

---

# MURI Team Meeting III

---

August 16-18, 2015, Carnegie Mellon University

## Meeting Schedule

<b>Sunday August 16, 2015</b>	<b>2</b>
[7:00PM - 9:00PM] Social get-together at the Wyndham hotel (bar area ground level) . . .	2
<b>Monday August 17, 2015, Wean Hall, Room 5421</b>	<b>2</b>
[8:55-9:00] Introductory Remarks [M. De Graef] . . . . .	2
[9:00-9:30] Growth and Coarsening of Si Particles in a Liquid: Insights from Four-Dimensional X-ray Microtomography [Ashwin J. Shahani, <sup>1</sup> Xianghui Xiao, <sup>2</sup> and Peter W. Voorhees <sup>1</sup> ] . . . . .	2
[9:30-10:00] Analysis of the Al-Cu Solidification Process Using 2-pt Statistics [Ahmet Cecen, <sup>1</sup> John W. Gibbs, <sup>2</sup> Peter W. Voorhees, <sup>2</sup> and Surya R. Kalidindi <sup>1</sup> ] . . . . .	3
[10:00-10:30] <b>Coffee Break</b> . . . . .	3
[10:30-11:00] Plug-and-Play Priors for 3D Reconstruction of Materials [Suhaz Sreehari and Charles A. Bouman] . . . . .	4
[11:00-11:30] Complex Diffraction Tomography (CODIT) [Aditya Mohan and Charles A. Bouman] . . . . .	5
[11:30-12:00] Vector Field Tomography for Materials Imaging [Aditya Mohan and Charles A. Bouman] . . . . .	6
[12:00-1:00] <b>Lunch Break</b> . . . . .	6
[1:00-2:00] Archetype-Blending Continuum (ABC) Stochastic Multiresolution Theory for Microstructure Based Predictive Materials Science: Application to Polymer Based Systems [L. Catherine Brinson, <sup>1,2</sup> Wei Chen, <sup>1</sup> Wing Kam Liu, <sup>1,3</sup> and Daniel Apley <sup>4</sup> ] . . . . .	7
[2:00-2:30] Quantify compatible interfaces for highly reversible phase transformation by Synchrotron Laue Micro diffraction [Xian Chen and Richard D. James] . . . . .	8
[2:30-3:00] Combining Image Compression with Digital Image Correlation [Jin Yang and Kaushik Bhat-tacharya] . . . . .	9
[3:00-3:30] <b>Coffee Break</b> . . . . .	9
[3:30-4:00] Sampling methods applied to material optimization problems with multiple microstructural solutions [Pinar Acar and Veera Sundararaghavan] . . . . .	10
[4:00-4:30] Dynamic Sampling [G.M. Dilshan Godaliyadda, Dong Hye He, Gregory Buzzard, Charles Bouman] . . . . .	11
[4:30-6:00] <b>Characterization Lab Tour / Free Time</b> . . . . .	11
[6:00-...] <b>Dinner at The Porch [short walk from campus]</b> . . . . .	11
<b>Tuesday August 18, 2015, Wean Hall, Room 5421</b>	<b>11</b>
[8:30-9:00] MATIN: An e-Collaboration Platform - Current State and Future Directions [Ahmet Cecen, David Brough and Surya Kalidindi] . . . . .	12
[9:00-9:30] Multi-Scale Microstructure-Property Modeling of Elastic Localization Relationships in High Contrast Composites [Rosanne Liu, Ankit Agrawal, and Alok Choudhary] . . . . .	13
[9:30-10:00] The marked point process for 3D datasets [Dae Woo Kim and Mary Comer] . . . . .	14
[10:00-10:30] <b>Coffee Break</b> . . . . .	15
[10:30-11:00] Application of Forward Models for Indexing of Electron Diffraction Modalities [Saransh Singh and Marc De Graef] . . . . .	15
[11:00-11:30] Extracting Grain Boundary Inclination Angles from 2D EBSD and PFIB Analysis of AlSiCu [Michael Chapman and Marc De Graef] . . . . .	16
[11:30-12:00] A New Joint Markov Random Field/Marked Point Process Image Model under the Bayesian Framework [Huixi Zhao and Mary Comer] . . . . .	17
[12:00-1:00] <b>Lunch</b> . . . . .	17

## Growth and Coarsening of Si Particles in a Liquid: Insights from Four-Dimensional X-ray Microtomography

Ashwin J. Shahani,<sup>1</sup> Xianghui Xiao,<sup>2</sup> and Peter W. Voorhees<sup>1</sup>

<sup>1</sup> Northwestern University; <sup>2</sup> Argonne National Laboratory

**Abstract:** Among the commercial aluminum alloy castings, hypereutectic Al-Si and Al-Si-Cu alloys are the most commonly used owing to their excellent hardness, corrosion resistance, and machinability. These properties depend strongly on the characteristics of the microstructure, e.g., the size, shape, and distribution of the highly anisotropic Si particles. The mechanisms controlling the growth and coarsening behavior of such particles above the eutectic temperature, which are critical to the semi-solid processing of the alloy, have been difficult to determine due to the lack of real-time experiments that can capture the 3D morphology of the particles. Thus, we probe the microstructural evolution of primary Si particles in an Al-32wt%Si-15wt%Cu alloy via synchrotron-based X-ray microtomography. In order to assess the extraordinary morphological and topological complexity of the Si particles, we calculate curvatures, orientations, and velocities from the four-dimensional (4-D, i.e., time and space resolved) data and track their evolution during the phase transformation. The results indicate that at long times, growth and coarsening are both diffusion-limited, despite the highly anisotropic particle morphology. This trend can be rationalized by postulating that twin defects provide the kink sites necessary for interfacial propagation. Other insights into the mechanisms responsible for the evolution of these complex systems that are attainable only through in situ 3D experiments will be given.

---

## Analysis of the Al-Cu Solidification Process Using 2-pt Statistics

Ahmet Cecen,<sup>1</sup> John W. Gibbs,<sup>2</sup> Peter W. Voorhees,<sup>2</sup> and Surya R. Kalidindi<sup>1</sup>

<sup>1</sup> Georgia Institute of Technology; <sup>2</sup> Northwestern University

**Abstract:** Spatial correlations in the form of n-point statistics have been previously demonstrated to be very effective in extracting structural information from complex datasets. This work leverages the established concepts of 2-pt statistics in order to gain otherwise obscure physical insights regarding the spatial arrangement of the solid-liquid interfaces in an Al-Cu mixture. Identification of particular spatial patterns in the interface curvature and velocity arrangements is expected to improve our understanding of the underlying phenomena governing the evolution of the solid-liquid mixture.

It is important to note the massive scale of data involved in such an undertaking. Through the evolution of the mixture, one time snapshot of the experimentally measured structure dataset contains more than 1.8B floating point numbers, each capturing the local state in a spatial voxel. Extracted information about the structure also depends on the specific set of choices taken during the processing of the data, such as the location and thickness of the interface, segmentation choices, identification of particular curvature-curvature, velocity-velocity and curvature-velocity relationships of interest. We will demonstrate the current status and discuss future directions regarding the analysis.

---

## Plug-and-Play Priors for 3D Reconstruction of Materials

Suhas Sreehari and Charles A. Bouman  
Purdue University

**Abstract:** Many important imaging problems in material science and structural biology involve reconstruction of 2D and 3D images containing repetitive non-local structures. Although model-based iterative reconstruction (MBIR) could in principle exploit the presence of such repetitive structures through the selection of a log prior probability term, in practice, determining such a log prior term is challenging. Denoising algorithms like non-local means (NLM) and BM3D are known to capture non-local similarities in images. But how do we make these denoising filters into prior models?

In this work, we answer this important question by presenting the “plug-and-play priors” technique that is based on the alternating direction method of multipliers (ADMM). ADMM decouples the forward and prior models through variable splitting and subsequent application of the augmented Lagrangian. In plug-and-play priors, we take a step further, and replace one of the ADMM minimizations with a denoising operator.

We also present a convergence theorem that outlines specific conditions that ensures convergence of the plug-and-play algorithm. It turns out NLM does not satisfy these conditions, so we modified NLM and call it the “doubly-stochastic gradient NLM” (DSG-NLM). Finally, we showcase 2D sparse interpolation and 3D bright field tomographic plug-and-play reconstruction results using multiple prior models. In both experiments, the DSG-NLM prior makes plug-and-play fully convergent, and provides high clarity, low artifact image reconstructions.

---

## Complex Diffraction Tomography (CODIT)

Aditya Mohan and Charles A. Bouman  
Purdue University

**Abstract:** In traditional absorption based X-ray tomography, the varying attenuation coefficient within the sample results in contrast variations in the reconstructed images. However, we cannot distinguish between materials with similar attenuation coefficients using this method. In material science, there is a need to image materials with similar attenuation coefficients but differing refractive indices. To image such samples, the detector and the sample are separated by a distance, which satisfies the condition for Fresnel diffraction. Unlike absorption-based tomography, the intensity variations on the detector are obtained by diffraction of the X-ray wave front in front of the object. The traditional approach to reconstruct the object is to use standard phase retrieval algorithms, which appropriately filter the measurements to get the phase of the wave front in front of the object. The reconstruction is then obtained by back-projecting the retrieved phase images. However, such an approach results in excessive smoothing of the edges in the reconstruction. Our approach to solve this problem is to integrate phase retrieval and the reconstruction algorithm in a MBIR framework. We model the propagation of the wave front within the object and combine it with a model for diffraction in the region between the object and the detector. The reconstruction is then formulated as a minimization of a cost function consisting of a forward model term, which models the X-ray propagation, and a prior model term, which is a model for image sparsity. Our algorithm enables simultaneous reconstruction of attenuation and refractive indices within the object.

---

## Vector Field Tomography for Materials Imaging

Aditya Mohan and Charles A. Bouman  
Purdue University

**Abstract:** In traditional vector field tomography, two components of the magnetic vector potential or the magnetic induction are reconstructed from the measured phase shifts of the electron wave. The third component of the vector is then computed analytically from the reconstructed images, which results in inaccuracies in the reconstruction of the overall vector potential. Furthermore, there is no accurate method to compute the magnetization from the vector potentials. Our model-based reconstruction algorithm (MBIR) directly reconstructs the magnetization and the charge density from the measured phase shifts. In our algorithm, we model the transformation from the magnetization and the charge density to the magnetic vector potential and the electrostatic potential and then its transformation to the measured phase shifts. We then combine this model with a prior model for image sparsity and formulate the reconstruction algorithm as an optimization problem.

---

# Archetype-Blending Continuum (ABC) Stochastic Multiresolution Theory for Microstructure Based Predictive Materials Science: Application to Polymer Based Systems

L. Catherine Brinson,<sup>1,2</sup> Wei Chen,<sup>1</sup> Wing Kam Liu,<sup>1,3</sup> and Daniel Apley<sup>4</sup>  
<sup>1</sup> Dept. Mech. Engg., <sup>2</sup> Dept. Mat. Sci. Engg., <sup>3</sup> Dept. Civil Engg., <sup>4</sup> Dept. Industrial Engg. and Mgmt Sc., Northwestern University

**Abstract:** Understanding structure-property relationships is a cornerstone of materials science, yet the ability to capture the dynamic relationship between structure and properties across space and time scales continues to be a grand modeling challenge to theoreticians, mathematicians, scientists, and engineers. In the realm of polymer composites, prediction is especially challenging due to the macromolecular nature of the polymer matrices and uncertainties in developing appropriate potentials at the small length scales and coarse graining connections toward macroscale properties. The presented work develops a comprehensive stochastic framework around a multiresolution continuum field theory to bridge statistically variable structural features and materials properties and performance, resulting in predictive materials modeling and discovery. Unlike homogenization approaches that lose key information on structural variability, the Archetype-Blending Continuum (ABC) multiresolution field theory is based on strong, concurrent coupling across spatial and temporal scales of interest with an embedded reduced-order approach, thus allowing mechanistically accurate predictions for complex deformation modes. To incorporate multiresolution random field microstructure/property models into the ABC field theory, both descriptor based and machine learning based methods are developed to render a mathematical representation of the material microstructure, probe variability across the data, and develop algorithms to generate statistically equivalent microstructures and provide efficient computation of a high order of geometric description. The microstructural representations are then analyzed via statistical learning using archetype level “local” physics-based simulations, applying uncertainty quantification (UQ) principles to studying the stochastic structure-property relations and producing a reduced set of descriptors, blending laws, and archetypal structure-property relationships to fully describe the material structures across the length scales. Data mapping algorithms are being developed to create libraries with which connections between the statistics of the microstructure can be connected to the final properties. The framework is applied to the prediction of properties for high-temperature polymer composites, accounting for details such as nanoparticles, fiber reinforcement, crosslinking, defects, and inhomogeneities at all length scales.

---

## Quantify compatible interfaces for highly reversible phase transformation by Synchrotron Laue Micro diffraction

Xian Chen and Richard D. James  
University of Minnesota

**Abstract:** Materials undergoing reversible phase transformation have tremendous potential for applications such as medical devices, microelectronic sensors, robotic actuators, solid-state refrigerators and energy conversion devices. These applications rely on the changes of crystal structure during phase transformation. However, the inevitable formation of microstructure introduces stressed transition layers due to the lattice misfit at phase interfaces. This, in turn, drives the nucleation of defects that leads to the degradation of the material under cyclic transformation. It has been revealed that conditions of compatibility play an important role in linking the formation of microstructure and material properties. Microstructures consisting of sets of interfaces that accommodate themselves elastically compatible and separate regions of different crystal structures. When the jump of the average deformations across these interfaces satisfies the “Cofactor Conditions” [Chen et al, JMPS (2013)] i.e. conditions of compatibility between phases, the material exhibits enhanced reversibility and “zero” hysteresis upon cyclic phase transformation. Two recent discoveries of highly reversible alloys in ZnAuCu [Song et al, Nature (2013)] and NiTiCu [Chluba et al, Science (2015)] showed the satisfaction of the conditions of interface compatibility results in ultra-low fatigue properties, i.e. the transition temperature, the latent heat and stress-strain response stay the same even after 10,000 thermal cycles or 10 million stressed-induced cycles, in sharp contrast to the most popular shape memory alloy NiTi, which suffers failure only after tens of cycles. To quantitatively study the morphology and coherency of the interface, here we would present an approach that constructs a spatial deformation mapping containing transitional interfaces by synchrotron X-ray Laue microdiffraction. Based on the gradient of deformations at the interface, we can directly calculate the jump conditions in-situ during the structural transformation of the  $Zn_{45}Au_{30}Cu_{25}$  that has been reported to satisfy the Cofactor Conditions closely.

---



## Combining Image Compression with Digital Image Correlation

Jin Yang and Kaushik Bhattacharya  
California Institute of Technology

**Abstract:** Digital image correlation (DIC) is a powerful experimental technique to obtain full-field displacements and strains. The basic idea of the method is to compare images of an object painted with a speckle pattern before and after deformation, and thereby to compute displacements and strains. Typical DIC requires high-resolution images. The massive size of images renders cost of digital storage expensive. We find that by combining subset DIC with image Discrete Cosine Transform (DCT) compression, we can obtain results which are in reasonable agreement with conventional DIC even though we use only 5% of the original image size. This is a promising tool, but DCT compression can introduce large noise into the dataset.

To overcome this problem, we are implementing a global regularized DIC method which incorporates displacement field compatibility. We also implement Augmented Lagrangian method with alternating direction method of multipliers (ADMM) scheme, which takes advantage of the best features of both local DIC (can be solved fast and in parallel) and global DIC (incorporate displacement compatibility).

---

## Sampling methods applied to material optimization problems with multiple microstructural solutions

Pinar Acar and Veera Sundararaghavan  
University of Michigan

**Abstract:** Microstructure optimization is important for improving the performance of critical components in numerous aerospace applications. In this work, the microstructure is quantified with the orientation distribution function (ODF). The ODF of polycrystalline alloys is represented in a discrete finite element form. The homogenized properties are computed through the ODF. The inverse problem of identifying optimal ODFs that leads to desired combinations of properties is then solved through sampling methods.

Two different sampling approaches are discussed: The first uses sampling in the ODF space using Latin hypercube method or incremental space filter. The optimal ODF is selected from these samples and then genetic algorithms are used to refine the results. The second approach uses sampling in the property space to find optimal property combinations. A direct linear solver is then employed so as to find multiple ODFs with the optimum solution. The first method is tested on a Titanium airframe thermal buckling problem. The objective of the optimization is to find the microstructure that maximizes the critical buckling temperature. The optimum solution of this approach is found to be same with as the data mining approach developed by Northwestern group. The second approach is tested on vibration frequency tuning of a Galfenol beam. This problem leads to multiple ODF solutions. We find that optimization using new techniques developed in this effort provide a considerable improvement in the computational time compared to traditional approaches.

---

## Dynamic Sampling

G.M. Dilshan Godaliyadda, Dong Hye He, Gregory Buzzard, Charles Bouman  
Purdue University

**Abstract:** In many imaging applications, it is very advantageous to find the samples that allow the highest fidelity reconstruction. Optimized sampling strategies generally fall into two categories: static and dynamic. In dynamic sampling, each new sample is chosen by using information obtained from previous samples. In this way, dynamic sampling offers the potential of much greater fidelity, but at the cost of greater complexity.

We present a framework for dynamic sampling where the objective is to find the pixel which when measured reduces the expected reconstruction error the most. In this framework, we use a training database to learn the relationship between measurements already made and the expected integrated interpolation error, an approximation to the expected reduction in reconstruction error. This framework is adapted for both continuously valued images and discrete (labeled) images (e.g. Electron back-scatter diffraction (EBSD) images). Furthermore, we have modified the algorithm for group sampling (i.e. selecting more than one sampling location in each iteration). We present results from simulated dynamic sampling experiments conducted on continuous images and on simulated EBSD images created using Dream3D.

---

## MATIN: An e-Collaboration Platform - Current State and Future Directions

Ahmet Cecen, David Brough and Surya Kalidindi  
Georgia Institute of Technology

**Abstract:** Highly productive cross-disciplinary collaborations cutting across materials science, manufacturing, product design, computational sciences, and data sciences are critically needed for the success of the emerging national strategic initiatives such as the Materials Genome Initiative (MGI) focused on the accelerated development of new/improved advanced materials and their deployment in emerging technologies. In response to these critical national needs, and with the guidance and support of AFOSR: MURI, GaTechs IMAT (Institute for Materials) and FLAMEL (NSF funded IGERT), we have initiated the development of an e-collaboration platform, whose primary purpose is to facilitate intimate exchange of ideas, data, codes, knowledge, and expertise between potential cross-disciplinary team members engaged in a diverse range of materials innovation efforts.

Called MATIN, this e-collaboration platform is aimed at nucleating an emergent community that is particularly adept at injecting customized materials data science and informatics tools into the ongoing materials innovation endeavours in an effort to dramatically enhance their productivity. Our current strategy is to seamlessly integrate and adapt a plethora of tools and paradigms already in place scattered across a variety of fields around this specific purpose, while minimizing the barrier to entry for a mainstream researcher. We will present the current status of this effort and discuss future plans.

---

## Multi-Scale Microstructure-Property Modeling of Elastic Localization Relationships in High Contrast Composites

Rosanne Liu, Ankit Agrawal, and Alok Choudhary  
Northwestern University

**Abstract:** This work attempts to develop statistical models that approximate materials science phenomena, with the help of advanced data science and informatics approaches. The focus is on the extraction of microstructure-property relationships that lies in three-dimensional voxel based microstructure volume elements (MVEs). More specifically, the elastic localization behavior in a 2-phase composite material is studied. A machine learning based multi-scale framework is able to extract the internal structure of a material system, where multiple hierarchical length scales exists. This talk is going to describe how an accurate modeling is achieved by 1) learning from a higher level abstraction of MVEs from 2-point correlation functions, and 2) representing the lower level information through novel geometrical features. Future works of applying convolutional neural networks that construct a nonlinear neighborhood relationship for each voxel to enhance the learning performance will also be discussed.

---

## The marked point process for 3D datasets

Dae Woo Kim and Mary Comer  
Purdue University

**Abstract:** The extension of the 2D marked point process (MPP) to three dimensions can be accomplished in several ways. The first is the straightforward extension of the model, and the corresponding optimization, from 2D to 3D. The problem with this approach is the high computational cost. To tackle this computational issue, in this research, we propose two alternative approaches. One is a multiresolution approach, which involves spatial subsampling of the data for initial processing. The other method consists of two steps: performing a 2D MPP first and then applying 3D object fitting to the clustered data of the 2D MPP result. The superellipsoid model is used for the experiments discussed in this presentation. The proposed methods are applied to synthetic and materials image data. The results show that these new methods can significantly reduce the computational complexity of detecting 3D objects.

---

## Application of Forward Models for Indexing of Electron Diffraction Modalities

Saransh Singh and Marc De Graef  
CMU

**Abstract:** Electron scattering is one of the fundamental tools for quantitative characterization of microstructure across a wide variety of material class. Even though the techniques have been around for some time, there are no reliable and accurate forward models for these modalities. In this contribution, we will describe the physics based forward models for a variety of electron diffraction modalities, specifically the Electron Backscatter Diffraction (EBSD), Electron Channeling Pattern (ECP) and Precession Electron Diffraction (PED). We will describe how the forward models are generated and the use of these forward models in indexing of experimental patterns using the normalized dot product approach. We will present results on a number of different datasets and compare them to the results from commercial packages. We will also present our efforts to port our existing code to the GPU platform and the performance gains we achieve.

---

## Extracting Grain Boundary Inclination Angles from 2D EBSD and PFIB Analysis of AlSiCu

Michael Chapman and Marc De Graef  
CMU

**Abstract:** To fully define a grain boundary, which is useful in grain boundary energy calculations, the misorientation between the grain orientations and the grain boundary plane need to be known. 2D EBSD easily gives the misorientation and a trace of the grain boundary plane, but typically 3D serial sectioning needs to be completed to obtain the inclination angle of the grain boundary into the sample to define the grain boundary plane. This work will show how the interaction volume of the electrons in EBSD give enough depth information to extract the grain boundary inclination angle from only a 2D scan. By calculating the proportion of a pattern that is from each grain in blended patterns near a grain boundary, and measuring the rate at which the proportion changes while translating over the boundary, the inclination angle can be recovered. AlSiCu samples from Peter Voorhees group have been examined using EBSD for sample preparation utilizing conventional polishing and slicing using the PFIB. Nanotwinned like structures have been observed near the curved edges of the Silicon plates.

---



## A New Joint Markov Random Field/Marked Point Process Image Model under the Bayesian Framework

Huixi Zhao and Mary Comer  
Purdue University

**Abstract:** Our previously proposed unified MRF/MPP model incorporates global and local constraints for image modeling, allowing simultaneous analysis of images at both the pixel level and the object level. However, there are two main drawbacks of the model: 1) Since we need to calculate both the object potential and the segmentation potential for each object, the computational complexity is large; and 2) For each object, the corresponding segmentation is obtained within a restricted image area of the object, which sometimes results in artifacts along the segmentation boundaries, especially when the object does not perfectly match the image data. We propose a joint MRF/MPP model to solve the above problems. Unlike the unified MRF/MPP model, which finds an optimized object configuration by minimizing an energy function, our new model obtains a joint object configuration and segmentation by maximizing a joint posterior probability, which models both the object field and the label field. We will describe the new model in detail and compare results with the unified MRF/MPP model.

---

## Directions to Wean Hall Room 5421

Wean Hall room 5421 is most easily reached as follows (look at the map on the next page).

- Starting at the Wyndham hotel, walk to Fifth Avenue, turn left, walk to intersection, turn right onto South Bellefield Avenue. Walk to the end and turn left on Forbes Avenue; follow Forbes past the lights at South Craig Street (cross the street here to continue on the right side of Forbes); cross a bridge (labeled **1**) on the map, and then turn right onto the CMU campus.
  - Walk in between Hamburg Hall and the Robert Mehrabian Collaborative Innovation Center, turn left at the end and walk to the main entrance of Newell-Simon Hall, labeled **2**.
  - Enter Newell-Simon Hall, walk to the curved stairs on the left and go one floor up. Turn left at the top and walk through a skywalk bridge into Wean Hall (labeled **3**). You will be on the fourth floor of Wean Hall.
  - Take the first right turn after entering Wean Hall; stairs will be on your left. Go up one floor to the fifth floor; turn right, another right, and then enter the 5400 corridor on the left; room 5421 will be towards the end on your left.
-