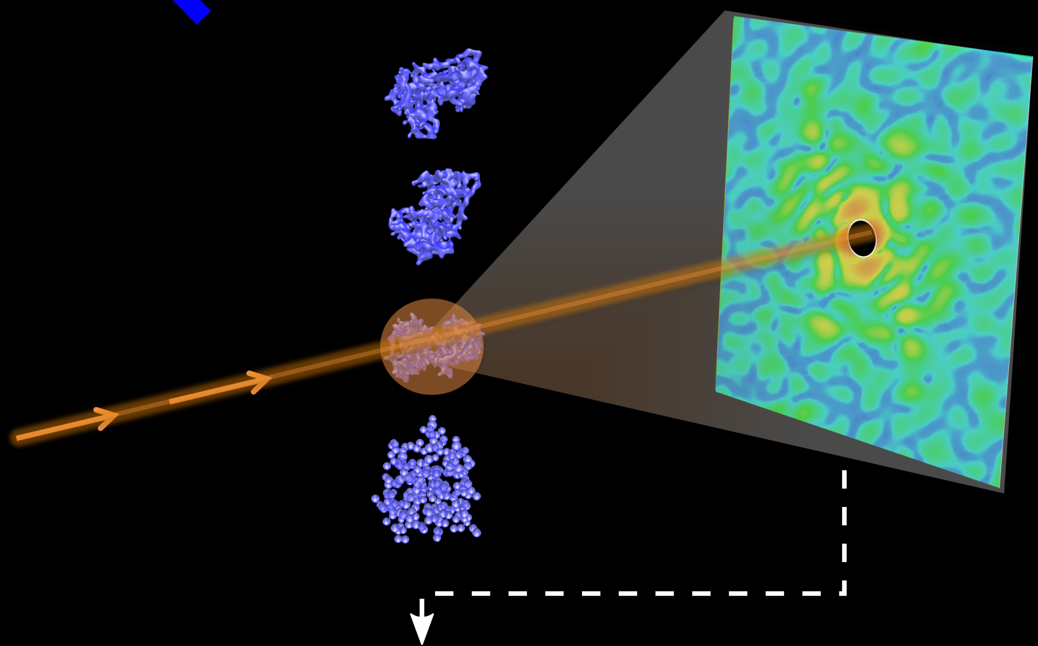
Center for Advanced Mathematics for Energy Research Applications

Summary Report 2018

CAMERA

Applied Math



$$I(\mathbf{q}) = \left| \int_{\mathbb{R}^3} \rho(\mathbf{r}) e^{-2\pi i \mathbf{q}\cdot\mathbf{r}} d\mathbf{r} \right|^2$$

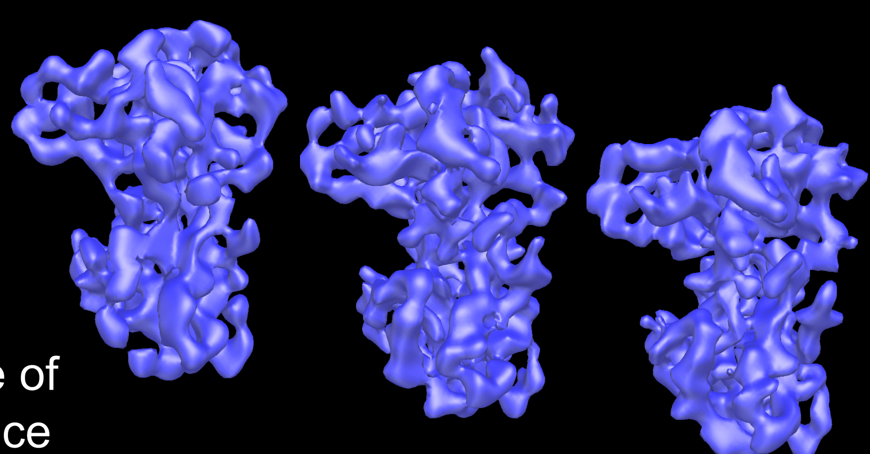
$$(\widehat{P_M(I)\rho})(\mathbf{q}) = \frac{\hat{\rho}(\mathbf{q})}{|\hat{\rho}(\mathbf{q})|}\sqrt{I(\mathbf{q})}$$

$$J_m^{(k)}(q) = \sum_{l=|m|}^{\infty} \sum_{m'=-l}^{l} D_{lmm'}(R_k) P_l^m(\cos\theta(q)) I_{lm'}(q)$$

$$\underset{R\in SO(3)}{\arg\min} \int_0^{q_{\max}} \int_0^{2\pi} \Big(J(q,\phi) - I^{(R)}(q,\theta(q),\phi) \Big)^2 w(q)\, d\phi\, dq$$

$$\rho^{(n+1)} = P_{S*} P_M (I^{(n+1)}) \rho^{(n)}$$

$$I(q,\theta,\phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} I_{lm}(q) Y_l^m(\theta,\phi)$$



U.S. DEPARTMENT OF ENERGY | Office of Science

CAMERA Applied Math

The Department of Energy supports a wide spectrum of experimental facilities to advance the fundamental science that will meet the nation's energy, environmental, and national security challenges. State-of-the-art applied mathematics can play a pivotal role in these investigations, transforming experimental science and furthering discovery.

Fundamental computational methods are needed to extract information from murky data, interpret experimental results, and provide on-demand analysis as data is generated. Advanced algorithms can screen candidate materials that are expensive and time-consuming to manufacture, rapidly find optimal solutions to energy-related challenges, and suggest new experiments for scientific discovery.

To address these growing needs, the Department of Energy established the Center for Advanced Mathematics for Energy Research Applications (CAMERA). Within this center, cross-disciplinary teams of applied mathematicians, software engineers, and facility scientists work together to formulate models, derive appropriate equations, develop algorithms, build and test prototype codes, and deliver useable software. Jointly funded by the Office of Advanced Scientific Computing Research (ASCR) and the Office of Basic Energy Sciences (BES), CAMERA is now a nationwide community resource in service of the DOE facilities.

This report provides a snapshot of some of CAMERA's current activities.

Glossary

ASCR Office of Advanced Scientific Computing Research, DOE

ALS Advanced Light Source

APS Advanced Photon Source

AMI Adolphe Merkle Institute

ALCF Argonne Leadership Computing Facility

ANL Argonne National Laboratory

BES Office of Basic Energy Sciences, DOE

BNL Brookhaven National Laboratory

CAMERA Center for Advanced Mathematics for Energy Research Applications

CD-GISAXS Critical Dimension Grazing Incidence Small Angle X-Ray Scattering

CD-SAXS Critical Dimension Small Angle X-Ray Scattering

CFN Center for Functional Nanomaterials

CLS Canadian Light Source

CWI Centrum Wiskunde & Informatica, Netherlands

DASK Library for dynamic task scheduling, `http://dask.pydata.org`

DESY Deutsches Elektronen-Synchrotron

Diamond Diamond Light Source at Harwell, UK

DOE US Department of Energy

EM Electron Microscopy

EMAT The Electron Microscopy for Materials Science (EMAT) Reseach group, Antwerp, Belgium

ESRF European Synchrotron Radiation Facility

FXS Fluctuation X-Ray Scattering

GISAXS Grazing Incidence Small Angle X-Ray Scattering

GUI Graphical User Interface

JBEI Joint Bio-Energy Institute

KIT Karlsruhe Institute of Technology

LDRD Laboratory Directed Research and Development

LANL Los Alamos National Laboratory

LLNL Lawrence Livermore National Laboratory

LBNL Lawrence Berkeley National Laboratory

LCLS Linear Coherent Light Source

MSRI Mathematical Sciences Research Institute

M-TIP Multi-Tiered Iterative Phasing

NSLS-II National Synchrotron Light Source

NIST National Institute of Standards and Technology

NCEM National Center for Electron Microscopy

NERSC National Energy Research Scientific Computing Center

NXCT National Center for X-Ray Tomography

OLCF Oak Ridge Leadership Computing Facility

ORNL Oak Ridge National Laboratory

PSI Paul Scherrer Institute, Switzerland

PAWS Platform for Automated Workflows (from SSRL)

Petra-IV Synchrotron at DESY

SciDAC Scientific Discovery through Advanced Computing

SAXS Small Angle X-Ray Scattering

SPD Single Particle Diffraction

SPI Single Particle Initiative

SLAC Stanford Linear Accelerator Center

SSRL Stanford Synchrotron Radiation Lightsource

TUM Technical University Munich

UCSF University of California, San Francisco

WAXS Wide Angle X-Ray Scattering

XFEL X-Ray Free Electon Laser

XPCS X-Ray Photon Correlation Spectroscopy

Xi-CAM CAMERA open source software for synchrotron experiments

The Center for Advanced Mathematics for Energy Research Applications (CAMERA)
Building 50A-2113, Lawrence Berkeley National Laboratory
1 Cyclotron Road, Berkeley, California 94720

The Center for Advanced Mathematics for Energy Research Applications (CAMERA)

Technological advances are opening doors to new experimental science, with scientific facilities collecting data at increasing rates and higher resolution. Analyzing this data is now a major bottleneck. New mathematics and algorithms are needed to extract useful information from experiments.

To address these growing needs, the Department of Energy established the Center for Advanced Mathematics for Energy Research Applications (CAMERA). Jointly funded by the Office of Advanced Scientific Computing Research (ASCR) and the Office of Basic Energy Sciences (BES) within DOE's Office of Science, CAMERA is comprised of coordinated teams of applied mathematicians, computer scientists, beam-line scientists, materials scientists, computational chemists, and software architects, all focused on solving challenging science problems.

CAMERA identifies areas in experimental science that can be aided by new mathematical insights, develops the needed algorithmic tools, and delivers them as user-friendly software to the experimental community.

Application areas include X-ray scattering and ptychographic imaging, reconstruction and analysis of imaged materials, chemical informatics for analysis of crystalline porous materials, fast methods for electronic structure calculations, reconstruction methods for emerging experiments at X-ray free-electron lasers, autonomous control of experiments, and real-time streaming for automatic feedback and reconstruction.

CAMERA has partnership projects with DOE light sources (ALS, APS, NSLS-II, SSRL, and LCLS), DOE Nanoscience Centers (Molecular Foundry and CFN), and a host of other national and international labs, including LANL, LLNL, NIST, DESY, BESSY, ESRF, E-XFEL, SSRF, CSC, CNS, Diamond, and industrial collaborators including Intel, GE, Dow, Bosch, and Samsung.

CAMERA focuses on four key questions:

- **How can mathematically correct inverse problems be formulated and effectively solved to extract information from different experimental techniques?**

  Recent work includes new methods for fluctuation scattering and single particle imaging for the LCLS, new methods for ptychographic reconstruction, and fast methods for SAXS, WAXS, and GISAXS.

- **Once this information is collected, how can it be effectively analyzed?**

  Recent work includes imaging algorithms to auto-detect fibers and breaks in materials, deep learning for X-ray diffraction and recognition, and new mixed-scale dense deep convolution neural networks for image classification.

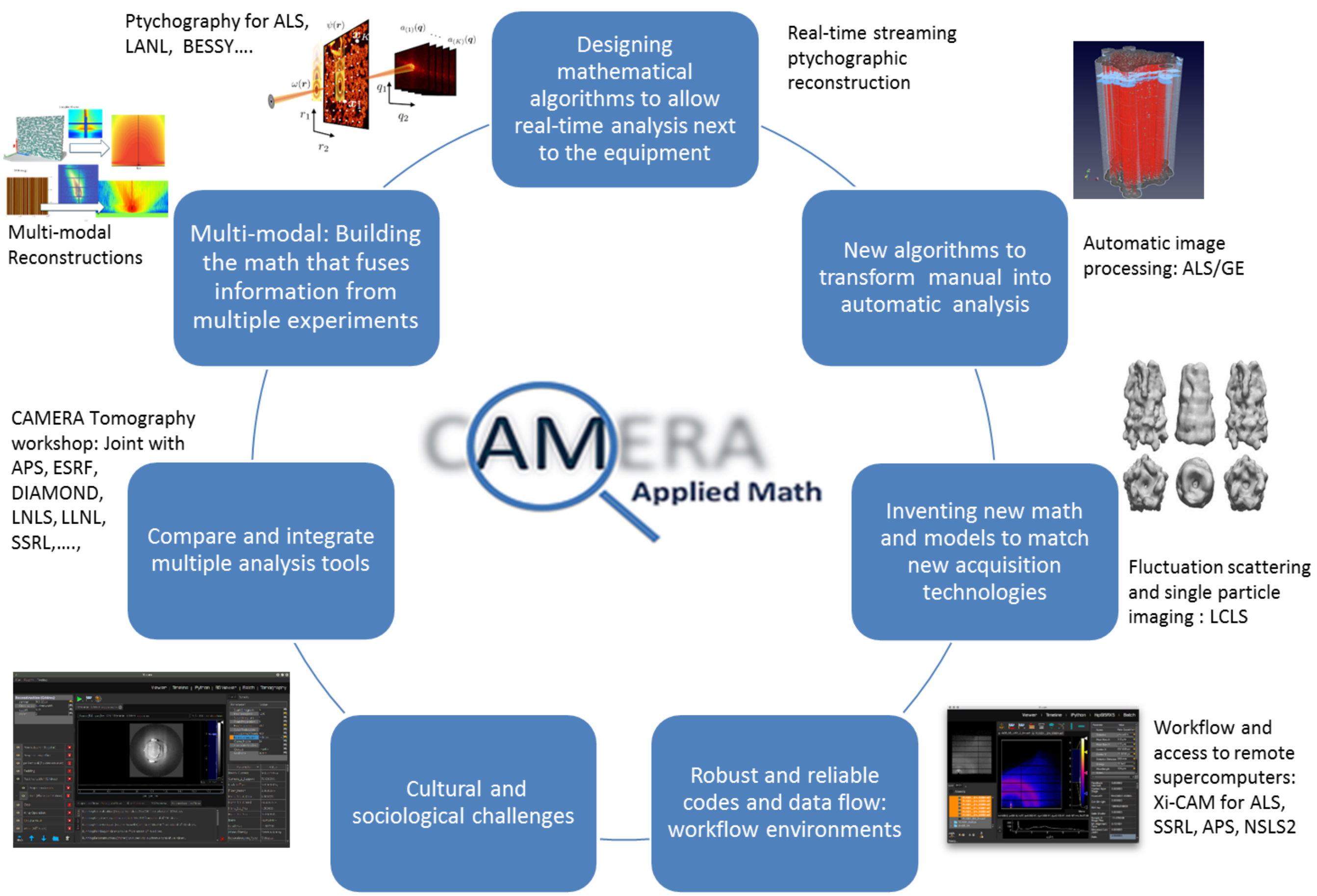
- **What is the best way to use computing resources (embedded in detectors vs. local hardware vs. remote supercomputers) to quickly analyze results and guide new experiments?**

  Recent work includes merging new algorithms, GPU accelerators and customized workflows for real-time streaming ptychography, and Kriging optimization to automatically steer autonomous X-ray scattering experiments.

- **How can algorithms, data, tools, and answers be shared across the community?**

  Recent work includes developing Xi-CAM, a combination GUI, python plugin environment and remote workflow manager for synchrotron data, now in use at multiple facilities.

Overview of Projects



CAMERA began in 2010 as a three year LDRD project at LBNL. It then expanded to a two year pilot project supported by ASCR and BES within DOE's Office of Science, mostly focused on work at the Advanced Light Source. Since 2015, it has been supported by DOE to work with multiple facilities. CAMERA now fosters collaborations across the DOE landscape of light sources, with growing interactions with nanoscience centers and international collaborators.

Current CAMERA projects include:

- **M-TIP for X-FEL fluctuation scattering and single particle imaging**

  Multi-tiered iterative phasing for reconstructing structure from X-ray free-electron laser data at the LCLS.

- **Surrogate model approach for optimizing autonomous experimentation**

  Kriging coupled to optimization and artificial intelligence for autonomous steering of experiments at NSLS-II.

- **Machine learning for biological and materials images**

  Mixed-Scale Dense convolution neural networks for automatic image segmentation at the NXCT and for sub-grid learning/reconstruction of missing phases and data in tomography at the ALS and CWI.

- **PEXSI for electronic structure**

  Pole Expansion and Selected Inversion (PEXSI) method for fast solutions to Kohn-Sham density functional theory for the Molecular Foundry and LLNL.

- **Ptychographic reconstruction**

  SHARP (Scalable Heterogeneous Adaptive Real-Time Ptychography) algorithms for ptychographic reconstruction leading to faster, brighter and sharper methods for the ALS, SSRL, and LCLS.

- **X-ray scattering and CD-SAXS/CD-GISAXS**

  Fast GPU-based methods using the Distorted Wave Born Approximation (DWBA) for CD-SAXS and CD-GISAXS for APS, NIST, and the ALS.

- **Automatic structure recognition for ceramic matrix composites and scattering experiments**

  Automatic structure identification for materials together with machine learning for scattering with the ALS and GE.

- **Algorithms and tools for accelerating nanoporous materials discovery**

  Fast methods for high-throughput material characterization for the Molecular Foundry, EFRC for gas separations relevant to clean energy technologies, Nanoporous Materials Genome Center, and the Hydrogen Materials Advanced Research Consortium.

- **Real-time streaming, analysis, and feedback of synchrotron data as it is being collected**

  An end-to-end environment in which data is collected from fast detectors and streamed to algorithms for on-the-fly reconstruction, displayed as the material is scanned. A ptychography version, Nanosurveyor, is currently in production use at the ALS.

- **Xi-CAM: A community platform for synchrotron experiments**

  Xi-CAM was developed as a GUI providing an applications plug-in environment and remote compute workflow manager for synchrotron experiments, using collaborative components from the larger community, including contributions from NSLS-II, SSRL, ESRF, APS, NIST, DESY, and ALS.

- **Bringing user communities together**

  CAMERA workshops brought together developers and installed their tomography packages in a common base for analysis, assessment, and further development. Participants included members from APS, ORNL, KIT, Diamond, LLNL, SSRL, NCEM, CWI, CSIRO, DMEA, UCSF, NSLS-II, Petra, Max IV, and SLS.

- **Summer schools for young scientists**

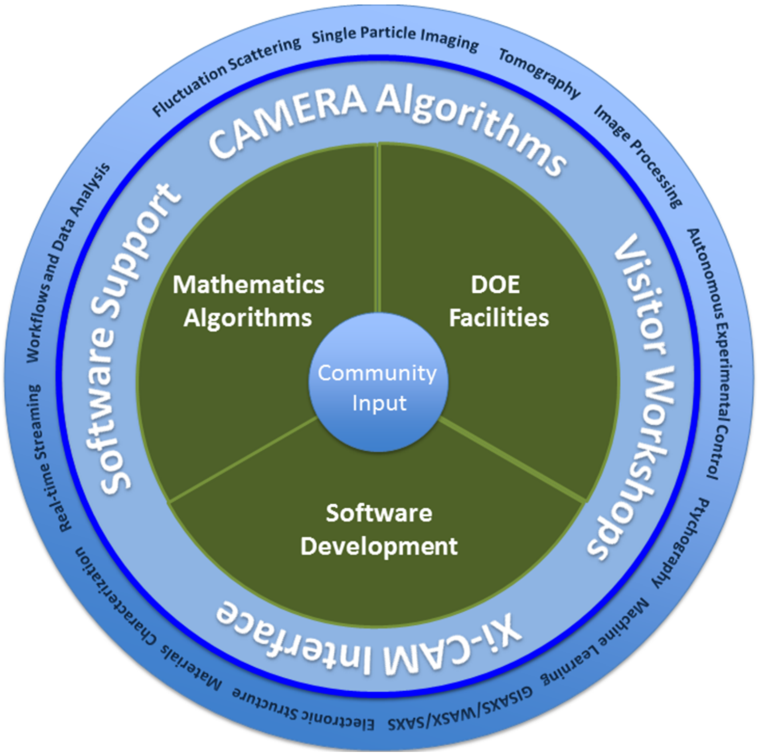
  CAMERA ran summer schools for young scientists to prepare them for cross-disciplinary work at DOE facilities: (1) 2016 Workshop: Experiment, algorithms, and computing for GISAXS; (2) 2016 Workshop: Fast and accurate new methods for electronic structure simulation.

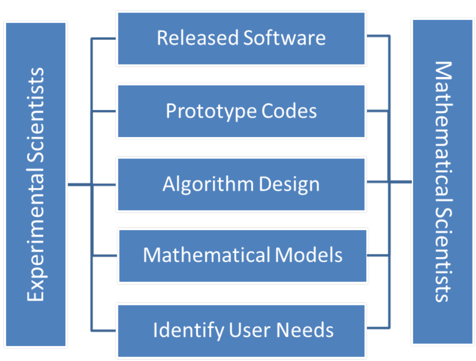
Structure, Organization, and Linkages

By reaching across traditional boundaries, brand-new mathematics can be built that can help analyze and characterize experimental data.

Traditionally, it takes considerable time for new mathematical ideas to migrate to user communities. Bringing mathematicians and experimentalists together accelerates the development and early adoption of new mathematics and algorithms. Including computer scientists ensures that the resulting codes will be efficient and make use of advanced compute resources. Engaging software engineers underscores that codes must be robust and maintainable.

CAMERA is structured around an inner core of scientists working on team projects, developed through the guidance of the larger community. Each cross-disciplinary team focuses on a particular application area. Participants are typically part of multiple teams, and vertical integration allows rapid feedback.





Vertical Integration of Tasks

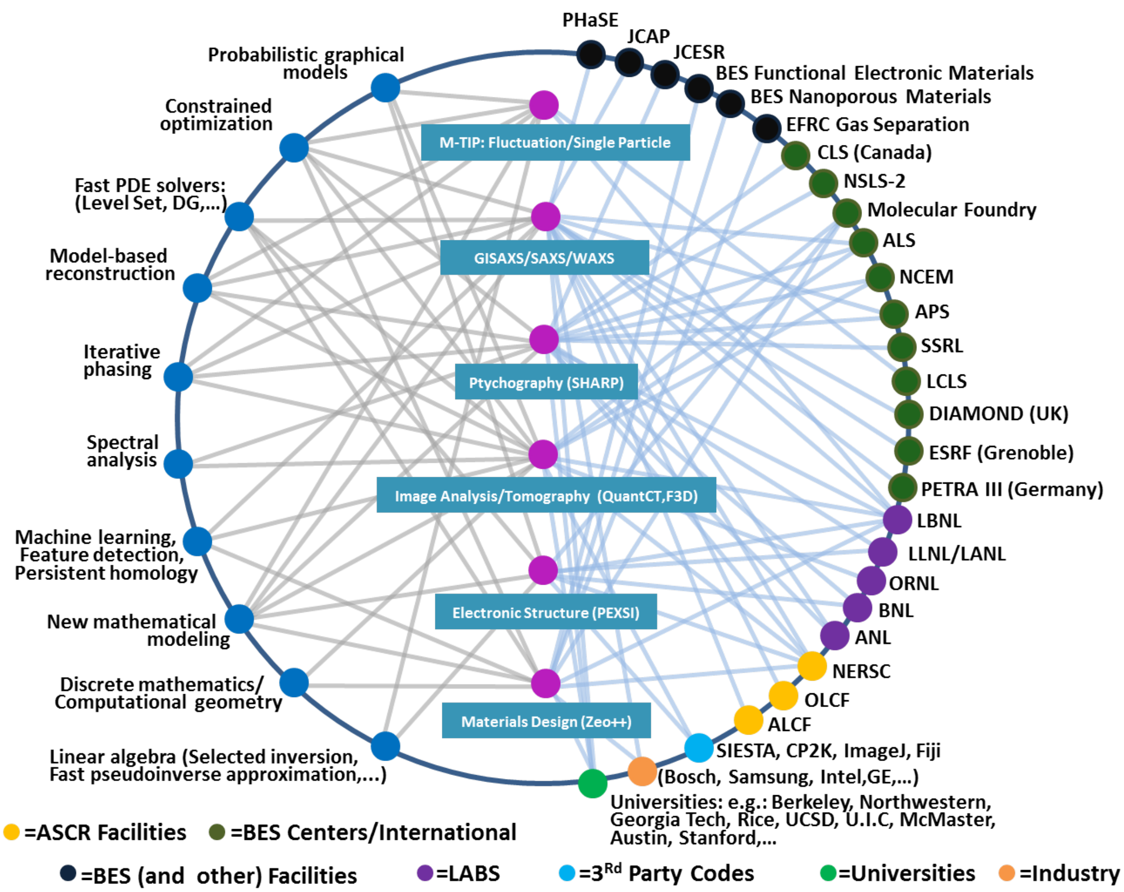
Close connection of mathematics, experimental expertise, and software development steers projects more efficiently toward meeting user needs.

Capitalizing on shared expertise

Sometimes seemingly different problems are in fact linked, and share common mathematical solutions. Matrixing mathematicians and scientists into more than one group creates cross-fertilization. Common questions emerge, and mathematics can be built that serves multiple projects.

Working together, we have seen that advances in such diverse fields as computational harmonic analysis, PDE-based techniques for image segmentation, graph theoretic approaches, dimensional-reduction and manifold embedding, diffusion maps and non-linear tensor schemes, sparse and compressed approximation methods, and new approaches to operator decompositions, can be cross-fertilized across challenges at the facilities.

This cross-fertilization is apparent in a node-edge graph showing how different types of mathematics come into play in more than one field, and how mathematics in one particular application can suggest new ideas when attacking a different area.



Interconnections between mathematics, applications, and collaborators

Building on core and applied research:

CAMERA builds and captilizes on a wide-spectrum of core and applied research supported and performed across DOE. ASCR base research in mathematics and computer science, BES work at facilities, and joint SciDAC efforts across the Office of Science are foundations on which CAMERA efforts are built. As just a few examples:

- **Core research on the M-TIP approach fluctuation scattering and on materials discovery:** developed under ASCR base math.
- **Core research work on image analysis:** developed under ASCR base math, base computer science, and a DOE early career award.
- **Core research work on PEXSI for density functional theory:** developed under ASCR base math, SciDAC partnerships, and a DOE early career award.
- **Core research on workflows in CAMLink:** developed under ASCR base computer science.
- **Core research on algorithms for inverse reconstruction for scattering and community software platforms:** developed under ASCR base math, at the light source facilities, and under a DOE early career award.

Fundamental support is crucial, and provides much of the initial insight, mathematical models and algorithmic tools that CAMERA then exploits.

CAMERA can be thought of as a graph with nodes and links. The nodes are people, performing research supported by many programs throughout DOE. CAMERA capitalizes on this work, and helps support and link together collaborations aimed at meeting the needs of DOE facilities.

Community Engagement and Project Selection

Engagement with the Community

Four types of engagements play valuable roles:

Teams
(appointed for project duration)
On-site cross-disciplinary teams. Scientists at other facilities may join a team project

Visitors
(short-term: days to weeks)
Visitors learn algorithms, attend workshops, bring data, try codes, and suggest new problems

Lab Exchange
(weeks to months)
CAMERA members sent to other facilities and scientists at other facilities come to CAMERA for joint development of new projects.

Community Software
(on-going)
CAMERA delivers algorithms and incorporates other people's algorithms into community software, and shares code across DOE

- **Teams:** Cross-disciplinary teams focus on developing the mathematics, algorithms, prototype codes, and robust software to tackle current and emerging facility challenges. Teams last for the duration of a project, and scientists at other facilities often collaborate on a specific project.

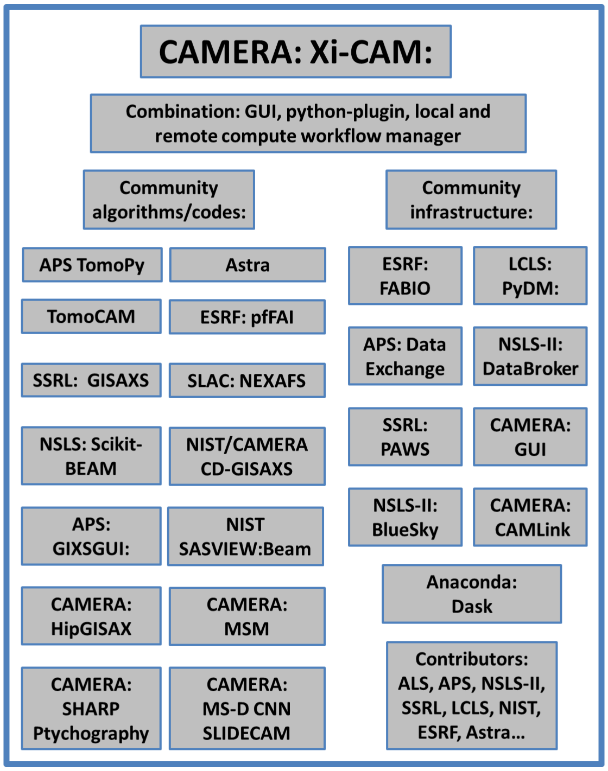
- **Visitors:** Short-term visitors attend workshops, learn how to run codes, and offer valuable insight into how to modify and extend the underlying mathematics, algorithms, and software to meet their own specific needs. Examples are the 2016 and 2017 tomography workshops.

- **Exchange with other Labs:** During a project's lifetime, collaborators are matrixed into CAMERA and into other DOE facilities in order to accelerate advancement. They communicate needs and help guide conversations in which people from different disciplines frame questions and goals.

- **Community Software:** Algorithms are delivered as software and shared across the DOE landscape. CAMERA's Xi-CAM is a GUI, connecting to multiple functionality through a plug-in environment, and executes remote compute workflow manager for synchrotron experiments. It embraces collaborative components from the larger community, including contributions from NSLS-II, SSRL, ESRF, APS, NIST, DESY, and ALS.

- **Additional Partners:** Additional institutions beyond DOE light sources, nano-science centers and other DOE Labs are valuable partners:

  - UC Berkeley is a rich resource of related research and people, including faculty, externally supported postdocs and new graduate students. CAMERA works closely with many Berkeley departments, including Computer Science, Statistics, Materials Science, Chemistry, and Mathematics.
  - Close ties with the Moore-Sloan Berkeley Institute for Data Science (BIDS) connect our efforts to data science. Several CAMERA members are also BIDS Fellows.
  - CAMERA has partnered with the NSF-funded MSRI to run joint summer schools, and shares researchers with the NSF STROBE Center.
  - Several international institutions have proposed linkage to their own efforts, including those in Germany, the UK, and China.



Xi-CAM: Synchrotron experiments analysis software: contributions from NSLS-II, SSRL, ESRF, APS, NIST, DESY, and ALS

How are projects selected?

CAMERA has focused on projects identified "from the ground up," visiting DOE light sources multiple times, gathering information from beamline scientists about their needs, and working together to understand the scientific challenges.

CAMERA tries to select projects that meet the following criteria:

- **Demand:** Is there a need and demand for the project from multiple groups?
- **Available Expertise:** Does CAMERA have, or can we connect to the needed expertise?
- **Time Scale for Success:** How long can the user wait? Is this urgent, or is there time to perform the required research to develop new, and potentially more powerful tools?
- **Disruption:** Do current solutions work well enough? Is there tolerance for transitioning to new technologies, which may cause interruptions?
- **Plausible Delivery:** Is there time and a reasonable plan to deliver useable software?
- **Support Infrastructure:** Are the people in place to support and maintain the sotware that results from new algorithms?

Cultural and sociological challenges: Getting teams to work together

Building effective teams has challenges. Language and cultural barriers between experimentalists, mathematical scientists and software engineers are obstacles. Each brings different requirements and different answers to questions such as:

- **When is something "done"?** What is the definition of success? A journal article? A prototype code? Working supported software?
- **How long should a project take?** Someone may want a slightly better algorithm sooner, rather than wait to develop the mathematics behind a new approach.
- **Should a new algorithm replace everything before it can be used?** Or, can multiple overlapping software exist side-by-side?
- **How should credit be shared among scientists from different communities?**

These questions are important. It can take many months for a team to learn to speak the same language and understand common questions and goals.

An essential element of success is the locality of these teams. Members work together at the same institution with offices close by. Questions can be answered quickly, and design decisions can be made rapidly as projects evolve.

Developing a cohesive strategy

The best results occur when the need is identified, the outcome is clearly defined, and when all parties are invested.

Projects need to align with the scientific strategy of the institution and support from management is important. At the same time, individual scientists need to be enthusiastic about the collaboration, so that they can drive direction and goals.

This is a delicate balance. Before undertaking a project, CAMERA tries to ensure that the project is relevant and needed. Input across multiple levels of management at an institution is encouraged.

Continuing Projects and New Paths Forward

CAMERA has had significant impact in the development and adoption of new mathematical technologies for DOE facilities, with particular attention on the light sources, and growing connections with the nanoscience centers. Looking to the future, several paths forward are apparent.

Blueprints for successful projects

Successful projects require participants and collaboration across fields, interests, and institutions. Different projects require different time scales and different amounts of research:

- **Some of the projects have required advanced, long-term core mathematical research in order to have practical implications for data analysis at advanced facilities.**

  One example is CAMERA's multi-tiered iterative phasing techniques (M-TIP), in which years of theoretical and algorithmic development were needed in advance, leading up to the now practical impact at the LCLS on fluctuation scattering and single particle imaging.

  Another example is the development of PEXSI for fast electronic structure simulations based on Kohn-SHAM DFT. This took years of work before it was able to have the large impact now occurring.

  These projects often build on core work initially supported by other DOE sources, such as base math, computer science, and SciDAC.

- **Conversely, for some projects, needed mathematics can be iteratively developed in close collaboration with facility scientists.**

  A good example is CAMERA's research on optimized experimental control, developed jointly with NSLS-II and CFN. Here, a CAMERA-supported and jointly-supervised postdoctoral fellow worked across labs to design a weighted Kriging algorithm to automatically steer experiments. Working together at the NSLS-II beam line, they devised multiple optimization weighting strategies.

- **Some projects require integration and guidance across facilities.**

  Xi-CAM software development has taken key pieces from a wide spectrum of collaborators (NSLS-II, APS, SSRL, LCLS, NIST, ALS, etc.). CAMERA's approach is not to reinvent or duplicate what is available from others, but instead to work together to build a community project.

Path forward: Capitalizing on momentum

Continuing the momentum of current CAMERA projects is important. As examples:

- **M-TIP.** The M-TIP approach is a powerful technique to analyze data coming from X-FELs. Future M-TIP mathematical development is needed to (a) build noise models in a systematic way, appropriate for the detector and collection mechanisms; (b) model more physical constraints in the algorithm to improve the reconstruction; and (c) accelerate the algorithms through remapping onto advanced emerging high performance computing architectures. These improvements will greatly improve the robustness and accuracy of reconstruction techniques for XFELs.
- **Autonomous Optimization of Experiments.** The joint NSLS-II/CFN/CAMERA project has immense potential, coupling advanced optimization, high-dimensional sampling, and artificial intelligence together to autonomously steer experiment and efficiently use resources. Much more needs to be done, including: (a) selected optimal weighting strategies; (b) coupling to more advanced optimization methods; and (c) adding more sophisticated constraints in the decision tree.

- **Mixed-Scale Dense Machine Learning CNNs.** CAMERA's MS-D is already being used by over 150 separate users across such fields as biology, pattern recognition, electron microscopy, tomography for metallic composites, MRI scans, segmentation of satellite images, and sonar imagery. One promising area is the reconstruction of sharp tomographic images from undersampled data. For time-varying tomography, reconstructing images from far fewer scans will reduce the time required and reduce radiation exposure.

- **Advanced Methods for Electronic Structure.** PEXSI is a powerful approach for ground-state calculations, and has been incorporated into a large number of packages. For KSDFT with high fidelity functionals such as the hybrid functional, the main challenge is the Fock exchange operator. Jointly with LBNL Math, we will continue development of the adaptively compressed exchange (ACE) formulation, which reduces the cost of hybrid functional calculations by 5-10 fold without loss of accuracy, and extend its capability to large scale ab initio molecular dynamics.

- **Automatic Techniques for Real-Time Image Analysis.** CAMERA image characterization methods, including methods that segment boundaries, extract fiber and crack structure in materials, and exploit machine learning to identify scattering patterns, are ripe for further development and application. This includes the addition of methods from topological data analysis exploiting persistence theory, and graph-theoretic classification techniques. New applications include NCEM applications on quantifying pore structure evolution, analyzing thin films, and capturing order and structure in colloidal nanocrystal films.

- **Real-time streaming analysis.** The CAMERA software environment for streaming, such as NanoSurveyor for ptychography, represents a future in which detectors, data collection, and algorithms come together at a beamline with local compute resources to provide on-the-fly real-time analysis and reconstruction. As more data is collected over shorter time scales, it becomes impractical to ship all the data to a remote resource and decide later what is worth keeping. Experimentalists need feedback as data is collected to make decisions and guide experiment. CAMERA is starting to export its real-time environment to other beamlines and facilities.

- **Xi-CAM.** The CAMERA Xi-CAM synchrotron platform is being used at a variety of beamlines around the country. New functionalities, including fluctuation scattering reconstruction, single particle M-TIP, autonomous experimental control using Kriging, new tomography tools (such as the Livermore Tomography Tools-LTT), are being incorporated. We are in the process of adding more automatic access to remote compute resources, including the DOE HPC resources (ALCF, OCLF, and NERSC). Our intent is to continue to grow this resource, welcoming contributors from across the community.

Path forward: New projects

Considerable community interest has been expressed in taking CAMERA algorithms to new areas. To name just two:

- **XPCS, powder diffraction, and electron microscopy:** While very different experimental techniques, we believe that CAMERA's multi-tiered iterative phasing (M-TIP) approach has applicability in these areas. The fundamental idea behind M-TIP, namely to decompose the reconstruction into several underdetermined subproblems that can be solved efficiently via application of carefully designed projection operators, can be targeted at multiple fields. These projection operators, once they are customized for the particular physics and constraints, are then applied in an iterative scheme which converges to the correct solution.

- **Machine learning for material characterization:** CAMERA's Mixed-Scale Dense convolution neural networks require far less tagged training data than other approaches and allow identification and categorization of materials. Using these techniques, a large number of biological applications, including cell classification, reconstruction of brain architecture, and crack identification, are now being explored by scientists world-wide.

More mathematics can be developed to meet the needs of BES facilities. For example, we have focused on only a few applications at two nanoscience centers, namely LBNL's Molecular Foundry and BNL's Center for Functional Nanomaterials. New mathematical opportunities can be explored at these and other DOE nanoscience centers.

Path forward: The software challenge

CAMERA is building software for the community, with many more algorithms and functionality in the pipeline.

- **Documentation and user support:** We need to provide documentation, available support, and development paths for contributors to add to existing codes.
- **Test data sets and examples:** Test data sets are needed, complete with examples and documentation of the accuracy and efficiency of computed results.
- **Curated repositories:** Codes must be sustained. They must always be accessible, compile, and embrace new features as they are developed, while maintaining back-compatibility whenever possible. Maintaining this software is important

Path forward: The data challenge

Profound data challenges are coming from the facilities, including capturing and storing increasing amounts of data, annotating and archiving this data, and providing accessibility across multiple institutions. Carefully targeted mathematics can play a key role:

- **Deciding what data to keep:** Forthcoming acquisition rates will make it hard to keep all data in raw, unprocessed form. Advanced mathematics will be needed to quickly analyze data, assess whether the experiment is as planned, and determine what data to keep.
- **Providing efficient and common descriptors for data:** Data will need to be analyzed and stored in reduced form, and this reduction will require new mathematics. Automatic tagging can be augmented by appropriate machine learning algorithms and characterization operators. Multi-modal analysis will require the design and development of multi-tiered projection operators that capitalize on applying simultaneously constraints across different experiments.

Fast networks, rapid data storage, and advanced computing facilities are critical. Their utility will be enhanced by complementary mathematics derived in tandem.

Path forward: New areas

Many interested parties have suggested expanding CAMERA to new areas, including biologists, earth scientists, and computer scientists. We have already been able to identify strong potential partners at JBEI where mathematics can make valuable contributions. CAMERA can have an impact on many other parts of the Office of Science.

At its core, this is an expression of interest in linking mathematics to more fields and an appreciation of what cohesive teams can accomplish.

Such expansions have potential, but need to be approached in the same systematic manner in which CAMERA was initially formed. Mathematical expertise and scientific interests need to be identified. Mathematical problems need to be well-formulated. Key people need to link together to attack clearly articulated problems within definable timeframes.

When appropriate, CAMERA can expand to these and other new and needed areas.

Path forward: Finding new people

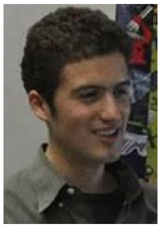
Sharing people and projects has advantages:

- Jointly supervising CAMERA-supported postdoctoral fellows works well, and these younger scientists help teams make progress together.
- Workshops bring people together on a common ground. Researchers are comfortable pointing out advantages and disadvantages of a wide collection of techniques, and help identify areas where new research is needed.
- Community projects such as Xi-CAM provide a mechanism in which algorithms and software can tested by the community.

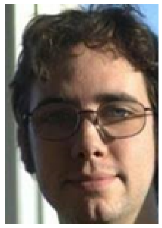
The CAMERA model

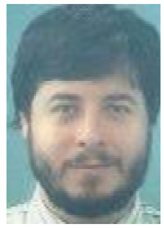
The CAMERA model requires people, commitment, and organization. With these components, it provides a way to focus teams to accelerate the application of mathematics to problems of DOE importance.

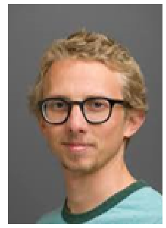
CAMERA Collaborators


D. Allan
(BNL)


A. Aquila
(SLAC)


T. Caswell
(BNL)


K. Champley
(LLNL)


B. Daurer
(Uppsala)


F. DeCarlo
(APS)


E. Dill
(BNL)

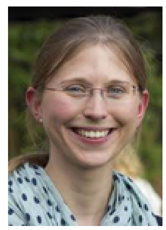

L. Fourcar
(Max Planck)

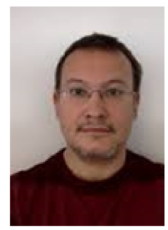

M. Fukuto
(BNL)

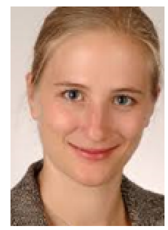

C. Gati
(SLAC)


C. Gheller
(CSCS)


A. Gorel
(Max Planck)

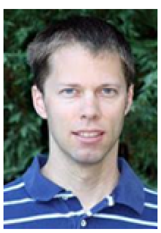

M. Grunbein
(Max Planck)


D. Gursoy
(APS)

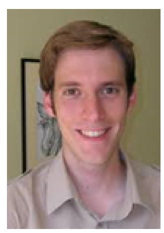

E. Herzig
(Bayreuth)

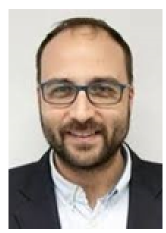

M. Hunter
(SLAC)


R. Kirian
(Arizona)

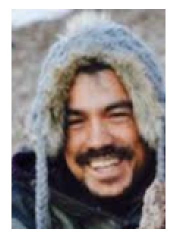

J. Klein
(NIST)


R. Kurta
(E-XFEL)

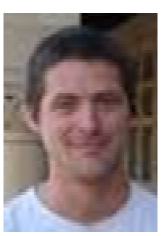

F. Maia
(Uppsala)

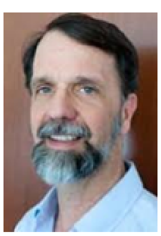

A. Mancuso
(E-XFEL)

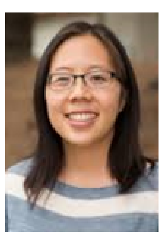

A. Mehta
(SSRL)


D. Mendez
(Arizona)

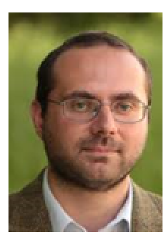

A. Perazzo
(LCLS)


L. Pellouchoud
(SSRL)

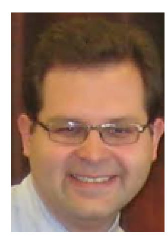

L. Richter
(NIST)


A. Sakdinawat
(SLAC)

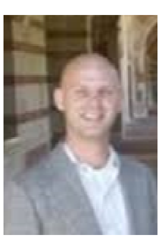

I. Schlichting
(Max Planck)


A. Sepe
(SSRF)

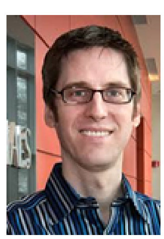

R. Sierra
(SLAC)


J. Strzalka
(APS)


C. Sweeney
(LANL)


C. Tassone
(SSRL)


S. Venkatakrishnan
(ORNL)

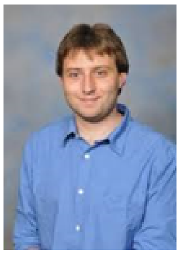

K. Yager
(BNL)


C. Yoon
(SLAC)


D. Prendergast
(Molecular Foundry)


J. Zhang
(APS)

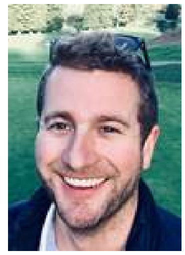
CAMERA Staff Members

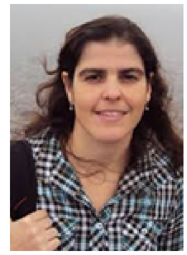

J.J. Donatelli
(A,B)

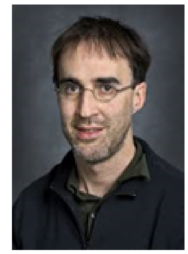

P.H. Zwart
(A,B)


K. Pande
(A,B)

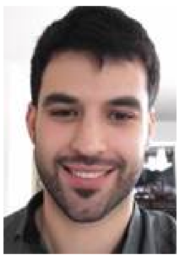

D. Ushizima
(C,G,I,L)


M. MacNeil
(C,G,I,L)

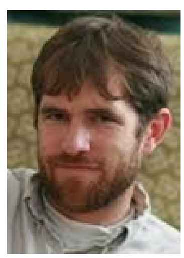

T. Perciano
(C,D,G)

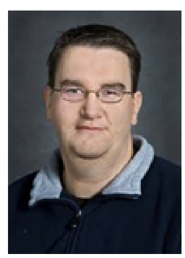

S. Marchesini
(D,E)

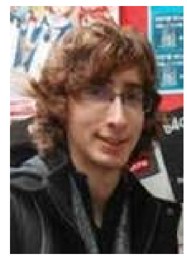

D. Shapiro
(D)


P. Enfedaque
(D)


H. Chang
(D)


D. Parkinson
(E,F)


A. Hexemer
(F,G,H)


R. Pandolfi
(F,G,H)

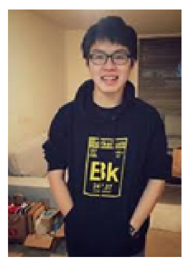

M. Noack
(M)

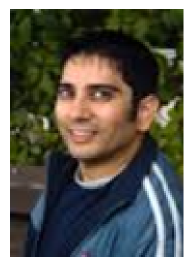

D. Kumar
(E,F,G)

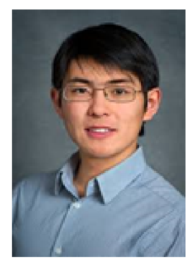

G. Freychet
(H,M)

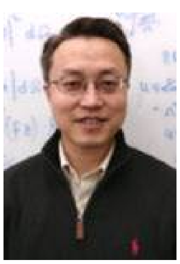

D. Pelt
(C,E,J)


O. Jain
(I)

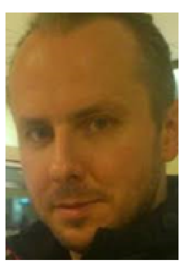

S. Mo
(I)


H. Krishnan
(C,D,E,F,G)

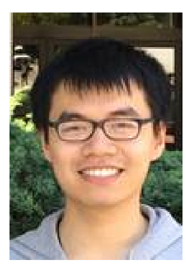

L. Lin
(J)


C. Yang
(J)


X. Li
(J)


M. Haranczyk
(K)

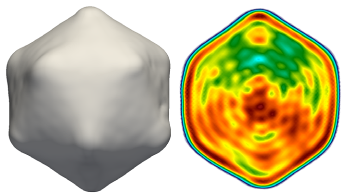

M. Shao
(B)


Z. Hu
(A)

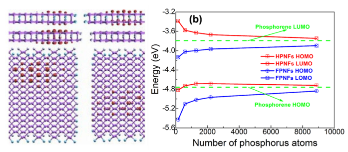

J.A. Sethian

A=Fluctuation scattering/Single particle, B=Exafel, C=Image Analysis, D=Ptychography/streaming, E=Tomography, F=Xi-CAM, G=GPU/Hardware acceleration, H=Scattering, I=Machine learning, J=Electronic Structure, K=Chemical Informatics, L=BioInformatics, M=Optimization

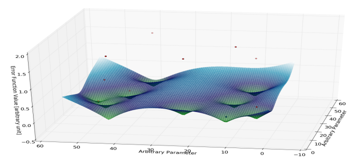
Technical Overview of Selected Projects



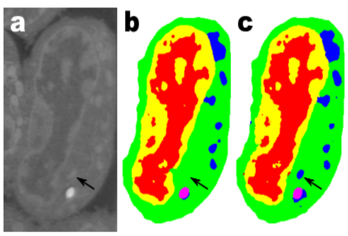
M-TIP for X-FEL fluctuation scattering



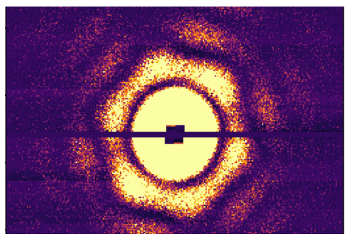
Electronic structure algorithms



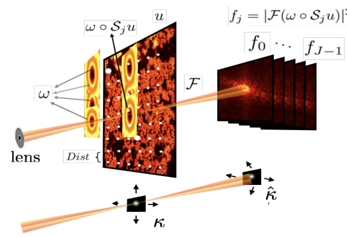
Autonomous experiments



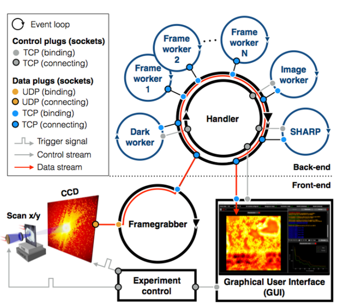
Mixed-Scale Dense Networks



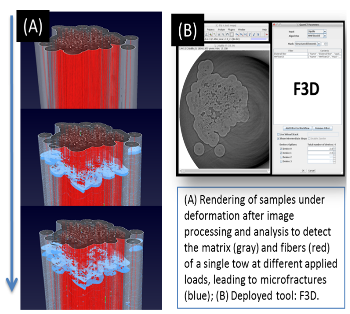
M-TIP for X-FEL single particle imaging



SHARP: Ptychography

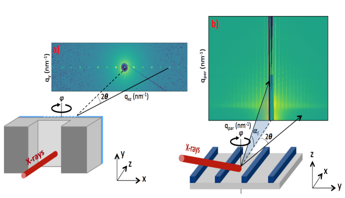


Real-time streaming



CMC structure recognition and Machine Learning

Materials discovery



X-ray scattering

Xi-CAM for synchrotrons

Community workshops

New Mathematics Enables Fluctuation X-ray Scattering at X-ray Free-Electron Lasers

(Joint Collaboration: LCLS, SLAC, Stanford, European XFEL, Max Planck Institute, Uppsala University, Arizona State University, and CAMERA)

Overview

The atomic structure and function of macromolecules, such as viruses and proteins, play fundamental biological roles, and probing their behavior has been a major challenge over the last century. Although traditional imaging techniques, such as X-ray crystallography, and more recent techniques, such as cryo-electron microscopy, have been successful at determining static structures to high resolution, many scientific questions cannot be efficiently studied with these methods.

One way to study the behavior of molecules in near-native environments is to collect X-ray diffraction patterns from particles directly in solution. However, in traditional solution scattering methods, such as small- and wide-angle X-ray scattering (SAXS/WAXS), the time it takes for the X-rays to interact and scatter off the particles is longer than the time it takes for the particles to undergo full rotation in the solution, resulting in "motion blur" that drastically reduces the information content.

The recent emergence of X-ray free-electron lasers (X-FELs), such as at the LCLS, have created an opportunity to overcome this challenge. X-FELs produce ultrabright and ultrashort X-ray pulses that can image particles at timescales far below rotational diffusion times, avoiding motion blur. Although experimental "fluctuation X-ray scattering (FXS)" was originally proposed in the 1970's, the challenge of determining 3D molecular structure from FXS data remained an open problem for over 40 years.

A New Approach

To address this problem, CAMERA mathematicians Jeffrey Donatelli and James Sethian, and physical bioscientist Peter Zwart developed a new mathematical algorithm called multi-tiered iterative phasing (M-TIP) which, for the first time ever, was able to determine *ab initio* 3D molecular structure from FXS data, solving the 40 year old open problem.

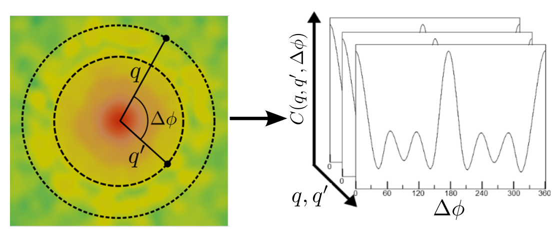
However, collecting and extracting accurate FXS data is itself challenging. Data is often corrupted with large degrees of noise, systematic issues, and incompleteness. To overcome this challenge, CAMERA physicist Kanupriya Pande developed data processing techniques to correct and extract robust FXS data from LCLS experiments and made them available in the Online Data Analysis (OnDA) software as a user-friendly GUI at X-FELs.

Using these techniques, CAMERA, working with an international team, demonstrated the first successful 3D reconstruction from both single particle and FXS data. As a result, FXS is now being looked at as a potential routine LCLS experiment, poised to tackle biological questions not answerable with other techniques.

Mathematical Approach

An FXS experiment takes a large number of independent X-ray diffraction snapshots $J^{(1)}, \ldots, J^{(N_{dp})}$, of a sample, with one or more particles in the beam per shot. From these images, for every pair of radii (q, q'), one calculates the average angular cross-correlation function

$$C(q,q',\Delta\phi) = \frac{1}{N_{dp}} \sum_{k=1}^{N_{dp}} \int_0^{2\pi} J^{(k)}(q,\phi) J^{(k)}(q',\phi+\Delta\phi) d\phi$$



Angular correlations of a diffraction image.

If orientations are uniformly sampled from the rotation group $SO(3)$ and X-ray exposures are taken below rotational diffusion times, then, when averaged over sufficiently many images, the correlation function can be directly related to the spherical harmonic coefficients of the 3D intensity function I via the Legendre polynomial decomposition

$$C(q,q',\Delta\phi) = \frac{1}{4\pi} \sum_{l=0}^{\infty} B_l(q,q') P_l(x(q,q',\Delta\phi)),$$

which, up to a scaling factor, the Legendre expansion coefficients B_l can be related to the intensity spherical harmonic coefficients via

$$B_l(q,q') = \sum_{m=-l}^{l} I_{lm}(q) I_{lm}^*(q'),$$

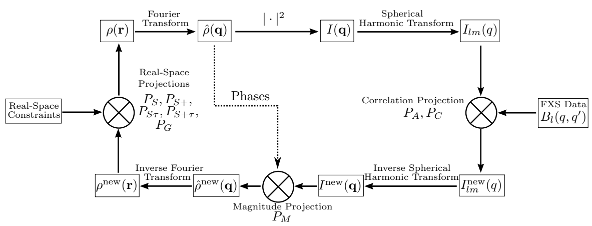
where

$$x(q, q', \Delta\phi) = \cos\theta_q \cos\theta_{q'} + \sin\theta_q \sin\theta_{q'} \cos\Delta\phi,$$

$\theta_q = \arccos(\frac{q\lambda}{2})$, and λ is the X-ray wavelength. The 3D intensity function is related to the electron density ρ of the molecular structure via $I = |\hat{\rho}|^2$, where $\hat{\rho}$ is the Fourier transform of ρ.

Determining 3D molecular structure from correlation data involves extracting the intensity function from the B_l coefficients, which can be cast as a hyper-phase problem, in addition to the classical phase problem of recovering the density ρ from its intensity function, both of which are challenging high-dimensional non-convex inverse problems.

CAMERA's M-TIP algorithm meets these challenges by decomposing the inverse problem into several underdetermined subproblems that can be solved efficiently via application of carefully designed projection operators. These projection operators are then applied in an iterative scheme which converges to the correct solution.



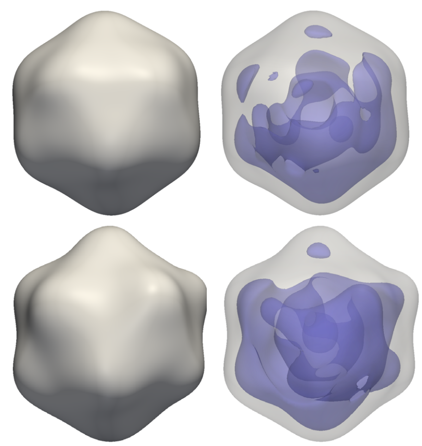
Flowchart description of the M-TIP algorithm.

Examples/Results

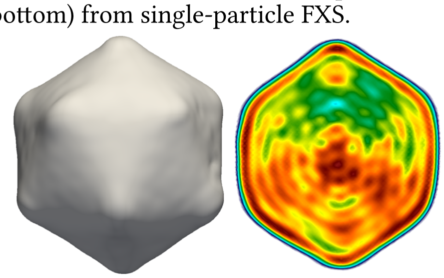
Determining 3D molecular structure from correlation data involves extracting the intensity. CAMERA used the above M-TIP algorithm to demonstrate the first successful 3D reconstruction of two viruses, RDV and PR772 from angular correlations of single-particle LCLS FXS data in a collaboration with an international team. Janos Hajdu's group at Uppsala performed sample preparation. The single-particle initiative, led by Andy Aquila at SLAC and with members from over 50 different universities and laboratories, organized data collection. Ruslan Kurta and Adrian Mancuso from the European XFEL performed part of the data processing.

CAMERA also used this approach to demonstrate the first successful 3D reconstruction of the PBCV-1 virus from angular correlations of multiple-particle LCLS FXS data, with 50-200 particles per shot. Ilme Schlichting's group from Max Planck provided the sample and initial data processing.

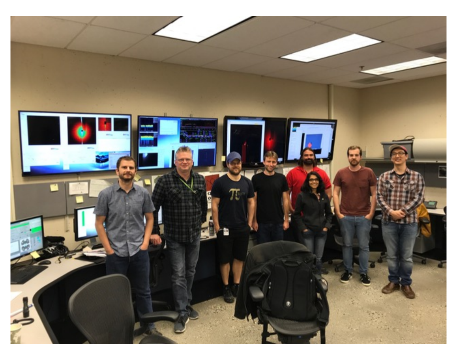
CAMERA is using these algorithms to: i) determine 3D molecular structure of the CroV virus from single-particle LCLS FXS data with members of Max Planck and ii) determine 3D molecular structure of the Trinity virus from single-particle LCLS FXS data with members of Uppsala and the European XFEL. CAMERA is leading the design and data collection strategies for FXS experiments at the LCLS, processing correlation data, providing software for FXS data analysis, and determining higher-resolution 3D structures of PBCV-1 and ribosomes with collaborators from SLAC, Stanford, and Arizona State.



M-TIP reconstructions of RDV (top) and PR772 (bottom) from single-particle FXS.



M-TIP reconstruction of PBCV-1 from multiple-particle FXS.



FXS experiment at LCLS: Richard Kirian (ASU), Peter Zwart (LBNL), Peter Walter (SLAC), Jeffrey Donatelli (LBNL), Mark Hunter (SLAC), Kanupriya Pande (LBNL), Cornelius Gati (SLAC and Stanford), and Chuck Yoon (SLAC).

Advanced Algorithms Significantly Boost Information Extracted from Single-Particle Diffraction Data

(Joint Collaboration: LCLS, SLAC, Stanford, LANL, NERSC, and CAMERA)

Overview

Biological structures are not static, and studying their inherent conformational flexibility is necessary in order to fully understand their behavior. However, fully probing the continuous landscape of conformations of important biological molecules is extremely challenging, requiring a vast amount of data in order to completely sample all possible configurations. Current imaging techniques study only tiny fractions of these conformational landscapes.

Upcoming powerful X-ray free-electron lasers (X-FELS) may provide an avenue for studying significant fractions of these conformational landscapes. Planned upgrades, such as at LCLS-II, promise to provide even brighter X-ray pulses with data collection rates at 10 KHz initially, and potentially up to 1 MHz in the future. Using this upcoming technology, single-particle diffraction (SPD) experiments, in which X-ray diffraction patterns are collected from individual molecules one at a time, may allow exploration of these conformational landscapes.

However, efficiently analyzing vast amounts of SPD data is challenging and complex, since orientations and conformations of the particles are unknown, complex phases are not measured, and data is often extremely noisy. Previous approaches are based on determining the orientations and conformations of the particles separately from the phases and the molecular structure, and thus are unable to make use of physical constraints on the molecular shape, such as size, symmetry, or positive density, to help in the orientation determination and conformational sorting step, ultimately limiting the structural features that can be resolved.

A New Approach

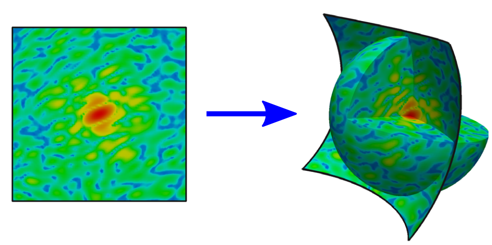
CAMERA mathematicians Jeffrey Donatelli and James Sethian and physical bioscientist Peter Zwart recently developed a new algorithmic approach to SPD reconstruction that significantly boosts the amount of information that can be extracted from these experiments, potentially allowing exploration of a much larger portion of the desired conformational landscapes. This approach, based on an extension of the multi-tiered iterative phasing (M-TIP) algorithm that they previously developed for fluctuation X-ray scattering reconstruction, makes maximal use of prior knowledge about what molecules look like throughout the reconstruction procedure. This algorithm was able to determine 3D structure of single- and multiple-state structures from a record-setting low number of diffraction images.

Mathematical Approach

An SPD experiment collects several X-ray diffraction patterns $J^{(1)}, \dots, J^{(N_{dp})}$ of individual molecules, with only one particle in the beam at a time. Each image samples the 3D intensity function I_s of the molecule along a 2D curved slice at a random conformational state s_k and orientation R_k, which can be expressed in polar coordinates as

$$J^{(k)}(q,\phi) = I_{s_k}^{(R_k)}(q,\theta(q),\phi),$$

where $I_s^{(R)}(\mathbf{q}) = I_s(R\mathbf{q})$, $\theta(q) = \arccos(q\lambda/2)$, and λ is the X-ray wavelength. The 3D intensity I_s is related to the electron density ρ_s of the s-th conformational state of the molecule via $I_s = |\hat{\rho}_s|^2$, where $\hat{\rho}_s$ is the Fourier transform of ρ_s.



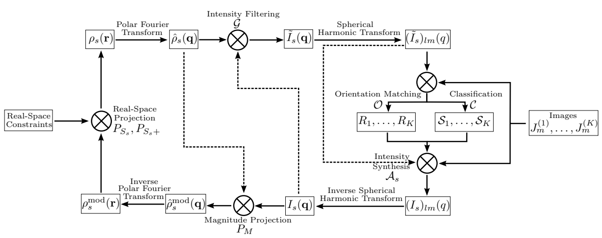
Each SPD image (left) samples a 2D curved slice of the 3D intensity function (right).

The goal of an SPD experiment is to determine 3D molecular structures of conformational states of the imaged sample. This requires determining orientations R_k and states s_k, corresponding to each image, assembling the oriented and classified images into their corresponding 3D intensity volumes, and determining missing complex phase information to retrieve the electron densities of the structure. Furthermore, SPD images are contaminated with significant noise, which must be treated.

CAMERA's M-TIP algorithm solves this problem by simultaneously solving all subproblems in an iterative projection framework, leveraging real-space constraints on electron densities of structures to significantly boost the amount of extractable information from the images. The algorithm exploits the mathematical relationship between the circular harmonic coefficients $J_m^{(k)}$ of an image and the spherical harmonic coefficients I_{lm}, given by

$$J_m^{(k)}(q) = \sum_{l=|m|}^{\infty} \sum_{m'=-l}^{l} D_{lmm'}(R_k) P_l^m(\cos\theta(q)) I_{lm'}(q),$$

where the $D_{lmm'}$ are Wigner-D functions and the P_l^m are associated Legendre functions. This formulation allows M-TIP to accelerate orientation matching through fast Wigner-D transforms and provides interpolation from the 3D intensity functions to the 2D images, and vice-versa, with spectral accuracy.

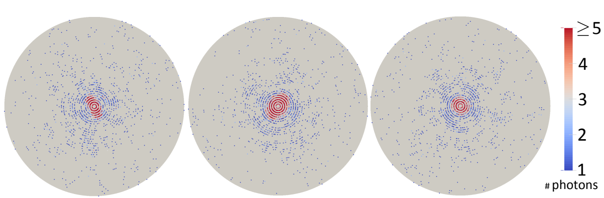


Flowchart of single-particle M-TIP algorithm.

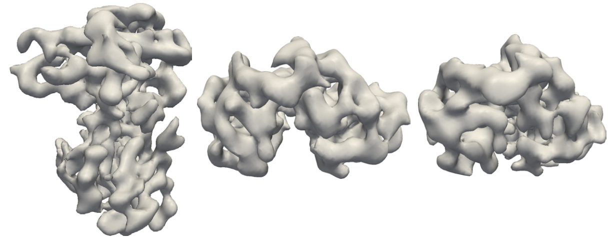
Examples/Results

CAMERA used the single-particle M-TIP algorithm to reconstruct the 3D structure of the retinoblastoma protein (prB) bound to E2F from only 192 photon-limited simulated single-state diffraction images, each with less than 0.1 photons per pixel at the image boundaries, setting a new record for the fewest number of images needed to determine 3D structure from shot-noise limited data.

M-TIP was also able to reconstruct the 3D structures of both the open and closed states of a sialic acid binding protein (SiaP), from only 384 noisy simulated diffraction images, which were randomly mixed between the two states.

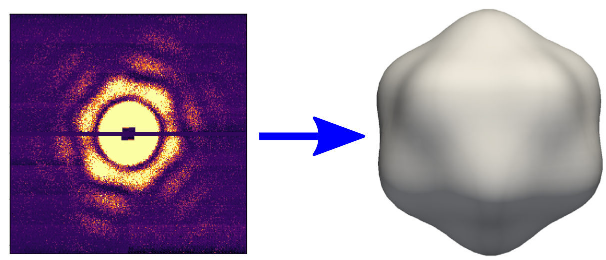


Examples simulated shot-noise contaminated SPD images for (left) prB bound to E2F and (right) the open and closed states of SiaP.



M-TIP reconstructions of (left) prB bound to E2F and (middle & right) the open and closed states SiaP.

This approach was used to analyze experimental SPD data of the PR772 virus, collected at the LCLS. Here, the single-particle M-TIP algorithm was able to exploit the icosahedral symmetry of the virus to determine 3D molecular structure from a single image, allowing a separate 3D view of each virus. The data was collected by the single-particle initiative and preprocessed by Chuck Yoon at SLAC.



M-TIP reconstructions of the PR772 virus from a single experimental SPD image by leveraging icosahedral symmetry.

CAMERA's single-particle M-TIP algorithm was identified as a key routine for single-particle imaging at the LCLS, as part of the Exascale Computing Project (ECP) "Data Analytics at Exascale for Free Electron Lasers". CAMERA is working with SLAC, Stanford University, LANL, and NERSC to port the single-particle M-TIP algorithm to exascale supercomputer architectures in order to provide real-time user feedback for LCLS SPD experiments.

CAMERA scientists P. Zwart, K. Pande, and J. Donatelli. Pande holds a 3D printed virus reconstructed by M-TIP from LCLS data.

Autonomous Steering of X-Ray Scattering Experiments through Optimization and Artificial Intelligence

(Joint Collaboration: NSLS-II, (BNL), CFN (BNL), and CAMERA)

Overview

X-ray scattering experiments are ofen lengthy procedures in which the experimentalist attempts to find the characteristics of a sample, subject to parameters like pressure and temperature. As the number of these parameters grow, the human experimentalist faces challenges visualizing the data and making informed decisions for the next experiment based on previous ones.

A common solution is to perform experiments randomly or at discrete predetermined points. Although "intuitively chosen", random or predetermined experiments turn out to be highly inefficient and biased. In addition, experimentalists have to observe the experiment constantly to react to changes when necessary. Beam line scientists work around the clock for days in a row to obtain a high-quality experimental result.

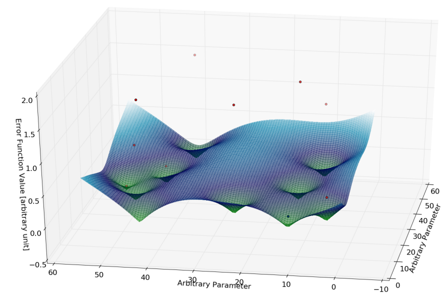
Steering through mathematical optimization

Instead, one can exploit mathematical optimization to make autonomous decisions based on past experiments and without human interaction. A mathematical formulation reveals that the desired parameters for future experiments are, in fact, optima of a complex high-dimensional error function. This error function depends on the previously performed experiments and their outcome. CAMERA brought Brookhaven scientists Kevin Yager and Masafumi Fukuto together with CAMERA members Marcus Noack and Alexander Hexemer to tackle this problem and find a solution.

Technical Summary

Based on previously collected data, Kriging creates a surrogate model, which explains the observed data optimally, and an error surface, which describes uncertainties in the unexplored regions.

The error surface defines the current estimated error depending on available data. Maxima of this error surface represent positions of the next experiments, and an evolutionary optimization algorithm finds the maxima. Minima represent positions where previous experiments have taken place.



Error surfaced computed by Kriging. Maxima represent next possible experiment positions. Minima represent positions of previous experiments. Dots show the data.

After the new experiment is executed, the data set is updated and the process starts over.

The error surface can be weighted to make computation sensitive to certain model features.

Mathematical Approach

Kriging computes an interpolant that inherently minimizes the uncertainty in between the data points and also returns a numerical value for the estimated error. Kriging estimates the function as a linear combination of weights w and data points $\rho(\mathbf{p}_i)$. The surrogate model is defined by

$$\rho_s(\mathbf{p}) = \sum_i w_i(\mathbf{p})\, \rho(\mathbf{p}_i),$$

where $\rho_s(\mathbf{p})$ is the surrogate model under investigation and $\rho(\mathbf{p}_i)$ are points of the model ρ at point $\mathbf{p_i}$, probed by the previous experiments.

The goal is now to minimize the mean squared prediction error

$$E\Big(\rho(\mathbf{p})\ -\sum_i w_i(\mathbf{p})\, \rho(\mathbf{p}_i)\Big)^2$$

given by $\sigma^2 = C_{00} - w^T \mathbf{C} w - 2w^T \mathbf{D}$, where

$$C_{ij} = 1 - \gamma(||\mathbf{p}_i - \mathbf{p}_j||_2),$$

$$D_i = 1 - \gamma(||\mathbf{p}_0 - \mathbf{p}_i||_2),$$

where $\mathbf{p}_0$ is the position of the point to be estimated and γ is the so-called variogram, which is an arbitrarily chosen function that optimally describes the dependence of points at a certain distance. The variogram is defined as $\gamma = 1 - e^{-ah}$, where h is the Euclidean distance between two points. The error surface can be multiplied by the gradient of the surrogate model to bias the procedure toward areas comprising a high rate of change.

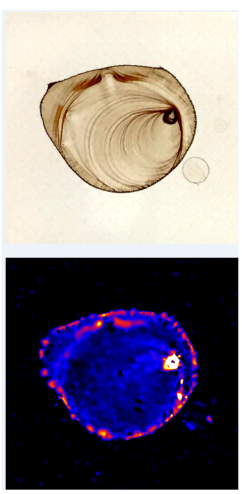
Results

The method has successfully been used to image several geometries autonomously at NSLS-II, drastically reducing the number of required experiments. At beamline 11-BM, autonomous steering algorithm was used to find the microscopic structure of the sample seen in the figure below.

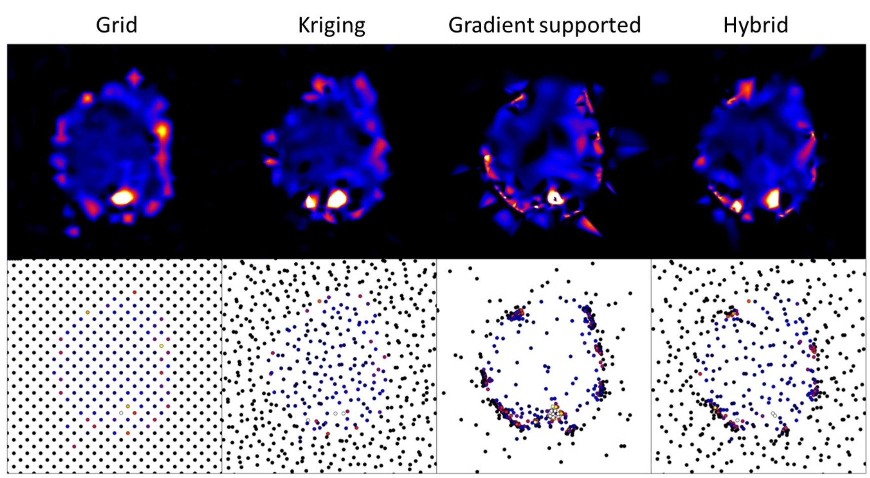
Collaborators:

The collaboration involves Kevin Yager and Masafumi Fukuto from Brookhaven National Laboratory and Marcus Noack from CAMERA.

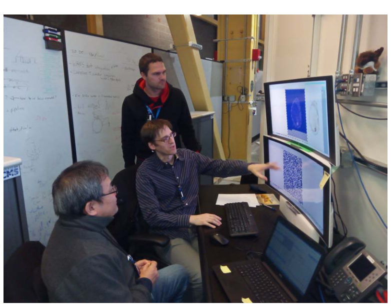
- *"Modern materials are increasingly complex, owing to the number of components and the wide range of possible processing histories. Exploring the phase/state diagrams of these materials is an enormous challenge. Working with the CAMERA project, we have been developing autonomous experimentation, wherein a machine can measure materials, and then automatically select and perform subsequent experiments. This has the potential to revolutionize materials discovery. CAMERA is developing the algorithms necessary for autonomous decision-making in an experimental context. Through this work, we have already performed first-of-a-kind autonomous x-ray scattering experiments."* Kevin Yager, BNL.
- *"Steve Jobs once said 'customers don't know what they want.' We believe the situation is similar for synchrotron experiments. Once the users realize that autonomous experiments are possible at synchrotron facilities, they will change the way they view and design their experiments at beam lines. This will give them an opportunity to tackle more complex materials design problems."* Masafumi Fukuto, BNL.

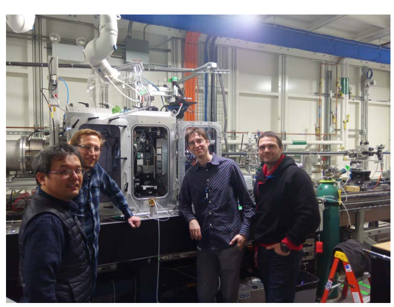


Top: Nanoparticle stain. Bottom=Autonomous investigation.



Each dot is an experiment. Far Left=uniform choices. Near left: Kriging choices. Near right: Gradient-supported choices. Far right: Hybrid scheme.





Left: M. Fukuto (BNL), K. Yeager (BNL), and M. Noack (CAMERA) running autonomous algorithm. Right: with G. Doerk (BNL).

CAMERA "Minimalist Machine Learning" Algorithms Analyze Images Using Very Little Data

(Joint Collaboration: NCXT, UCSF, CWI, and CAMERA)

Overview

Images are everywhere. Smart phones and sensors have produced a treasure trove of pictures, many tagged with pertinent information identifying content. Using this vast database of cross-referenced images, machine learning algorithms can quickly identify natural images that look like ones previously seen and catalogued. But what if you don't have so many tagged images?

In many research fields, a large database of tagged images is an unachievable luxury. For example, biologists record cell images and painstakingly outline the borders and structure by hand. It is not unusual for one person to spend weeks segmenting a single fully three-dimensional image. These few precious hand-curated images are nowhere near enough for traditional machine learning.

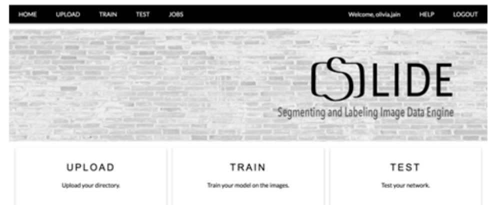
A New Approach

To meet this challenge, CAMERA mathematicians Daniël Pelt and James Sethian focused on machine learning with very limited amounts of data. Traditional machine learning algorithms "learn" by tuning a large set of hidden internal parameters, guided by millions of tagged images, and requiring large amounts of supercomputer time.

Instead, their goal was to figure out how to build efficient mathematical "operators" that could greatly reduce the number of parameters. The resulting "Mixed-Scale Dense Convolution Neural Network (MS-D)" requires far fewer parameters, converges quickly, and "learns" from a small training set.

This approach is already being used to extract biological structure from cell images, and is poised to provide a major new computational tool to analyze data across a wide range of research areas.

To make the algorithm accessible to a wide set of researchers, a CAMERA team led by Olivia Jain and Simon Mo built a web portal "Segmenting Labeled Image Data Engine (SlideCAM)" as part of the CAMERA suite of tools for DOE.



slidecam-camera.lbl.gov

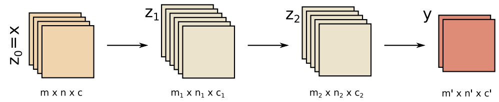
Brief Technical Description

Many applications of machine learning for imaging problems use deep convolutional neural networks (DCNNs), in which the input image and intermediate images are convolved in a large number of successive layers, allowing the network to learn highly nonlinear features. CAMERA researchers realized that the usual downscaling and upscaling that capture features at various image scales could be replaced by dilated convolutions. Furthermore, algorithms could be built that employ multiple scales within a single layer, and densely connect all intermediate images. Their new approach achieves accurate results with few intermediate images and parameters, eliminating both the need to tune hyperparameters and additional layers or connections to enable training. Furthermore, the algorithm automatically adapts to different problems, making it easier to implement and use in real-world problems.

Mathematical Approach

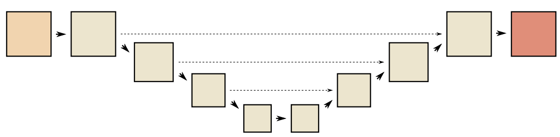
Imagine training a network to classify images. View an image as pixels $\boldsymbol{x} \in \mathbb{R}^{m \times n \times c}$ with m rows, n columns, and c *channels*, with image $\boldsymbol{x}^j$ corresponding to a single channel j of $\boldsymbol{x}$. Many image processing problems boil down to finding a function f that takes a certain image $\boldsymbol{x}$ and produces an output image $\boldsymbol{y}$, i.e. $f : \mathbb{R}^{m \times n \times c} \to \mathbb{R}^{m' \times n' \times c'}$.

Convolutional neural networks (CNNs) model the unknown f through connected *layers*. Each layer i produces an output image $\boldsymbol{z}_i \in \mathbb{R}^{m_i \times n_i \times c_i}$, called a *feature map*, using the previous layer's output as input. The input image $\boldsymbol{x}$ is the first layer $\boldsymbol{z}_0$, with final layer the output image $\boldsymbol{y}$.



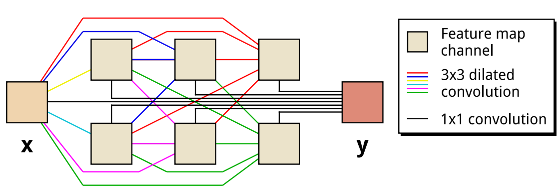
A schematic representation of a two-layer CNN with input $\boldsymbol{x}$, output $\boldsymbol{y}$, and feature maps $\boldsymbol{z}_1$ and $\boldsymbol{z}_2$. Arrows represent convolutions with nonlinear activation.

Deep convolutional neural networks (DCNNs) use a similar network architecture, but consist of a larger number of layers, which enables them to model more complicated functions. In addition, DCNNs often include downscaling and upscaling operations between layers, decreasing and increasing the dimensions of feature maps to capture features at different image scales.



A common DCNN architecture: Downward (upward) arrows represent downscaling (upscaling). Dashed arrows represent skip connections.

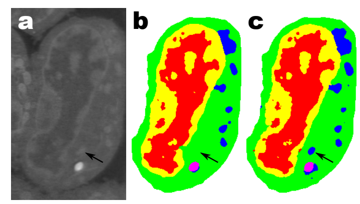
Mixed-Scale Dense networks: As an alternative, CAMERA mathematicians introduced a "Mixed-Scale Dense (MS-D)" architecture which (a) mixes scales within each layer and (b) densely connects all feature maps. Instead of downscaling and upscaling to capture features at different scales, the MS-D architecture uses *dilated convolutions*, capturing additional features. Instead of each layer operating at a certain scale, each individual *channel* of a feature map within a single layer operates at different scale.



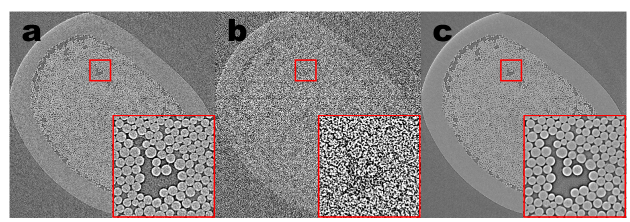
Schematic representation of an MS-D network. Colored lines represent 3×3 dilated convolutions: each color represents a different dilation.

This mixed-scale approach alleviates many traditional stumbling blocks. First, large-scale image information quickly becomes available in early network layers through relatively large dilations, and improves the results of deeper layers. Second, information at a certain scale can be used directly to inform decisions at other scales without having to pass through intermediate scales. No additional parameters have to be learned, resulting in smaller networks that are easier to train. Finally, the network can learn which combinations of dilations to use during training, making identical Mixed-Scale DCNNs applicable across different problems.

Cell classification: Using CAMERA's MS-D algorithm, researchers at NXCT automatically determined the internal structure of biological cells. Avoiding countless hours required to hand-segment cells to extract structure and differences between healthy vs. diseased cells, the MS-D algorithm determined structures automatically, training with data from seven cells. The figure shows raw data (a); manual segmentation (b); and MS-D output with 100 layers (c) (Data: A.Ekman, C. Larabell)



Improving Tomographic Images: The MS-D algorithm is also being used to improved tomographic images. To minimize damage to samples and enable advanced dynamic experiments, one goal is to acquire tomographic scans at a very low X-ray dose, however resulting images are typically noisy. The MS-D network takes noisy input data and reconstruct higher resolution images.



Tomographic images of a fiber-reinforced mini-composite, reconstructed using 1024 projections (a) and 128 projections (b). In (c), the output of an MS-D network with image (b) as input is shown. Small region indicated by red square is enlarged in bottom-right corner (Data: N. Larson).

Collaborators

Collaborators include researchers around the world, including the National Center for X-ray Tomography (NCXT), CWI, the Paul Scherrer Institute, and EMAT, where it is being used to improve the tomographic reconstruction of nanomaterials.

"This new approach has the potential to radically transform our ability to understand disease, and is a key tool in our new Chan-Zuckerberg-sponsored project to establish a Human Cell Atlas, a global collaboration to map and characterize all cells in a healthy human body." Carolyn Larabell, UCSF and Director of NXCT.

CAMERA and Electronic Structure: Fast Methods for Solving Density Functional Theory

(Joint collaboration: Molecular Foundry, Argonne, UC Berkeley, Duke, Imperial College London, Institut de Ciencia de Materials de Barcelona, and CAMERA)

Overview

Detailed understanding of electronic properties at the nanoscale is critical to developing new energy materials at DOE facilities. The electronic structure of an atomistic system can be determined from the solution of a quantum many-body problem described by the Schrödinger equation for the many-body wavefunction. However finding the exact solution of Schrödinger's equations is not computationally feasible except for systems with a handful of atoms, due to the exponential increase in the numbers of degrees of freedom with respect to the number of atoms.

The widely used Kohn-Sham density functional theory alternatively reformulates the problem as one involving non-interacting electrons moving in an effective potential, which must be determined. The advantage is that the ground-state properties of a many-electron system are now determined by an electron density in R^3, regardless of the number of electrons. This is a significant computational advantage.

While KS-DFT makes computation of electronic structure feasible for many quantum systems of practical interest, it is still computationally demanding, especially for nanoscale systems and beyond (with a large number of electrons $N \sim 10^3 - 10^6$). The challenge is to understand the mathematical properties of these approaches in order to design efficient numerical algorithms. The most widely used algorithms are based on matrix diagonalization, with computational cost $\mathcal{O}(N^3)$ (N is the number of atoms), which severely limits applicability to large scale systems especially for metallic systems.

A New Approach

To overcome this problem, CAMERA scientists Lin Lin and Chao Yang have developed the *pole expansion and selected inversion* (PEXSI) method as a new, reliable, and efficient method for accelerating KS-DFT systems for large scale systems. The key idea is that, instead of finding the eigenvalues and eigenfunctions as originally required by DFT, the PEXSI method instead evaluates the most important physical quantities such as the electron density, the energy, and the atomic force directly through the computation of selected elements of a series of inverses of shifted Hamiltonian matrices.

The PEXSI method has been built into a versatile, massively parallel software package, and has now been integrated into electronic structure software packages such as BigDFT, CP2K, DGDFT, FHI-aims, QuantumWise ATK, SIESTA, and is part of the "Electronic Structure Infrastructure" (ELSI) project to be integrated into many more codes.

Mathematical Approach

The Kohn-Sham density functional theory requires the solution of the following nonlinear eigenvalue problem.

$$
\begin{gathered}
H[\rho]\psi_i(x) \equiv \\
\left(-\frac{1}{2}\Delta + \int dx' \frac{m(x') + \rho(x')}{|x - x'|} + V_{xc}[\rho]\right)\psi_i(x) \\
= \epsilon_i \psi_i(x).
\end{gathered}
$$

Here the eigenvalues ϵ_i and the eigenfunctions ψ_i depend on the electron density ρ, given by summing up the eigenfunctions, namely

$$
\begin{gathered}
\rho(x) = 2\sum_{i=1}^{N/2} |\psi_i(x)|^2 \quad \int dx \psi_i^*(x)\psi_j(x) = \delta_{ij}, \\
\epsilon_1 \le \epsilon_2 \le \ldots
\end{gathered}
$$

reflecting the orthogonality of the eigenfunctions.

The PEXSI approach avoids the evaluation of the eigenvalues or eigenfunctions all together, and instead directly evaluates the density matrix $\hat{\gamma}(x, x')$, whose diagonal elements give the electron density as $\rho(x) = \hat{\gamma}(x, x)$. In this sense, the PEXSI approach directly focuses on physical observables of interest.

More specifically, the density matrix is expanded as

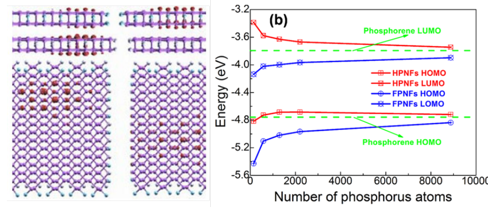
$$\hat{\gamma}(x, x') = \Phi(x)\mathrm{Im}\left(\sum_{l=1}^{P} \frac{\omega_l^{\rho}}{H - (z_l + \mu)S}\right)\Phi^T(x') \equiv \Phi(x)\Gamma_P\Phi^T(x').$$

Here $\Phi(x)$ represents a basis set. Each term $G_l = \left((z_l + \mu)S - H\right)^{-1}$ is called a Green's function. PEXSI's contributions are two-fold. First, PEXSI provides an efficient discretization scheme for evaluating the Cauchy contour integral for approximating the Fermi-Dirac operator (i.e. the density matrix). This technique gives by far the lowest cost for expanding the Fermi-Dirac operator. Second, PEXSI provides the selected inversion method accurately and efficiently computes selected elements of a Green's function for a Kohn-Sham system, and significantly reduces the computational complexity from $\mathcal{O}(N^3)$ to at most $\mathcal{O}(N^2)$ *without loss of accuracy* for generic systems, including the difficult metallic systems. The PEXSI method also offers much higher scalability when exploiting high performance computing than previous methods. CAMERA scientists have developed a massively parallel selected inversion method, as well as an efficient selected inversion method for heterogeneous computer architectures.

One remaining difficulty in the PEXSI method, and the Fermi operator expansion (FOE) method in general, is the evaluation of chemical potential. To overcome this problem, we recently developed an efficient and robust strategy for determining chemical potential based on rigorous numerical analysis. The method's efficiency stems from the fact that it always requires one iteration per self-consistent field iteration step. The accuracy of the chemical potential is automatically refined as the self-consistent field iteration proceeds, and eventually becomes accurate. This significantly increases the efficiency as well as the robustness of the PEXSI method.

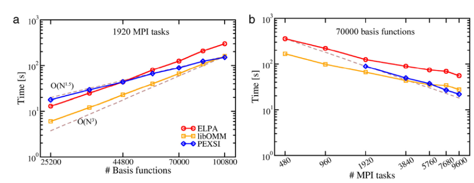
The PEXSI technique has been successfully used to tackle challenging electronic structure problems for systems of large sizes: the SIESTA-PEXSI method was used to calculate electronic structure properties of a graphene nanoflake for more than $10,000$ atoms from first principles, far beyond previous efforts. CAMERA scientists have used DGDFT-PEXSI to study large scale phosphorene nanoflakes, and predicted the edge reconstruction of armchair edged phospherene nanoribbons at room temperature.

SIESTA-PEXSI was used to predict new solar cell material candidates based on large scale edge modified phosphorene heterojunctions and a new way was proposed to construct a heterojunction from a single type of material derived from only phosphorene.



Left: Phosphorene nanoribbons. Right: HOMO and LUMO energies of large PNF monolayers in different system sizes and edge types computed from SIESTA-PEXSI.

The PEXSI method has been benchmarked within the ELSI framework, which is a multi-institutional collaboration for pushing forward the frontier of numerical methods to solve Kohn-Sham density functional theory. Using a large scale graphene system with 5000 atoms for example and tested in the community software package FHI-aims, PEXSI has been demonstrated to have lower asymptotic complexity and is more scalable than previous methods.



Scaling of the repeated steps in ELPA, libOMM, and PEXSI solvers with respect to (a) the number of basis functions and (b) the number of MPI tasks.

Collaborators

PEXSI and its CAMERA developers (L. Lin and C. Yang) are a key component of ELSI: a multi-institutional effort to build a unified software interface for Kohn-Sham electronic structure solvers. ELSI aims to simplify the implementation and optimal use of the different strategies, by offering: (a) a unified software framework designed for the electronic structure solvers in Kohn-Sham density functional theory; (b) reasonable default parameters for a chosen solver; (c) automatic conversion between input and internal working matrix formats; and, in the future, (d) recommendation of the optimal solver depending on the specific problem.

Faster, Brighter, Sharper X-ray Ptychography

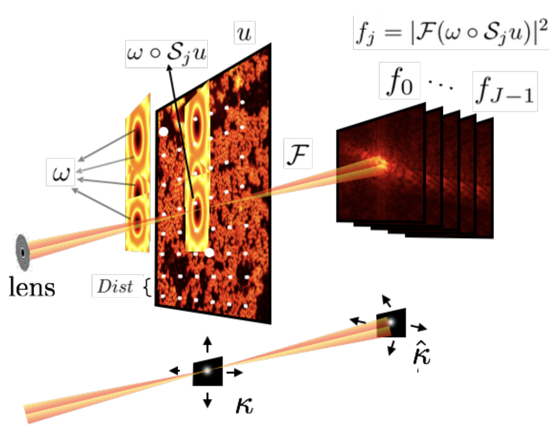
(Joint Collaboration: Uppsala, Michigan, Chicago, Toronto, Duke, U Texas, Tianjin Normal U., Peking U. with LANL, ALS, SSRL, LCLS, SLAC, and CAMERA)

Overview

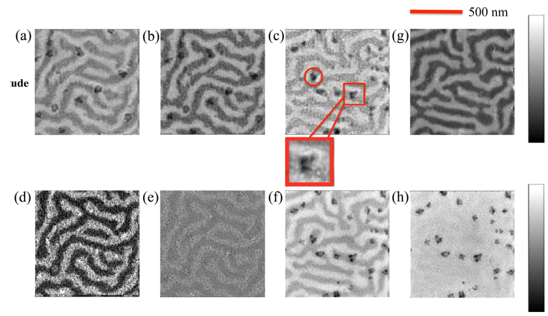
To characterize structure and properties of new materials, a new generation of microscopes are being pioneered, commissioned, and planned at several DOE user facilities. These new facilities couple together the brightest sources of tunable X-rays, nanometer positioning, nanofocusing lenses, and fast detectors.

These new microscopes utilize ptychography invented 50 years ago to improve the resolution of an electron microscope. Initially the process was impractically slow, and prohibitively data and computation intensive.

Today, faster detectors and several X-ray microscopes at the brightest light sources can measure a ptychographic dataset in a few seconds. The reconstruction of millions of phases per second at various microscopes and light sources is enabled by an algorithmic framework and computer software known as “SHARP” (Scalable Hetereogeneous Adaptive Real-time Ptychography), developed in collaboration between scientists from around the world and members of CAMERA, and used in production every day at the ALS, and is also used at other US light sources.



Ptychographic experiment (Far-field): A stack of intensities $f_j = |\mathcal{F}(\omega \circ \mathcal{S}_j u)|^2$ are collected. ω is the localized coherent probe and u is the image of interest (or specimen). White dots on the image represent probe center or scanning lattice points with $Dist$ denoting the sliding distance between centers of two successive frames. Frames are extracted out of the image by the linear operator S_j, κ and $\hat{\kappa}$ represent translational and angular convolution kernels respectively. (H. Chang et al. Acta Cryst. A (2018))



Magnetic state mapping in thin $SmCo_5$ films at nanoscale resolution obtained using SHARP, collaboration with University of Oregon, LBNL (ALS, CRD, MSD, Engineering), UC Santa Cruz, Institute for Metallic Materials, Helmholtzstr. Dresden, (NSRRC) Taiwan, X. Shi, et al. Appl. Phys. Lett. (2016).

Mathematical Challenges and Results

Ptychographic reconstruction is challenging because it involves solving a difficult phase retrieval problem, calibrating optical elements, and dealing with experimental outliers and noise. For 3D nanotomography, sample drifts occur at high resolution and sample rotation may be limited.

To meet these challenges, CAMERA scientists Huibin Chang, Pablo Enfedaque, and Stefano Marchesini exploited state-of-the-art mathematical aspects of phase retrieval, as well as the complexities of “background noise” optimization and detector denoising specific to a variety of instrumentation. This has led to some notable successes in the analysis of magnetic thin films, magnetozomes, and three-dimensional battery materials.

Faster Ptychography

Coherent ptychographic imaging experiments often discard the majority of the flux from a light source to define the coherence of an illumination. Even when coherent flux is sufficient, the stability required during an exposure is another important limiting factor. A new model developed by CAMERA scientists, the Univ. of Texas, and Tianjin University can use more light than before, opening the entrance slits of a ptychographic microscope, and reducing the number of frames required to obtain sufficient data to reconstruct a meaningful image. Fast analysis is ensured by using a simple and efficient model with only one coherent probe, and the variance of a convolution kernel. The illumination is described by the superposition of a single coherent illumination convolved with a separable translational kernel, so that partially coherent effects in ptychography are addressed by using a simple and efficient model with only one coherent probe, its gradient and the variance of a convolution kernel.

The starting point is the now standard blind ptychographic phase retrieval problem, namely:

Find $\omega \in \mathbb{C}^{\bar{m}}$ and $u \in \mathbb{C}^n$, $s.t.\ |\mathcal{F}(\omega \circ \mathcal{S}_j u)|^2 = f_j$.

ω is a complex matrix describing the wavefront of the illumination, u is a complex matrix describing the image, S and $\mathcal{F}$ extract frames and perform a DFT operation. Taylor expansion of ω yields:

$$f_j(q) \simeq \int \left|\mathcal{F}\left(\mathcal{S}_j u \left(\omega - \xi^T \nabla \omega + \tfrac{1}{2} \xi^T \nabla^2 \omega \xi\right)\right)\right|^2 \kappa(\xi) \mathrm{d}^2 \xi$$

which can be simplified as

$$f \simeq |\mathcal{F}(\omega \circ \mathcal{S}_j u)|^2 + \sigma_1^2 |\mathcal{F}(\nabla_1 \tilde{\omega} \circ \mathcal{S}_j u)|^2 + \sigma_2^2 |\mathcal{F}(\nabla_2 \tilde{\omega} \circ \mathcal{S}_j u)|^2,$$

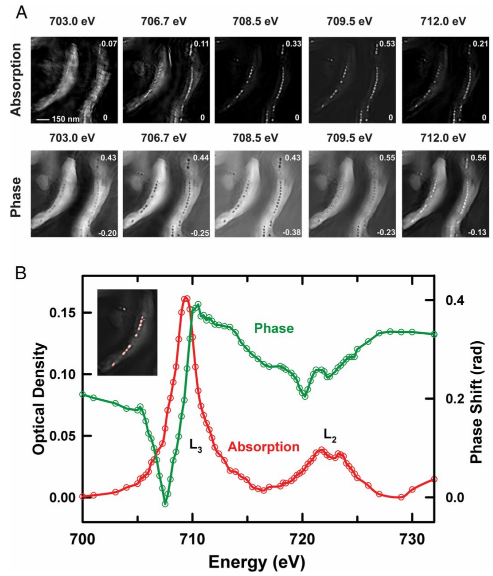
where $\boldsymbol{\sigma} := (\sigma_1, \sigma_2)$ with variance adjusted probe

$$\tilde{\omega} := \omega + \tfrac{1}{2}(\sigma_1^2 \nabla_{11} \omega + \sigma_2^2 \nabla_{22} \omega + 2\sigma_{12} \nabla_{12} \omega).$$

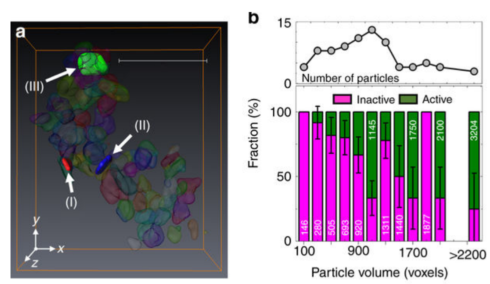
The collaboration developed the Gradient Decomposition of the Probe (GDP), a model that exploits translational kernel separability, coupling the variances of the kernel with the transverse coherence, and developed an efficient first-order splitting algorithm GDP-ADMM to solve the proposed nonlinear optimization problem. Numerical experiments demonstrate the effectiveness of the proposed method with Gaussian and binary kernel functions in fly-scan measurements.

Remarkably, GDP-ADMM using nano-probes produces satisfactory results even when the ratio between kernel width and beam size is more than one, or when the distance between successive acquisitions is twice as large as beam width: these qualities reduce acquisition and exposure times.

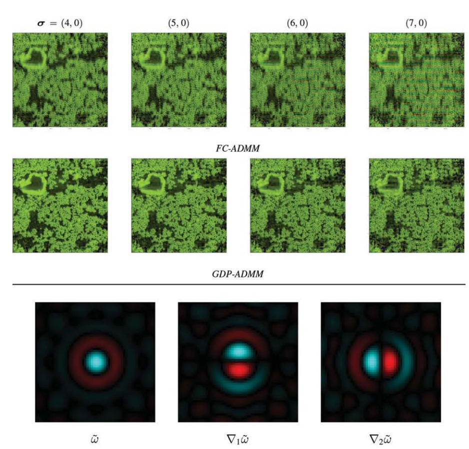
CAMERA scientists are building a high performance implementation of new advanced calibration algorithms for metrology, tomography, background removal, dictionary learning denoising, and are working in collaboration with the Beamline Experiment Analysis and Reconstruction project at LANL and the LCLS, to bring beam characterization of coherent light source experiments to LCLS.



Magnetic state mapping magnetozome bacteria at nanoscale resolution obtained using SHARP, collaboration with McMaster, Universidade Federal do Rio de Janeiro, (NSRRC) Taiwan. X. Zhu, PNAS (2016).



3D chemical state mapping of a battery material obtained using SHARP. Voxel segmentation to define individual particles, and distribution of particles. Collaboration with LBL, UI Chicago, Chungnam Nat. Univ., South Korea Chunjoong Kim, SLAC, Cambridge, Stony Brook, Uppsala. From Y-S. Yu, Nat. Comm (2018).



Comparison between standard ptychographic analysis (top row) using partially coherent illumination and blurring due to sample motion and the analysis using the gradient decomposition of the probe (second row). The illuminating beam and its gradient (third row). H. Chang et al. Acta Cryst. A (2018)

X-ray Scattering for Reconstruction of Form-factors in Line Etched Patterns

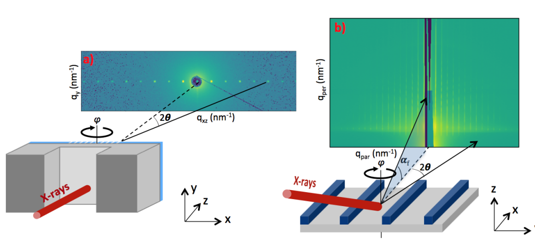
(Joint collaboration: NIST, APS, NSLS-II, ALS, and CAMERA)

Overview

Moore's law has been a guiding principle for the semiconductor industry and has helped to push manufacturing to even smaller feature sizes. Photolithography, followed by chemical etching, is the fundamental process of producing the required transistor sizes. With feature sizes now ranging down to a few nanometers, new measuring techniques are required to ensure quality control across manufacturing processes. Many traditional techniques, such as scanning force microscopy, are reaching the resolution limit or lack the required contrast. In the last few years, X-ray scattering has started to emerge as a possible contender to fill the required metrology gap, since it provides a fast and non-destructive method to investigate nanostructures with potentially high resolution and accuracy.

Fast algorithms and analyses are needed be able to convert Fourier patterns captured on detectors at a rate and accuracy that can handle emerging X-ray scattering measurements. One of the most successful techniques, *Critical Dimension Small Angle X-ray Scattering* (CD-SAXS), was developed at NIST and recovers the morphology of gratings in a transmission geometry. CAMERA, employing a similar framework, has developed a technique to use Grazing-Incidence geometry.

Critical Dimension GISAXS



(a) CD-SAXS in Transmission geometry and b) CD-GISAXS in Grazing-Incidence geometry.

CAMERA scientists Guillaume Freychet, Dinesh Kumar, and Alexander Hexemer have worked in close collaboration with the NIST group to accelerate the CD-SAXS analysis code by porting the code onto GPUs resulting in a code ten times faster. CAMERA has also embedded CD-SAXS in Xi-CAM for ease of access. CAMERA then extended the method to work in reflection geometry, thus eliminating the need for thin substrates and high energy X-rays. The technical requirements for measuring CD-GISAXS are quite minimal. GISAXS is a technique for measuring the Fourier components of surface morphologies. The characteristics of line patterns morphologies exhibit strong Fourier rods, that are perpendicular to the surface and are equally spaced. The Fourier rods, also known as Bragg rods, intersect with the momentum transfer vector of the elastic X-ray scattering at a single point above the horizon. The Bragg rods can be scanned by rotating the moment transfer vector, and therefore the sample. The intensity of the recorded Bragg rods is modulated by the of Fourier transform of the shape, i.e. the form factor of the individual grating.

Mathematical Formulation and Algorithm

If we assume that the etched line gratings are infinitely long, the mathematical problem of resolving the shape of the gratings is reduced to a 2-D cross-section:

$$I(q) \propto \|F(q)S(q)\|^2$$

Focusing on the cross-section reduces the complexity of the approach. However, the commonly used approximation for X-ray transmission, *Born Approximation*, is no longer valid in the GISAXS regime, because of multiple scattering occurrences. One must use the *Distorted Wave Born Approximation* (DWBA), to calculate the form-factor $\mathcal{F}$,

$$\mathcal{F}(\mathbf{q}) = \sum_{n=1}^{4} C_n(\alpha^f, \alpha^i; \eta, t) F_n(q_x, q_y, \pm k_z^f \mp k_z^i; \ell)$$

where Cs are the Fresnel coefficients for a given medium with complex refractive index η and thickness t. Fs are the Fourier transforms of a shape with dimensions ℓ. If the medium is air (or vacuum), i.e. $\eta = 0$, the calculation of Fresnel coefficients is simplified to:

$$C = [1, r(\alpha^i), r(\alpha^f), r(\alpha^i)r(\alpha^f)]^T$$
$$r = \frac{k_z - \tilde{k}_z}{k_z + \tilde{k}_z}$$
$$\tilde{k}_z = -\sqrt{\eta_s^2 k_0^2 - |k_{||}|^2}$$

where η_s is complex refractive index of the substrate, and the Fourier transform of the trapezoid is given by

$$F(q_y, q_z) = \frac{1}{q_y}\left[-me^{jh\frac{q_y L}{2}}\left(1 - e^{-jh\frac{q_y + mq_z}{m}}\right) + me^{-jh\frac{q_y L}{2}}\left(1 - e^{-jh\frac{q_y + mq_z}{m}}\right)\right]$$

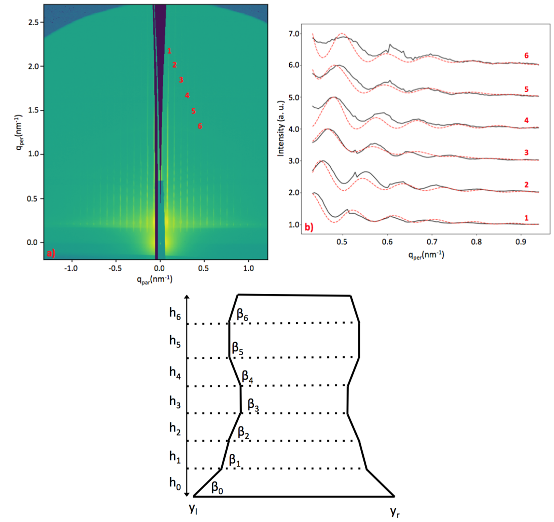
Here, m is the tangent of the side-wall angle. A complex shape can be approximated by stacking multiple trapezoids. In order to reduce the number of parameters, all the trapezoids are restricted to be of same height.

Exploiting High-Performance GPUs

The minimization problem is inherently non-convex, making it difficult to use gradient-based methods. A genetic algorithm is used to search for the optimal parameters. Such global optimization methods can be very expensive as one need to evaluate objective function multiple times. CAMERA has implemented a GPU version of the required form factor calculation in pure CUDA and archived a 10x speedup on a single graphics card. CAMERA is planning to expand the code to a multi-GPU version to be able to match coming measurement times and provide full automated real-time feedback for CD-GISAXS.

Experimental Results

The GISAXS experiment is performed while the stage is spinning, in the sample-plane. The figure below shows analysis of data obtained at the beamline 8-ID-E at the Advanced Photon Source.



CD-GISAXS images recording with a rotation of the gratings and the corresponding profiles obtained from a vertical 1D cut with the simulation and the line profile extracted CD-GISAXS and CD-SAXS

Summary

CAMERA has developed an algorithm that solves full DWBA to fit complex shapes. Previous attempts to solve this problem have either used SAXS to avoid DWBA or have fitted simpler shapes. The experimental setup results in scattering patterns that eliminates the need to solve for full 2-D images. All that is required is to simulate 1-D scattering profiles along the Bragg rods. The experimental setup allows 1D simulations along the Bragg rodes, instead of expensive 2D simulations. Additionally, if the incoming angle does not change during the experiment, there is no need to calculate Fresnel coefficients and q-values for every minimization iteration. This reduces the cost of solving DWBA.

Collaborators

This work was done in collaboration with J. Kline, D. Sunday and D. Delongchamp from NIST. Experiments were performed in collaboration with J. Strzalka from APS at the Argonne National Lab, M. Fukuto from NSLS-II, at the Brookhaven National Lab and E. Schaible at the Advanced Light Source.

Initial experiments performed on line gratings were provided by the Center of X-Ray Optics (P. Naulleau), INTEL, and Imec, and future developments and experiments are being planned. IBM and Applied Materials have expressed interest in future collaborations,

Algorithms and Tools for Accelerating Nanoporous Materials Discovery

(Joint collaboration: Molecular Foundry, EFRC for Gas Separations Relevant to Clean Energy Technologies, Nanoporous Materials Genome Center, Hydrogen Materials Advanced Research Consortium, and CAMERA)

Overview

The last decade has seen a surge of interest in the synthesis, characterization and understanding of the structure and design principles of advanced porous materials such as metal-organic frameworks (MOFs), covalent organic frameworks (COFs), porous polymeric networks (PPNs), and porous organic cages (POCs). These materials hold promise for application in many energy-related technologies, most prominently in separations (e.g., separating carbon dioxide from other gases in power plant exhaust), gas storage (e.g., methane and hydrogen storage in vehicular applications), and catalysis.

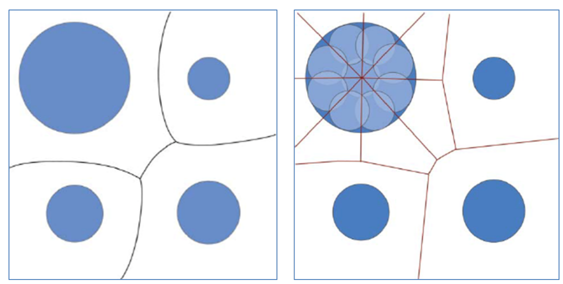
The huge space of possible organic and inorganic building blocks of these materials, along with the simple, tinkertoy-like assembly principles, gives rise to a vast combinatorial space of possible materials. CAMERA teams of applied mathematicians and chemists, led by Maciek Haranczyk, have built algorithms to describe and efficiently explore this complex space. This has led to: a) methods to build 3D models of materials; b) pore structure characterization and comparison; c) advanced pore design and discovery via optimization algorithms and machine learning, respectively; and (d) automatic, high-throughput characterization methods.

A New Approach

A material structure is defined by positions of atoms. Hence, calculating geometrical parameters describing the void space in terms of its size, shape, and connectivity requires introducing a representation of its void space. Tessellation techniques, where three-dimensional cells are constructed around atoms so that the boundaries of cells serve as a representation of the voids in the structures, are well suited for this task.

In the Voronoi tessellation, the space surrounding atoms is divided into irregular polyhedral cells such that the cell for a given atom comprises the space that is closer to that atom than any other. This Voronoi tessellation is appropriate for the case when all atoms have the same atomic radius, and is not suitable for a realistic model where the atoms have radii that are unequal.

One approach is to invoke curved, hyperboloidal faces as boundaries, which is an expensive approach. To avoid this prohibitive cost, CAMERA researchers capitalized on an approximation in which large atoms are replaced by clusters of smaller particles with radii equal to the radius of the smallest atom present in the system. This then reduces to a standard Voronoi tessellation, and the increased quantity of equal-sized particles provide additional degrees of freedom to better approximate the idealized curved-boundary Voronoi cell network.



Voronoi tessellation around four particles: (left) tessellation with curved boundaries around atoms of unequal radii; (right) tessellation after replacing the largest atoms with smaller atoms.

This approach, together with efficient implementations of Voronoi tessellation in CAMERA's Voro++ library, provides a framework for specialized algorithms to find parameters describing the void space, its geometry and topology, within the material.

For example, voids inaccessible to a given molecular probe can be identified. This information can be used to calculate accessible surface area, accessible volume, pore size distributions, and other descriptors that can be utilized in building complex material discovery approaches. All algorithms have been implemented in the Zeo++ software suite, which offers sub-0.1 angstrom resolution and throughput allowing characterization of millions of structures within hours on a workstation.

Results:

Some examples of successful use of CAMERA screening and discovery tools include:

• Zeo++ screening of databases of approximately 500k experimental and predicted materials structures of zeolite, MOF, COF, ZIF, and other families to identify optimal porous materials, and performance limits for each family, in applications in methane storage, hexane separations, and carbon capture.

• New structure descriptors, which were used in a machine learning-based approach to discover optimal materials for xenon/krypton separations, for example, at the conditions relevant to nuclear fuel reprocessing technology. One of the top performing structures, SBMOF-1, was later synthesized and characterized at PNNL to confirm that it is indeed an outstanding material.

• Application of Zeo++ in analysis of dynamic porosity in porous organic cage materials, which helps interpret experimental observations.

• Development of optimization-based design approach for porous materials, showing targeted materials with specific properties such as methane uptake and internal surface area (gravimetric and volumetric).

CAMERA developed Zeo++ has provided unique functionalities and enabling technologies, which contributed to the success of a number of DOE-funded research centers. Figure: Six journal covers highlighting contributions enabled by Zeo++.

Tools under development

There is growing interest in porous molecular materials, which include crystalline materials, porous molecular alloys, and porous molecular liquids. Analysis of their porosity is more challenging as compared to 3D framework materials such as MOFs or COFs. For porous molecular materials, there is interest in determining the characteristics of each molecule comprising the material as well as the ability to track the dynamic changes of flexible structures. CAMERA's current focus is on developing new tools aimed specifically at molecular porous materials, built in hybrid approaches that combine Voronoi tessellations with alpha-shape analysis. These tools will provide basic characteristics for any molecule that form porous material, e.g. for a given molecule, calculate its internal and external surface area, internal volume, shape and size of openings leading to its molecular internal cavity, and qualitative measure the non-convex character of the molecule. The challenge is to identify the boundary of the internal void of the molecule that would agree with an intuitive definition used by chemists.

Collaborators

The algorithms implemented in Zeo++ have been utilized thus far by approximately 1000 researchers from both academia and industry, and is an important tool at a number of DOE-funded research centers, including

- The DOE Basic Energy Sciences-funded "Nanoporous Materials Genome Center."
- The Energy Frontier Research Center for gas separations for clean energy technologies.
- The DOE Fuel Cell Technologies Office's "Hydrogen Materials-Advanced Research Consortium."

These collaborations have resulted in methods to predict novel crystal structures as well as enumerate, characterize and screen porous material databases, design of novel materials with properties tailored to specific applications, and exploit optimization-based porous materials design.

Recognizing Structure from Image Data: Enhancement, Extraction, and Identification

(Joint collaboration: ALS, GE, BIDS, and CAMERA)

Overview

Given reconstructed images produced from scanning experiments, a major task is to detect and extract characteristics of imaged structures. This is typically done through painstaking manual segmentation: a costly and time-consuming procedure which cannot handle high-throughput experiment.

CAMERA researchers, in collaboration with the ALS, NCEM, and BIDS, have built automatic algorithms to quickly extract and analyze image data. These algorithmic tools, which include classical image processing, geometric priors, and template matching, and generalized physics-specific machine learning, are in use across a field of applications.

A. Analyzing micro-CT images

A major task in processing microtomography (micro-CT) is to detect and quantify properties of imaged solids, as a step toward assessing the quality of materials and measuring microstructures. Challenges include dealing with corrupted scans, reconstruction artifacts, and multiphase volumes. Much of this metrology requires tools that offer both flexibility of use, a variety of algorithms, and efficient implementations fo allow for fast iterations and scability to data streams.

To address materials metrology through microCT experiments, CAMERA scientists have built tools to automatically extract structure. In the context of analyzing ceramic material composites (CMC) for micro-structure damage, these automatic tools can process large numbers of images to assess:

- Number of components and detected defects.
- Deformation and failure under tension.
- Damage in ceramic matrix composites.

Outline of technical approach

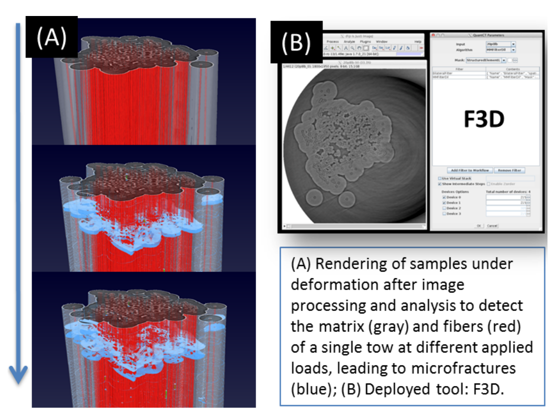
Three main steps in analyzing micro-CT reconstructed images are:

• Enhancement of image quality by designing scalable 3D filtering algorithms based on anisotropic diffusion and mathematical morphology to emphasize contrast and edge maps. These algorithms handle both data streaming and can load from out-of-core sources, and the resulting software tool enables large datasets to be processed in parallel, removing RAM-based constraints.

• Separation of the dense material from the background involves volume partitioning into solid phase and interstitial regions, using graph-based models based on an adaptive statistical merging predicate on intensity levels and voxel vicinity that runs in linear-time. These methods are combined with non-supervised algorithms (fast clustering approaches such as k-means and histogram-based thresholding) and supervised algorithms (including random forest, neural networks, and convolutional neural networks).

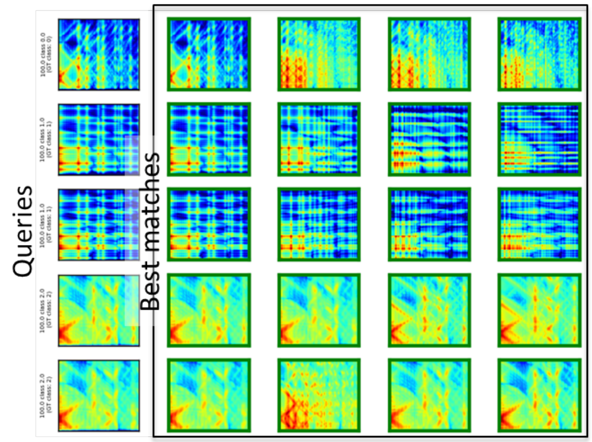
• Extraction of target microstructure, using priors and geometric constraints to reduce the size of the search space with regard to the pattern to be detected. For example, when analyzing ceramic matrix composites, to identify fibers, we model fiber cross-sections as an ellipse and define the fiber detection as a search problem. Since similarity of the fiber cross-section is consistent, a variant of template matching is used to search for fibers, and depends on two main steps: first, to define similarity metrics between prototypes and local regions, and second, to determine the best matches.

These algorithms are used at ALS beamlines to extract micro-fiber data, and have been coupled to a virtual reality environment to allow 3D navigation. They reduce the time to analyze a material from days with manual segmentation to a few minutes.



(A) Rendering of samples under deformation after image processing and analysis to detect the matrix (gray) and fibers (red) of a single tow at different applied loads, leading to microfractures (blue); (B) Deployed tool: F3D.

DOE Secretary Perry using 3D virtual imagery of ALS-imaged and CAMERA-reconstructed fiber data



pyCBIR output. Left column: Queries. Right columns: Closest matches.

B. PyCBIR: Content Based Image Retrieval

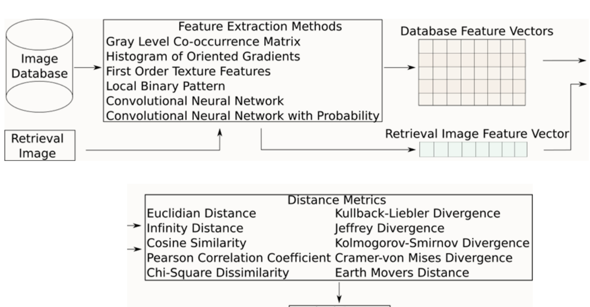
CAMERA researchers have built a new visual search engine (pyCBIR) for scientific image retrieval based on pictorial similarity. This tool is capable of retrieving relevant images using datasets across science domains. CAMERA's package has been used to find closest matches of scattering data to a trained library of stored images.

PyCBIR provides real-time image retrieval using a compact data representation which leverages historical data tagged by domain experts, and provides an associated confidence metric for each image. It exploits convolution neural network-based tools for pattern pattern recognition using optimized libraries, such TensorFlow, cuDNN, and cuFFT.

Results

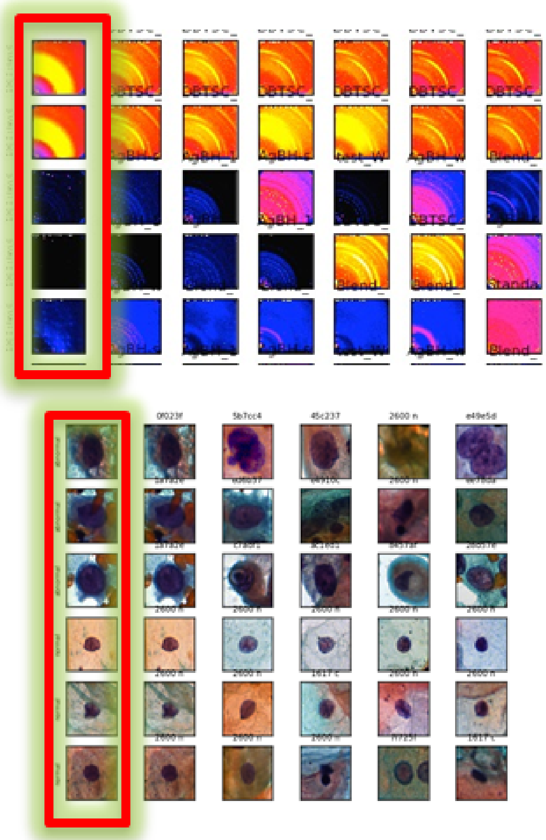
As an example, pyCBIR was used to search and rank materials imaged using X-ray diffraction. Scattering patterns were generated taking input structures and running CAMERA's HipGISAXS forward simulator to produce the output scattering patterns.

Then, a network was trained with simulated images of X-ray diffraction designed to match regions and patterns of appropriate crystal structures.



PyCBIR flow chart for scattering image recognition

In a different application, pyCBIR was used to find closest texture matches from samples against a large public database.



pyCBIR Output. Left column: Queries. Right Columns: Closest matches.

CAM-Link: Real-Time Streaming and Workflows

(Joint collaboration: SSRL, ALS, and CAMERA)

Overview

Imagine trying to "get the most" from data coming out of a beamline. At one extreme, this might involve real-time streaming that processes data as it is being collected and then provide instant feedback and "on-the-fly" experimental steering. At the other extreme, one might post-process terabytes of data.

It is tempting to write customized software for a given set of experimental requirements. However, many beamlines share a mix of workflow and algorithms for data analysis.

What is needed is a scalable solution that, for a given experimental requirements, connects together the best combination of detectors, experimental controls, algorithms, and compute resources, from local dedicated resources to supercomputing facilities.

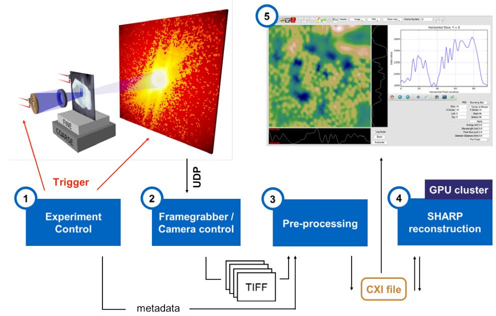
To address this range of needs, a CAMERA project built a distributed generator that enables execution of customized workflows algorithms together into an end to end processing pipeline which

- Executes tasks and moves data across distributed environments. (from beamline to local environment to remote execution.);
- Enables client-server workflow, from executing static graphs to dynamic tasks.
- Enables streaming, in-situ workflow.

This workflow environment is available independently, and is also built into Xi-CAM. It has been used to execute GiSAXS code at supercomputing facilities and execute remote tomography pipelines. The infrastructure seamlessly moves data and access remote computing while providing a comprehensive visual interface.

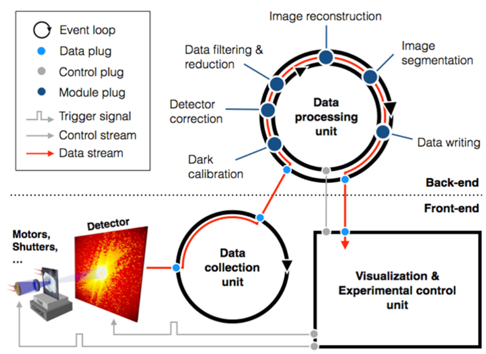
Case Study: Ptychography

A good example is provided by CAMERA's Nanosurveyor streaming workflow environment for ptychography at the ALS. It links and drives efficient algorithms and workflow to run the experiment, executes framegrabbers and camera control, performs data pre-processing, and uses CAMERA's SHARP ptychography algorithm executing on a local GPU cluster for on-the-fly image reconstruction.

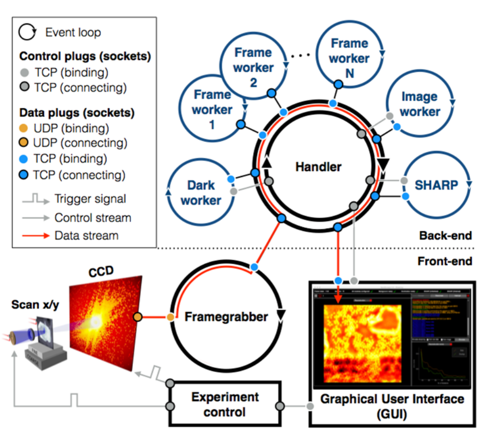


Ptychography steps

The figure below shows the data workflow: flow from the framegrabber to the SHARP reconstruction algorithm and GUI display is shown at bottom.



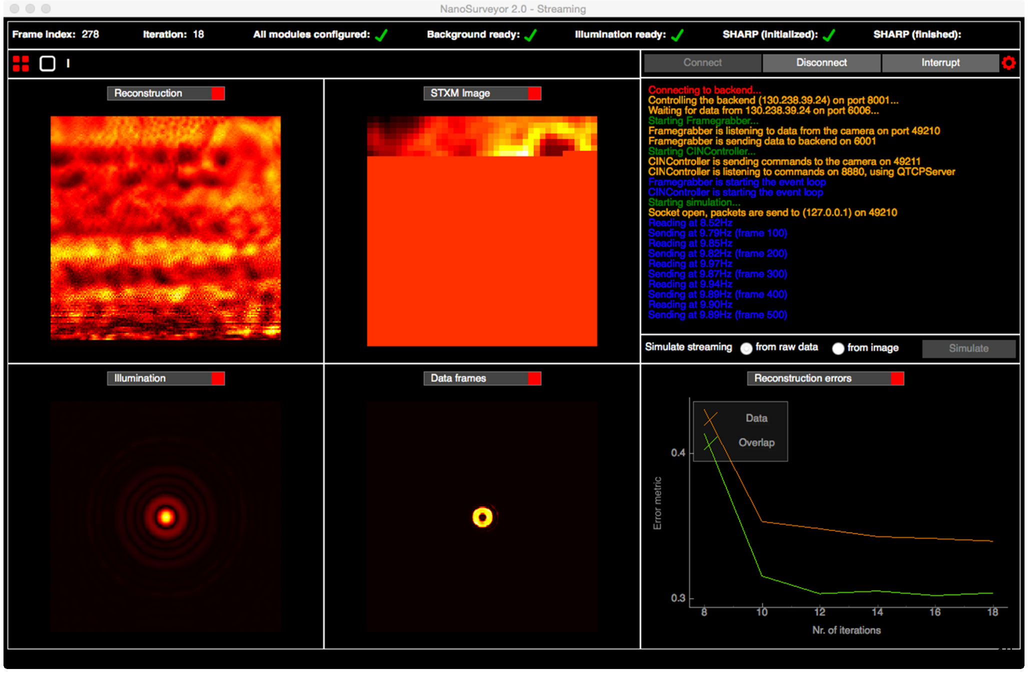
Nanosurveyor: Data Workflow



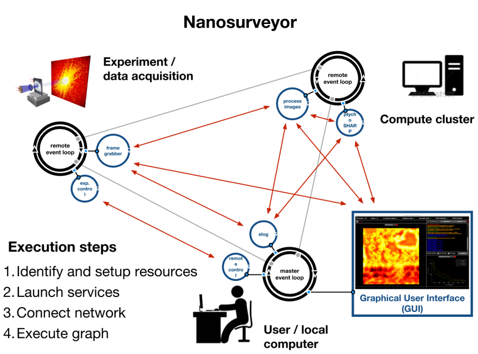
Real-time ptychography

CAMERA's CAM-Link: Flexible Workflows

At the core is CAMERA's "CAM-Link", which is an underlying low level library to launch tasks and move data between remote machines and propagate results back to the host (which is either executed by Xi-CAM or some other environment).



The CAM-Link library, launched either standalone or within Xi-CAM, enables developers to describe the ecosystem required for executing tasks that best matches the desired criteria, such as quickest response, best performance, or least data movement. CAM-Link's setup performs four steps:



CAM-Link and Nanosurveyor

- **Identify and setup resources:** Connect to each remote resource: launch event loops that perform proper connection and coordination;
- **Launch services:** Start tasks within each resources and ensure proper setup;
- **Connect network: Pass relevant information between each task**, such as level of parallelism, communication ports, etc.;
- **Execute graph:** The entire graph is executed to ensure no data is lost during analysis potentially due to any race conditions.

For example, the ptychography streaming analysis pipeline launches 6 tasks over 3 machines. The user's machine serves as the master control and visualizes results, while the data acquisition machine samples the frames from the CCD and performs clean up while saving raw frames to disk, and the compute cluster performs parallel ptychographic reconstruction using SHARP and forwards the reconstructed image to the user's desktop.

Second, the Xi-CAM Workflow API enables construction of graphs that describes execution of an end-to-end analysis pipeline. The API supports connections between task inputs and outputs as well as methods to subscribe to changes in state. These two ways of describing connections between tasks supports both real time updates within a task as well as dependency based execution across tasks.

CAM-Link/Xi-CAM supports client-server workflows and converts internal plugins into static graphs, dynamic graphs, and graphs that provide real-time updates. Using the Dask backend scheduler paired with the Cam-Link library enables Xi-CAM to launch tasks locally or remotely. This transparent movement of the analysis pipeline enables computation wherever the data is located by simply providing credentials to any given remote machine.

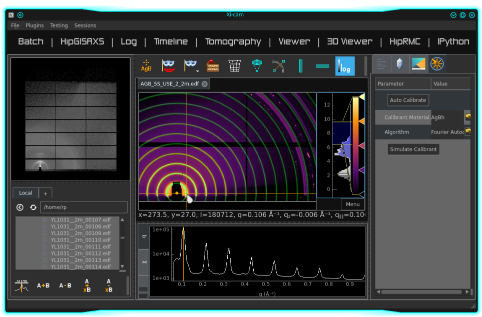
Xi-CAM: A Community-Driven Platform for Multimodal Analysis in Synchrotron Science

(Joint Collaboration: SSRL, NSLS-II, APS, NIST, ALS, and CAMERA)

Overview

Synchrotron scientists and users require new software tools for growing needs as data volume and complexity of analysis/experiment increases. Faster detectors and streamlined automation require a sustainable path towards managing this data.

In a cooperation across lightsources, CAMERA scientists Ron Pandolfi, Hari Krishnan, Dinesh Kumar and Alex Hexemer have developed a versatile interface "Xi-CAM" for visualization, data analysis, workflow for local and remote computing, data management, and seamless integration of plugins.



Xi-CAM screenshot

A Community Resource Across Facilities

Xi-CAM is pure Python, BSD open-source, and community integrated, with growing contributions from across the synchrotron community:

Unified GUI:

Xi-CAM has a unified GUI to access many external technique-specific algorithm libraries, including

• *APS: TomoPy:* Xi-CAM has incorporated APS's TomoPy software for tomography reconstruction.

• *Antwerp: Astra:* Xi-CAM has incorporated Astra's tomography software.

• *ALS: TomoCAM:* Xi-CAM has incorporated CAMERA's tomography software.

• *ESRF: pyFAI:* Xi-CAM incorporates ESRF's pfFAI for high-throughput SAXS analysis.

• *ALS: HipGISAXS and HipRMC:* Xi-CAM uses ALS's packages for GISAXS/SAXS simulations.

• *UCHI: Larch:* Xi-CAM uses Larch for NEXAFS corrections and analysis, including Kramers-Kronig complex refractive index estimations.

• *ALS: MSM:* Xi-CAM includes CAMERA's MSM for materials analysis.

• *NIST/CAMERA: CD-SAXS and CD-GISAXS:* Xi-CAM includes the joint NIST/CAMERA packages for CD-SAXS and CD-GISAXS.

• *SSRL: HiTp:* Xi-CAM includes SSRL's high throughput GIWAXS algorithms for combinatorial analyses.

• *NSLS-II: Scikit-Beam:* Xi-CAM uses the scikit-beam library for XPCS data analysis algorithms.

• *NIST: SASVIEW* Xi-CAM uses many form factor models in the SASVIEW-models library for fitting 1D spectra

• *APS: GIXSGUI:* Xi-CAM has a Python port of this package's GISAXS crystal structure simulator.

• *DESY: DPDAK:* Xi-CAM can call this library's geometric refinement algorithm for calibration.

Data Handling:

• *NSLS-II: DataBroker:* Xi-CAM data management is mediated through NSLS-II's DataBroker.

• *ESRF: FabIO:* Xi-CAM's data formats are abstracted from ESRF's FabIO scattering data formats.

• *APS: DataExchange:* Xi-CAM uses this abstraction library to unify loading of tomographic data.

Abstracted Controls Interface:

• *LCLS-II: PyDM:* Xi-CAM's rapid controls interface design uses this GUI widget library.

• *NSLS-II: Bluesky and Ophyd:* Xi-CAM's uses NSLS's Bluesky/Ophyd to provide controls interface across LCLS-II, NSLS-II, ALS and APS beamlines.

Remote Processing:

• *ALS: CAM-link:* Xi-CAM integrates with ALS's CAM-link's rapid compute resource deployment system for high throuput processing.

• *Anaconda: DASK:* Xi-CAM uses Anaconda's Distributed package for scalable remote execution.

• *SSRL: PAWS:* Xi-CAM incorporates SSRL's PAWS for remote processing of custom workflows.

Design Principles

Xi-CAM is not limited to a specific technique, facility/instrument, data format, or OS operating system. The intent is to provide a software stack for multiple instruments in multiple environments. The plugin-based approach supports extensibility, allowing new techniques to be added to Xi-CAM. Multiple data formats and hardware profiles are supported, and can easily be extended to cover new devices.

By making a variety of techniques available in a single platform, cross-plugin communication can direct multi-modal analysis. Xi-CAM exposes libraries to researchers without requiring programming experience or deep technical knowledge. Xi-CAM developers collaborate with the authors of these libraries and contribute back to external packages.

Xi-CAM Features

Current features and functionality include:

• *Automated calibration:* With minimal user direction, the complete experimental geometry can be fitted to ensure correct translation of the real space image to Q-space. Multiple options are available for calibrant materials. Automated techniques include Fourier auto-correlation, circular wavelets, and DPDAK's refinement algorithm. An interactive alignment interface is also available for tomography.

• *Data formats:* A wide variety of data formats is available including community standard formats (NeXUS, dxchange), legacy formats (TIF, fits, etc.), device-specific formats (EDF etc.) and more.

• *Fast azimuthal integration:* Xi-CAM uses the community package pyFAI (ESRF) for high-throughput SAXS data analysis with optional optimizations for GPUs.

• *GIWAXS remeshing:* A special geometric correction necessary for GIWAXS experiments is included, properly correcting for projection of the Ewald sphere, and resulting inaccessible Q-space.

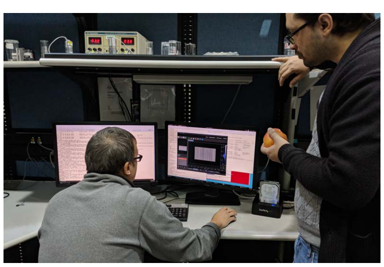
• *Timeline mode:* Xi-CAM provides unique tools to interactively analyze series data. With timeline mode, users scroll through time-series data and quickly identify key structural changes, or compare properties across a parameter space.

• *Data infill:* SAXS often has missing data resulting from masked or inactive regions on a detector. Multiple approaches are provided to fill in missing data to clean up artifacts.

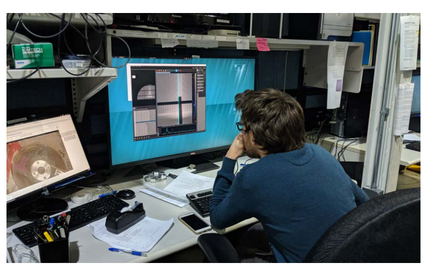
• *Visual parameter optimization:* When exploring effects of parameters in processing algorithms, Xi-CAM allows users to select a range of values, and then scroll through results and select the ideal value for use in analysis or reconstruction.

• *IPython console:* All internal variables of Xi-CAM are exposed in an embedded Python console. Custom processing can easily be applied to loaded data with some programming experience.

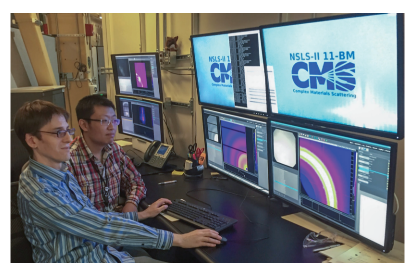
Current Installations



At APS 2-BM (micro-CT)



At APS 8-ID-E (Scattering)



At BNL 11-BM (Scattering)

Xi-CAM is currently installed at:

- APS: Two beamlines: 2-BM, 8-ID-E
- BNL: Three beamlines: 11-BM, 6-BM, 12-ID
- SSRL: Two beamlines: 2-1, 1-5
- ALS: Five: 7.3.3, 5.3.1, 11.0.1.2, 6.3.1.2, 8.3.2i

Other research facilities: NIST: One beamline:
Universities: Fribourg, Berkeley, Colorado, Kent State, TU Munich, Bayreuth, Stanford, UCSF, Tufts, TU Denmark, Penn State, UC Davis
Industry: DOW, Rivera, GE.

CAMERA Workshop: Bringing the Synchrotron Tomography Community Together

(Joint Collaboration: ALS/LBNL, LLNL, SSRL, APS/ANL, NSLS-II/BNL, ORNL, NIST, LANL, KIT, MAX IV, ANKA, SLS, Petra III, Australian Synchrotron, Diamond, NCEM/LBNL, ALCF/ANL, CWI, and CAMERA)

Overview

In November 2016 and 2017, a CAMERA-sponsored workshop was held at LBNL with a focus on current state-of-the-art tomographic reconstruction algorithms. The goal of the workshop was to bring together users, practitioners, and developers to assess the current landscape of available algorithms, to investigate commonalities and differences among the various techniques, and to discuss a range of topics, from required theoretical and algorithmic advancements on through to practical issues of implementation and deployment. Participants included beamline scientists, developers and users. Talks included:

- Developers describing their current algorithms, capabilities, and potential.
- Users discussing successes and unmet needs, and trying to find common goals.
- Beamline scientists presenting recent and future instrumentation developments.

Three working groups emerged: "Performance Benchmarking", "Image Quality" and "Web Portal and Sharing", chaired by Singanallur Venkatakrishnan (Oak Ridge National Laboratory), Doga Gursoy (Argonne National Laboratory), and Daniël Pelt (CWI Amsterdam), respectively.

A key component of both workshops was the demonstration sessions.

- In advance of the meeting, nine different software packages were sent to CAMERA. These packages included: TomoPy, the ASTRA Toolbox, UFO, Savu, PyHST2, TXM-Wizard, Livermore Tomography Toolbox (LTT), Xi-CAM, and TomoCam.
- The packages were all installed on LBNL machines, with a log kept of challenges involved in installing working versions.
- Machines were made available to run these packages during the workshop, including workstations, GPU clusters, and supercomputing facilities at NERSC.

Participants in the Nov 2016 Meeting

Ample time was included to demonstrate each package and to discuss various strengths. One of the highlights of the meeting was CAMERA's Dinesh Kumar's closing talk of the first meeting:

What I learned installing 10 different tomography packages in less than 10 days

Participants all commented that watching someone else go through the process of deploying their demos was one of the most valuable parts of the workshop: it revealed aspects of their software that users experience in actuality, but never come up during a rehearsed standard presentation. The shared experience led to conversations and interactions produced ideas for improvement. A user who wished to remain anonymous commented:

It was nice to finally meet the architects of some of the packages I have been using. Now that I have met them, I can no longer send nasty e-mails.

Shared Observations

- *The explosion in data:* Due to the high flux of light and neutron sources, the size and speed of new detectors, the increasing level of automation, and the increasing bandwidth of networking infrastructure, we are increasingly seeing very high data rates and volumes at DOE tomography beamlines.

– Fast feedback is needed to confirm that an experiment is working, and that the data will yield the information needed.
– Data analysis and acquisition protocols need to be improved so that experimental errors can be detected as soon as possible, desirably in real-time, to maximize utilization and productivity.

- *Algorithms:* It is hard for beamlines to take advantage of published algorithms. Algorithm developers should package their new work within the tools, software, or frameworks already in use at the beamlines to make it easy for beamline users to try new techniques. Preprocessing is a key part of reconstruction, and these methods should also be shared. Adoption of new algorithms will also be encouraged when developers benchmark software using shared data sets and then share information about their work on the portal. However, there is an intrinsic challenge:
  – Developers want to optimize a particular component: benchmarks that include the entire chain are not useful.
  – However, from the user perspective, what matters is overall performance.

Critical Needs

• *The need for performance benchmarks and metrics:* The explosion in data rates leads to a major push to increase speed and performance of tomography code. Beamline scientists want to make decisions about which software will have the highest performance. However, it is difficult to compare timing benchmarks between software, because tomographic reconstruction is just one step in a data chain that must include data management and a processing workflow to manage the required computing steps, from input/output, to preprocessing, postprocessing, visualization, and output.

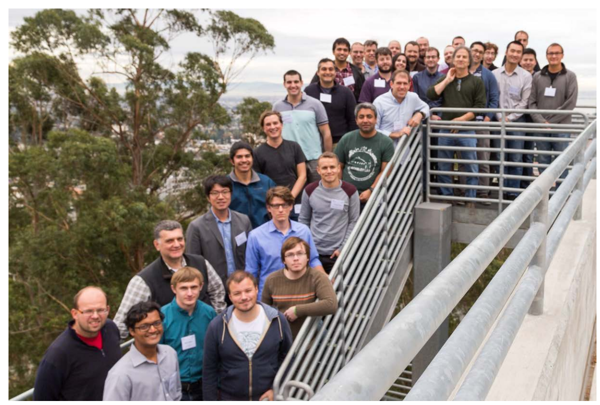
• *The need for image quality benchmarks and metrics:* There are no common approaches nor common language to talk about image quality, or to be able to compare different approaches beyond visually inspecting them and saying, "that one looks better." For the community to make more rapid progress towards improving the image quality of tomographic reconstruction, and then to automate those improvements, it is critical that we develop appropriate image metrics and the ability to benchmark image quality in different ways.

Results: Paths forward

Several paths forward were laid out and are now being pursued:

• To improve the process of collaboration and sharing, workshop participants agreed to contribute to a shared web portal focused on the process of tomographic reconstruction, "TomoPedia" `https://tomopedia.github.io/`, which complements "TomoBank" `http://tomobank.readthedocs.io/`, a public repository of tomography raw data, and in particular data sets representing those that give particular challenges to tomographic reconstruction codes.

•Several tomography packages committed to being incorporated into Xi-CAM: the CAMERA GUI-Python software environment. Plans to incorporate LTT (the Livermore Tomography Tools) into Xi-CAM are underway.



Participants in the Nov 2017 Meeting

Comments

"Great concept, a long-needed push to promote synergies that have been itching to coalesce, and fill knowledge gaps that stymie many researchers. Particularly useful to bolster/bootstrap the young investigators we really need in this field." B. Ward, LANL

"It has been great for me to see some of the software packages that are available and their features and strengths. I hope this becomes a re-occurring workshop to keep everyone talking and collaborating." A. Kiss, SLAC.

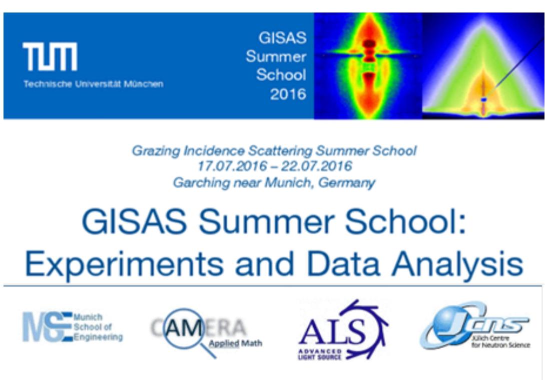
"There are many meetings on tomographic algorithms every year, but I have never attended a meeting dedicated to tomographic software. It was good to bring all of these groups together; this will improve the collaborative environment." K. Champley, LLNL.

Training the Next Generation: CAMERA Schools

Overview

Part of CAMERA's mission is to train the next generation of young scientists to tackle problems at DOE synchrotron light sources and nano-science centers. What is required are skills at the intersection of applied mathematics, computational science, software engineering, scattering physics, materials science, and experimental measurement. People seldom come with experience in all of these fields and it is important that they gain common understandings across these disciplines. To meet these needs, CAMERA has sponsored a set of summer schools and conferences to bring communities together to work on common problems.

2016 GISAS Summer School at TU Munich



CAMERA co-sponsored a summer school on the interplay between experiments and theory in grazing incidence scattering (GISAS), remote workflows, and high performance computing. The GISAS summer school was designed to kick-start beginners and introduce new data analysis tools for students with scattering experience.

The summer school invited Masters and PhD students to join with their own thin film samples suitable for grazing incidence small angle X-ray scattering (GISAXS) and grazing incidence small angle neutron scattering (GISANS) measurements. The program consisted of lectures on experiment design and scattering theory, necessary to understand the method and to choose experimental parameters.

CAMERA designed a true "superfacility" for use by students in the summer school:

- During the workshop X-ray experiments were carried out remotely at the ALS using a remote-controlled robot.
- Data was streamed from ALS into CAMERAfis Xi-CAM and reduced for processing.
- Students then used the Xi-CAM interface to design workflow (using Dask) to execute HIPGISAXS in GPU acceleration mode in realtime at the Swiss CSCC supercomputer center 200 miles away.
- Visualization was performed using CAMERAfis Xi-CAM interface.

The supercomputing facility at CSCS performed a full synchrotron dataset simulation in about 100 seconds, rather than several hours. This allowed students to fully analyze their datasets in just one week, rather than the typical 3 to 6 months.

"Future developments of the CAMERA potentials are followed with great interest and expectations, as it is likely to become a comprehensive supercomputing framework for the synchrotron community. A novel collaboration with CAMERA is in fact now under consideration at the SSRF, Chinese Academy of Sciences, where we are developing a very large scale unified infrastructure for Synchrotron Big Data.". Alessandro Sepe, Head of the Big Data Science, SSRF, Chinese Academy of Sciences, Shanghai, China.

2016 Summer School on Electronic Structure

CAMERA co-sponsored, jointly with MSRI, a 2016 summer school on electronic structure.

Ab initio or first principle electronic structure theories, particularly represented by Kohn-Sham density functional theory (KS-DFT), have been developed into workhorse tools with a wide range of scientific applications in chemistry, physics, materials science, and biology, etc. What is needed are new techniques that greatly extend the applicability and versatility of these approaches.

Many of the challenges that need to be addressed are essentially mathematical. The purpose of the workshop was to provide graduate students a self-contained introduction to electronic structure theory, with particular emphasis on frontier topics in aspects of applied analysis and numerical methods.

The two-week lectures co-taught by CAMERA's Lin Lin and by Duke's Jianfeng Lu gave a mathematical introduction to the field of electronic structure theory, in particular the density functional theory. The lectures covered spin-1/2 particle, Schrödinger equations for spin systems and in the real space, hydrogen atom and identical particles, many-body Hamiltonian, Hartree-Fock theory, Kohn-Sham density functional theory, self-consistent field iteration, density matrix and Green's function, density matrix algorithms, crystal and k-point sampling, localization of Green's function, perturbation theory and density functional perturbation theory, time-dependent density functional theory, time-dependent perturbation theory, and RPA correlation energy.

The first week lecture started from the basic quantum mechanics, and provided a self-contained introduction to the density functional theory for many-electron quantum systems. The second week lecture focused on two aspects of mathematical study of electronic structure theory: (1) Analysis and algorithms based on the density matrix formulation of DFT and (2) Linear response theory on time-independent and time-dependent systems.

Four one hour talks gave brief introductions to electronic structure theory in chemistry and materials science and other related topics:

- "Large scale quantum mechanical simulations of nanosystems": Lin-Wang Wang (Materials Science Division, LBNL)
- "Numerical methods for solving the Kohn-Sham problem": CAMERA's Chao Yang (Computational Research Division, LBNL)
- "NWChem: Pushing the scientific envelope": Bert de Jong (Computational Research Division, LBNL)
- "Beyond DFT: predicting excited-state properties of materials using Green's function formalisms": Felipe H. da Jornada (Department of Physics, UC Berkeley).
- "Fast algorithms for localization of Kohn-Sham orbitals": Anil Damle (Cornell)
- "Orbital Minimization Method": Kyle Thicke (Duke)

"Students found (it) useful to see how the mathematical formulation they learned can be used for real materials applications and to connect to experimental investigation at ALS." (From the MSRI-LBNL closing report.)

Publications: 2010-2018

X-ray Free-Electron Lasers

Structure Determination from Experimental Fluctuation X-ray Scattering Data, Pande K. et al., 2018 (In preparation).

Free Electron Laser based Multiple Particle Fluctuation Scattering Data, Pande K. et al., 2018 (In preparation).

Filtering techniques for small/wide-angle and fluctuation X-ray scattering, Donatelli J.J., Pande K., and Zwart P.H., 2018 (In preparation).

Interparticle coherence effects in fluctuation X-ray scattering, Donatelli J.J., Pande K., and Zwart P.H., 2018 (In preparation).

Correlations in Scattered X-Ray Laser Pulses Reveal Nanoscale Structural Features of Viruses, Ruslan P. Kurta, Jeffrey J. Donatelli, Chun Hong Yoon, Peter Berntsen, Johan Bielecki, Benedikt J. Daurer, Hasan DeMirci, Petra Fromme, Max Felix Hantke, Filipe R.N.C. Maia, Anna Munke, Carl Nettelblad, Kanupriya Pande, Hemanth K.N. Reddy, Jonas A. Sellberg, Raymond G. Sierra, Martin Svenda, Gijs van der Schot, Ivan A. Vartanyants, Garth J. Williams, P. Lourdu Xavier, Andrew Aquila, Peter H. Zwart, and Adrian P. Mancuso, Phys. Rev. Lett. 119, 158102, 2017.

Reconstruction from limited single-particle diffraction data via simultaneous determination of state, orientation, intensity, and phase, Jeffrey J. Donatelli, James A. Sethian and Peter H. Zwart, Proc. National Acad. Sciences, 114(28), 7222-7227, 2017. http://www.pnas.org/content/114/28/7222.

Structural enzymology using X-ray free electron lasers, Christopher Kupitz, Jose L. Olmos Jr., Mark Holl, Lee Tremblay, Kanupriya Pande, Suraj Pandey, Dominik Oberthr, Mark Hunter, Mengning Liang, Andrew Aquila, Jason Tenboer, George Calvey, Andrea Katz, Yujie Chen, Max O. Wiedorn, Juraj Knoska, Alke Meents, Valerio Majriani, Tyler Norwood, Ishwor Poudyal, Thomas Grant, Mitchell D. Miller, Weijun Xu, Aleksandra Tolstikova, Andrew Morgan, Markus Metz, Jose M. Martin-Garcia, James D. Zook, Shatabdi Roy-Chowdhury, Jesse Coe, Nirupa Nagaratnam, Domingo Meza, Raimund Fromme, Shibom Basu, Matthias Frank, Thomas White, Anton Barty, Sasa Bajt, Oleksandr Yefanov, Henry N. Chapman, Nadia Zatsepin, Garrett Nelson, Uwe Weierstall, John Spence, Peter Schwander, Lois Pollack, Petra Fromme, Abbas Ourmazd, George N. Phillips Jr., and Marius Schmidt, Structural Dynamics, 4, 044003, 2017, https://doi.org/10.1063/1.4972069.

Femtosecond structural dynamics drives the trans/cis isomerization in photoactive yellow protein, Kanupriya Pande, Christopher D. M. Hutchison, Gerrit Groenhof, Andy Aquila, Josef S. Robinson, Jason Tenboer, Shibom Basu, Sbastien Boutet, Daniel P. DePonte, Mengning Liang, Thomas A. White, Nadia A. Zatsepin, Oleksandr Yefanov, Dmitry Morozov, Dominik Oberthuer2, Cornelius Gati, Ganesh Subramanian, Daniel James, Yun Zhao, Jake Koralek, Jennifer Brayshaw, Christopher Kupitz, Chelsie Conrad, Shatabdi Roy-Chowdhury, Jesse D. Coe, Markus Metz, Paulraj Lourdu Xavier, Thomas D. Grant, Jason E. Koglin, Gihan Ketawala, Raimund Fromme, Vukica rajer, Robert Henning, John C. H. Spence, Abbas Ourmazd, Peter Schwander, Uwe Weierstall, Matthias Frank, Petra Fromme, Anton Barty, Henry N. Chapman, Keith Moffat, Jasper J. van Thor, Marius Schmidt, Science, 352(6286), 725-729, 2016. http://science.sciencemag.org/content/352/6286/725

The linac coherent light source single particle imaging road map, Andrew Aquila, Anton Barty, Christoph Bostedt, Sebastien Boutet, Gabriella Carini, P Drell, S Doniach, KH Downing, T Earnest, H Elmlund, V Elser, M Ghr, J Hajdu, J Hastings, SP Hau-Riege, Z Huang, EE Lattman, FRNC Maia, S Marchesini, A Ourmazd, C Pellegrini, R, Santra, I Schlichting, C Schroer, JCH Spence, IA Vartanyants, S Wakatsuki, WI Weis, GJ Williams, Structural Dynamics 2 Issue 4, Pages 041701, 2015/7/1

Iterative phasing for fluctuation X-ray scattering J.J. Donatelli, P.H. Zwart, and J.A. Sethian, Proc. National Acad. Sciences, 112(33), 10286-10291, 2015. http://www.pnas.org/content/112/33/10286.

Operational properties of fluctuation X-ray scattering data, E. Malmerberg, C.A. Kerfeld, and P.H. Zwart, IUCrJ, 2(3), 309-316, May 2015.

Simulations on time-resolved structure determination of uncrystallized biomolecules in the presence of shot noise, K. Pande, M. Schmidt, P. Schwander, and D.K. Saldin, Struct Dyn, 2(2), 024103, 2015.

https://aca.scitation.org/doi/10.1063/1.4916980.

Deducing fast electron density changes in randomly oriented uncrystallized biomolecules in a pump-probe experiment, K. Pande, P. Schwander, M. Schmidt, and D.K. Saldin, Philos Trans R Soc Lond B Biol Sci, 369(1647), 20130332, 2014.

Time-resolved serial crystallography captures high-resolution intermediates of photoactive yellow protein, Jason Tenboer, Shibom Basu, Nadia Zatsepin, Kanupriya Pande, Despina Milathianaki, Matthias Frank, Mark Hunter, Sbastien Boutet, Garth J. Williams, Jason E. Koglin, Dominik Oberthuer, Michael Heymann, Christopher Kupitz, Chelsie Conrad, Jesse Coe, Shatabdi Roy-Chowdhury, Uwe Weierstall, Daniel James, Dingjie Wang, Thomas Grant, Anton Barty, Oleksandr Yefanov, Jennifer Scales, Cornelius Gati, Carolin Seuring, Vukica Srajer, Robert Henning, Peter Schwander, Raimund Fromme, Abbas Ourmazd, Keith Moffat, Jasper J. Van Thor, John C. H. Spence, Petra Fromme, Henry N. Chapman, Marius Schmidt, Science, 346(6214), 1242-1246, 2014.

New Light on Disordered Ensembles: Ab-Initio Structure Determination of One Particle From Scattering Fluctuations Of Many Copie, D. K. Saldin, H. C. Poon, M. J. Bogan, S. Marchesini, D. A. Shapiro, R. A. Kirian, U. Weierstall, and J. C. H. Spence, Phys. Rev. Lett. 106, 115501 (2011). (viewpoint in Physics). (ALS highlight)

Structure of a single particle from scattering by many particles randomly oriented about an axis: toward structure solution without crystallization?, D. K. Saldin, V. L. Shneerson, M. R. Howells, S. Marchesini, H. N. Chapman, M. Bogan, D. Shapiro, R. A. Kirian, U. Weierstall, K. E. Schmidt and J. C. H. Spence, New J. Phys. 12, 035014, (2010).

Algorithmic framework for X-ray nanocrystallographic reconstruction in the presence of the indexing ambiguity, Donatelli, J.J. and Sethian, J.A., Proc. National Acad. Sciences, 111, 2, pp. 593-598, 2014. http://www.pnas.org/content/111/2/593.full.pdf+html

Component Particle Structure in Heterogeneous Disordered Ensembles Extracted from High-Throughput Fluctuation X-Ray Scattering, G. Chen, P.H. Zwart, and D. Li, Phys. Rev. Lett., 110(19), May 2013.

Three-dimensional single-particle imaging using angular correlations from X-ray laser data, H. Liu, B.K. Poon, D.K. Saldin, J.C.H. Spence, and P.H. Zwart, Acta Cryst. A, 69(4), 365-373, July 2013. https://scripts.iucr.org/cgi-bin/paper?sc5058

Computation of fluctuation scattering profiles via three-dimensional Zernike polynomials, H. Liu, B.K. Poon, A.J.E.M. Janssen, and P.H. Zwart, Acta. Cryst. A, 68(5), September 2012. https://scripts.iucr.org/cgi-bin/paper?sc5051

Structure determination of Pt-coated Au dumbbells via fluctuation X-ray scattering, G. Chen, M.A. Modestino, B.K. Poon, A. Schirotzek, S. Marchesini, R.A. Segalman, A. Hexemer, and P.H. Zwart, 19(5), 695-700, September 2012. https://scripts.iucr.org/cgi-bin/paper?co5018

Phasing of coherent femtosecond X-ray diffraction from size-varying nanocrystal, J. C. H. Spence, R. A. Kirian, X. Wang, U. Weierstall, K. E. Schmidt, T. White, A. Barty, H. N. Chapman, S. Marchesini, and J. Holton, Optics Express 19(4), pp. 2866-2873, 2011. http://dx.doi.org/10.1364/OE.19.002866 .

Compressive auto-indexing in femtosecond nanocrystallography, F. R. N. C. Maia, C. Yang, and S. Marchesini, Ultramicroscopy 111(7), 807-811. 2011. http://arxiv.org/abs/1011.3072

Orientation determination for 3D single molecule diffraction imaging, Chao Yang, Zhen Wang, and Stefano Marchesini, Proc. SPIE Vol. 7800, 78000P (2010).

Electronic Structure

Accelerating Optical Absorption Spectra and Exciton Energy Computation via Interpolative Separable Density Fitting, W. Hu, M. Shao, A. Cepellotti, F. H. da Jornada, L. Lin, K. Thicke, C. Yang and S. G. Louie, accepted, Intern. Conf. Computational Science, 2018.

PSelInv: A distributed memory parallel algorithm for selected inversion: the non-symmetric case, M. Jacquelin, L. Lin and C. Yang, Parallel Comput. 74, 84, 2018

Highly efficient photocatalytic water splitting over edge-modified phosphorene nanoribbons, W. Hu, L. Lin, R. Zhang, C. Yang and J. Yang, J. Amer. Chem. Soc. 139, 15429, 2017

Interpolative separable density fitting decomposition for accelerating hybrid density functional calculations with applications to defects in silicon, W. Hu, L. Lin and C. Yang, J. Chem. Theory Comput. 13, 5420, 2017

Projected Commutator DIIS Method for Accelerating Hybrid Functional Electronic Structure Calculations,

W. Hu, L. Lin and C. Yang, J. Chem. Theory Comput. 13, 5458, 2017

Accelerating selected columns of the density matrix computations via approximate column selection, A. Damle, L. Lin and L. Ying, SIAM J. Sci. Comput. 39, 1178, 2017

Robust Determination of the Chemical Potential in the Pole Expansion and Selected Inversion Method for Solving Kohn-Sham density functional theory, W. Jia and L. Lin, J. Chem. Phys. 147, 144107, 2017

A posteriori error estimates for discontinuous Galerkin methods using non-polynomial basis functions. Part II: Eigenvalue problems, L. Lin and B. Stamm, Math. Model. Numer. Anal. 51, 1733, 2017

Localized spectrum slicing, L. Lin, Math. Comp. 86, 2345, 2017

Randomized estimation of spectral densities of large matrices made accurate, L. Lin, Numer. Math. 136, 183, 2017

Adaptively compressed exchange operator for large scale hybrid density functional calculations with applications to the adsorption of water on silicene, W. Hu, L. Lin, A. Banerjee, E. Vecharynski and C. Yang, J. Chem. Theory Comput. 13, 1188, 2017

Adaptively compressed polarizability operator for accelerating large scale ab initio phonon calculations, L. Lin, Z. Xu and L. Ying, Multiscale Model. Simul. 15, 29, 2017

SCDM-k: Localized orbitals for solids via selected columns of the density matrix, A. Damle, L. Lin and L. Ying, J. Comput. Phys. 334, 1, 2017

Adaptive local basis set for Kohn-Sham density functional theory in a discontinuous Galerkin framework II: Force, vibration, and molecular dynamics calculations, G. Zhang, L. Lin, W. Hu, C. Yang and J.E. Pask, J. Comput. Phys. 335, 426 2017

PSelInv: A distributed memory parallel algorithm for selected inversion : the symmetric case, M. Jacquelin, L. Lin and C. Yang, ACM Trans. Math. Software 43, 21, 2016

Chebyshev polynomial filtered subspace iteration in the Discontinuous Galerkin method for large-scale electronic structure calculations, A. S. Banerjee, L. Lin, W. Hu, C. Yang, J. E. Pask, J. Chem. Phys. 145, 154101, 2016

Adaptively compressed exchange operators, L. Lin, J. Chem. Theory Comput. 12, 2242, 2016

Low rank approximation in G0W0 calculations, M. Shao, L. Lin, C. Yang, F. Liu, F. Jornada, J. Deslippe and S. G. Louie, Sci. China Math., 59 1593, 2016

Decay estimates of discretized Green's functions for Schrodinger type operators, L. Lin and J. Lu, Sci. China Math., 59, 1561, 2016

Approximating spectral densities of large matrices, L. Lin, Y. Saad and C. Yang, SIAM Rev. 58, 34, 2016

A proximal gradient method for ensemble density functional theory, M. Ulbrich, Z. Wen, C. Yang, D. Klockner, Z. Lu,, SIAM J. Sci. Comp., June 20, 2015, 37:A1975–A20,

Edge-modified phosphorene nanoflake heterojunctions as highly efficient solar cells, W. Hu, L. Lin, C. Yang, J. Dai and J. Yang, Nano Lett. 16 1675, 2016

Enhancing the scalability and load balancing of the parallel selected inversion algorithm via tree-based asynchronous communication, M. Jacquelin, L. Lin, N. Wichmann and C. Yang, IEEE IPDPS, 192, 2016

A posteriori error estimates for discontinuous Galerkin methods using non-polynomial basis functions. Part I: Second order linear PDE, L. Lin and B. Stamm, Math. Model. Numer. Anal. (M2AN) 50, 1193, 2016

Large-scale ab initio simulations based on systematically improvable atomic basis, P. Li, X. Liu, M. Chen, P. Lin, X. Ren, L. Lin, C. Yang and L. He, Comput. Mater. Sci. 112 503, 2016

Fast algorithms for estimating the absorption spectrum within linear response time-dependent density functional theory, J. Brabec, L. Lin, M. Shao, N. Govind, C. Yang, Y. Saad, E. Ng, J. Chem. Theory Comput. 11, 5197, 2015

A massively parallel method for large scale density functional theory calculation, W. Hu, L. Lin and C. Yang, DGDFT. Chem. Phys. 143, 124110, 2015

Edge reconstruction in armchair phosphorene nanoribbons revealed by discontinuous Galerkin density functional theory, W. Hu, L. Lin and C. Yang, Phys. Chem. Chem. Phys. 17, 31397, 2015

Compressed representation of Kohn-Sham orbitals via selected columns of the density matrix, A. Damle, L. Lin and L. Ying, .Chem. Theory Comput. 11, 1463, 2015

Electronic structure of large-scale graphene nanoflakes, W. Hu, L. Lin, C. Yang and J. Yang,,J. Chem. Phys. 141, 214704, 2014

SIESTA-PEXSI: Massively parallel method for efficient

and accurate ab initio materials simulation without matrix diagonalization, L. Lin, A. Garcia, G. Huhs and C. Yang, J. Phys. Condens. Matter 26, 305503, 2014

A posteriori error estimator for adaptive local basis functions to solve Kohn-Sham density functional theory, J. Kaye, L. Lin and C. Yang, Commun. Math. Sci. 13, 1741, 2015

Elliptic preconditioner for accelerating the self-consistent field iteration in Kohn-Sham Density Functional Theory, L. Lin and C. Yang, SIAM J. Sci. Comp., 35(5), S277-S298, 2013.

Accelerating Atomic Orbital-based Electronic Structure Calculation via Pole Expansion and Selected Inversion, L. Lin, M. Chen, C. Yang and L. He,J. Phys.: Condens. Matter, 25, pp. 295501, 2013.

Element orbitals for Kohn-Sham density functional theory, L. Lin and L. Ying, Phys. Rev. B, 85:235144, 2012.

Optimized local basis set for Kohn-Sham density functional theory, L. Lin, J. Lu, L. Ying and W. E, J. Comput. Phys., 231:4515, 2012,

Adaptive local basis set for Kohn-Sham density functional theory in a discontinuous Galerkin framework I: Total energy calculation, L. Lin, J. Lu, L. Ying and W. E, J. Comput. Phys., 231:2140, 2012.

Materials Informatics

A Surrogate Model Approach to Autonomous Experimentation and Applications to X-Ray Imaging, Noack, M., Fukuto, M., Yager, K., Hexemer, A., 2018 (In preparation).

A High-Performance QED Ray Tracer for X-Ray Scattering Computations, Noack, M., Fukuto, M., Yager, K., Sethian, J., 2018 (In preparation).

Accurate Characterization of the Pore Volume in Microporous Crystalline Materials, D. Ongari, P. Boyd, S. Barthel, M. Witman, M. Haranczyk, B. Smit, Langmuir 33 (2017), 14529-14538. (featured on cover)

Computationally-Guided Synthetic Control over Pore Size in Isostructural Porous Organic Cages, A. Slater, P. Reiss, A. Pulido, M. Little, D. Holden, L. Chen, Linjiang, S. Chong, B. Alston, R. Clowes, M. Haranczyk, M. Briggs, T. Hasell, G. Day, A. Cooper, ACS Central Science 3 (2017) 734-742.

The Influence of Intrinsic Framework Flexibility on Adsorption in Nanoporous Materials, M. Witman, S. Ling, S. Jawahery, P. Boyd, M. Haranczyk, B. Slater, B. Smit, Journal of the American Chemical Society 139 (2017) 5547-5557.

Scanning electron microscopy as a source of morphological data on nanoparticles: image representativeness, K. Odziomek, D. Ushizima, P. Oberbek, K. Kurzydlowski, T. Puzyn, M. Haranczyk, Journal of Microscopy 265 (2017) 34-50

Metal-Organic Framework with Optimal Adsorption, Separation, and Selectivity towards Xenon, D. Banerjee, A.M. Plonka, C.M. Simon, R.K. Motkuri, J. Liu, X. Chen, B.Smit, J.B. Parise, M. Haranczyk, P.K. Thallapally , Nature Communications 7 (2016)

Tunable porosity through cooperative diffusion in a multicomponent porous molecular crystal, R. Manurung, M. Miklitz, D. Holden, L. Chen, T. Hasell, S.Y. Chong, M. Haranczyk, A.I. Cooper, K.E. Jelfs, Journal of Physical Chemistry C 119 (2015) 22577-22586

Understanding Small-Molecule Interactions in MetalfiOrganic Frameworks: Coupling Experiment with Theory, J.S. Lee, B. Vlaisavljevich, D. K. Britt, C. M. Brown, M. Haranczyk, J.B. Neaton, B. Smit, J.R. Long, W.L. Queen, Advanced Materials (2015), DOI: 10.1002/adma.201500966

Design of Three-Dimensional Porous Covalent Organic Frameworks via Known Synthesis Routes and Commercially Available Species, R.L. Martin, C. Simon, B. Medasani, D. Britt, B. Smit, M. Haranczyk, Journal of Physical Chemistry C 118, pp. 23790-23802, 2014,

Exploring frontiers of high surface area metal-organic frameworks, R.L. Martin, M. Haranczyk, Chemical Science 4, pp. 1781-1785, 2013,

High accuracy geometric analysis of crystalline porous materials, M. Pinheiro, R.L. Martin, C.H. Rycroft, M. Haranczyk, CrystEngComm 15, pp. 7531-7538, 2013.

Insights into Multi-Objective Design of Metal-Organic Frameworks, R.L. Martin, M. Haranczyk , Crystal Growth and Design 13, pp. 4208-4212, 2013.

Algorithms and tools for high-throughput geometry-based analysis of crystalline porous materials, T.F. Willems, C.H. Rycroft, M. Kazi, J.C. Meza, M. Haranczyk, Microporous and Mesoporous Materials, 149, pp. 134-141, 2012.

Addressing challenges of identifying geometrically diverse sets of crystalline porous materials, R.L. Martin, B. Smit, M. Haranczyk. Jour. Chem. Information and Modeling 52, pp. 308-318, 2012, http://pubs.acs.org/doi/abs/10.1021/ci200386x.

Accelerating analysis of void space in porous materials on multicore and GPU platforms, R.L. Martin, Prabhat, Donofrio, J.A. Sethian, M, .Haranczyk, International Journal of High Performance Computing, Feb., 2012, 1094342011431591

Automatic Structure Analysis in High-Throughput Characterization of Porous Material, M. Haranczyk and Sethian, J.A., J. Chem. Theory Comput., 2010, 6 (11), pp 3472-3480,

Navigating molecular worms inside chemical labyrinths, Haranczyk, M. and Sethian, J.A., Proc. National Acad. Sciences, 106, pp. 1472-21477, 2009.

GISAXS

Computational Analysis of Grazing Incidence Small Angle X-Ray Scattering Data, A. Sarje, S. Chourou, D. Kumar, S. Venkatakrishnan, X. Li, and A. Hexemer, submitted to J. Applied Crystallography, 2018 (in revision).

Accurate Multi-slice Grazing-Incidence X-ray Simulation, S.V. Venkatakrishnan, Jeffrey Donatelli, Dinesh Kumar, Abhinav Sarje, Sunil K. Sinha, Xiaoye S. Li, Alexander Hexemer, J. Applied Crystallography, Vol.49, Part 6, December 2016.

Pursuing the critical dimension using Grazing Incidence Small Angle X-ray Scattering, G. Freychet, D. Kumar, R. Pandolfi, P. Naulleau, I. Cordova, J. Strzalka, M. Fukuto, and A. Hexemer, Proc. Vol. 10585, Metrology, Inspection, and Process Control for Microlithography XXXII, SPIE Advanced Lithography 2018.

DOE Scientists Team up to Demonstrate Scientific Potential of Big Data Infrastructure, LBNL News Feb. 3, 2015.

Organic Photovoltaics Experiments Showcase "Superfacility" Concept, LBNL News March 17, 2015.

Real-Time Data Pipeline and analysis using SPOT and HIPGISAXS, A. Hexemer and C.E.Tull, OLCF Users meeting June 24, 2015.

HIPGISAXS for fast analysis, A. Hexemer, canSAS 8 meeting in Tokai, Japan. 2015.

HIPGISAXS, A. Hexemer, Kyoto Institute of Technology, Japan, May 2015.

Fast Analysis for Scattering, A. Hexemer, ISPAC, Houston, May 2015.

Fast Analysis of Time-Resolved Scattering Data, A. Hexemer APS March Meeting 2015.

Inverse Modeling Nanostructures from X-ray Scattering Data through Massive Parallelism, A. Sarje, X.S. Li, D. Kumar, S. Venkatakrishnan, A. Hexemer, SC15 conference, Nov. 2015.

Recovering Nanostructures from X-ray Scattering Data, A. Sarje, X.S. Li, D. Kumar, A. Hexemer, NVIDIA GPU Technology Conference, San Jose, Calif., May 2015.

Scalable Particle Swarm Optimization for Nanostructure Discovery, A. Sarje, X. Li and A. Hexemer, submitted to Euro-Par 2015 Conference, Aug. 24-28, 2015, Vienna.

High-Performance Inverse Modeling with Reverse Monte Carlo Simulations, A. Sarje, X. Li and A. Hexemer, 2014 Intern. Conf. on Parallel Processing (ICPP-2014), Sept 9-14, 2014, Minneapolis, Minn.

PbS Nanoparticles Capped with Tetrathiafulvalenetetracarboxylate: Utilizing Energy Level Alignment for Efficient Carrier Transport, M. Scheele, D. Hanifi, D. Zherebetskyy, S.T. Chourou, S. Axnanda, B.J. Rancatore, K. Thorkelsson, T. Xu, Z. Liu, L.-W. Wang, Y. Liu, and A. P. Alivisatos, ACS Nano, ACS Nano, 2014, 8 (3), pp. 2532-2540.

An In Situ Grazing Incidence X-Ray Scattering Study of Block Copolymer Thin Films During Solvent Vapor Annealing, Xiaodan Gu, Ilja Gunkel, Alexander Hexemer, Weiyin Gu and Thomas P. Russell, , Advanced Materials, Volume 26, Issue 2, pp. 273-281. January 15, 2014.

HipGISAXS: A High-Performance Software for Simulating GISAXS Data, S. T. Chourou, A. Sarje, X. Li, E. Chan, and A. Hexemer, J. Applied Crystallography, Vol. 46, Part 6, Dec. 2013.

Tuning HipGISAXS on Multi and Many Core Supercomputers, A. Sarje and X.S. Li, Proc. of 4th International Workshop on Performance Modeling, Benchmarking and Simulation of High Performance Computer Systems (PMBS13), SC13, Denver, Colorado, November 2013.

Synchrotron Light-Source Data Analysis through Massively-Parallel GPU Computing, A. Sarje, X.S. Li, S. Chourou, A. Hexemer, NVIDIA GPU Technology Conference, San Jose, Calif., May 2013.

Massively Parallel X-ray Scattering Simulations, A. Sarje, X.S. Li, S. Chourou, E. Chan, and A. Hexemer, Proc. of The International Conference for High Performance Computing, Networking, Storage and Analysis (SC12), Salt Lake City, Nov. 10-16, 2012.

Pursuing the critical dimension in etched patterns using x-ray scattering, G. Freychet, D. Kumar, R. Pandolfi, D. Staacks, P. Naulleau, R. J. Kline, D. Sunday , M. Fukuto, J. Strzalka and A. Hexemer, Proceeding SPIE Advanced Lithography, Vol. 10585, pp. 10585 -10585-7, 2018.

Programmed LWR metrology by multi-techniques approach, J. Reche, M. Besacier, P. Gergaud, Y. Blancquaert, G. Freychet and T. Labbaye, Proceeding SPIE Advanced Lithography, Vol. 10585, pp. 105850F, 2018.

Tomography

Ring artifact reduction in synchrotron X-ray tomography through helical acquisition, D.M. Pelt, & D. Y. Parkinson, Measurement Science and Technology, Volume 29, Number 3 (2018).

Machine learning for micro-tomography, Parkinson, D. Y.; Ushizima, D. M.; Perciano, T.; Krishnan, H.; Barnard, H. S.; MacDowell, A. A.; Pelt, D.; Sethian, J. A. , Dev. X-Ray Tomogr. XI 18 (2017).

Insight into 3D micro-CT data: convergence of segmentation algorithms through evaluation metrics, T. Perciano, D. Ushizima, H. Krishnan, D. Parkinson, N. M. Larson, Daniel M. Pelt and F. W. Zok, Journal of Synchrotron Radiation, 24(5): 1065-1077, Sept. 2017

Improved tomographic reconstruction of large-scale real-world data by filter optimization, D. M. Pelt and V. De Andrade. Advanced Structural and Chemical Imaging 2016 2:17.

Insight into 3D micro-CT data: convergence of segmentation algorithms through evaluation metrics, T. Perciano, D. Ushizima, H. Krishnan, D. Parkinson, N. M. Larson, Daniel M. Pelt and F. W. Zok, Journal of Synchrotron Radiation, 24(5): 1065-1077, Sept. 2017

Improved tomographic reconstruction of large-scale real-world data by filter optimization, D. M. Pelt and V. De Andrade. Advanced Structural and Chemical Imaging 2016 2:17.

Model:Based Iterative Reconstruction for Synchrotron X:Ray Tomography, Mohan, K. A., Venkatakrishnan, S. V, Drummy, L. F., Simmons, J., Parkinson, D. Y., & Bouman, C. A,, ICASSP, 2014.

Scientific data exchange: a schema for HDF5:based storage of raw and analyzed data, De Carlo, F., G ́ursoy, D., Marone, F., Rivers, M., Parkinson, D. Y., Khan, F., Jacobsen, C, Journal of Synchrotron Radiation, 21(Pt 6), 1224fi?!30.

High performance data management and analysis for tomography, Parkinson D. Y., Blair, J., Canon, R. S., Deslippe, J., Essiari, A., Hexemer, A., MacDowell, A. A., ... others, In SPIE Optical Engineering and Applications (p. 92121G - 92121G).

Image Analysis

Gradient Boosting Decision Trees for Echo Images, Melo, Ushizima, Barachio, Coelho, IEEE World Congress on Computational Intelligence, International Joint Conference on Neural Networks (IJCNN) 2018 (accepted).

Active contours for overlapping cell segmentation, Araujo, Silva, Medeiros, Farias, Calaes, Bianchi, Ushizima, International Journal of Biomedical Engineering and Technology 2018 (accepted).

Xi-cam: A versatile interface for data visualization and analysis, Pandolfi, Allan, Arenholz, Barroso-Luque, Campbell, Caswell, Blair, Carlo, Fackler, Fournier, Freychet, Fukuto, Gursoy, Jiang, Krishnan, Kumar, Kline, Li, Liman, Marchesini, Mehta, N'Diaye, Parkinson, Parks, Pellouchoud, Perciano, Ren, Sahoo, Strzalka, Sunday, Tassone, Ushizima, Venkatakrishnan, Yager, Zwart, Sethian, Hexemer, Journal of Synchrotron Radiation 2018 (accepted).

Mathematics in Pattern Recognition for Scientific Investigations, T. Perciano, B. Loring, H. Krishnan, J. Michael L. MacNeil, D. Ushizima, position paper in the DOE Scientific Machine Learning Workshop, 2018.

Maximal clique enumeration with data-parallel primitives, B. Lessley, T. Perciano, M. Mathai, H. Childs and E. W. Bethel, IEEE 7th Symposium on Large Data Analysis and Visualization (LDAV), Phoenix, AZ, 2017, pp. 16-25, 2017 doi: 10.1109/LDAV.2017.8231847

Data Efficient X-ray Phase Tomography with Self-calibrated Sandpaper Analyzer,Chen, M., Parkinson, D., Venkatakrishnan, S., Marchesini, S. & Waller, L., Computational Optical Sensing and Imaging CW2B–2 (2017).

Machine learning for micro-tomography, Parkinson, D. Y.; Ushizima, D. M.; Perciano, T.; Krishnan, H.; Barnard, H. S.; MacDowell, A. A.; Pelt, D.; Sethian, J. A. , Dev. X-Ray Tomogr. XI 18 (2017).

Nearest-Neighbour Nanocrystal Bonding Dictates Framework Stability or Collapse in Colloidal Nanocrystal Frameworks, Williams, Ushizima, Zhu, Anders, Milliron, Helms, Chemical Communica-

tions, Royal Society of Chemistry, 2017.

Automating Cell Detection and Classification in Human Brain Fluorescent Microscopy Images Using Dictionary Learning and Sparse Coding, Alegro, Theofilas, Nguy, Castruita, Seeley, Ushizima, Grinberg, Journal of Neuroscience Methods, 2017.

Detection and Classification of Cervical Cells, Ushizima, D. in The Practice of Reproducible Research: Case Studies and Lessons from the Data-Intensive Sciences, Kitzes, J., Turek, D., & Deniz, F. (Eds.), Oakland, CA: Univ. Calif. Press 2017. [book chapter]

Convolutional Neural Networks with Tensor Flow: theory and practice, Araujo, Carneiro, Silva, Medeiros, Ushizima, p. 382-406. Brazilian Society of Computation Press 2017. [book chapter]

Computer Vision in python with libraries scikit-image & scikit-learn, Silva, Lopes, Araujo, Medeiros, Ushizima, p. 407-428. Brazilian Society of Computation Press 2017. [book chapter]

A multi-objective approach for calibration and detection of cells nuclei, Oliveira, Moreira, Ushizima, Carneiro, Medeiros, Araujo, Silva, Bianchi, IEEE Congress on Evolutionary Computation, 2017.

Portable Learning Environments for Hands-On Computational Instruction Using Container- and Cloud-Based Technology to Teach Data Science, Holdgraf, Rokem, Culich, Alegro, Deniz, Ushizima, Practice & Experience in Advanced Research Computing Conference, PEARC'17.

Distributed Memory Parallel Markov Random Fields using Graph Partitioning, C. Heinemann, T. Perciano, D. Ushizima, and E. Wes Bethel, Fourth International Workshop on High Performance Big Graph Data Management, Analysis, and Mining (BigGraphs 2017), in conjunction with IEEE BigData 2017, December 11-14, 2017, Boston MA, USA.

Insight into 3D micro-CT data: convergence of segmentation algorithms through evaluation metrics, T. Perciano, D. Ushizima, H. Krishnan, D. Parkinson, N. M. Larson, Daniel M. Pelt and F. W. Zok, Journal of Synchrotron Radiation, 24(5): 1065-1077, September 2017

Improved tomographic reconstruction of large-scale real-world data by filter optimization, D. M. Pelt and V. De Andrade. Advanced Structural and Chemical Imaging 2016 2:17.

Robust model-based phase ptycho-tomography, Singanallur V. Venkatakrishnan, Maryam Farmand, Young-Sang Yu, Hasti Majidi, Klaus Van Benthem, Stefano Marchesini, David Shapiro, and Alexander Hexemer, IEEE Signal Processing Letters, Vol. 23, no. 7, pp. 944-948, July 2016

Scanning electron microscopy image representativeness: morphological data on nanoparticles, Odziomek, K., , Ushizima, D., Oberbek, P., Kurzydlowski, K., Puzyn, T., and Haranczyk, M., Jour. of Microscopy, 265(1), 2017

Ammonia gas sensor based on the frequency-dependent impedance characteristics of ultrathin polyaniline films, Santos, Bianchi, A., Ushizima, D., Pavinatto, Bianchi, Sensors and Actuators A: Physical, 2016

Evaluation of Three Algorithms for the Segmentation of Overlapping Cervical Cells, Lu, Carneiro, Bradley, Ushizima, Nosrati, Bianchi, Carneiro, Hamarneh, IEEE Journal of Biomedical and Health Informatics, 99, pp. 2168-2194, 2016.

Scaling Analytics for Scientific Images from Experimental Instruments, Ushizima, Hexemer, Parkinson, Yang, IEEE Applied Imagery Pattern Recognition October, 2016

Searchable datasets in Python: images across domains, experiments, algorithms and learning, Araujo, Silva, Ushizima, Medeiros, PyData, San Francisco 2016;

Pathway toward diagnosing and monitoring prodromal Alzheimer's Disease using novel imaging biomarkers, Ushizima, Grinberg, California Initiative for the Advancement of Precision Medicine Workshop 2016

A two-level Markov random field for road network extraction and its application with optical, SAR, and multitemporal data, T. Perciano, F. Tupin, R. Hirata Jr., and R. M. Cesar Jr., International Journal of Remote Sensing, 37(16):3584-3610, July 2016

Making advanced scientific algorithms and big scientific data management more accessible, S.V. Venkatakrishnan, K. Aditya Mohan, K. Beattie, J. Correa, E. Dart, J.R. Deslippe, A. Hexemer, H. Krishnan, A. A MacDowell, S. Marchesini, S.J Patton, T. Perciano, J.A Sethian, R. Stromsness, B.L Tierney, C.E. Tull, D. Ushizima, and D.Y. Parkinson. Electronic Imaging, 2016(19):1-7, February 2016

IDEAL: Images Across Domains, Experiments, Algorithms and Learning, D. M. Ushizima, H. A. Bale, E. W. Bethel, P. Ercius, B. A. Helms, H. Krishnan, L. T. Grinberg, M. Haranczyk, A. A. Macdowell, K. Odziomek, D. Y. Parkinson, T. Perciano, R. O. Ritchie, and C. Yang. JOM - The Journal of The Minerals, Metals & Materials Society (TMS), pages 1-10 2016

Model:Based Iterative Reconstruction for Synchrotron X:Ray Tomography, Mohan, K. A., Venkatakrishnan, S. V, Drummy, L. F., Simmons, J., Parkinson, D. Y., & Bouman, C. A,, ICASSP, 2014.

Scientific data exchange: a schema for HDF5:based storage of raw and analyzed data, De Carlo, F., Gufkrsoy, D., Marone, F., Rivers, M., Parkinson, D. Y., Khan, F., Jacobsen, C, Journal of Synchrotron Radiation, 21(Pt 6), 1224-30. doi:10.1107/S160057751401604X

High performance data management and analysis for tomography, Parkinson D. Y., Blair, J., Canon, R. S., Deslippe, J., Essiari, A., Hexemer, A., MacDowell, A. A., … others, In SPIE Optical Engineering Applications (p. 92121G-92121G).

CAMERA: The Center for Advanced Mathematics for Energy Research Applications, Donatelli, J; Haranczyk, M; Hexemer, A; Krishnan, H; Li, X; Lin, L; Maia, F; Marchesini, S; Parkinson, D; Perciano, T, Sethian, J.A., Synchrotron Radiation News 28 2 9-Apr 2015

Evaluation of Algorithms for the Segmentation of Overlapping Cervical Cells, Z Lu, G Carneiro, A Bradley, D Ushizima, MS Nosrati, A Bianchi, IEEE Journal of Biomedical and Health Informatics 2016.

Fast Detection of Material Deformation through Structural Dissimilarity, D. M. Ushizima, T. Perciano, D. Y. Parkinson, IEEE Big Data 2015.

Cell reconstruction under Voronoi and enclosing ellipses from 3d microscopy, GLB Ramalho, DS Ferreira, AGC Bianchi, CM Carneiro, FNS Medeiros, IEEE Intern. Symp. Biomedical Imaging (ISBI) 2015.

Investigating Pill Recognition Methods for a New National Library of Medicine Image Dataset, D Ushizima, A Carneiro, M Souza, F Medeiros, Advances in Visual Computing, 410-419.

Reduced-complexity Image Segmentation under Parallel Markov Random Field Formulation using Graph Partitioning, T. Perciano, D. M. Ushizima, Y. Mizrahi, E. W. Bethel, J. A. Sethian, IEEE ICIP, 2016

Block Copolymer Packing Limits and Interfacial Reconfigurability in the Assembly of Periodic Mesoporous Organosilicas, Andrew W. Wills, David J. Michalak, Peter Ercius, Ethan L. Rosenberg, Rory Runser, Talita Perciano, Daniela Ushizima, Brett Helms, Advanced Functional Materials, 25 (26), pp 4120-4128, 2015,

Real-time Data Intensive Computing, D.Y. Parkinson, K. Beattie, X. Chen, J. Correa, E. Dart, B. J. Daurer, J.R. Deslippe, A. Hexemer, H. Krishnan, A. MacDowell, F.R.N.C. Maia, S. Marchesini, H.A. Padmore, S.J. Patton, T. Perciano, J.A. Sethian, D.A. Shapiro, R. Stromsness, N. Tamura, B.L. Tierney, C.E. Tull2, D. Ushizima, Synchrotron Radiation Instrumentation 2015.

Aperture imaging for fluorescent x-ray,, A. Haboub, A. A. MacDowell, S. Marchesini, D. Y. Parkinson, Rev. Sci. Instrum. 85, 063704, 2014.

Structure recognition from high resolution images of ceramic composites, D.M. Ushizima, T. Perciano, H. Krishnan, B. Loring, H. Bale, D. Parkinson, and J. Sethian., IEEE International Conference on Big Data, October 2014.

Toward quantitative structure activity relationship (qsar) models for nanoparticles, K. Odziomek, D.M. Ushizima, M. Haranczyk, and T. Puzyn. American Chemical Society National Meeting - Scientific Excellence Award, August 2014.

Segmentation of subcellular compartments combining superpixel representation with voronoi diagrams, D.M. Ushizima, A.G.C. Bianchi, and C. Carneiro. IEEE International Symposium on Biomedical Imaging (ISBI) - 1st place in Code Competition, April 2014.

Corner Detection in Planar Shapes, Paula Jr., I.C., Medeiros, F.N.S., Bezerra, F.N. and Ushizima, D.M., Journal of Mathematical Imaging and Vision, March 2013.

Challenges and New Developments in Imaging with Large Data Sets, Ushizima, D.M., Bianchi, A.G.C., Krishnam, H., Joint Statistical Meeting (JSM2013), Montreal, Aug 2013 (oral presentation).

"Multiscale Corner Detection in Planar Shape, Paula Jr., I.C., Medeiros, F.N.S, Bezerra, F.N. and Ushizima, D.M., Journal of Mathematical Imaging and Vision, March 2013.

Material science image analysis using quant-CT in ImageJ, Ushizima, D.M., Bianchi, A.G.C., deBianchi, C. and Bethel E.W.,in: ImageJ User and Developer Conference 2012, Oct, Luxembourg, LX.

Augmented topological descriptors of pore network, Ushizima, D.M., Morozov, D, Weber, G.H., Bianchi, A.G.C. and Bethel E.W., in: VisWeek 2012, Oct, Seattle, WA, USA.

Algorithms for Microstructure Description applied to

Microtomography, Ushizima, D.M., Weber, G., Morozov, D., Bethel, W., Sethian, J.A., Carbon Cycle 2.0 Symposium, LBNL, Feb. 2012.

Compressive phase contrast tomography, F. Maia, A. MacDowell, S. Marchesini, H. A. Padmore, D. Y. Parkinson, J. Pien, A. Schirotzek, and C. Yang, Proc. SPIE Vol. 7800, 78000F, 2010

Ptychography

Three-dimensional localization of nanoscale battery reactions using soft X-ray tomography, Yu, Y. S., Farmand, M., Kim, C., Liu, Y., Grey, C. P., Strobridge, F. C., ... & Krishnan, H. Nature communications, 9(1), 921. (2018).

Variational Phase Retrieval with Globally Convergent Preconditioned Proximal Algorithm, Huibin Chang, Stefano Marchesini, Yifei Lou, and Tieyong Zeng, SIAM Journal on Imaging Sciences, 11(1), 2018

Total variation based phase retrieval for Poisson noise removal, Huibin Chang, Yifei Lou, Yuping Duan, and Stefano Marchesini, SIAM Journal on Imaging Sciences, 11(1), 2018

GPU-based implementation of Ptycho-ADMM for high performance X-ray imaging, Pablo Enfedaque, Stefano Marchesini, Hari Krishnan and Huibin Chang, International Conference on Computational Science, 2018 (accepted)

Partially Coherent Ptychography by Gradient Decomposition of the Probe, Huibin Chang, Pablo Enfedaque, Yifei Lou and Stefano Marchesinifi, Acta Crystallographica Section A: Foundations and Advances, to appear (2018). https://arxiv.org/abs/1710.07382

Data Efficient X-ray Phase Tomography with Self-calibrated Sandpaper Analyzer, Chen, Michael, et al. Computational Optical Sensing and Imaging. Optical Society of America, 2017.

Nanometer-resolved spectroscopic study reveals the conversion mechanism of CaOttAl2O3tt10H2O to 2CaOttAl2O3tt8H2O and 3CaOttAl2O3tt6H2O at an elevated temperature, G. Geng, et al, Crystal Growth and Design, 17 (8), 4246-4253, 2017

Ptychographic imaging of nano-materials at the Advanced Light Source with the Nanosurveyor Instrument, Shapiro, D.A., Celestre, R., Peter Denes, Maryam Farmand, John Joseph, A.L.D. Kilcoyne, Stefano Marchesini, Howard Padmore, Singanallur V. Venkatakrishnan, Tony Warwick and Young-Sang Yuet al, IOP Conference Series: Journal of Physics 849 012028 (2017)

Correlative cellular ptychography with functionalized nanoparticles at the Fe L-edge, M. Gallagher-Jones, et al, Scientific Reports, 7, 4757 (2017)

Near-edge X-ray refraction fine structure microscopy, M Farmand, R Celestre, P Denes, ALD Kilcoyne, S Marchesini, et al, Applied Physics Letters 110 (6), 063101 (2017)

A general framework for denoising phaseless diffraction measurements, Huibin Chang, Stefano Marchesini, arXiv preprint arXiv:1611.01417, 2016

Denoising Poisson Phaseless Measurements via Orthogonal Dictionary Learning, Huibin Chang, Stefano Marchesini, arXiv:1612.08656, 2016

Robust X-ray Phase Ptycho-Tomography, Venkatakrishnan, V., et. al., IEEE Signal Processing Letters, 10.1109/LSP.2016.2562504 (2016)

Measuring spectroscopy and magnetism of extracted and intracellular magnetosomes using soft X-ray ptychography, X. Ahu, et. al., PNAS, 2016, 113(51), E8219-E8227.

Nanosurveyor: a framework for real-time data processing, B.J. Daurer, H. Krishnan, T. Perciano, F. R.N.C. Maia, D.A. Shapiro, J.A. Sethian, Stefano Marchesini, Advanced Structural and Chemical Imaging 20173:7,

SHARP: a distributed GPU-based ptychographic solver, S. Marchesini, H. Krishnan, B. J. Daurer, D. A. Shapiro, T. Perciano, J. A. Sethian and F. R. N. C. Maia, J. Appl. Cryst. (2016). 49,

ALS User Meeting Highlights Accomplishments and Challenges, K Troutman, E Arenholz, S Marchesini, D Shapiro, C Zhu, A Lanzara, Synchrotron Radiation News 29 (1), 7-11, 2016

Imaging nanoscale magnetic and structural correlations in thin SmCo5 films using soft x-ray ptychography, P. Fischer, X. Shi, V. Neu, D. Elefant, J.C.T. Lee, D.A. Shapiro, M. Farmand (ALS LBNL Berkeley CA 94720), W. Shiu, S. Marchesini, S. Roy, S.D. Kevan X. Shi, Applied Physics Letters, 2016

Nanoscale Chemical Imaging of an Individual Catalyst Particle with Ptychography, Anna M. Wise, Johanna Nelson Weker, Sam Kalirai, Maryam Farmand, David A. Shapiro, Florian Meirer, and Bert M. Weckhuysen, ACS Catalysis, 2016.

Soft Xfi...ray Ptychographic Imaging and Morphological Quantification of Calcium Silicate Hydrates

(CfiSfiH), Sungchul Bae, Rae Taylor, David Shapiro, Peter Denes, John Joseph, Journal of the American Ceramic Society 98 (12), 4090-4095

Effect of Particle Size, Electronic Connectivity, and Incoherent Nanoscale Domains on the Sequence of Lithiation in LiFePO4 Porous Electrodes, Yiyang Li, Sophie Meyer, Jongwoo Lim, Sang Chul Lee, William E Gent, Stefano Marchesini, Harinarayan Krishnan, Tolek Tyliszczak, David Shapiro, Arthur L David Kilcoyne, William C Chueh, Advanced Materials 27 (42), 6591-6597

Magnetic studies of magnetotactic bacteria by soft X-ray STXM and ptychography, X. H. Zhu, T. Tyliszczak, H.-W. Shiu, D. Shapiro, D. A. Bazylinski, U. Lins and A. P. Hitchcock, AIP Conf. Series, AIP 1696, 020002, 2016

Dependence on crystal size of the nanoscale chemical phase distribution and fracture in LixFePO4, Y.-S. Yu et al, Nano Letters, 15 (7), pp 4282-4288 (2015)

Alternating Projection, Ptychographic Imaging and Phase Synchronization, Stefano Marchesini, Yu-Chao Tu, Hau-tieng Wu, Applied and Computational Harmonic Analysis, 41 (2016), pp. 815-851, technical report LBNL-6583E (2014)

Chemical composition mapping with nanometre resolution by soft X-ray microscopy, David A. Shapiro, Young-Sang Yu, Tolek Tyliszczak, Jordi Cabana, Rich Celestre, Weilun Chao, Konstantin Kaznatcheev, A. L. David Kilcoyne, Filipe Maia, Stefano Marchesini, Y. Shirley Meng, Tony Warwick, Lee Lisheng Yang & Howard A. Padmore, Nature Photonics, Sept. 2014.

Rank-1 accelerated illumination recovery in scanning diffractive imaging by transparency estimation, Stefano Marchesini, Hau-tieng Wu, Technical report LBNL-6734E 2014. http://arxiv.org/abs/1408.1922

Efficient algorithms for Ptychographic Phase Retrieval, Jianliang Qian, Chao Yang, A. Schirotzek, F. Maia, and S. Marchesini, Inverse Problems and Applications, Contemporary Mathematics, 615, 261 2014.

Augmented projections for ptychographic imaging, Stefano Marchesini, Andre Schirotzek, Chao Yang, Hau-tieng Wu, Filipe Maia, Inverse Problems 29, 115009 2013.

Alternating Direction Methods for Classical and Ptychographic Phase Retrieval, Zaiwen Wen, Chao Yang, Xin Liu, S. Marchesini, Inverse Problems 28 115010, 2012. http://dx.doi.org/10.1088/0266-5611/28/11/115010

Iterative Algorithms for Ptychographic Phase Retrieval C. Yang, J. Qian, A. Schirotzek, F. Maia, S. Marchesini, 2011. technical report LBNL-4598E

Massively parallel X-ray holography, S. Marchesini, S. Boutet, A. E. Sakdinawat, M. J. Bogan, S. Bajt, A. Barty, H. N. Chapman, M. Frank, S. P. Hau-Riege, A. Szoke, C. Cui, M. R. Howells, D. A. Shapiro, J. C. H. Spence, J. W. Shaevitz, J. Y. Lee, J. Hajdu, M. M. Seibert, Nature Phot. 2, 560 - 563 (2008),

Phase Retrieval and Saddle-Point Optimization, S. Marchesini, J. Opt. Soc. Am. A 24,32890-3296 (2007),

A unified evaluation of iterative projection algorithms for phase retrieval, S. Marchesini, Rev. Sci, Inst. 78, 011301 (2007),

Phase Aberrations in Diffraction Microscopy, S. Marchesini, H. N. Chapman, A. Barty, C. Cui, M. R. Howells, J. C. H. Spence, U. Weierstall, A. M. Minor, IPAP Conf. Series 7 pp.380-382, 2006,

Coherent X-ray Diffractive Imaging; applications and limitations, S. Marchesini, H. N. Chapman, S. P. Hau-Riege, R. A. London, A. Szoke, H. He, M. R. Howells, H. Padmore, R. Rosen, J. C. H. Spence, U. Weierstall, Optics Express 11(19), 2344 (2003),

X-ray fluorescence holography: beyond the diffraction limit, S. Marchesini, C. S. Fadley, PRB 67, 024115 (2003),

X-ray image reconstruction from a diffraction pattern alone, S. Marchesini, H. He, H. N. Chapman, S. P. Hau-Riege, A. Noy, M. R. Howells, U. Weierstall, J.C.H. Spence, PRB 68, 140101(R) (2003), [arXiv:physics/0306174].

X-ray microscopy by phase-retrieval methods at the advanced light source, M.R. Howells, H. Chapman, S. Hau-Riege, H. He, S. Marchesini, J. Spence and U. Weierstall, J. Phys. IV 104 Pr2-557 (2003)

XiCAM, User Interfaces, Workflows, Remote Execution

Xi-cam: A versatile interface for data visualization and analysis, Pandolfi, R., et al, submitted to J. Synchrotron Radiation, Jan., 2018.

On-the-fly data assessment for high throughput X-ray diffraction measurement, Ren, F., Pandolfi, R., Van Campen, D., Hexemer, A., and Mehta, A.: ACS Comb. Sci. 19, 377-385, 2017.

Nanosurveyor: a framework for real-time data processing, B.J. Daurer, H. Krishnan, T. Perciano, F. R.N.C. Maia, D.A. Shapiro, J.A. Sethian, S. Marchesini, arXiv:1609.02831. Advanced Structural and Chemical Imaging 20173:7.

Talks: 2010-2018

X-ray Free-Electron Lasers

Structure determination from experimental multi-particle fluctuation scattering data, Zwart, Petrus H, 5th Ringberg Meeting on Structural Biology with FELs, Max Planck Geselschafft Ringberg Castle, February 2018

Structure determination from experimental multi-particle fluctuation scattering data, Zwart, Petrus H, PETRA-IV planning meeting, Hamburg, DESY, February 2018

Structure determination from experimental multi-particle fluctuation scattering data, Zwart, Petrus H, Netherland Cancer Institute, Amsterdam, February 2018

Fluctuation X-ray Scatteringfi, Zwart, Petrus H, LCLS-II-HE First experiments meeting, Stanford Linear Accelerator Center, October 2017

Fluctuation X-ray scattering at the ALSu, Zwart, Petrus H. fiALS-U: Solving scientific challenges with coherent soft X-raysfi, January 2017.

From Blobology to Biology: How advanced mathematics and algorithms can enable new high-resolution studies of uncrystallized biomolecules at the LCLS-II-HE, Donatelli, Jeffrey, LCLS-II-HE fiFirst Experiments" Meeting: AMO, Biology, and Quantum Materials, SLAC National Accelerator Laboratory, Menlo Park, CA, November 2017.

New Mathematics for Next-Generation X-ray Imaging, Donatelli, Jeffrey, 2017 ASCR Applied Mathematics Principal Investigators Meeting, Rockville, MD, September 2017.

Reconstruction Algorithms for Next-Generation Imaging: Multi-Tiered Iterative Phasing for Fluctuation X-ray Scattering and Single-Particle Diffraction, Donatelli, Jeffrey, AI-at-SLAC Seminar, SLAC National Accelerator Laboratory, Menlo Park, CA, August 2017.

Femtosecond Structural Dynamics of Photoactive Yellow Protein, Pande, Kanupriya, IUCr Congress, Hyderabad, India, August 2017.

New approaches to structure determination from uncrystallized biomolecules, Donatelli, Jeffrey, UWM Colloquium, Milwaukee, WI, April 2017.

Reconstruction of RDV and PR772 from angular correlations via multi-tiered iterative phasing, Donatelli, Jeffrey, Single Particle Initiative Data Analysis Meeting, March 2017.

Analysis of XFEL Scattering Data from Nanocrystals and Biomolecules, Pande, Kanupriya, CRD Postdoc Seminar, LBL, Berkeley, CA, March 2017.

Data analysis challenges for next-generation imaging, Donatelli, Jeffrey, CS Strategy for Data, Berkeley, CA, December 2016.

Fluctuation X-ray Scattering, Zwart, Petrus H, LCLS-II-HE First experiments meeting, Stanford Linear Accelerator Center, SSRL user meeting, October 2016

Fluctuation X-ray scattering analysis of single particle RDV data, Donatelli, Jeffrey, Single Particle Initiative Data Analysis Meeting, February 2016.

Macromolecular Reconstruction from Fluctuation X-ray Scattering and Single-Particle Diffraction, Donatelli, Jeffrey, 2016 Linac Coherent Light Source User Meeting, SLAC National Accelerator Laboratory, Menlo Park, CA, October 2016.

Multi-tiered iterative phasing for fluctuation X-ray scattering and single-particle diffraction, Donatelli, Jeffrey, 12th International Conference on Biology and Synchrotron Radiation, SLAC National Accelerator Laboratory, Menlo Park, CA, August 2016.

Multi-tiered iterative phasing for fluctuation X-ray scattering and single particle imaging, Donatelli, Jeffrey, BioXFEL 3rd International Conference, San Juan, Puerto Rico, January 2016.

New Mathematics for Single and Multiple Particle Analysis from XFEL Data, Donatelli, Jeffrey, Future Electron Microscopy at LBNL Workshop, Berkeley, CA, October 2016.

Reconstruction algorithms for next generation imaging: Multi-tiered iterative phasing for fluctuation X-ray scattering and single-particle diffraction, Donatelli, Jeffrey, The Center for Advanced Mathematics for Energy Research Applications (CAMERA) Seminar, Lawrence Berkeley National Laboratory, Berkeley, CA, May 2016.

Structure determination from fluctuation X-ray scattering and single-particle diffraction via multi-tiered iterative phasing, Donatelli, Jeffrey Biological Physics Seminar, Arizona State University, Tempe, AZ, November 2016.

Fluctuation X-ray Scattering, Zwart, Petrus H, Janelia Crystallography Conference, Janelia Farm / HHMI, October 2015

Fluctuation X-ray Scattering, Zwart, Petrus H, LCLS-II Scientific Opportunities Workshops, February 2015

Macromolecular reconstruction from fluctuation X-ray scattering, Donatelli, Jeffrey, External Computing Sciences Strategic Plan Review, Lawrence Berkeley National Laboratory, Berkeley, CA, September 2015.

Multi-tiered iterative phasing for fluctuation X-ray scattering reconstruction, Donatelli, Jeffrey, 2015 Advanced Light Source User Meeting, Lawrence Berkeley National Laboratory, Berkeley, CA, October 2015.

Algorithms for X-ray nanocrystallography in the presence of the indexing ambiguity, Donatelli, Jeffrey, BES Triennial Ops Review, Lawrence Berkeley National Laboratory, Berkeley, CA, March 2014.

Algorithms for X-ray nanocrystallography in the presence of the indexing ambiguity, Donatelli, Jeffrey, Mathematics and Statistical Methodologies for DOE Data-Centric Science at Scale, Lawrence Berkeley National Laboratory, Berkeley, CA, March 2014.

An algorithmic framework for X-ray nanocrystallographic reconstruction in the presence of the indexing ambiguity, Donatelli, Jeffrey, Applied Mathematics Seminar, UC Berkeley, Berkeley, CA, April 2014.

Fluctuation Scattering, Zwart, Petrus H., Gordon Research Conference: Diffraction Methods in Structural Biology, Lewiston, Maine, July 2014.

Biological Solution Scattering with an FEL: challenges and opportunities, Zwart, Petrus H. Photon Sciences Seminar, SLAC, October 2013.

Compressive phase retrieval for X-ray nanocrystallography, Donatelli, Jeffrey, 2013 DOE CSGF Annual Program Review, Arlington, VA, July 2013.

Orientation recovery in single particle X-ray imaging: A diffusion map approach, Donatelli, Jeffrey, Applied Mathematics Seminar, UC Berkeley, Berkeley, CA, April 2012.

New Light on Disordered Ensembles: Ab Initio Structure Determination of One Particle from Scattering Fluctuations of Many Copies, Marchesini, Advanced Light Source, Berkeley CA, 2011.

Orientation determination for 3D single molecule diffraction imaging, C. Yang, S. Marchesini, SPIE Conference San Diego 2011.

Ab Initio Compressive Phase retrieval, S. Marchesini IUCR conference Osaka, Japan, 2008.

Inverse problems for ultrafast high resolution x-ray imaging, S. Marchesini, SIAM Conference on Imaging Science, San Diego, CA, July 7-9, 2008.

Computational Lenses, S. Marchesini, The International Workshop on Phase Retrieval and Coherent Scattering, Asilomar, California, USA, June 2007.

Electronic Structure

Numerical methods for Solving Coulpled Cluster Equations, Yang, Chao, Oberwolfach Workshop on Mathematics and Quantum Chemistry, March 2018.

Variational formulation for finding Wannier functions with entangled band structure, Lin, L., MaX Conference on the Materials Design Ecosystem at the Exascale: High-Performance and High-Throughput Computing, Trieste, January 2018

DGDFT: A massively parallel electronic structure calculation tool for electronic structure calculations, Yang, Chao, Workshop on Massively Parallel Computational Chemistry, Kobe, Japan, Jan 2017.

Electronic Structure Calculations for Large Systems, Lin, L., Workshop on Density-Functional Theory and Beyond: Accuracy, Efficiency, and Reproducibility in Computational Materials Science, Berlin, August, 2017

Electronic Structure Calculations for Large Systems, Lin, L., Computational Physics at the Petascale and Beyond (invited talk), APS March Meeting, New Orleans, March, 2017

Fast Algorithms for Estimating Optical Absorption Spectrum, Yang, Chao, IMA Workshop on Nanooptics, Minneapolis, Apr, 2017.

Iterative Methods for Solving Coupled Cluster Equations, Yang, Chao, SIAM Conference on Optimization, Vancouver, May, 2017.

Fast algorithm for estimating optical absorption spectrum via linear response TDDFT, Yang, Chao, Workshop on Mathematical and Computational Methods in Quantum Chemistry, Yale, May 2016

Fast algorithms for hybrid functional electronic structure calculations, Lin, L., International Conference on Algorithms and Applications for Excited State Electronic Structure Theories, CSRC, Beijing, August 2016

Fast algorithms for hybrid functional electronic structure calculations, Lin, L., Workshop on Mathematical and Computational Methods in Quantum Chemistry, Yale, May 2016

Fast electronic structure calculation methods for studying low dimensional nanomaterials, Yang, Chao, SIAM Conference on Mathematical Aspects of Materials, Philadelphia, May 2016

Low-rank approximation in G0W0 Calculation, Yang, Chao, Workshop on Mathematical and Numerical Analysis for Electronic Structure Calculations, Roscoff, Jun, 2016.

Recent Advances in Numerical Methods for Electronic Structure Calculations, Yang, Chao, International Conference on Algorithms and Applications for Excited State Electronic Structure Theories, CSRC, Beijing, August 2016.

Electronic Structure Calculations for Large Systems, Lin, L., Upscaling Electronic Structure: Reduced-Scaling and Multi-Scale Methods (invited talk), Psi-k 2015, San Sebastian, September 2015

Electronic Structure Calculations for Large Systems, Lin, L., Minisymposium on Recent Progress in Multiscale Modeling at the Intersection of Ab-initio Methods, Mechanics and Mathematics, 13th U.S. National Congress on Computational Mechanics (USNCCM13), San Diego, July 2015

A posteriori error estimates for discontinuous Galerkin methods using non-polynomial basis function, Lin, L., Workshop on Mathematical and Numerical Methods for Complex Quantum Systems, Chicago, March 2014

A posteriori error estimates for discontinuous Galerkin methods using non-polynomial basis function, Lin, L., Workshop on Numerical Solution of PDE Eigenvalue Problems, Oberwolfach, November 2013

Electronic Structure Calculations for Large Systems, Lin, L., Materials defects: Mathematics, Computation, and Engineering Workshop I: Quantum and Atomistic Modeling of Materials Defects, IPAM, October 2012

Electronic Structure Calculations for Large Systems, Lin, L., Thematic Minisymposia: Quantum modeling in molecular simulation, International Council for Industrial and Applied Mathematics (ICIAM 2011), Vancouver, July 2011

GISAXS/WAXS/SAXS

Strategies for X-ray Analysis Hexemer, Alexander, GISAS Workshop Munich February 2018

Pursuing the critical dimension in the etched patterns using x-ray scattering Freychet, Guillaume, APS March Meeting 2018, Los Angeles CA, March 2018.

Critical-Dimension Grazing Incidence Small Angle X-ray Scattering Freychet, Guillaume, SPIE advanced lithography 2018, San Jose CA, February 2018.

Towards Real-Time Analysis of Morphologies using Scattering Hexemer, Alexander, APS March meeting 2018

Influence of Molecular Structure Hexemer, Alexander, DOW Chemicals, October 2017

Towards real-time analysis of morphologies using x-ray scattering Freychet, Guillaume, EUVL Workshop 2017, Berkeley CA, June 2017.

Strategies for Multi-Modal Analysis Hexemer, Alexander, APS March meeting 2017

Strategies for Multi-Modal Analysis Hexemer, Alexander, UC Irvine seminar 2017

Strategies for Multi-Modal Analysis Hexemer, Alexander, Air Force Research Lab Dayton Ohio seminar 2017

Strategies for X-ray Analysis Hexemer, Alexander, Columbia University November 2017

Strategies for X-ray Analysis Hexemer, Alexander, NYU November 2017

Xi-CAM: Pursuing the critical dimension using x-ray scattering Freychet, Guillaume, ALS User Meeting 2017, Berkeley CA, October 2017.

Addressing the data challenge at the ALS Hexemer, Alexander, Pandaas2 meeting ESRF July 2016

Addressing the data challenge at the ALS Hexemer, Alexander, AMI seminar Switzerland July 2016

An Automated, High-Throughput System for GISAXS and GIWAXS measurements of thin films Hexemer, Alexander, APS March meeting 2016

X-ray Studies of Nano Composites Hexemer, Alexander, APS March meeting 2016

Addressing the data challenge in Small Angle Scattering Hexemer, Alexander, SOLEI France 2015

Addressing the data challenge in Small Angle Scattering Hexemer, Alexander, MRS meeting 2015

Addressing the data challenge in Small Angle Scatter-

ing Hexemer, Alexander, Plenary Talk Small Angle Scattering Meeting September 2015

Addressing the data challenge in Small Angle Scattering Hexemer, Alexander, BACATECH Meeting September 2015

Addressing the data challenge in Small Angle Scattering Hexemer, Alexander, NSLS II seminar November 2015

Addressing the data challenge in Small Angle Scattering Hexemer, Alexander, WSU seminar 2015

DOE Date Demos and SPOT Hexemer, Alexander, OLCF User Meeting, 2015

Fast Analysis of Time-Resolved Scattering Data Hexemer, Alexander, APS March meeting 2015

High Performance Toolkit for Photon Science Hexemer, Alexander, Oak Ridge National Lab, 2015.

High Performance Toolkit for Photon Science Hexemer, Alexander, canSAS Meeting Kyoto, 2015.

High Performance Toolkit for Photon Science Hexemer, Alexander, Kyoto Institute of Technology, 2015.

High Performance Toolkit for Photon Science Hexemer, Alexander, ISPAC Houston, 2015.

SAXS and WAXS of Soft and Functional Materials hexemer, Alexander, Shanghai Synchrotron Seminar, October 2015

Slot-die printing at the Synchrotron Hexemer, Alexander, NIST seminar, May 2015

Towards Automated Analysis of X-ray Scattering Data Kumar, Dinesh, CSCS Swiss National Supercomputing Center, November 2015

Towards Automated Analysis of X-ray Scattering Data Kumar, Dinesh, Adolphe Merkle Institute, October 2015

Automation of Data Calibration for SAXS/WAXS Scattering Experiments Kumar, Dinesh, 2014 Advanced Light Source User Meeting, October 2014.

Beyond Petascale with the HipGISAXS Software Suite Hexemer, Alexander , APS March Meeting 2014

Beyond Petascale with the HipGISAXS Software Suite Hexemer, Alexander , SC14, 2014

High Perfromance GISAXS Hexemer, Alexander, ACA meeting 2014

Mathematics for grazing incidence small angle X-ray scattering: Accurate form factor computation and automatic peak detection Donatelli, Jeffrey, 2014 Advanced Light Source user Meeting, October 2014.

HipGISAXS: A Massively Parallel Code for GISAXS Simulation Chourou, Slim, APS March Meeting 2013

High performance GISAXS Hexemer, Alexander, GISAXS 2013 Hamburg, 2013

GISAXS simulation and analysis on GPU clusters Chourou, Slim, APS March Meeting 2012

Tomography

Energy Materials by integrating MicroCT with microscopy, spectroscopy, and scattering, Parkinson DY, American Chemical Society, Symposium on Multimodal Characterization of Energy Materials, Washington, DC, August 2017

A survey of available algorithms and software for synchrotron microCT, Pelt, D.M., CAMERA Workshop: Algorithms and Software for Tomographic Reconstruction for Beamlines, November 2017

Efficiently parallelizable approximations to regularized iterative reconstruction algorithms, Pelt, D.M., CAMERA Workshop: Algorithms for Tomographic Reconstruction: State-of-the-Art and Future Goals, November 2016

Tomography Software at LBNL, Parkinson, DY, Algorithms for Tomographic Reconstruction, Berkeley, CA, Nov. 9-11, 2016.

Optimizing tomographic reconstruction for specific analysis tasks, Pelt, D.M., 2016 Advanced Light Source User Meeting, October 2016.

Case Studies in Multi-Modal Imaging, Parkinson DY, Multi-modal Data Analysis Workshop and Hackathon, Argonne National Laboratory, April 4-8, 2016

3D Imaging of Energy Materials, Parkinson DY, The 1st Workshop on Synchrotron Radiation Research and Energy Science between FUNSOM and ALS, Soochow University, Suzhou, China. October 28-31, 2015,

Time-resolved High Temperature Tomography, Parkinson DY, XRM2014, 12th International Conference on X-ray Microscopy, Melbourne, Australia, October 27-31, 2014.

Quantification of microstructures from microtomography images, Parkinson DY, Machine Learning for Science, November 4, 2013.

Multi-scale x-ray tomography at the ALS, Parkinson DY, ALS/CXRO Seminar, 24 August 2011

Automating image registration, reconstruction, and *segmentation at the ALS tomography beamlines*, Parkinson DY, Stanford Synchrotron Radiation Lightsource Users Meeting, 20 October 2010

Image processing for synchrotron-based hard and soft x-ray tomography, Parkinson DY, Xradia Seminar, 1 December 2010

Image Analysis

Searching images: characterization, retrieval and ranking for pictures across domains, D. Ushizima, Expanding Your Horizons Technical Career Workshops for Young Women (EYH - Sonoma County Chapter): motivating young women in science + mathematics, Sonoma State University, April 2018.

Computer-Aided Design and 3D Printing Workshop, D. Ushizima, Black Girls Code: Bay Area Chapter, San Francisco CA, April 2018.

Scientific Image Analysis with Convolutional Neural Networks, D. Ushizima, CoDA, Santa Fe, March 2-4, 2018.

Machine learning for image across domains, D. Ushizima, Spring 2018 Internships Brown Bag Series, Berkeley Lab, March 2018.

Machine Learning for Transformative Scientific Discovery, D. Ushizima, Silicon Valley Community Foundation Visit, Berkeley Lab, February 2018.

Image across Domains, Algorithms, Experiments and Learning: a DOE ECRP in pattern recognition, D. Ushizima, Early Career Enrichment Program, Berkeley Lab, February 2018.

Deep learning for billion-pixel digital pathology analysis: application in mapping Tau protein in the human brain, M. Alegro, D. Ushizima, Deep Learning in Biomedicine. UCSF, San Francisco, February 2018.

Predictive brain imaging, L. Grinberg, D. Ushizima, DOE officials visit UCSF, San Francisco CA, January 2018.

Mathematics in Pattern Recognition for Scientific Investigations, T. Perciano, DOE Scientific Machine Learning Workshop, January 2018.

Data Science in practice: dealing with image across domains using machine learning, D.Ushizima, Unified Meeting of Computer Scientists (ENUCOMP), Parnaiba PI, Brazil, November 2017.

Data Science in practice: dealing with image across domains using machine learning, D.Ushizima, Unifesp Computer Science Seminars, Federal University of Sao Paulo, Sao Paulo, Brazil, November 2017.

Science impact, visibility and networking at LBNL, D. Ushizima, CRD Training Workshop, Berkeley Lab, November 2017.

Computer vision and deep learning for experimental observational images, D. Ushizima, Workshop on Xi-CAM and other New Software for Synchrotron Users, from the ALS, CAMERA, and Collaborators, ALS Annual User Meeting, Berkeley Lab October 2017.

Science, Technology & Engineering womenfis career within the UC system and new resources, D. Ushizima and R. Chakraborty, Women in Science and Technology Council (WSEC) Meeting, October 2017.

Data Science for Image across Domains, Experiments, Algorithms and Learning, D. Ushizima, Data Science at Scale School, Los Alamos National Laboratory, Aug 2017.

Quantitative microscopy applied to diverse specimens: materials and cells, Biotechnology Graduate Seminars, Federal University of Ouro Preto, Brazil June 2017.

High Throughput Reverse Image Search with pyCBIR: Quantification, Search, Retrieval and Ranking for Multi-modal Imaging, D. Ushizima, Workshop in Multi-dimensional and Multi-modal X-ray Imaging and Analysis, Making and Measuring in 4-Dimensions, NSLS-II and CFN Userfis Meeting, Brookhaven National Laboratory, May 2017.

Building the analytical instrumentation for microscopy image analysis, D. Ushizima, 4D Advanced Microscopy of Brain Circuits Course, Zeiss Microscopy Center, UC Berkeley April 2017.

Searching images with images: characterization, retrieval and ranking, D. Ushizima, Microsoft Research Seattle March 2017.

Image Segmentation Across Domains using Parallel Markov Random Field Technique, ImageXD, T. Perciano, March 2017

Modeling Energy Materials by integrating MicroCT with microscopy, spectroscopy, and scattering, Parkinson DY, American Chemical Society, Symposium on Multimodal Characterization of Energy Materials, Washington, DC, August 2017

Using convnets to find relevant cells, D. Ushizima, California Cognitive Science Conference, UC Berkeley, May 2017.

Future Directions & Areas of Joint Interest in Data Science, D. Ushizima, Computational Health Science

Symposium, Institute for Computational Health Sciences, UC San Francisco, April 2017.

Images Across Domains, Experiments, Algorithms and Learning, D. Ushizima, DOE ASCR Computer Science Principal Investigators' (PI) Meeting: Resilience, SSIO, Design Space and SDMAV, Bethesda MD March 2017.

Women in STEM during the digital revolution, D. Ushizima, TechWomen Program, Mount Kenya University, Kenya February 2017.

Breaking the glass ceiling, D. Ushizima, TechWomen Program and Safaricomm, Tribe Hotel, Nairobi, Kenya, February 2017.

Identifying visual cues to enable searching of 3D images, D. Ushizima, ALS Annual Usersfi Meeting, Berkeley Lab, Oct 2016.

Scaling Analytics for Scientific Images from Experimental Instruments, D. Ushizima, IEEE Applied Imagery Pattern Recognition, Washington DC, Oct 2016.

TechWomen Program Debriefing, D. Ushizima, TechWomen Panel at the U.S. Dept of State, Washington DC, October 2016.

3D image analysis and impact on Alzheimers disease, D. Ushizima, Moore-Sloan Foundation Data Science Environments Workshop, NY October 2016.

Searching for images across domains with CBIR, D. Ushizima, CAMERA Seminars, Berkeley Lab, September 2016.

Searching for images across domains with convolutional neural networks, D. Ushizima, Computational Sciences and Engineering Conference - the integration of experiment, big data, and modeling and simulation into instruments for discoveries in science and engineering, Gatlinburg, TN, Aug 2016.

From Face Detection to the Faces of Scientific Images, D. Ushizima, ImageXD Inaugural Workshop. UC Berkeley June 2016.

Robot Expo - building with NXT, D. Ushizima, Black Girls Code: Bay Area Chapter, UC Berkeley, Dec 2016.

Searchable datasets in Python: images across domains, experiments, algorithms and learning, D. Ushizima, PyData San Francisco October 2016.

DOE Early Career Program D. Ushizima, Panel with Director of the Office of Science Department of Energy Cherry Murray at Berkeley Lab Aug 2016.

Accelerating discovery from image-based experiments D. Ushizima, NCEM User Meeting Symposium, Berkeley Lab Aug 2016.

An overview of my research career and its challenges, T. Perciano. BLUFF Student, BLUR, CCI, SULI and VFP Student: Brown Bag Meeting, LBNL, June 2016

Gaining insight into image-based data collected from experimental science projects, T. Perciano, Computer Science Seminar, LBNL, June 2016

Picture is worth 1,000 words, but how to extract information from them? D. Ushizima, SULI, CCI and BLUR: Brown Bag Meeting March 2016.

Unveiling information from scientific images D. Ushizima, Pub-tech, Stanford CA, March 2016.

Mathematical tools for analysis of high resolution, time-resolved 3D X-ray images T. Perciano, Conference on Data Analysis 2016. March 2016.

Recognizing Patterns from Experimental Data D. Ushizima, Driving Discovery: Integration of Multi-Modal Imaging and Data Analysis, TMS Annual Meeting & Exhibition, Feb 2016

Investigating recognition methods for a new National Library of Medicine Image Dataset, D. Ushizima, Advances in Visual Computing: 11th Int. Symp, ISVC 2015, Las Vegas, NV, USA, Dec 14-16, 2015.

Fast detection of material deformation through structural dissimilarity T. Perciano, IEEE International Conference on Big Data, November 2015.

Real-Time data pipeline and analysis using SPOT and HipGISAXS Hexemer, Alexander, GISAS Nice 2015.

Scaling Analytics for Image-based Experimental Data D. Ushizima, 3D Image Visualization and Analysis Tutorial, 2015 ALS User Meeting, October 2015.

Multi Platform image processing tools for micro-CT T. Perciano, 3D Image Visualization and Analysis Tutorial at the 2015 ALS User Meeting, October 2015.

CRIC Hackathon for Cell Recognition and Materials Analyses CRIC Conference, Fortaleza CE, Brazil, July 2015.

Image Processing and Visualization using R, T. Perciano, Postdoc Seminars Series at LBL, June 2015

Picture is worth 1,000 words, but how to extract information from them? D. Ushizima, CRD Summer Students Brown Bag, Berkeley Lab Mar 2015.

Scalability of Scientific Image Analysis, D. Ushizima, Informs Annual Meeting: Bringing Data and Decisions, San Francisco, CA, Nov 2014.

Structure Recognition from High Resolution Images of Ceramic Composites, D. Ushizima, T. Perciano, 2014 IEEE International Conference on Big Data, October 2014.

Visualization and analysis of high throughput experiments D. Ushizima, I Imaging Initiative Workshop: Tomography and Ptychography, Argonne National Laboratory, Chicago IL, September 2014.

Image Processing and Analysis Challenges: An Overview of Different Applications, T. Perciano, Data Analytics and Visualization Group Seminar Series, September 2014

Teaching machines and machine learning D. Ushizima, NERSC Brown Bag, July 2014.

Image analysis and statistics: an introduction using R and RIPA T. Perciano, The International R Users Conference, June 2014.

Delving into R Analytics for Image Analysis T. Perciano, Workshop on Algorithms for Modern Massive Data Sets, June 2014.

Dynamic Tomography at the Advanced Light Source, Parkinson DY APS user meeting, 4D Imaging Applications in Dynamic Studies Workshop, May 14, 2014

Mathematics of Computer Vision D. Ushizima. Outreach Program Bay Area Schools, HRS Oakland CA, March 2014.

Segmentation of subcellular compartments combining superpixel representation with Voronoi diagrams - awarded 1st place in code competition, D. Ushizima, IEEE International Symposium on Biomedical Imaging, Beijing, China April 2014.

How images shape your life, and shapes from images D. Ushizima, LBNL Workforce Development and Education Seminar, Berkeley, February 2014.

Analysis and visualization of image-based experiments D.Ushizima, Current Challenges in Computing (C3) Conference, Napa CA, August 2013.

Challenges and New Developments in Imaging with Large Data Sets, D. Ushizima, Joint Statistical Meeting (JSM2013), Montreal, Aug 2013.

Data analysis and management D. Ushizima, LBNL Brain Workshop, Berkeley Lab, July 2013.

Image analysis of experimental data D. Ushizima, Workshop of the Program on Statistical and Computational Methodology for Massive Datasets, Statistical and Applied Mathematical Sciences Institute (SAMSI), Research Triangle, MD, 2013.

Characterization of MRI brain scans associated to Alzheimer's disease through texture analysis D. Ushizima, IEEE International Symposium on Biomedical Imaging, New York NY, April 2013.

science image analysis using quant-CT in ImageJ, D. Ushizima, ImageJ User and Developer Conference, Luxembourg, LX, Oct 2012.

Algorithms for Microstructure Description applied to Microtomography, D. Ushizima, Carbon Cycle 2.0 Symposium, LBNL, Fev. 10. 2012.

I/O Workload Analysis with Server-side Data Collection, D. Ushizima, SuperComputing 2011 (SC11), Seattle, WA, Nov. 13 2011.

Statistical segmentation and porosity quantification of 3D x-ray microtomography, D.Ushizima, SPIE Optics and Photonics: XXXIV Applications of Digital Image Processing, Vol.8135-1, pp.1-14, San Diego, CA, Aug 2011.

Tracking cell dynamics from time-lapse laser scanning microscopy imagery D. Ushizima, Physical Sciences - Oncology Centers Annual Site Visit, Berkeley, CA, Aug 2011.

Computed tomography analysis in multiscale control of geologic CO2 D. Ushizima, Free University of Berlin, Germany: Institute of Computer Science and Konrad Zuse Institute of Information Technology, Berlin, June 2011.

Statistical regions in porous media and 3D structure characterization, D. Ushizima, Bay Area Vision Meeting, Google, Apr 2011.

Analysis and visualization for multiscale control of geologic CO2 D. Ushizima, Scidac Conference, Denver CO, July 2011.

Minimizing I/O contention at NERSC using data analysis, D. Ushizima, Workshop on Algorithms for Modern Massive Data Sets (MMDS'10), Stanford, CA, June 15-18, 2010

Vessel Network Detection Using Contour Evolution and Color Components, D. Ushizima, 32nd Annual International Conference of the IEEE Engineering in Medicine and Biology Society, Buenos Aires, Argentina. Sept 2010.

Retinopathy diagnosis from ocular fundus image analysis, D. Ushizima, Modeling and Analysis of Biomedical Image, SIAM Conference on Imaging Science (IS10), Chicago, Il, April 12-14th, 2010.

Ocular fundus and retinopathy characterization, D. Ushizima, Bay Area Vision Meeting, Feb 5th, Berkeley, CA 2010.

Materials Informatics

Discovery of nanoporous materials for energy applications, Maciej Haranczyk, Pacifichem, 2015, Dec 15-20, Honolulu, HI

Exploring Frontiers of Advanced Porous Materials, Maciej Haranczyk, Denver, CO, March 2015

Discovery of Porous Materials for Energy Applications, Maciej Haranczyk, MOF 2014 meeting, Kobe, Japan, Sept-Oct 2014

Exploring Frontiers of the Material Space of Metal-Organic Frameworks, Telluride, CA, July 2014

Similarity Searching and Screening for Porous Materials, Sheffield Cheminformatics Conference, Sheffield, UK, July 2013

Exploring frontiers of high surface area MOFs, EUROMAT 2013, Sevilla, Spain, September 2013

Ptychography

A Look into the Future of X-Ray Imaging: When Ptychography Meets GPU Acceleration Stefano Marchesini, Pablo Enfedaque, GPU Technology Conference (GTC), San Jose, CA, March 2018

High Throughput Phase Retrieval Stefano Marchesini, in Phaseless Imaging in Theory and Practice: Realistic Models, Fast Algorithms, and Recovery Guarantees, Institute for Mathematics and Its Applications, University of Minnesota, August 14 - 18, 2017

Fast convergent splitting algorithms for (blind) phase retrieval with/without sparse prior Huibin Chang, LBNL, Berkeley, June 2017

X ray Scattering and Phase Retrieval Stefano Marchesini , Optical Imaging and Inverse Problems, Institute for Mathematics and Its Applications, University of Minnesota, February 13 - 17, 2017

Lens design for X-ray imaging, Huibin Chang, Stefano Marchesini, Anne Sakdinawat, (SSRL/SLAC), Joint Mathematics Meeting Special Session on the Mathematics of Signal Processing, Jan. 7th, 2017

Streaming Ptychography,, Workshop on Control Systems for Next Generation Experiment Control at X-Ray Light Sources,S. Marchesini, Lawrence Berkeley National Laboratory, September 12-14, 2016

Nanoscale coherent X-ray imaging,, S. Marchesini, Los Alamos National Laboratory, New Mexico, May 23-26, 2016

Ptychography in real time,, S. Marchesini, SIAM conference on Imaging Science (Albuquerque, New Mexico, May 23-26), 2016

High throughput Coherent X-ray imaging, S. Marchesini, Coherence 2016, SAINT MALO France, June 7-10 2016

Nanoscale coherent X-ray imaging, S. Marchesini, Stanford Pulse Institute, December, 2015 https://ultrafast.stanford.edu/events/pulse-special-seminar-nanoscale-coherent-x-ray-imaging

CAMERA-SHARP Software tools for real-time ptychographic imaging, T. Perciano, Ultra-high Resolution X-ray Imaging for the Energy Sciences at the COSMIC Beamline, at the 2015 ALS User Meeting, 2015.

Frame-wise synchronization for blind ptychography, S. Marchesini , Mathematics and Computer Science, Argonne National Lab, Aug 27 2015.

Multi Platform image processing tools for micro-CT, T. Perciano, 3D Image Visualization and Analysis Tutorial at the 2015 ALS User Meeting, 2015.

Soft x-ray ptychography of nanomaterials at the Advanced Light Source, David Shapiro (contributed), Synchrotron Radiation Instrumentation 2015

High-dimensional imaging with nanometer resolution using soft x-rays, David Shapiro , Gordon Research Conference on X-ray Science, July 2015

Phase retrieval in high dimensions, S. Marchesini, Colloquium CFEL DESY, Hamburgy 19 Dec 2014

Soft x-ray microscopy with wavelength limited spatial resolution, Davud Shapiro, invited talk, Elettra Workshop on Advances in X-ray imaging, December 2014,

X-ray ptychography for nano-materials research, David Shapiro, The international conference on X-ray microscopy (XRM2014), October 2014, Melbourne

Soft x-ray microscopy with wavelength limited spatial resolution, David Shapiro, Workshop in support of the Australian Center of Excellence in Synchrotron Science, November 2014, Melbourne

Diffractive x-ray imaging, David Shapiro, Workshop on soft x-ray science at diffraction limited synchrotrons, LBNL, Berkeley October 2014,

Sharp workshop, (Fast Scalable Methods for Ptychographic imaging, Soft X ray ptychography, Kernels *and cxi file format, Architecture*, S. Marchesini, D. Shapiro, H. Krishnan F. Maia, Berkeley October 2014.

Detector needs for soft x-ray ptychography, David Shapiro , ALS User Meeting, Better Detectors for the ALS - Today and Tomorrow, invited talk, LBNL October 2014

Pairwise relationships in scanning diffractive imaging, S. Marchesini Mathematical Signal Processing and Phase Retrieval Gttingen, Sept 1-3, 2014.

Soft x-ray microscopy with wavelength limited spatial resolution, Argonne Imaging Initiative workshop, David Shapiro, invited talk, "September 2014

The international workshop on phase retrieval and coherent scattering, (Coherence 2014), David Shapiro contributed talk, September 2014.

Chemical composition mapping at nanometer resolution using soft x-ray microscopy, David Shapiro, Northwestern Univ. September 2014.

Phase retrieval in high dimensions, S. Marchesini, RACIRI summer school, Stockholm area, Sweden. Aug 24-31, 2014

Phase retrieval in high dimensional data space, S. Marchesini HT Wu* (invited) in Advances in Phase retrieval, SIAM imaging conference, Hong Kong, May 12-14 2014,

Phase retrieval in high dimensional coherent diffraction data space, S. Marchesini, Gordon Research Conference, X-ray Science, August 4-9, 2013

Ptychography and high dimensional phase retrieval, S. Marchesini 97th Frontiers in Optics, Orlando, Floorida, Oct 2013

Robust signal recovery in ptychography, S. Marchesini, Ptycho2013, Hohenkammer Castle Bavaria, Germany, May 4-7, 2013

Multi-GPU real-time ptychographic x-ray image reconstruction, F. Maia , Ptycho2013, Hohenkammer Castle Bavaria, Germany, May 4-7, 2013

Coherent imaging, S. Marchesini , APS March Meeting 2013 Baltimore, Maryland. March 18fi?!22, 2013;

Multiscale algorithms for mesoscale diffractive imaging, S. Marchesini, Real and reciprocal space X-ray imaging, The Royal Society at Chicheley Hall, Buckinghamshir UK, Feb 2013

Inverse problems in x-ray science, S. Marchesini, Progress on Statistical Issues in Searches, A Conference Involving Statistical Issues in Astrophysics, Particle Physics and Photon Science, SLAC National Accelerator Laboratory, Menlo Park, June 4 - 6, 2012

Coherent diffractive imaging, S. Marchesini, ESI 2012 Modern Methods of Time-Frequency Analysis II: Phase Retrieval, Monday, October 8. - Friday, October 12. 2012,

Multi-GPU real-time ptychographic x-ray image reconstruction, F. Maia, GTC conference, San Jose, May 2012.

Cuda Accelerated X-Ray Imaging, F. Maia , Manycore and Accelerator-based High performance Scientific Computing workshop, International Center for Computational Science (ICCS) Berkeley, 2011.

Compressive Phase Contrast, Tomography, S. Marchesini, SPIE Conference San Diego 2011.

Massively Parallel Holography, Ptychography and Diffractive imaging, S. Marchesini, Science at the hard X-ray diffraction limit: Diffraction microscopy, holography and ptychography using coherent beams, Cornell Laboratory, Ithaca NY, June 2011.

Coherent Imaging at ALS, S. Marchesini, X-ray microscopy cross cutting review, ALS 2011.

Detector Denoising, S. Marchesini, ALS User's Meeting workshop 2011.

Ptychography at ALS, S. Marchesini, ALS User's Meeting workshop 2011.

The Nanoscale Surveyor, S. Marchesini S. Marchesini , Carbon Cycle 2.0 Seminar, Lawrence Berkeley Lab, Oct 6 2011

Inverse Problems in X-Ray Science, S. Marchesini Neyman Seminar, Statistics, Berkeley, Nov 9. 2011

Inverse Problems in X-Ray Science, S. Marchesini, (4 lectures), Math Dept., Berkeley, 2011

Soft X-ray Ptychography with a fast CCD, S. Marchesini , ALS User meeting workshop 2009.

Ab Initio Compressive Phase retrieval, S. Marchesini IUCR conference Osaka, Japan, 2008.

Inverse problems for ultrafast high resolution x-ray imaging, S. Marchesini, SIAM Conference on Imaging Science, San Diego, CA, July 7-9, 2008.

Computational Lenses, S. Marchesini, The International Workshop on Phase Retrieval and Coherent Scattering, Asilomar, California, USA, June 2007.

Xi-CAM, User Interfaces, Workflows, Remote Execution

CAMERA tomographic reconstruction and analysis capabilities, available within Xi-cam, Pandolfi, RJ, CAMERA Tomography Workshop 2017, Berkeley CA, November 8 2017

Xi-CAM and other new software for synchrotron users, from the ALS, CAMERA, and collaborators, Pandolfi, RJ (organizer), ALS User Meeting 2017, Berkeley CA, October 4 2017

Xi-cam: Platform for Synchrotron Data Reduction, Visualization, and Management, Pandolfi, RJ, Materials Data Infrastructure Integration Workshop, Dayton OH, September 11 2017

Data Management and Analysis at the Advanced Light Source, Parkinson DY, Molecular Foundry User Meeting, Berkeley, August 2017

Xi-cam: Platform for Synchrotron Data Reduction, Visualization, and Management, Pandolfi, RJ, canSAS IX, Berkeley CA, June 6 2017

Xi-cam: Flexible High Throughput Data Processing for GISAXS, Pandolfi, RJ, APS March 2017, New Orleans, March 15 2017

Gathering, linking, organizing, and mining data at the ALS, Parkinson, DY, The Future of Materials Exploration ALS user meeting workshop, Berkeley, CA, October 5, 2016

Challenges of Computing for Light-source Science, Parkinson, DY, CHEP, Computing in High Energy Physics, San Francisco, CA, 11 October 2016

Xi-cam: Addressing the Data Challenge for X-Ray Scattering, Pandolfi, RJ, 2016, ALS User Meeting 2016, Berkeley, October 4, 2016

GISAXS data reduction with Xi-cam, Pandolfi, RJ, GISAS Summer School 2016, Garching, Germany, July 17-22, 2016

HipIES: platform for synchrotron data analysis, Pandolfi, RJ, CCP-SAS, Gaithersburg, MD, 23 May 2016

HipIES: High performance integrated environment for scattering, Pandolfi, RJ, SAS 2105, Berlin, 16 September 2015

Real-Time Data-Intensive Computing, Parkinson DY, 12th International Conference on Synchrotron Radiation Instrumentation, New York City. July 5-10, 2015

Tomography data demo, Parkinson DY, SC14, The International Conference for High Performance Computing, Networking, Storage, and Analysis, Department of Energy Exhibition Area, New Orleans, November 17-20, 2014.

High performance tomography, Parkinson DY, Workshop at ALS User Meeting, fiHigh Performance Algorithms, Software, Workflows, and Visualization for Synchrotronsfi, October 2014

High performance algorithms and data management for tomography at the ALS, Parkinson DY, Big Data in X-ray Microscopy Workshop, XRM 2014, Melbourne, Australia, October 25-26, 2014

End users's perspective on Data Challenges, Parkinson DY, BES Facilties Computing Working Group Technical Meeting, Berkeley, February 20th 2014.

Web interfaces and High-Performance Computing: Solutions to Data Management, Processing, and Analysis Challenges at the Advanced Light Source X-ray Facility, Parkinson DY, IEEE Big Data and Science: Infrastructure and Services Workshop, 6 October 2013,

Performance Tomography, NERSC brown bag talk, Oakland, CA, Aug. 13, 2013

Dealing with data, Parkinson DY, National User Facilities Organization, Berkeley, June 2013

Towards an end-to-end solution for light source data, Parkinson DY, CASIS workshop, Livermore, 22 May 2012

High Performance Tomography, Parkinson DY, International workshop on high-volume experimental data, computational modeling and visualization (Beijing), 18 October 2011

CAMERA

CAMERA: The Center for Advanced Mathematics for Energy Research Applications, Sethian, J.A., Five-way Light Source Directors Meeting, April 2018

CAMERA: The Center for Advanced Mathematics for Energy Research Applications, Sethian, J.A., US Department of Energy, September 2017

CAMERA: The Center for Advanced Mathematics for Energy Research Applications, Sethian, J.A., NanoCenter Directors, December 2016

CAMERA: The Center for Advanced Mathematics for Energy Research Applications, Sethian, J.A., Diamond Light Source, Harwell, UK, September 2016

CAMERA: The Center for Advanced Mathematics for Energy Research Applications, Sethian, J.A., US Department of Energy, June 2016

CAMERA: The Center for Advanced Mathematics for Energy Research Applications, Sethian, J.A., APS, Argonne National Lab, April 2016

CAMERA: The Center for Advanced Mathematics for Energy Research Applications, Sethian, J.A., DOE Secretary Moniz Panel, LBNL, Jan 2016

CAMERA: The Center for Advanced Mathematics for Energy Research Applications, Sethian, J.A., ASCAC, July 2015

CAMERA: The Center for Advanced Mathematics for Energy Research Applications, Sethian, J.A., BESAC, Feb 2015

CAMERA: The Center for Advanced Mathematics for Energy Research Applications, Sethian, J.A., ALS Users Meeting, Oct 2014