

Applied Mathematics For Experimental Science

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Want to do two things:

Provide an overview of CAMERA

Discuss detectors, data, mathematics, and models.





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

Mission: Build the applied mathematics that can accelerate scientific discovery at DOE experimental facilities

Execution: Coordinated team of applied mathematicians, beam scientists, computational chemists, computer scientists, materials scientists, statisticians, image and signal processors, ...

Initial set of partners:



Advanced Light Source



Molecular Foundry



NCEM

Initial Support: LBNL LDRD

(P. Alivasatos, H. Simon, D. DePaolo, R. Falcone, D. Brown, J. Neaton, H.A. Padmore, M.J. Banda, K.A. Yelick)

Now: Joint ASCR-BES Pilot Project



(Steve Lee, P. Lee, B. Harrod, S. Binkley, H. Kung)



Overview of CAMERA

Build the advanced mathematics that can:

Extract information from murky data, and help interpret experimental results Provide on-demand analysis as results are being generated Steer experiment and suggest optimal solutions Decrease turn-around time/save money: More experiments and more users Extend the capabilities of existing and future experimental facilities

To do so, we need to:

Have experimental scientists/applied mathematicians work together Develop common language Build new mathematical models, invent algorithms, build prototype codes Test on "shop floor", iterate until codes are solid and useful

Goal: Deliverables users can use (without becoming mathematicians): Advanced mathematics embedded in useable software tools





CAMERA: Organization



CAMERA: Original/Current Projects

Pytchography (ALS/MATH) Coherent Diffraction with Microscopy







Stars Stars

Automatic Image Analysis (ALS/MATH)





GISAXS (ALS/MATH)

Grazing incidence small angle x-ray scattering

BERKELEY LA



Designer Materials (Molecular Foundry/Math)



(ALS/MATH)

CAMERA: End Goal: Released Software: (camera.lbl.gov)

HipGISAXS: (http://camera.lbl.gov/software/hipgisaxs_software)

Flexible grazing-incidence small-angle X-ray scattering (GISAXS) Distorted wave Born approximation

Speed: graphics processors and multicore processors.

PEXSI (http://camera.lbl.gov/software/pexsi)

Fast method for electronic structure calculation: Kohn-Sham DFT. Can regularly handle systems with 10,000 to 100,000 electrons. Achieves scalability on more than 10,000 processors..

SHARP-CAMERA (http://camera.lbl.gov/software/sharp_camera_download) Multi-GPU Accelerated Ptychography Software . Combines diffraction + microscopy + high performance GPUS Advanced acceleration algorithms for convergence and analysis Freely available, open environment for collaboration/customization

QUANT-CT (http://camera.lbl.gov/software/)

Image enhancement, filtering, segmentation and feature extraction Currently on ALS beamline 8.3.2, multi GPU. Open source: FiJi plugin

Zeo++ (http://camera.lbl.gov/software/zeo/)

Analysis/assembly of crystalline porous materials. Geometry-based analysis of structure/topology of material void space Current users: EFRC Nanoporous Materials Genome Center, EFRC Materials Project, Bosch, SABIC and Samsung.



Outline of Talk

How did this start? History and Motivation

Why mathematics? Math/Data/Computing

What is being delivered? Four models for delivery

Where is it going?

A DOE Resource





Background: LBNL/UCB Mathematics: Long Standing DOE Program: (LBNL+UC Berkeley)



Example: Semiconductor Algorithms: Samsung, Intel, Motorola, Infineon, Synopsis...





Look broadly at mathematical needs of Office of Science facilities, starting with the ALS, Molecular Foundry, NCEM, Joint BioEnergy Institute (JBEI), and future facilities

Question: How can applied mathematics help facilities do More science More efficiently (users, materials, turn-around time...)?



DOE Facilities in 2025: More Data, More Users, More Discovery

Experimental facilities will be transformed by highresolution detectors, advanced mathematical analysis techniques, robotics, software automation, and programmable networks.



Mathematics for accelerating the analysis of experimental data



Computational tools for analysis, data reduction & feature extraction *in situ*, using advanced algorithms and special-purpose hardware.

Post-processing: reconstruction, intercomparison, simulation, visualization.

Mathematics for each can be quite different:

What is the minimum/fastest computational model/algorithm that gives (at least some) useful information?

Can you quickly determine if data is useful, not useful, or in between?

Can you quickly do analysis and steer experiment to more optimal configurations or output?



What is the maximal amount of information you can get out of the data?

Can data be measured, processed, organized and displayed to help understand/suggest further experiment?

Can data be transformed to initialize computational models, and output framed to complement experiment?



Why is this so interesting (and challenging?)

(a) Problems have not yet been "mathematicized".(b) No "equations of motion"

(c) Deep connections between the science and math

To tackle these problems requires new mathematics that bridges across mathematical disciplines.

Fortunately, Applied Mathematics is Undergoing a Profound Transformation

Traditional walls between continuous math, discrete math, analysis, probability and statistics, topology, algebra, geometry **are all breaking down.**





Mathematics and (or versus!) "Big Data"



Mathematics

Mathematics is what changes data into information





Challenges are growing:

More data, more resolution More complexity Less obvious relational linking More noise More false signals

Mathematics is what changes data into information

Going to need mathematics more than ever...



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CAMERA: Center for Applied Mathematics for Energy Research Applications



Goal: Build the applied mathematics that helps transform experimental data



 Key: Leverage
 Spectral clustering
 Maximum likelihood estimators
 Graph theory
 Machine learning
 Mori-Zwanzig theory

 state-of-the-art
 Clique analysis
 PDE-based image segmentation
 Statistical sampling
 Discrete/continuous shape descriptors

 mathematics
 Hamilton-Jacobi solvers
 Voronoi methods
 Representation theory
 Bayesian analysis
 Optimization methods



CAMERA: Personnel Who is working on this?

Advanced Light Source (ALS):

- A. Hexemer (Beam Scientist/GISAXS)
- S. Marchesini (Ptychography)
- D. Parkinson (Beamline Scientist, Hard X-ray tomography)
- D. Shapiro (Beamline scientist)

Molecular Foundry

- D. Britt (Organic and Macromolecular Synthesis)
- J. Neaton (Electronic Structure)
- W. Queen (Inorganic Nanostructures)

National Center for Electron Microscopy (NCEM)

P. Ercius (Scanning transmission electron microscope)

Computational Research Division (CRD)

- M. Haranczyk (Materials Design)
- X. Li (GISAXS/)

- T. Perciano (Image Analysis)
- H. Krishnan (Image Analysis/HPC)
- L. Lin (Electronic Structure)
- R. Martin (Materials Design)
- C. Yang (Electronic Structure)
- D. Ushizima (Image Analysis)

- **CRD Mathematics Department:**
 - J. Donatelli (X-Ray Nanocrystallography)
 - C. Rycroft (Optimal Chemical Design)
- J.A. Sethian (Director)

•Opportunity: Steady stream of new Berkeley faculty/postdocs/grad students







Office of Science

What Does CAMERA Deliver?







"Long-distance Delivery": SPOT-Suite Led by C. Tull, LBNL

Towards an End-to-End Solution for Light Source Data, Analysis, & Simulation

• Combining...

- scalable software systems.
- HPC/HTC/network resources.
- advanced algorithms & analysis.
- advanced simulation.
- realtime feedback.
- Multi-division team: CRD, ALS, Math, CAMERA, ESNet, MSD, & NERSC.
- Extending to include SAXS, µDiff, and Ptychography beamlines.
 Focus on in-situ, time-resolved experiments, new algorithms, data sharing & collaboration.
- SC14 Demos include LCLS, APS, NSLS datasets.

Research into generalizable real time workflows and metadata already yielding valuable insight for photon scientists.









EC Who is using CAMERA's deliverables?

Ptychography:	CXRO/SEMETEC, LLNL/NASA, UI Chicago, UC San Diego, UC Davis, UCB, McMaster, Stanford. ALS, BNL, F. Maia, Uppsala, BYU, multiple workshops, tutorials	
QuantCT:	Advanced Light Source Users, available on "shop floor". Downloadable FiJi Plugin (world-wide user base).	
PEXSI:	Accelerated Kohn-Sham Density Functional Algorithms Embedded in SIESTA (Spanish Initiative for Electronic Simulations with Thousands of Atoms): Next: CP2K	
Zeo++:	Open-source package - <u>www.zeoplusplus.org</u> . Zeo++ : a default tool for two BES Materials Genome Centers (Nanoporous Materials Genome Center (Minnesota) and Center for Functional Electronic Materials (LBNL)) and LBNL EFRC for Gas Separations Roughly 200 registered users world-wide in both academia/industry (e.g. Bosch, Samsung)	
HipGISAXS:	ORNL, ANL, ALS, Molecular Foundry, numerous universities,	









AN OVERVIEW OF SOME OF THE WORK UNDERWAY



(Describe problem, emphasize new mathematics, describe deliverables)





SHARP

(Scalable Heterogeneous Adaptive Robust Ptychography)

Fast scalable methods for ptychographic reconstructions

S. Marchesini, D. Shapiro (Advanced Light Source)H. Krishnan (LBNL Computing Sciences)F. Maia (LBL/Uppsala)H-T Wu (LBNL/Stanford, now Toronto)







CAMERA: Ptychographic Imaging



S. Marchesini, D. Shapiro, H. H. Krishnan (LBL) F. Maia (LBL/Uppsala), H-T. Wu (Stanford))

Fundamental idea: combine:

- High precision scanning microscope with
- High resolution diffraction measurements.
- Replace single detector with 2D CCD array.
- Measure intensity distribution at many scattering angles

Each recorded diffraction pattern:

- contains short-spatial Fourier frequency information
- only intensity is measured: need phase for reconstruction.
- phase retrieval comes from recording multiple diffraction patterns from same region of object.

Pytchography:

- uses a small step size relative to illumination geometry to scan sample.
- diffraction measurements from neighboring regions related through this geometry
- Thus, phase-less information is replaced with a redundant set of measurements.

Lots of ptychographic equipment/codes throughout DOE, universities, world-wide









CAMERA: Ptychography Mathematical and Algorithmic Issues



When does it (not) work?

(no convergence proof yet available for method)

Existing algorithms may have trouble converging on large data sets:

(iterative methods intrinsically operate by interchanging information between nearest neighbor frames (diffraction patterns) at each step, so it might take many iterations for frames far apart to communicate.)

Effects of noise and physical uncertainties:

(how do reconstruction algorithms perform with uncertainties in photon statistics, lens perturbations, illumination positions, incoherent measurements, detector response and discretization, time fluctuations, etc.)

What is the best lens and illumination scheme for arbitrary specimens?

(given a detector, with a limited rate, dynamic range and response function, what is the best scheme to encode and extract more information per detector channel?)







Phase retrieval in high dimensional space



Tackling Efficiency: Challenges with basic alternating projection algorithm:

Poor scaling:

long range interactions among frames decay exponentially with distance.

Poor initial guess:

can significantly delay convergence.

Ultimately, an overdetermined problem in high dimensional space.







How can we speed this up?





Graph Theory/Graph Laplacians



Building a better starting guess:

(1) View every pixel of every frame as a dimension. Each data point lives on a torus (complex plane)



 (3) Construct Graph Laplacian of RN: defined as difference between the degree matrix D and the adjacency matrix A: GL = D - A

(4) The largest eigenvector of the Connection graph provides the most aligned phases encoding the (approximate) data topology.

This provides a strong starting guess.







measurement graph



G=(V,E) V: illuminated pixels E: overlapped windows



Approximate torus with ball

Diffraction data manifold



Released Code: SHARP: Scalable Ptychography Solver



Code: Open source, downloadable package

■release
□prototype □under way/testing

- •Scalable code, (\blacksquare source package, \blacksquare remote interface, \square web interface, \square API).
- \Box real time feedback by reducing latency
- ☑ 80x speedup with algorithms
- 🗷 30x speedup with GPUs
- 🗷 >16x speedup with distributed GPU
- 🗷 Optimal Network fabric design for throughput
- I Optimal lens design for SNR
- ☑ Iterative tomography (□ network/bandwidth optimized)
- ☑ Chemical mapping (robust PCA/SVD)

"**Compute design**" SHARP real time specs:

- 3D torus p2p fabric
- CCD/RDMA streaming
- instrument calibration

Intercalation Battery Research: Mechanisms in Lithium Ion Phosphate ALS BL 5.3.2 (Nat. Phot. /in press)





Partners:

CXRO/SEMETEC, LLNL/NASA, UI Chicago, UC San Diego, UC Davis, UCB, McMaster, Stanford. ALS, BNL, F. Maia, Uppsala, BYU

Software presentations: Ptycho 2013, FIO/LS, SIAM IM14, MSPPR, XRM, Coherence 14 Software tutorials: Coming: SSRL/CAMERA xx/2014, CAMERA/ALS/BNL AUG 2014 CAMERA/ALS/APS Sep 10/14, COHERENCE, XRM , SIAMIM, FIO/LS, RACIR summer school, ALS Users workshop



Toward real-time feedback



Currently

the user interface starts processing at the end of a full scan. (1 minute each)

In the future low Latency (<5 ms) feedback by streaming detector frames on distributed direct memory access fabric.

Real time enables smart self-calibrating, autotuning feedback of the microscope control system.

Two Weeks Ago: Finished a prototype "Real Time" version-code directly off of CCD





Processing: 60x60 (1024^2) frames/minute





QuantCT

Automatic image analysis tools for micro-CT

D. Ushizima, D. Morozov, H. Krishnan, T. Perciano (LBNL Computing Sciences) D. Parkinson (Advanced Light Source)







CAMERA: Quantitative Image Analysis of Micro-CT Samples



Goal: Develop algorithms for 3D/4D quantitative analysis of experiments, addressing challenges posed by noise, artifacts, sheer size, and heterogeneous materials.

Analyze structure: porosity, pathways, interior voids, ...

- Application: High-resolution synchrotron-based X-ray absorption microtomography.
- Suitability of materials and biomineralization processes for carbon sequestration.
- Acquire projection views at equi-spaced angles: produce 2D cross-sections.
- Gray level value of image voxels reflects x-ray attenuation and density.
- Compute pathways through materials:





Imaging Pipeline Requires:

- Filtering: remove noise, sharpen contrasts (bi-lateral and non-linear filters)
- Segmentation to isolate, and extract shapes from images (PDE-VIIM methods)
- Feature detection/analysis (Reeb graphs, topological analysis, channel detection)







QuantCT: Timeline of Mathematics/ Algorithm Development







QuantCT: B. PDE-based Automatic Segmentation and Extraction



 (1) Mumford-Shah functional for image segmentation of two phases (index i indicates separate phases, Find interface G to minimize E)

$$E(G, I_1, I_2) = \check{0}_A (I(x, y) - I_1)^2 d\mathbf{x} + \check{0}_B (I(x, y) - I_2)^2 d\mathbf{x} + M \check{0}_G g(G(s)) ds$$

(2) Becomes PDE transport method using level set methodology:

$$f_t + F |\nabla f| = 0$$
, where $F = [((I - I_1)^2 + ((I - I_2)^2) - M \nabla \cdot (g \nabla f / |\nabla f|)]$

(3) New approach: Extend the Mumford-Shah energy

functional to multi-phase multi-interface

Voronoi Implicit Interface Method (VIIM) $F_i = [((I - I_i)^2 - m\nabla \cdot (g\nabla f/|\nabla f|)]$

(combination implicit embedding plus dual Eikonal Voronoi reconstruction)

(4) Allows simultaneous extraction of multiple structures in 3D.



Calcite precipitation: "pore clogging"







QuantCT: C. Determination of Connectivity and Channel Pathways



Augmented Topological Descriptors: Max Flow Graphs and Persistence Diagrams



Void Space





Reeb graph

Edge capacities





• Reeb graph: Evolution of level sets of function on manifold.

Wide pathways

- Use to detect pathways for particle of size a
- Edge capacities = Intersection area between slices
- Flow between source/sink without exceeding capacities
- Family of graphs: Vary α

Persistence Diagram:

- Track components in superlevel set of distance function
- When component merge: "younger" component merges into "older" component







QuantCT: Results





QuantCT

software for microCT analysis (0.33 images/s)



Pore network through porous material







Automatic detection of 3D fibers and matrix cracking from assembled 2D slices





QuantCT: Workflow





Figure 1: Flow diagram of Quant-CT segmentation workflow: yellow indicates user-interaction event and blue indicates a program action.

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







QuantCT: Delivery Mechanisms

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Training subset: 5



Cancel

OK

Delivery mechanisms:

Current:

- (1) Browser/computer at ALS
- (2) Available as FiJi plugin
- (3) Prototype source downloadable.

Code Specifics:

- Implemented in Java.
- Part of *Fiji* framework.
- Implemented in OpenCL.
- Called from Java code through JOCL.
- Dedicated thread assigned to each OpenCL device to handle multiple accelerators on any given node.
- Each thread requests unprocessed slices up to the maximum allowed



)	3	QuantCT - splitting volumes into VOID and DENSE MATERIA		
er parameter:	s to p	rocess, segment and analyze microCT images:		
Stack folder:	/Volumes/Macintosh HD 2/data/ALS/xray/reconstructed/original/			
utput folder:	/Volumes/Macintosh HD 2/data/ALS/xray/reconstructed/original/seg/			
ename radix:	calcite_f_bot_port_			
ages: paramet	ters to	o subset stack with 484 images		
First slice at:	1	max=484		
ting subset:	10	max=484 <= SUBSET SUGGESTED		

Slab size: 5 images

Algorithm: parameters to filter and segment stack

max = 50

QuantCT

Sigma range:	50	[0,255]
Sigma spatial:	3	-1 for interactive tuning
Minimum area:	200	pixels
Complexity of SRM:	32	[2,64]

- Soolean classification? * Multiclass under construction
- Keep previous settings? ** Use file settings.txt in the specified folder
- Subset stack with cylinder? *** Consider only portion inside the cylinder
- Considerable brightness variation accross slices? **** Normalization applies

Ref. **Ushizima**, Parkinson, Nico, Ajo-Franklin, Macdowell, Kocar, Bethel and Sethian, Statistical segmentation and porosity quantification of 3D X-ray microtomography. Applications of Digital Signal processing XXXIV, Vol. 8135, pp.1-14 (2011).

Fluctuation X-Ray Scattering

Mathematics for structure reconstruction

J. Donatelli, J.A. Sethian (LBNL Computing Sciences) P. Zwart (LBNL Advanced Light Source and Physical Biosciences)







Fluctuation X-Ray Scattering (Brand-new work)

(1) Fluctuation X-Ray Scattering:

Extension of Small- and Wide- angle X-Ray Scattering X-Ray snapshots taken below rotational diffusion times Significantly more experimental information than traditional techniques Powerful technique for modern synchrotrons and free electron lasers (FEL)

(2) Going from real space structure to fluctuation scattering data is straightforward.

- (3) But the reverse "inverse" problem is tough.
- (4) A joint CAMERA collaboration between LBNL Physical Biosciences, ALS, and Computing Sciences has produced a new technique: **"M-TIP**", which exploits multi-tiered iterative phasing and solves this inverse problem.

(5) The new method figures out structure of objects that cannot be crystallized, at a far higher resolution than previously available (to appear: PNAS in few weeks)

(6) Example: Using M-TIP, was able to reconstruct 3D profile of pentameric ligand-gated ion channel (pLGIC), from Protein Data Bank entry 4NPP





CAMERA: Where is this going? Reaching out:

Positive response from the community

BESAC Committee Presentation (June 2014)
Oak Ridge/SNS Joint NSRC Workshop (June 2015)

"Big, Deep, Smart Data Analytics in Materials Imaging"
Brookhaven and NSLS (May 2015)

Invited Seminar Talk

Argonne/APS Joint Workshop (March 2015)

"Frontiers in Data, Modeling, and Simulation
LBNL/Advanced Light Source (Oct. 2014)

"CAMERA Workshop on Real-Time Robust Ptychography"

Many software requests:

Download, use CAMERA codes Requests for CAMERA to house, curate, and host algorithms and software across the light sources

New Joint Projects starting up:

GISAXS and extensions to neutron sources (ORNL/SNS) Ptychography (BNL, ANL) Fluctuation scattering (LCLS)







CAMERA: Take Home Messages

Knowing <u>what to build</u>, <u>how to build it</u>, and <u>how to use it</u> requires close-knit, coordinated teams with many different skills.



With careful attention to mathematics and algorithms, we can build codes and software tools that can transform data into the information that users really want.









