine structure signals from adjacent columns to allow a more direct and meaningful comparison with standard first-principles simulations of energy loss fine structure. However, both approaches require the basic structure of the specimen to be known. The outstanding challenge is whether the same quantitative rigour can be achieved on samples when the structure is not known in advance. Some ideas will be given as to how this might be achieved as the potential for simultaneous collection of multiple imaging modes is increasingly being realized.

Tuesday, 14:00 – 14:30

Exploring the limitations of energy dispersive X-ray mapping of nanomaterials with the Titan ChemiSTEM

Sarah Haigh

University of Manchester

Our Titan "ChemiSTEM" aberration corrected scanning transmission electron microscope (STEM) is optimised for high efficiency energy dispersive X-ray (EDX) spectroscopy with high spatial resolution. In this talk I will discuss recent results using this high spatial resolution elemental mapping to better understand variations in the physical and electronic properties of nanomaterials. I will focus on applications that have demanded the development of novel experimental approaches:

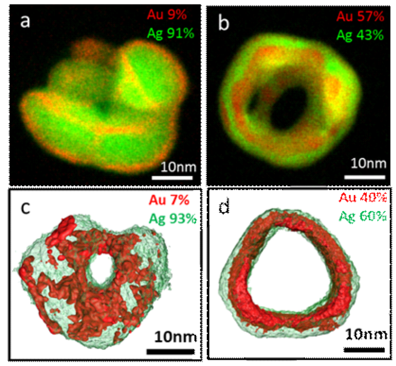
1) Two dimensional materials like graphene are widely studied using plan-view TEM/STEM imaging. However, this approach cannot be applied after the various individual atomic layers are used encapsulated so as to fabricate a complex heterostructured device. I will demonstrate how a side-view approach to imaging these materials has facilitated new insights into electrical device performance including the use of elemental mapping to locate atomic layers [Haigh et al, Nature Materials, 2012; Georgiou et al, Nature Nano, 2013].

2) The vast majority of STEM imaging is in vacuum. In-situ liquid cell experiments are increasingly popular but these have not generally been considered compatible with elemental analysis due to the cell geometry. I report on the first use of a redesigned liquid cell that has allowed us to perform the first elemental mapping of nanostructures submerged in liquid with nanometer spatial resolution [Zaluzec et al, Microscopy and Microanalysis, 2014].

3) I will also report on recent results using tomography to obtain full elemental distributions in three dimensions with nanometer spatial resolution for different nanoparticle compositions. This has allowed us to overcome the limitations of interpretation associated with two dimensional projections [Slater et al Nanoletters, 2014] providing a much clearer understanding of catalytic performance (fig 1).

Figure 1: a,b) Two dimensional EDX spectral images showing differing Au and Ag distributions within nanoparticles with varying Au content.

c,d) Surface visualisations of reconstructed 3D tomograms of Au and Ag in nanoparticles displaying transition from Au to Ag surface segregation



Tuesday, 13:30 – 14:00

Image denoising using directional separable complex tight framelets

Bin Han

University of Alberta

Real-valued separable wavelets and framelets are known to have some shortcomings for high dimensional problems such as image processing, for example, they lack directionality and cannot capture edges very well. In this talk, we introduce directional separable complex tight framelets and show that directionality can be greatly improved by using separable complex tight framelets. While keeping the efficient tensor product structure, our approach has the advantages of much better improved directionality and the use of finitely supported complex tight framelets. For the image denoising problem, we show that separable complex tight framelets have significant performance gains (typically, 0.5db to 1db improvement) compared with several state-of-the-art image denoising methods such as undecimated wavelet transform, dual tree complex wavelet transform, shearlets, curvelets, total variation based method, and etc. We are looking forward for other applications of separable complex tight framelets in image processing.

Friday, 10:45 – 11:30

Multidimensional Compressive Imaging with a Two-Dimensional Modulator

Kevin F. Kelly

Rice University

We have been successful in translating the mathematical breakthroughs of compressive sensing into optical imaging systems from the ultraviolet to the infrared portions of the spectrum. These cameras rely on making many multiplexed measurements over time summed into a single or a few detectors. In the case of video, the motion in the scene during acquisition disrupts the scene reconstruction. To overcome this, we have designed and developed various algorithms to successfully reconstruct both the background and foreground. Lastly, a few comments will be made on how we exploit this in the design of compressive optical microscopy instrumentation for sum-frequency generation imaging of molecular vibrations and darkfield imaging of plasmon resonances.

Friday, 8:45 – 9:40

A partial derandomization of phase retrieval via PhaseLift

Felix Krahmer

University of Göttingen

The problem of retrieving phase information from amplitude measurements alone has appeared in many scientific disciplines over the last century; for example x-ray crystallography and electron microscopy measurements can be modeled in this way. PhaseLift is a recently introduced algorithm for phase recovery that is computationally tractable, numerically stable, and comes with rigorous performance guarantees. PhaseLift is optimal in the sense that the number of amplitude measurements required for phase reconstruction scales linearly with the dimension of the signal. However, it specifically demands Gaussian random measurement vectors - a limitation that restricts practical utility and obscures the specific properties of measurement ensembles that enable phase retrieval.

In this talk, we present two partial derandomizations of PhaseLift. First we consider a construction that only requires sampling from certain polynomial size vector configurations, called t-designs. Such configurations have been studied in algebraic combinatorics, coding theory, and quantum information. We prove reconstruction guarantees for a number of measurements that depends on the degree t of the design. If the degree is allowed to grow logarithmically with the dimension, the bounds become tight up to polylog-factors. Second, we consider Fourier measurements with random masks as they are encountered in x-ray crystallography. Here the number of measurements is optimal up to a single logarithmic factor.

This is joint work with David Gross and Richard Kueng.

Wednesday, 8:45 – 9:40

A Compressed Sensing Approach to Component Separation in Imaging

Gitta Kutyniok

Technische Universität Berlin

Modern imaging data are often composed of several geometrically distinct constituents. For instance, neurobiological images could consist of a superposition of spines (pointlike objects) and dendrites (curvelike objects) of a neuron. A neurobiologist might then seek to extract both components to analyze their structure separately for the study of Alzheimer specific characteristics. However, this task seems impossible, since there are two unknowns for every datum.

Utilizing the novel methodology of Compressed Sensing, this geometric separation problem can indeed be solved both numerically and theoretically. For the separation of point- and curvelike objects such as in the neurobiological example, we choose a deliberately overcomplete representation system made of wavelets (suited to pointlike structures) and shearlets (suited to curvelike structures). The decomposition principle is to minimize the ℓ_1-norm of the representation coefficients or to perform iterative thresholding. Our theoretical results, which are based on microlocal analysis considerations, show that at all sufficiently fine scales, nearly-perfect separation is indeed achieved.

This project was done in collaboration with David Donoho (Stanford University) and Wang-Q Lim (TU Berlin).

Thursday, 10:35 – 11:30

Solving the Regularized Reconstruction Problems Arising in Limited-Angle Tomography

Philipp Lamby

Texas A&M University

In many tomographic applications, including STEM tomography, the view angle is severely limited due to mechanical restrictions. In this situation standard image reconstruction methods produce reconstructions with notorious streaking artifacts. Recently, motivated by the advances in the theory of sparse recovery, several algorithms have been developed that regularize the reconstruction problem using range constraints, the $\ell_1$norm and (possibly anisotropic) versions of the total variation semi-norm as priors.

To solve the resulting typically underdetermined constrained optimization problems one needs iterative solvers which however converge only slowly because the data matrix A is badly conditioned. For example, with the regularized ART algorithm from [HD08] one can often observe notable improvements of the reconstruction even after thousands of iterations which is computationally unacceptable for 3D reconstructions. Many algorithms developed for compressed sensing, like the Augmented Lagrangian Method [Li09] or Bregman iterations [MFOM10] accentuate the problem since they require iterative solution of the normal equation involving the matrix $A^T A$ which is even worse behaved. These algorithms typically work only well, if the full range of angles is accessible.

In this talk we explore the idea to combine the above mentioned algorithms with multigrid techniques, similar to the ones that have been proposed in [KPPR06] for overdetermined problems. Multigrid naturally acts as preconditioning of the system and one can hope for accelerated convergence. However, because of the structure of the system matrix the standard multigrid theory is not applicable. We discuss the theoretical challenges and present some experimental results with synthetical and real data.

References

[HD08] G. T. Herman and R. Davidi. Image reconstruction from a small number of projections. *Inverse Problems,* 24, 2008.

[KPPR06] Harald Köstler, Constantin Popa, M. Prümmer, and Ulrich Rüde. Towards an algebraic multigrid method for tomographic image reconstruction improving convergence of ART. In P.Wesseling, E. Onate, and J. Periaux, editors, *European Conference in Computational Fluid Dynamics ECCOMAS CFD,* TU Delft, The Netherlands, 2006.

[Li09] Chengbo Li. An efficient algorithm for total variation regularization with application to the single pixel camera and compressive sensing. Masters thesis, Rice University, Houston, Texas, 2009.

[MFOM10] Yu Mao, Benjamin P. Fahimian, Stanley J. Osher, and Jianwei Miao. Development of optimization of regularized tomographic rconstruction algorithms utilizing equally-sloped tomography. *IEEE Transactions on Image Processing,* 19(5):12591268, 2010.

Wednesday, 9:40 – 10:10

On accurate modeling of electron scattering factors for TEM, STEM and diffraction

Ivan Lobato

University of Antwerp

In this work we present a new parameterization of the electron scattering factor using five analytic non-relativistic hydrogen electron scattering factors as a basis functions. This new parameterization for the elastic electron scattering factors and its derived quantities such as the X-ray scattering factor, the electron charge density distribution and the atomic potential obey all the correct physical constraint conditions, have the correct asymptotic behavior and can be calculated analytically.

We also investigate the accuracy of the main parameterized electron scattering factors for large variety of diffraction experiments including reflection that lies on the Zero Laue zones and Higher order Laue zones. Comparison of all these results allows us to draw reliable conclusions about the range of applicability of the different parameterizations.

Friday, 9:40–10:10

PICO – Chromatic Aberration Correction in TEM and its impact on new experiments and signals

Joachim Mayer[1,2], *Juri Barthel*[2], *Lothar Houben*[2], *Maryam Beigmohamadi*[1,2] *and Knut Urban*[2]

[1]RWTH Aachen, [2]Research Centre Juelich

The invention of aberration correctors has revolutionized the development of TEM and STEM instrumentation. Only shortly after the development and installation of the first TEM with a corrector for the spherical aberration [1], commercial instruments with aberration correctors are now offered by all major manufacturers. In order to provide a platform for these novel developments and based on the experience with the first aberration corrected TEM [2-4], Research Centre Juelich and RWTH Aachen University have jointly founded the Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons (ER-C) [5]. At the Ernst Ruska-Centre we have recently installed the FEI Titan 60-300 PICO. PICO is a fourth-generation transmission electron microscope capable of obtaining high-resolution transmission electron microscopy images approaching 50 pm resolution in the CC- and CS-corrected mode at 300 keV. It is currently one of only two microscopes in the world capable of chromatic aberration correction [6].

In the present contribution we will report on the initial results obtained with the PICO instrument. In the PICO instrument, HRTEM images can be obtained with simultaneous correction of the spherical and the chromatic aberration. Furthermore, a spherical aberration corrector also exists in the illumination system for Cs-corrected STEM imaging. The benefits of chromatic aberration corrected imaging are particularly large for HRTEM imaging at low accelerating voltages and for energy filtered (EFTEM) imaging with large energy window width [7]. In the present contribution we will focus on these two applications and will present results from our recent work.

References:

[1] M. Haider, H. Rose, S. Uhlemann, E. Schwan, B. Kabius, and K. Urban, Nature 392 (1998) 768.

[2] M. Lentzen, B. Jahnen, C.L. Jia, K. Tillmann, and K. Urban, Ultramicroscopy 92 (2002) 233.

[3] C.L. Jia, M. Lentzen, and K. Urban, Science 299 (2003) 870.

[4] C.L. Jia, K. Urban, Science 303 (2004) 2001.

[5] http://www.er-c.org

[6] B. Kabius, P. Hartel, M. Haider, H. Müller, S. Uhlemann, U. Loebau, J. Zach, and H. Rose, J. Electron Microsc. 58, 147 (2009).

[7] K. Urban, J. Mayer, J. Jinschek, M. J. Neish, N. R. Lugg, and L. J. Allen, PRL 110, 185507 (2013)

Tuesday, 15:20 – 16:10

Non-local Means based Denoising and Reconstruction of STEM Images

Niklas Mevenkamp, Benjamin Berkels

RWTH-Aachen

We propose modifications of the classical non-local means algorithm (NLM) to certain characteristics typical for Scanning Transmission Electron Microscopy (STEM) imaging. We focus on three aspects: periodic recurrence of patterns, local horizontal distortions and the noise type.

The periodic distribution of the objects within the image is exploited to formulate an efficient strategy to search for similar patches. A periodic search grid is approximated from the image's Fourier transform.

The local horizontal distortions inherent to STEM images cause difficulties to recognize self similarities with the classical patch similarity measure. We propose to counter these horizontal distortions by allowing line shifts that improve patch regularity.

The most dominant source of noise in STEM imaging is typically Poisson distributed. However, the NLM algorithm was originally designed to remove additive Gaussian noise. We introduce corresponding modifications that increase the denoising performance on STEM images, especially in high intensity regions.

In addition to this, we discuss a method to correct the horizontal distortions in STEM images based on the NLM weights. This is joint work with Ronny Bergmann (TU Kaiserslautern), Wolfgang Dahmen (RWTH Aachen University), Joachim Mayer (RWTH Aachen University, Jülich Research Center), Paul Voyles (University of Wisconsin-Madison) and Andrew B. Yankovich (University of Wisconsin-Madison).

Thursday, 16:30 – 17:00

Greedy algorithms in super-resolution

Deanna Needell

Claremont McKenna College

Super-resolution refers to the problem of identifying a high resolution image from a subsampled, or lower resolution image. The problem can me modeled as a sparse recovery problem when the measurement operator has a pre-defined specific structure. In this talk we present some new work on greedy algorithms which can handle the structure in the measurement operator for super-resolution. We present experimental results as well as theoretical guarantees.

Monday, 14:40 – 15:10

Movie Mode Dynamic Transmission Electron Microscopy

B. W. Reed[1,2], *T. LaGrange*[1,2], *J. T. McKeown*[1], *M. K. Santala*[1], *and G. H. Campbell*[1]

[1]Lawrence Livermore National Laboratory, [2]Integrated Dynamic Electron Solutions, Pleasanton, CA

With the widespread availability of aberration correction, the frontier of transmission electron microscopy (TEM) has shifted away from the push to ever-higher spatial resolution and towards expanding the class of things that can be done with the instruments. The idea of doing experiments inside the microscope, of actually capturing the crucial "during" moments instead of merely "before" and "after", is now one of the biggest growth areas in TEM. An essential difficulty with this is time resolution, the importance of which derives from general physical scaling laws. Simply put, small things tend to move fast. The nanometer- and micrometer-scale processes most relevant to materials science typically happen on nanosecond to microsecond scales, far faster than the multi-millisecond scales of conventional TEM.

This need inspired the development of Movie-Mode Dynamic Transmission Electron Microscopy (MM-DTEM), exemplified by the prototype instrument at Lawrence Livermore National Laboratory which is capable of capturing nine TEM images or diffraction patterns in the span of less than one microsecond. MM-DTEM enables direct visualization of details of phase transformations, microstructural evolution, and propagating chemical reactions at the actual time, length, and temperature scales of the real-world applications. MM-DTEM works by coupling a unique arbitrary-waveform laser, a photoemission-based TEM, and a high-speed fully programmable electrostatic deflector system.

The development of such an instrument raises both challenges and opportunities. DTEM experiments must make maximal use of the information provided by every single precious electron, for any wasted beam current implies performance degradation because of finite brightness, space charge, and stochastic blur effects. There is little doubt that DTEM can benefit greatly from recent developments in applied mathematics. Yet the arbitrary-waveform laser and the extremely low duty cycle of the DTEM's electron beam enable entirely new operating modes, such as laser-driven ponderomotive phase plate imaging, that are difficult or impossible with conventional instruments.

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Tuesday, 17:00 – 17:30

Spectro-microscopy of 2D materials: challenges and perspectives

Jerzy T. Sadowski

Brookhaven National Laboratory

The ongoing miniaturization in technological devices and the progress in surface science demand novel instrumental methods for surface characterization on a length scale of only a few atomic distances. Typically, the state-of-the-art instruments for that purpose are scanning electron microscopes (SEM), with a resolution limit of several nanometers, and scanning probe microscopes (SPM). The latter can investigate the morphology and geometric structure of surfaces on an atomic scale. However, the disadvantages, especially of scanning probe microscopes, are (a) the relatively slow data acquisition due to serial detection, (b) the restriction to the topmost surface layer, and especially (c) the fact that they do not allow sufficient spectroscopic information, i.e. electronic and chemical analysis. Alternative techniques are the direct imaging photoelectron emission microscope (PEEM) or low-energy electron microscope (LEEM) combined with an imaging analyzer and a tunable high-brilliance synchrotron radiation source (XPEEM mode).

LEEM is a powerful technique for studying the dynamic and static properties of surfaces and thin films including growth and decay, phase transitions, reactions, surface structure and morphology. It utilizes low energy electrons to image surfaces with < 5nm lateral resolution and atomic layer depth resolution (see: E. Bauer, Rep. Prog. Phys. 57, 895 (1994); and R. M. Tromp, IBM J. Res. Develop. 44, 503 (2000)).

In the LEEM/XPEEM setup, when using the electron irradiation, the elastically and inelastically backscattered electrons, Auger and secondary electrons may be used, while photoelectrons, Auger and secondary electrons are utilized for imaging when sample is irradiated with photons. The choice of the imaging, diffraction or spectroscopy mode depends upon the information to be obtained: structural, chemical, magnetic or electronic, from the topmost or rather deeper layers. The strength of the technique lies in the combination of the real-time structural and spectroscopic measurements in a single analytical system.

In this talk I will present examples of application of the LEEM/XPEEM technique to the in situ, real-time investigations of the 2D layered materials, including few-layer graphene on transition metals and dichalcogenides.

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Tuesday, 14:30 – 15:00

Compressed sensing approaches for novel 3D imaging modes in the TEM

Zineb Saghi, Rowan K. Leary and Paul A. Midgley

University of Cambridge

Electron tomography (ET) has become an important technique for the 3D characterization of nanomaterials [1]. Recently, significant advances in transmission electron microscopy have allowed spatial, temporal and spectroscopic imaging at unprecedented resolution. Extending these innovative techniques to 3D is of great interest for many nanotechnology applications. It necessitates, however, the development of powerful tomography algorithms that are capable of producing reliable reconstructions from datasets that are often limited due to constraints about e.g., sample geometry, total electron dose, total acquisition time and beam damage [2,3].

In this work, we will present the latest algorithmic developments with emphasis on the recent introduction of compressed sensing ET (CS-ET) [4,5]. By using the prior knowledge that the signal is sparse or compressible in a chosen transform domain (e.g. pixel or gradient domains), CS-ET employs a non-linear optimization algorithm to recover the sparsest solution consistent with the acquired projections. Based on simulations and experimental data, we will compare CS-ET with traditionally employed algorithms and show that artifacts related to the limited number and angular range of available projections can be greatly reduced, making the segmentation and subsequent quantitative analysis much more reliable.

Applied to innovative imaging modes, we expect CS-ET to have a significant impact in the field of nanotechnology with unprecedented ability to follow changes in space and time, generate chemically-sensitive 3D reconstructions, and provide high quality 3D data that can be used as reliable starting point for detailed nanometrology and further simulations of the properties and behaviour of nanodevices. We also forsee great potential in the 3D study of beam-sensitive materials, and in atomic scale ET using aberration-corrected microscopes and a small number of well-oriented projections [6].

[1] P A Midgley et al, Chemical Society Reviews 36 (2007) p.1477.

[2] P.A. Midgley and R.E. Dunin-Borkowski, Nature Materials 8 (2009) p.271.

[3] Z Saghi and P Midgley, Annual Review of Materials Research 42 (2012) p.59.

[4] Z Saghi et al, Nano Letters 11 (2011) p. 4666.

[5] R. Leary et al., Ultramicroscopy 131 (2013) p.70.

[6] The research leading to these results has received funding from the European Research Council under the European Union's Seventh Framework Programme (FP7/2007-2013)/ERC grant agreement 291522-3DIMAGE.

Monday, 16:00 – 16:30

Practical 3-D Reconstruction Techniques for Electron Tomography

Toby Sanders[1,2], *Peter Binev*[2], *Ilke Arslan*[1]

[1]Pacific Northwest National Laboratory, [2]University of South Carolina

In recent years, the field of electron tomography is finding applications to more beam sensitive materials. For these beam sensitive materials, we are challenged to recover accurate 3D morphologies from as few measurements and tilt angles as necessary. Unfortunately, classical back projection methods, such as weighted back projection (WBP), and simultaneous iterative reconstruction technique (SIRT), are not designed to handle this lack of information, and in particular, they do not handle well the case of the "missing wedge". Therefore, more advanced techniques for reconstruction have been introduced in recent years, namely, compressed sensing (CS) based total variation minimization (TVM) and the discrete algebraic reconstruction technique (DART), both of which we investigate.

Each of these techniques approaches reconstruction by including some characterization of the solution into the method. DART enforces a tight grip on this characterization, and restricts the class of solutions to have only a few a priori selected gray values, through iterative segmentation and refining. The technique of TVM formulates the reconstruction into CS problem applying a regularization penalty onto the solution, which encourages the solution to take larger jumps in the intensities of adjacent pixels to reduce blurring affects and create clear boundaries. While these techniques are gaining more popularity, lacking is a complete understanding of the limitations, consequences of the characterizations, and practicality of use in varying scenarios. In addition, particularly with DART, with this characterization of the images comes the task of delicate parameter selection, to which even a semi-automated parameter selection procedure is nontrivial.

We attempt to tackle some of these issues and give potential improvements in the techniques. In addition, we discuss each step in the 3D reconstruction, from the original data to the final reconstruction. In doing so, we give some general considerations for alignment and preprocessing of the tilt series, which can potentially improve the results of the reconstruction techniques.

This research has been partially supported by the NSF grant DMS 1222390.

Thursday, 15:30 – 16:00

Optical Flow Decomposition on Evolving Surfaces

Otmar Scherzer

University Vienna and Radon Institute of Computational and Applied Mathematics

Optical flow is traditionally computed from a sequence of flat images and used for motion estimation. We extend the concept of optical flow to a dynamic non-Euclidean setting and provide a concept for decomposition of flows. It is the purpose of this talk to introduce variational motion estimation and decomposition for images that are defined on an evolving surface. An application to biological imaging is presented.

This is joint work with Lukas Lang and Celemens Kirisits (Univ. of Vienna).

Monday, 14:10 – 14:40

Image Restoration: Wavelet Frame Approach, Total Variation and Beyond

Zuowei Shen

National University of Singapore

This talk is about the wavelet frame-based image and video restorations. We start with some of main ideas of wavelet frame based image restorations. Some of applications of wavelet frame based models image analysis and restorations will be shown. Examples of such applications include image and video inpainting, denoising, decomposition, image deblurring and blind deblurring, segmentation, CT image reconstruction, 3D reconstruction in electronmicroscopy, and etc. In all of these applications, spline wavelet frames derived from the unitary extension principle are used. This allows us to establish connections between wavelet frame base method and various PDE based methods, that include the total variation model, nonlinear diffusion PDE based methods, and model of Mumford-Shah. In fact, we will show that when spline wavelet frames are used, right chosen models of a wavelet frame method can be viewed as a discrete approximation at a given resolution to the corresponding PDE based models. A convergence analysis in terms of objective functionals and their approximate minimizers as image resolution increases will be discussed.

Thursday, 14:30 – 15:00

Viewing Direction Estimation in cryo-EM Using Synchronization

Yoel Shkolnisky

Tel-Aviv University

A central stage in recovering the structure of large proteins (3D density maps) from their 2D cryo-electron microscopy (cryo-EM) images, is to determine a three-dimensional model of the protein given many of its 2D projection images. The direction from which each image was taken is unknown, and the images are small and extremely noisy. The goal is to determine the direction from which each image was taken, and then to combine the images into a three-dimensional model of the molecule.

We present an algorithm for determining the viewing directions of all cryo-EM images at once, which is robust to extreme levels of noise. The algorithm is based on formulating the problem as a synchronization problem, that is, we estimate the relative spatial configuration of pairs of images, and then estimate a global assignment of orientations that satisfies all pairwise relations. Information about the spatial relation of pairs of images is extracted from common lines between triplets of images. These noisy pairwise relations are combined into a single consistent orientations assignment, by constructing a matrix whose entries encode the pairwise relations. This matrix is shown to have rank 3, and its non-trivial eigenspace is shown to reveal the projection orientation of each image. In particular, we show that the non-trivial eigenvectors encode the rotation matrix that corresponds to each image.

This is a joint work with Amit Singer from Princeton University.

Tuesday, 8:45 – 9:40

Covariance Matrix Estimation for the Cryo-EM Heterogeneity Problem

Amit Singer

Princeton University

In cryo-electron microscopy (cryo-EM), a microscope generates a top view of a sample of randomly-oriented copies of a molecule. The cryo-EM problem is to use the resulting set of noisy 2D projection images taken at unknown directions to reconstruct the 3D structure of the molecule. In some situations, the molecule under examination exhibits structural variability, which poses a fundamental challenge in cryo-EM. The heterogeneity problem is the task of mapping the space of conformational states of a molecule. It has been previously shown that the leading eigenvectors of the covariance matrix of the 3D molecules can be used to solve the heterogeneity problem. Estimating the covariance matrix is however challenging, since only projections of the molecules are observed, but not the molecules themselves.

In this talk we show that this problem can be viewed as a noisy matrix completion problem, and we derive an estimator for the covariance matrix as a solution to a certain linear system. While we prove that the resulting estimator for the covariance matrix is consistent in the classical limit as the number of projection images grow indefinitely, an interesting open question regarding the sample complexity of the problem remains. Namely, how many images are required in order to resolve heterogeneous structures as a function of the volume size and the signal to noise ratio? We will see that solving this question requires us to extend the analysis of the spike model in principal component analysis (PCA) in high dimensions, as we encounter limiting distributions that differ from the classical Marcenko-Pastur distribution.

Joint work with G. Katsevich and A. Katsevich.

Tuesday, 10:35 – 11:30

Machine Learning and Compressive Sensing for Electron Microscopy

Andrew Stevens

Duke University

Techniques in machine learning and compressive sensing have many applications in electron microscopy. The contribution of compressive sensing is twofold– it can be used to reduce dose (spatial compression) and increase acquisition speed (time compression). In the case of spatial compressive sensing, Bayesian dictionary learning was used. This method infers the underlying basis space and a sparse representation from the compressed measurements. For temporal compressive sensing the Gaussian mixture model is used. Both of the approaches are relatively recent developments from statistical machine learning. Computational experiments in spatial and temporal compressive sensing will be presented.

Monday, 16:30 – 17:00

Addressing Feynmans Challenge The 3D Shape of NanoCrystals from Single Projections at Atomic Resolution

F-R. Chen[1], *C. Kisielowski*[2], *D. Van Dyck*[3]

[1]National Tsing-Hua University, Taiwan, [2] Lawrence Berkeley National Laboratory, [3]University of Antwerp

Already in the late 50th Richard Feynman pointed out1 that, "It would be very easy to make an analysis of any complicated chemical substance; all one would have to do would be to look at it and see where the atoms are." since all structure-property relations are encoded in the 3D atom positions for a given set of elements. Nowadays, resolution and sensitivity of the latest generation aberration-corrected Transmission Electron Microscopes (TEM) suffice to detect even single light atoms from the Periodic Table of Elements2-5 and to pinpoint their position with a lateral precision that reaches the 2pm wavelength of the imaging electrons at 300kV of acceleration voltage6 but the depth (z) information remains less certain. In the past, only a few favorable cases allowed for an extraction of atom positions in beam (z) direction with high precision. They included the study of a graphene double layer7 and the study of nanocrystals of which the surfaces were protected by embedding in a sacrificial matrix8. Also, the combination of projections from different viewing directions yields remarkable results9 as long as linear models for the interaction between the electron beam with the object apply and beam-induced sample alterations are ignored. However for the study of nanoparticles such as for catalysts there is a need for a tomographic method that allows a fast characterization of the shape of pristine particles at atomic resolution. Here we present a new approach to atomic resolution tomography that meets these demands.

References

1. R.P. Feynman, Engineering and Science, 23, 22 - 36 (1960)
2. Ç. Ö. Girit, J.C. Meyer, R. Erni, M.D. Rossell, C. Kisielowski, L. Yang, C.-H. Park, M.F. Crommie, M.L. Cohen, S.G. Louie, A. Zettl, Science 323, 1705-1708 (2009)
3. O.L. Krivanek, M. F. Chisholm, V. Nicolosi, T.J. Pennycook, G. J. Corbin, N. Dellby, M.F. Murfitt, S. S. Own, Z. S. Szilagyi, M. P. Oxley, S. T. Pantelides, S. J. Pennycook, Nature 464, 571-574 (2010)
4. K. Suenaga, Y. Sato, Z. Liu, H. Kataura, T. Okazaki, K. Kimoto, H. Sawada, T. Sasaki, K. Omoto, T. Tomita, T. Kaneyama, Y. Kondo, Nature Chemistry 1, 415 - 418 (2009)
5. P. Y. Huang, S. Kurasch, J. S. Alden, A. Shekhawat, A. A. Alemi, P. L. McEuen, J. P. Sethna, U. Kaiser, and D. A. Muller, Science 342, 224-227 (2013)
6. X. Xu, S. P. Beckman, P. Specht, E. R. Weber, D. C. Chrzan, R. P. Erni, I. Arslan, N. Browning, A. Bleloch, C. Kisielowski, PHYSICAL REVIEW LETTERS 95, 145501 (2005)
7. D. Van Dyck, J.R. Jinschek, F.R. Chen, Nature 486 243 (2012)
8. S. Van Aert, K. J. Batenburg, M. D. Rossell, R. Erni, and G. Van Tendeloo, Nature 374 470 (2011)
9. M. C. Scott, C.-C. Chen, M. Mecklenburg, C. Zhu, R. Xu, P. Ercius, U. Dahmen, B. C. Regan, and J. Miao, Nature, 483, 444 (2012)

Wednesday, 10:35 – 11:30

From Picture to Data - the iconoclastic struggle in materials science

Thomas Vogt

University of South Carolina - NanoCenter

The use of scanning transmission electron microscopy data and images in materials science will be discussed and a case will be made to better integrate STEM with other analysis techniques. The dangers of 'cartoon science' and the use of 'selective imaging' could dominate the use of STEM in the near future.

Monday, 9:00 – 9:40

Linear dimension reduction in the L_1 norm: When and how is it possible?

Rachel Ward

University of Texas

Through the Johnson-Lindenstrauss Lemma and related results, it is known that a small set of points in a high-dimensional space can be linearly embedded into a space of much lower dimension in such a way that Euclidean distances between the points are nearly preserved, and that a random projection can be used for such embeddings. At the same time, it is known that a result of this kind is not possible if we replace Euclidean distance by the ℓ_1 norm, at least not for arbitrary sets of points. Certain sets, such as sparse vectors, can be linearly embedded in low dimension with respect to the ℓ_1 norm, and sparse random matrices work well for such embeddings. In this talk, we present a general framework which aims to address: for which sets of points, using what randomized linear maps, and to what extent is dimensionality reduction in ℓ_1 possible?

Monday, 15:30 – 16:00

Applications of NR registration for enhanced signal to noise ratio, spatial precision, and standardless atom counting in STEM images

Andrew B. Yankovich[1], *Benjamin Berkels*[2,3], *W. Dahmen*[2,4], *P. Binev*[2], *S. I. Sanchez*[5], *S. A. Bradley*[5] *and Paul M. Voyles*[1]

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Atomic-resolution imaging by transmission electron microscopy (TEM) and scanning TEM (STEM) has become routine in the last decade. Now that atoms are easily resolved, one important question is how precisely can their positions be measured? Precision smaller than the resolution is routinely attainable, but in the STEM, precision in limited by practical problems, such as image distortions caused by instabilities of the electron probe and the sample, before reaching the fundamental signal to noise ratio (SNR) precision limit. We have used non-rigid registration of a series of STEM images [1] to undo the effect of instabilities and enable averaging to improve the SNR and thus the precision. NR registration and averaging results in reproducible sub-pm precision [2], 5-7 times better than what is attainable with rigid registration and the best ever reported in electron microscopy. We have applied this high precision STEM method to measuring the surface atom distortions on a Pt nanocatalyst, for which the catalytic activity of the nanoparticles is determined by their atomic surface structure.

Another important problem is determining three dimensional atomic structures of materials from the acquired two dimensional images. NR registration of STEM images enables extraction of 3D atomic structure information using the standardless atom counting method with the best-reported uncertainties. Previous results using the same method reported a few atom uncertainty and were limited by image Poisson noise. The extremely high SNR images resulting from NR registration allows for standardless atom counting with < 1 atom uncertainty for a majority of the atomic columns in the Pt nanocatalyst, with no limitation from Poisson noise.

[1] Berkels et al, Ultramicroscopy 138, 46 (2014).

[2] Yankovich et al, *Picometer-Precision Analysis of STEM Images of Pt Nanocatalysts*, Nature Communications, to appear (2014).

Thursday, 9:40 – 10:10

A Semidefinite Programming Approach to 3D Reconstruction of Macromolecules

Teng Zhang

Princeton University

We propose a semidefinite programming approach to determine the 3D structure of small macromolecules by extending Kam's theory for single particle reconstruction in cryo-electron microscopy. The 3D reconstruction requires us to solve for U and V in the equation $Z = XU + YV$, where X, Y, Z are matrices of size $n \times d$, and U, V are d by d orthogonal matrices. We relax this to a semidefinite program, and show that when $n > d$, we can recover U and V exactly. A phase transition is observed at $n = d$.

Based on this, we propose a new method that would potentially enhance the capabilities of three-dimensional electron microscopy techniques by being able to answer biological questions related to small protein structures that have so far remained unresolved. We test our method by numerical experiments on the simulated data of the Kv1.2 potassium channel complex.

Thursday, 17:00 – 17:30

DISCUSSIONS

How can Mathematics help Electron Microscopy?

Nigel Browning and Peter Binev

- ▷ Compressive sensing for faster/low-dose image acquisition
- ▷ Noise reduction/image alignment/statistics
- ▷ Data rates and sampling the big data problem for electron microscopy

Monday, 19:30 – 20:30

Elemental quantification using energy dispersive x-ray spectrometry in the STEM

Sarah Haigh and Zineb Saghi

The opportunities, limitations and challenges of:

- ▷ different specimen geometries including compensating for absorption effects within the sample;
- ▷ accuracy of quantification when using new larger collection angle and multiple x-ray detector geometries;
- ▷ in situ experiments including the effects of elevated temperature, absorption within the in situ liquid or gaseous medium and/or effect of the Si3N4 environmental cell windows;
- ▷ EDX tilt series acquisition including optimisation of acquisition time, effect of beam damage, thickness increase and also processing of limited-angle EDX datasets;
- ▷ accurate quantification in three dimensions.

Tuesday, 16:10 – 17:00

Improving Precision and Signal to Noise Ratio in Electron Micrographs

Paul Voyles and Wolfgang Dahmen

- ▷ What we want is information about the sample, not pictures. What are the best ways to extract information (atom positions, structural patterns or deviations from patterns) from electron scattering without having nice-looking, or even human-interpretable pictures?
- ▷ For lots of important problems, every scattered electron counts. What are the best ways to make use of physical prior knowledge and redundant information in electron microscopy experiments to extract the most knowledge from the least number of electrons?
- ▷ What challenges do the specific noise sources in electron microscopy (Poisson distributed noise, Fano noise, dark current noise) pose in the mathematics needed to answer the above two questions?

Thursday, 13:30 – 14:30
