MURI: Managing the Mosaic of microstructure

Surya R. Kalidindi
Georgia Tech

AFOSR-FA9550-12-1-0458
PI: Marc DeGraef (CMU)

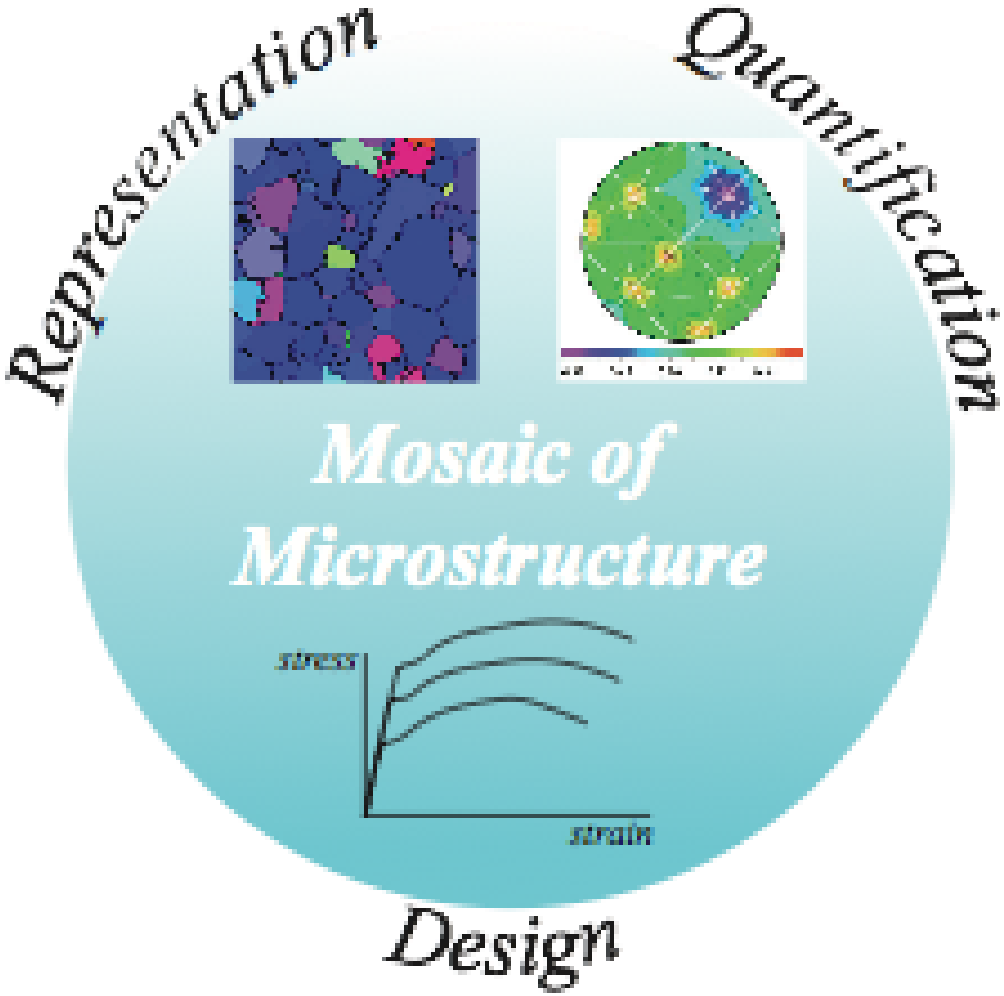
Program Managers
Ali Sayir and Fariba Fahroo

The Call (BAA 11-026)

- *Topic: Managing informational complexity in predictive materials science*
- "This MURI is to establish mathematical approaches for a stochastic and statistical framework for multiscale materials modeling that leads to discovery of new materials."
- "The ultimate aim is to create a platform of new scientific enterprise to successfully resolve issues of complexity, variability across time and length scales, and allow for a dynamic integration and validation of mathematical predictions through new experimental methods that can enable rapid interrogation of structure and properties at different scales."

School	co-PI(s)		#GS/PD
CalTech	Kaushik Bhattacharya		0/1
Minnesota	Richard James		2/0
Northwestern	Peter Voorhees, Alok Choudhary, Ankit Agrawal		2/1
Purdue	Charles Bouman, Mary Comer		4/0
Michigan	Veera Sundararaghavan		2/0
Georgia Tech	Surya R. Kalidindi		1/0.5
Carnegie Mellon	Marc De Graef		2/1
Neetha Khan	Michael Jackson		

The Mosaic of Microstructure



Team Expertise

Microstructure Characterization

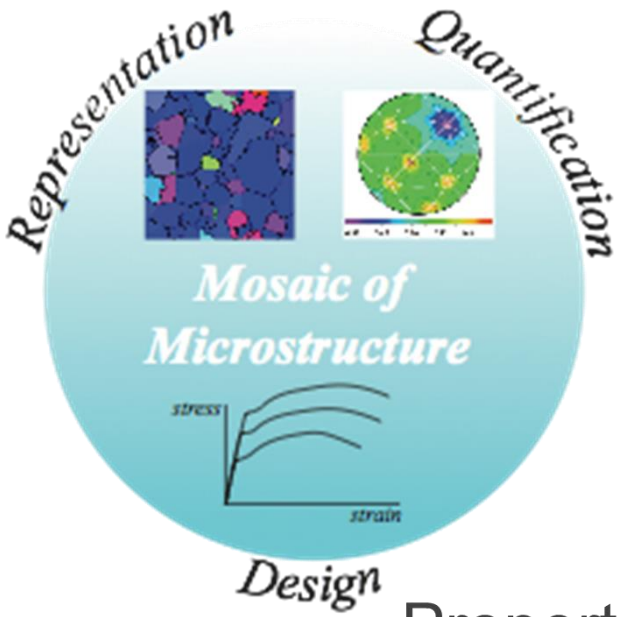
Statistical & Probabilistic Signal Processing

Microstructure Evolution

Microstructure Property Stochastic Models

Mathematical Theory of Microstructure

High Performance Computing



Data Mining

Materials Informatics

Property/Microstructure Modeling

Planned Budget

- CMU is the lead institution; all others are sub-awards from CMU

Period	CMU	CalTech	G. Tech	Michigan	Minnesota	Northwestern	Purdue
Yrs 1-3	978,105	459,926	424,285	444,787	435,000	900,000	780,000
Yrs 4-5	686,501	328,317	282,855	193,446	290,000	600,000	520,000
Total	1,664,606	788,243	707,140	638,233	725,000	1,500,000	1,300,000

Grand Research Challenges

- The main objectives of our research are:
  - *to establish a standardized methodology, grounded in sound mathematics, for acquiring, storing, analyzing, modeling, and querying "beyond 3-D" materials data, taking full account of the potential sparsity of such data as well as the associated uncertainties and variabilities;*
  - *to employ advanced stochastic/probabilistic models that allow not only for the description of the "average" microstructure, but also for the inclusion of rare events (large deviations), and to set up the proper data structures to enable such a stochastic description;*
  - *to employ advanced data mining approaches, constrained by accurate mathematical models and accounting for variability, to instantiate large numbers of digital microstructures to search for an optimal microstructure and its process path, to achieve a desired property combination.*

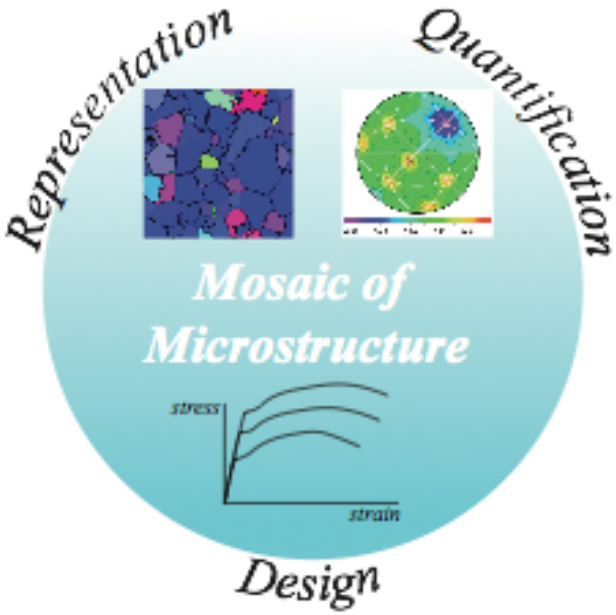
Research Thrust areas

T1: *Representation of structure and time evolution in microstructures*: what can we measure and how can we compactly represent microstructure?

Peter Voorhees

T2: *Mathematical quantification of microstructures for bridging scales*: what information about a micro-structure is relevant for its properties?

Dick James



T3: *Multi-scale materials design using informatics*:
how can we use microstructure information for design?

Surya R. Kalidindi

Project outcomes

- The MURI project will produce *algorithms*, *mathematical models*, and *methodologies or frameworks* for microstructure design and microstructure-property relations modeling.

— *algorithms for:* optimal design of magnetoelastic and energy conversion devices; optimization of multiferroic microstructure; reconstruction and generalized forward projectors for FIBSS, VFET, and time-dependent XCT; reconstruction code capable of detecting/identifying rare events; extraction of accurate interface curvatures from 3D time-dependent data sets; data storage and retrieval, compatible with high-end data mining approaches; optimal sampling of microstructure space; robust importance samples for stochastic modeling of rare events.

— *mathematical models for:* microstructure-property relations in multiferroics; time-dependent tomographic reconstructions; thin-manifold description of microstructures; PGM adapted to materials microstructures and data acquisition;

— *methodologies/frameworks for:* microstructure-sensitive design in multiferroic alloys, Ni-based superalloys and α–β Ti alloys; robust process design of polycrystalline materials for customized performance; experimental validation of process designs.

4D Measurements of Microstructural Evolution

J. Gibbs, A. Mohan[+], A. Shahani, B. Gulsoy, C. Bouman[+], M. De Graef**, X. Xiao*, P. Voorhees

Materials Science and Engineering
Northwestern University

**Materials Science and Engineering
Carnegie Mellon University

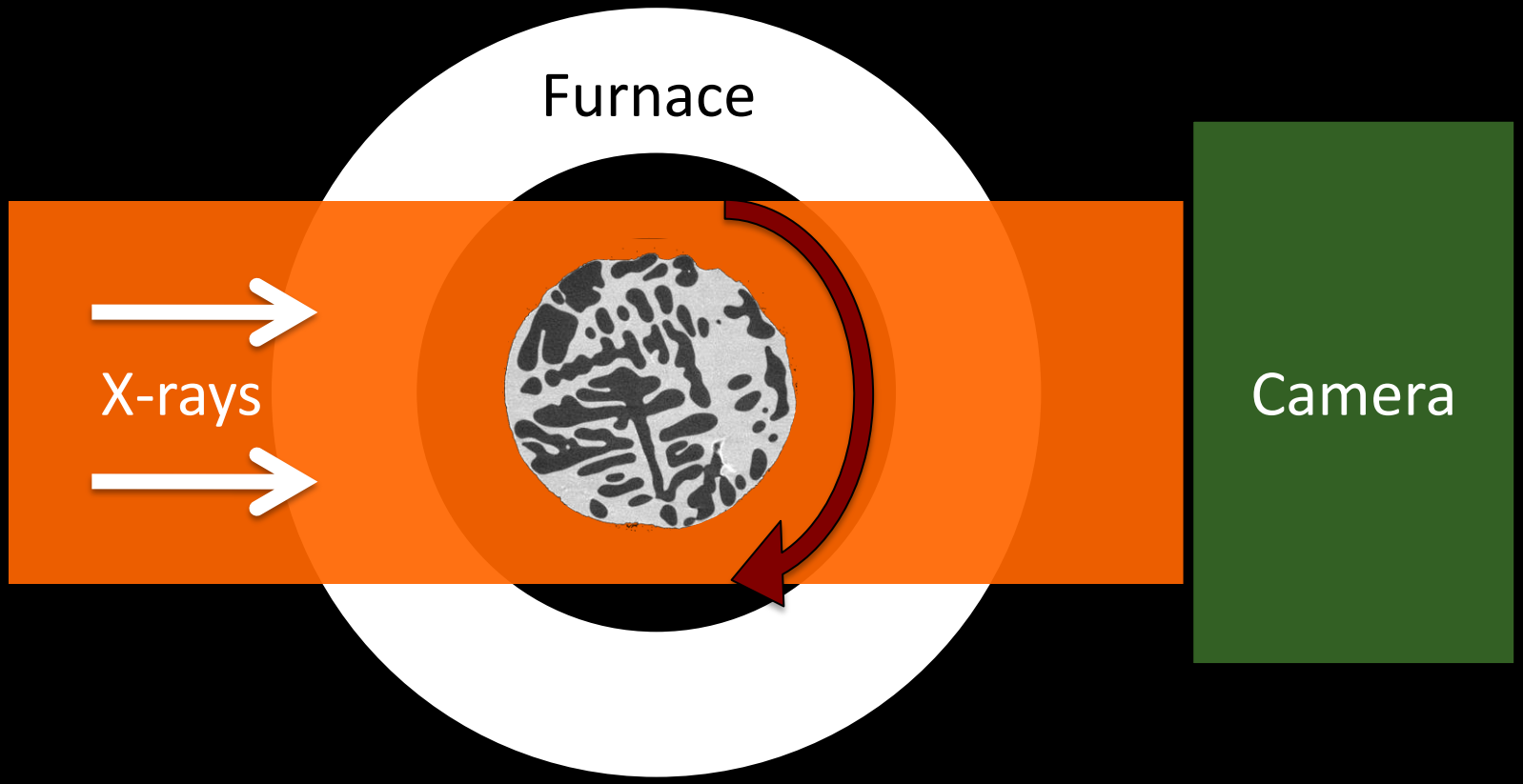
[+]Electrical Engineering and Computer Science
Purdue University

* Advanced Photon Source,
Argonne National Laboratory

AFOSR MURI Program

Insitu X-Ray tomography: 4D

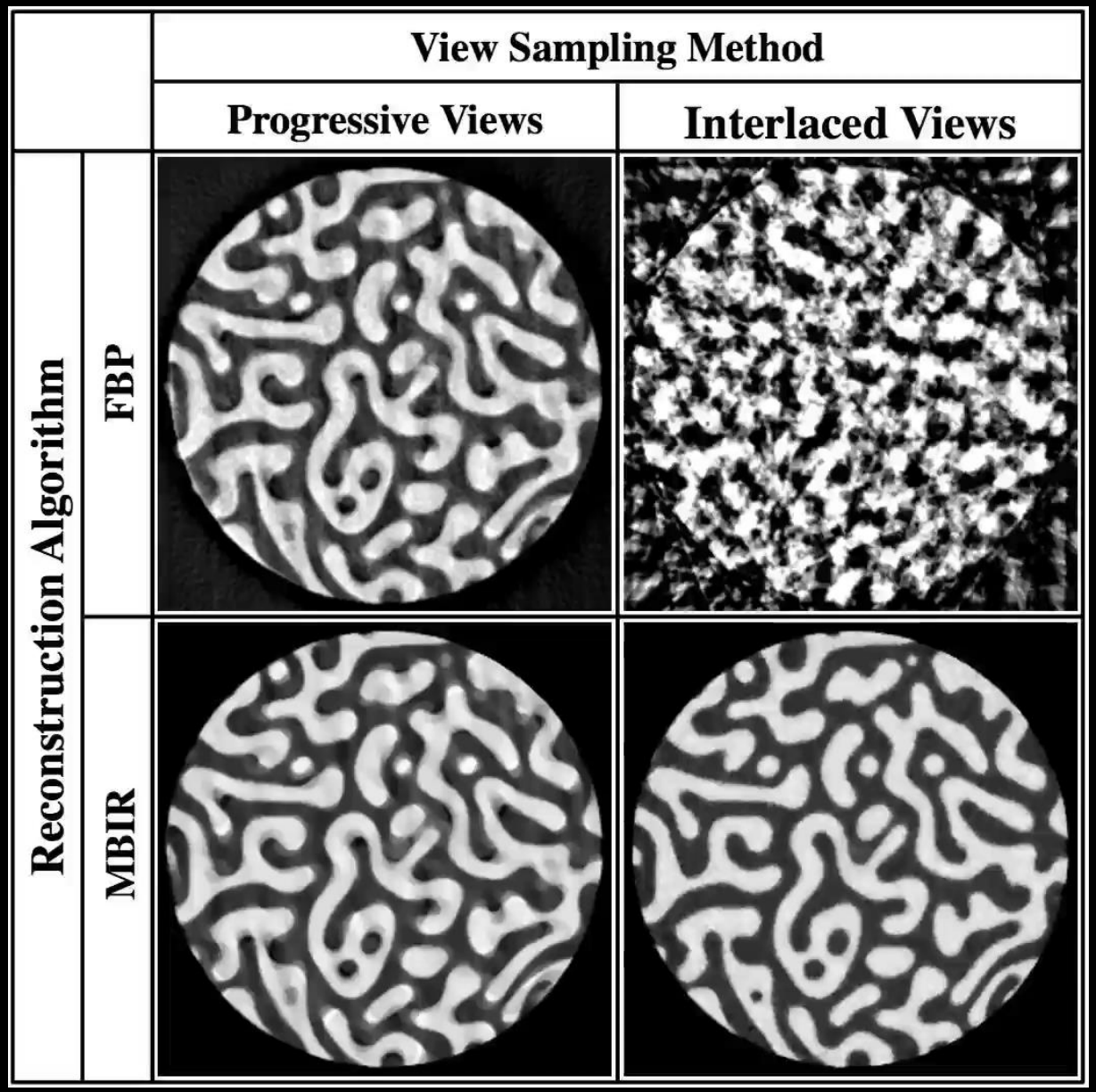
X-ray computed tomography



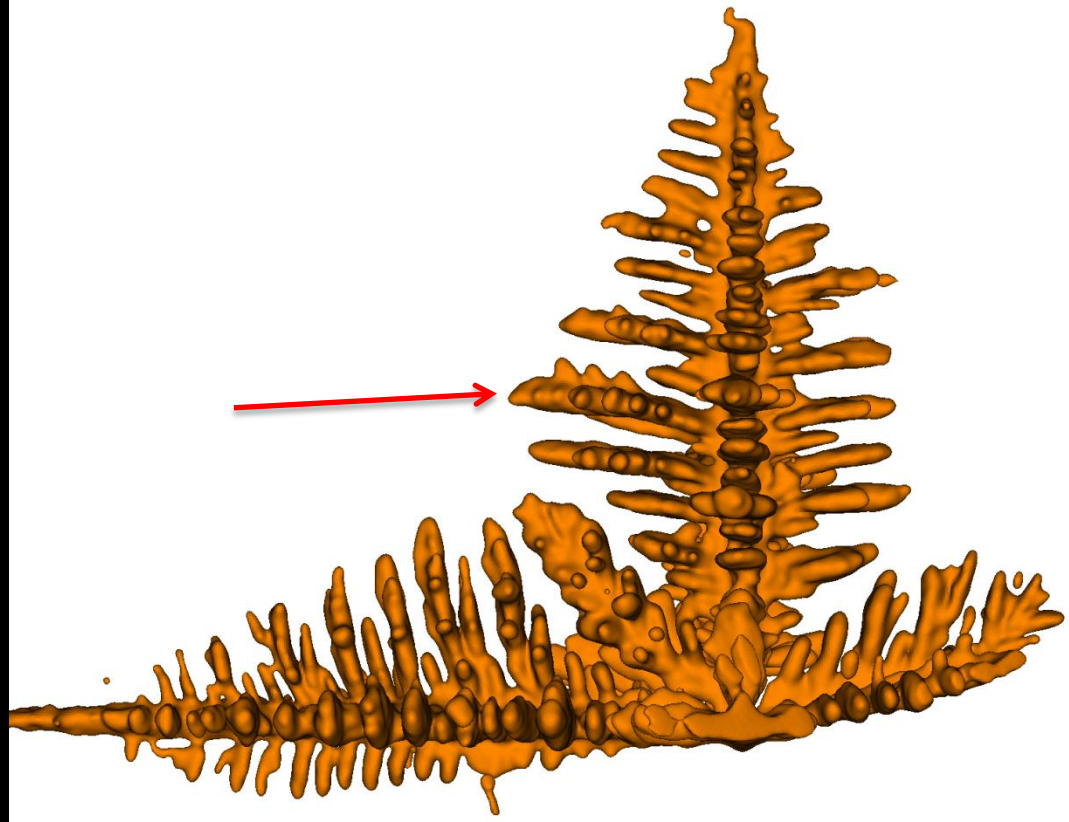
TIMBIR

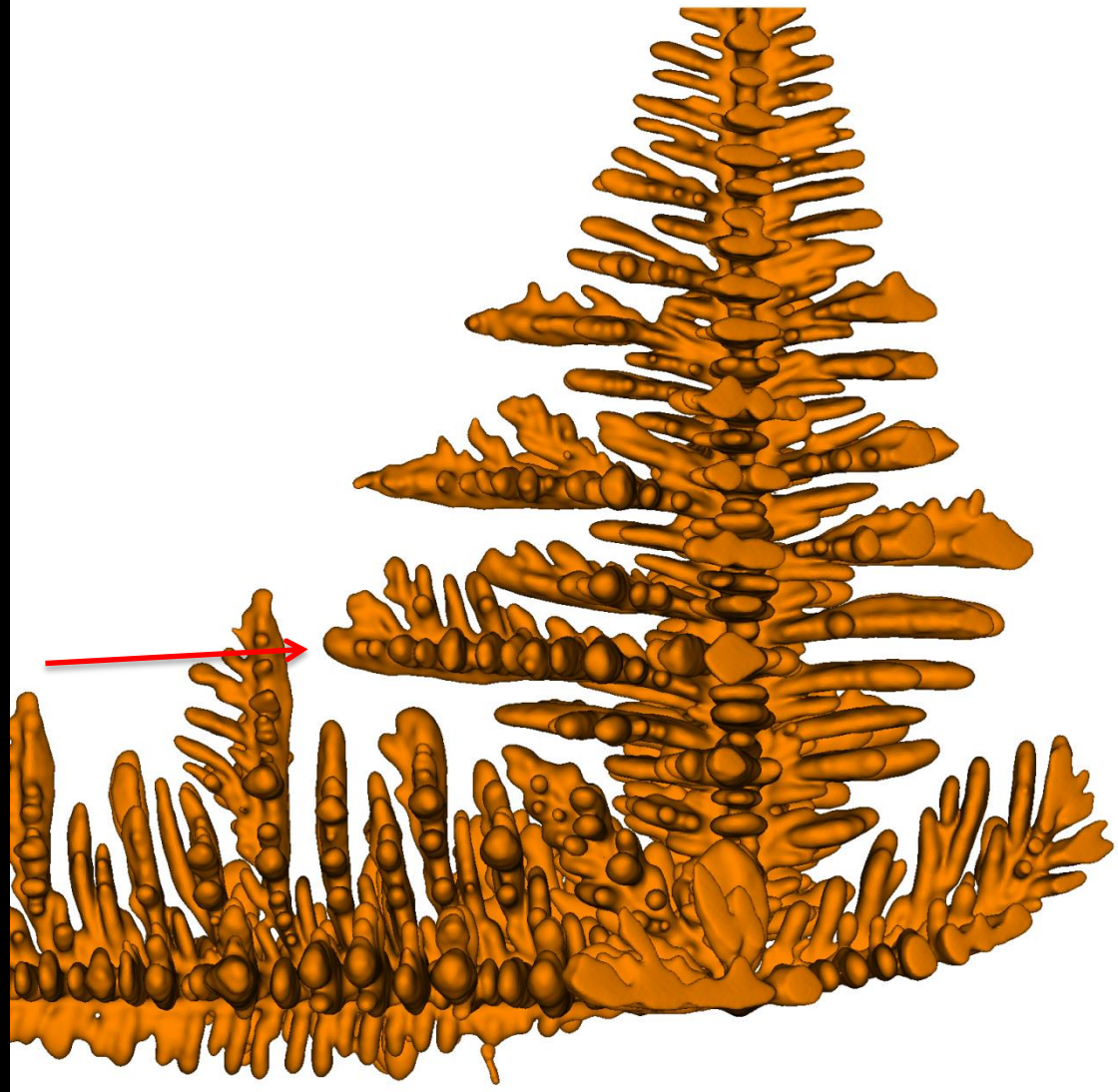
Cahn-Hilliard phantom, ground truth

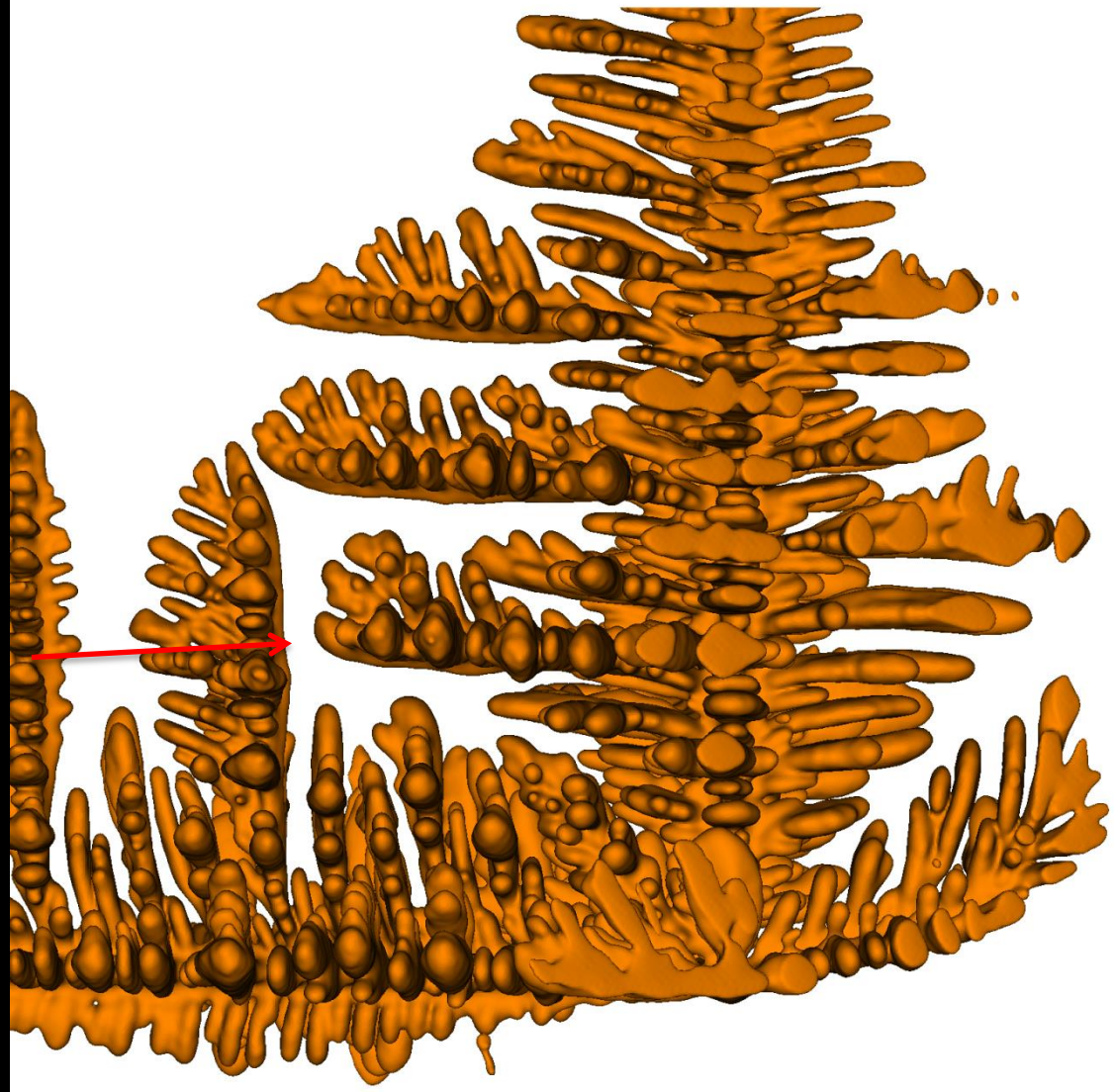
Method	Root Mean Squared Error (mm^{-1})
FBP/progressive	0.258
FBP/interlaced	0.5867
MBIR/progressive	0.1032
TIMBIR	0.0853



Remove one dendrite, and orient the <100> along a coordinate axis.







Conclusions

- New methods for destructive 3D analysis with the goal of routine automated acquisition of 3D datasets
- A new method for 4D tomography: Time-Interlaced Model-Based Iterative Reconstruction (TIMBIR). Improvements are possible
- Quantified the morphology of a growing dendrite using the ISD $V_v, A_s, S_v, \langle C \rangle$, benchmark data for simulation. Doublon formation surprisingly common
- Large datasets: sharing, storing, and computing

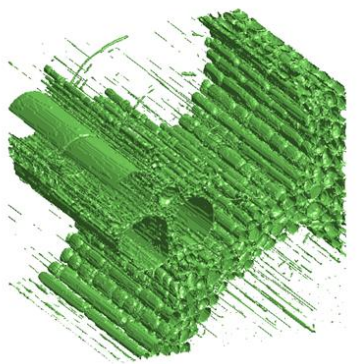
Georgia Institute of Technology

Microstructure Quantification using Spatial Statistics

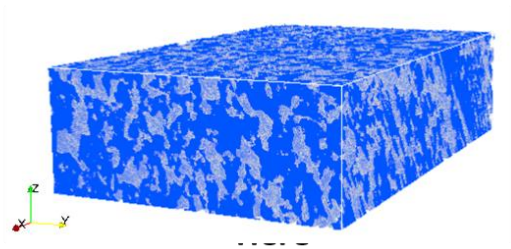
Surya R. Kalidindi, Tony Fast, Ahmet Cecen

Funding: AFOSR MURI

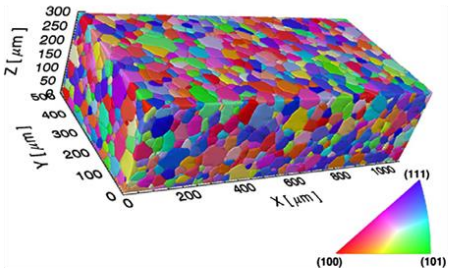
Microstructure Quantification



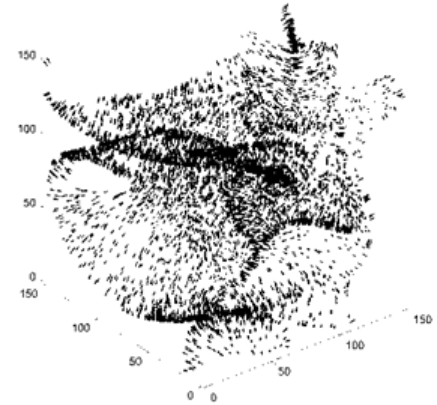
Bamboo
X-Ray Tomography



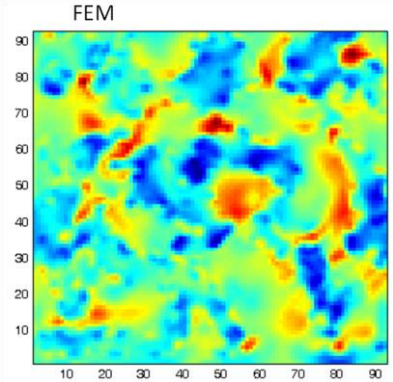
Fuel Cell Micro Porous Layer
FIB SEM



Beta Titanium
Mechanically Polished
SEM+EBSD

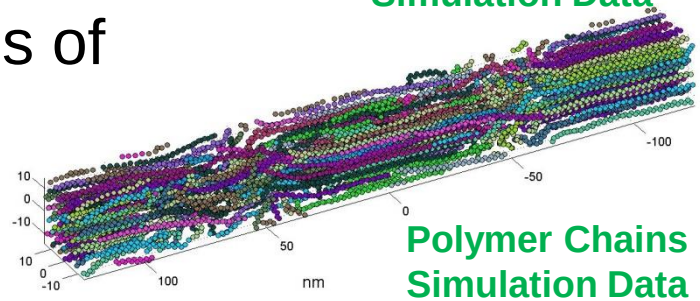


Surface Curvature data



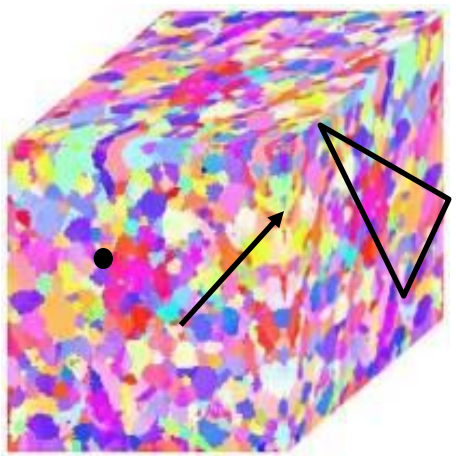
Strain Distribution
Simulation Data

- Thinking of microstructure as a digital signal allows a generalized treatment at multiple hierarchical length/structure scales: m_s^h
- Ad-hoc measures of microstructure: average grain size, average spacing, ODF, MODF, ...
- Naturally organized extensible measures of microstructure: n-point statistics
- Data Analytics: seek objective low-dimensional representations



Polymer Chains
Simulation Data

Microstructure Statistics



$f(h)$ 1-point correlations (Volume Fraction)

$f_2(h, h'|\mathbf{r})$ 2-point correlations

$f_3(h, h', h''|\mathbf{r}, \mathbf{r}')$ 3-point correlations

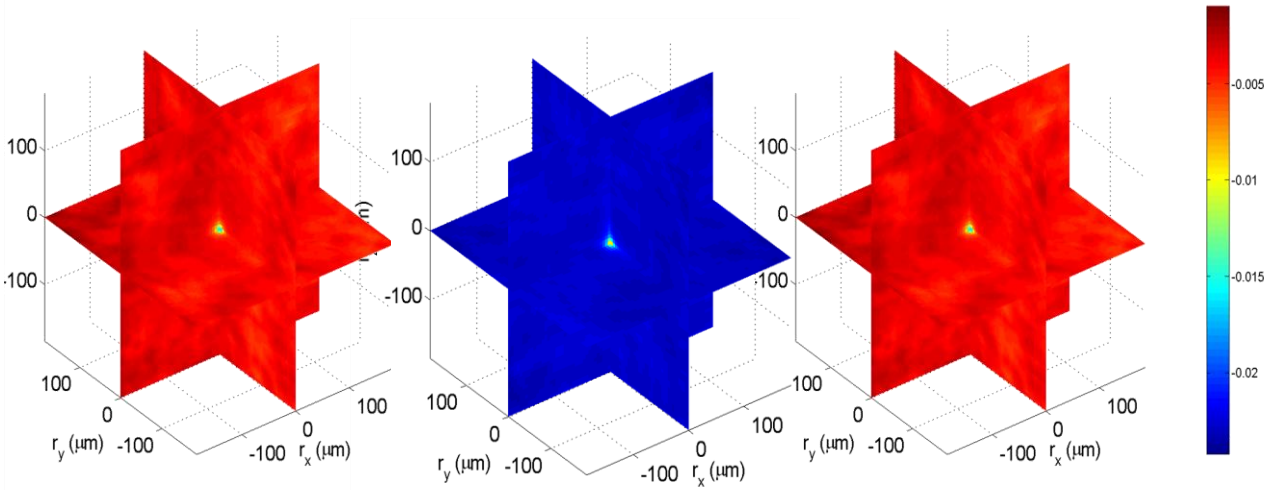
...

Conveniently computed using FFT algorithms

PCA: $$f_2(h, h'|\mathbf{r})^n = \sum_{i=1}^{N-1} \alpha_i^n \phi_i + \overline{f}_2$$

Hypothesis: PCA weights of *n*-point statistics provide objective measures of microstructure

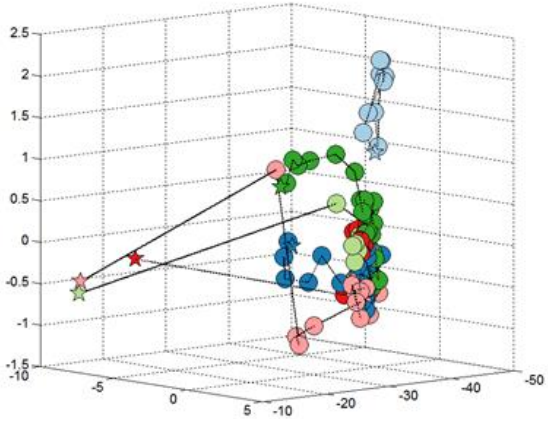
New Advances in Computation of 2-pt Statistics

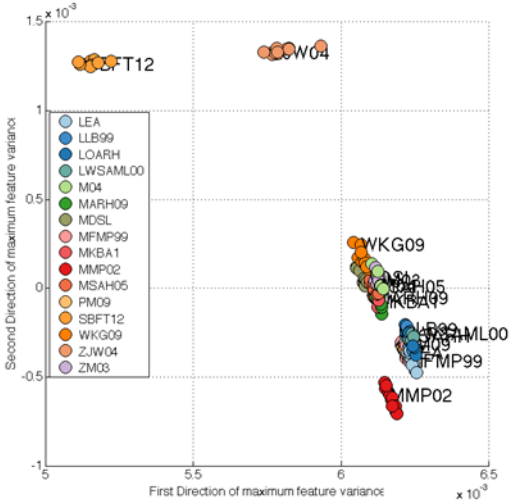


2-pt. Statistics for Al-Cu solidification datasets (Vorhees Group)

- Generalization of the computational framework for gridded and point cloud datasets
- Allow treatment of various mixed assumptions on the boundaries (e.g., periodic, non-periodic)
- Extension to include complex local states (e.g., continuous variables, tensorial variables)
- Extension to include partial and/or incomplete datasets (e.g., non-standard boundary geometries, low confidence in selected measurements)

Degree of crystallinity in polymer molecular dynamics



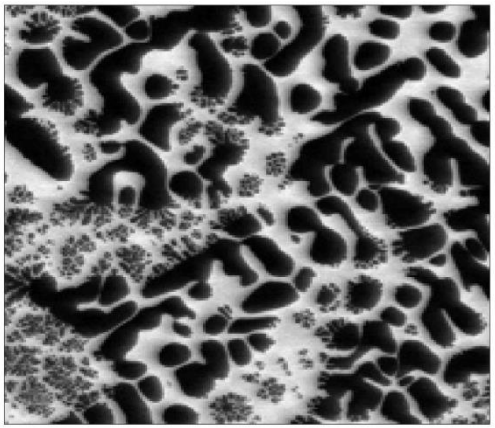


Potential model comparison in Al molecular dynamics

Data Science Protocols for Microstructure Engineering

Data Generation (Collaborator: Bouman)

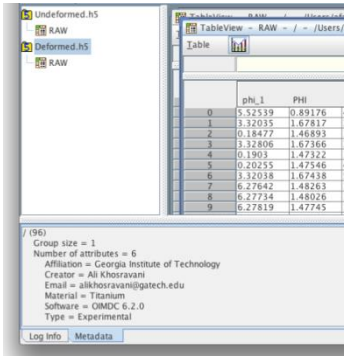
Bayesian Dynamic Sampling



Data Curation (Potential Collaborators: All)

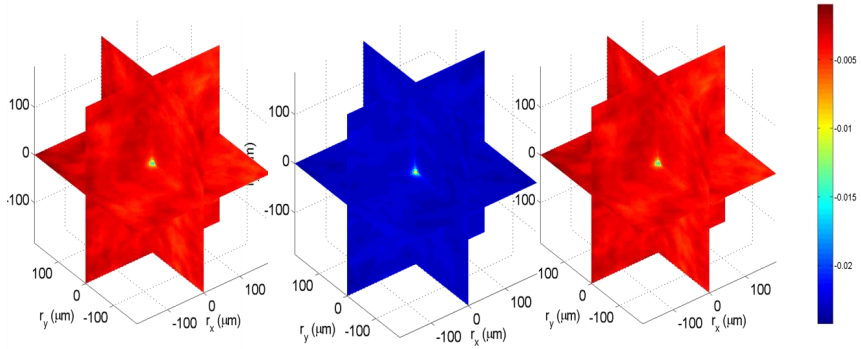
Metadata Wiki

High Value Data shared in real time



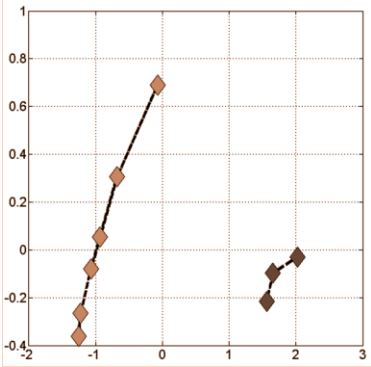
HDF5 file organization for nearly all spatial materials data and metadata

Data Analytics

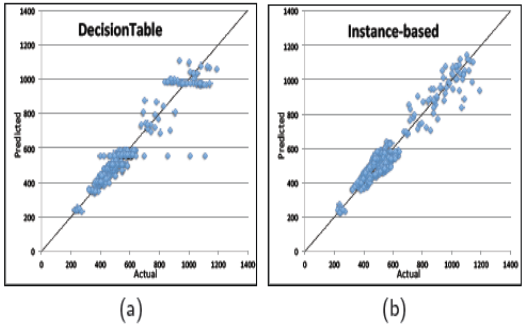


Matlab codes for 2-point statistics on nearly all datasets vetted and made available on GitHub

Data Mining (Collaborators: Vorhees, Choudhary)



Low-dimensional Visualization of spatiotemporal X-CT datasets



Process-Structure-Property Linkages