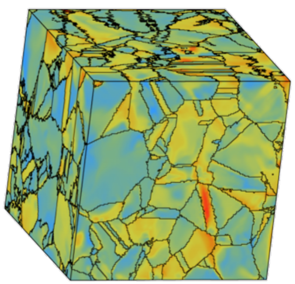
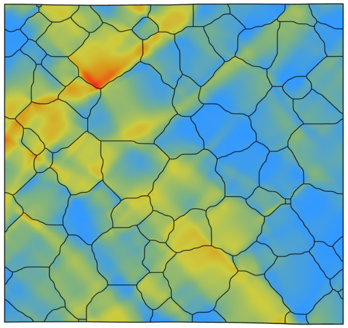
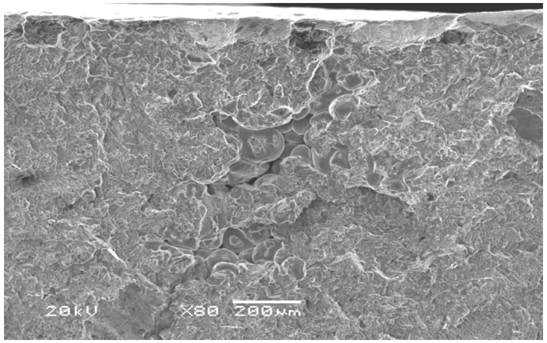
SAND2015-4510PE

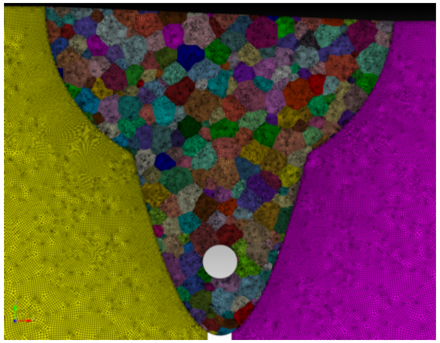
Exceptional service in the national interest

Sandia National Laboratories









Probabilistic Modeling of Crystallographic Texture

R. Field, 01523, rvfield@sandia.gov

U.S. DEPARTMENT OF ENERGY

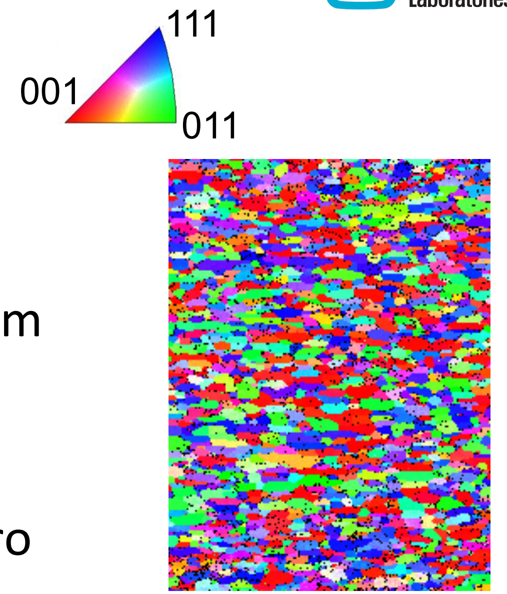
NNSA National Nuclear Security Administration

Outline

- Motivation
  - What is texture? Why do we want to model it?
- Euler angles
  - One measure of texture
  - Inherently random and spatially dependent
- Random field model for Euler angles in a material microstructure
  - Marginal cumulative distribution functions (CDFs)
  - Spatial correlations
- Implementation – "EulerRF" code
  - My goal: A tool for analysts
- Example

Motivation

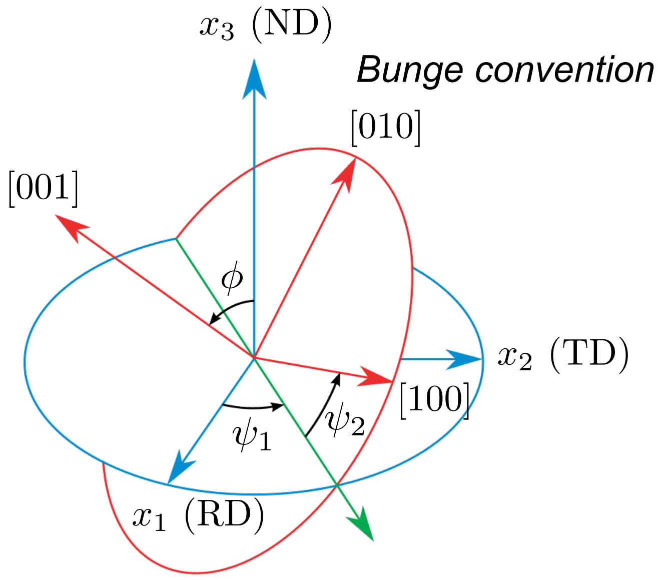
- Texture is the distribution of crystallographic orientations of a polycrystalline sample
  - Crystallographic orientation is an inherently random phenomena that varies spatially
  - Originates from processing
  - When orientations are “fully random” we have zero texture; else there is some preferential orientation and we have non-zero texture
  - Texture is known to affect material strength, weldability, deformation behavior, cracking,…
- <u>Objective</u>: Develop approach to supply FE models with accurate samples of texture
  - Calibrate to data if available (match statistics)
  - Make tool available to analysts
  - Address both “micro” and “macro” texture

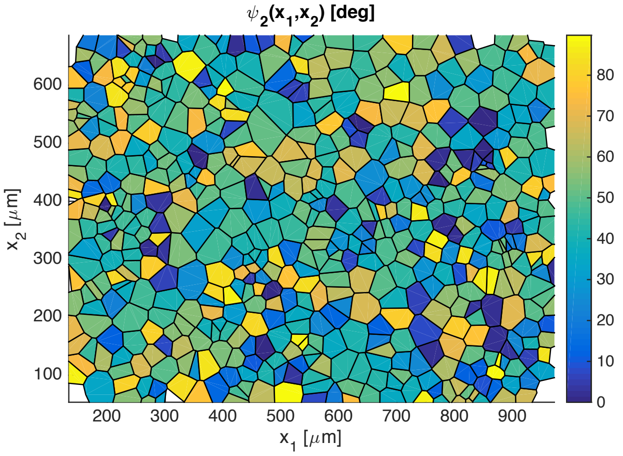


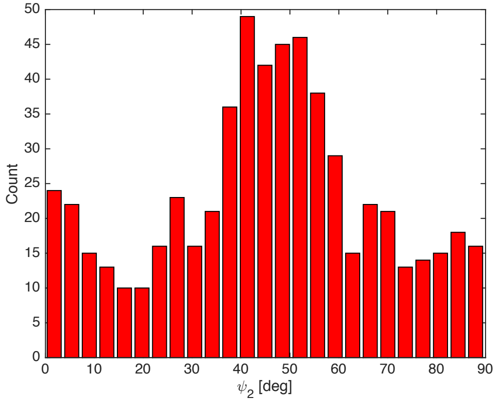
Taken from http://en.wikipedia.org/wiki/Texture_(crystalline)

Euler Angles – One Measure of Texture

- Three angles $\{\psi_1, \phi, \psi_2\}$ used to describe crystallographic orientation of material microstructures
- Transform specimen coordinate system C_s ($x_1x_2x_3$) onto the crystal coordinate system C_c
- Can be measured in each individual grain using EBSD







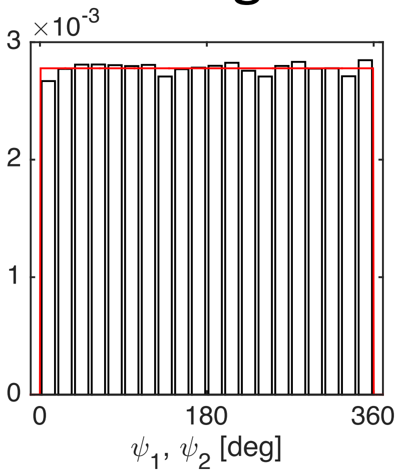
EBSD measurements of ψ_2 in Ta specimen (J. Carroll, 5/17/13)

"Zero Texture" Case

- A 3x3 orientation matrix *g* can be obtained from the Euler angles

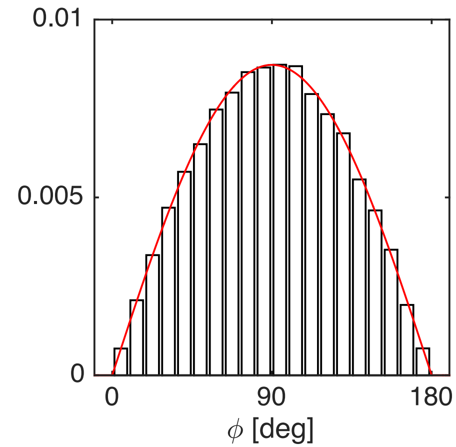
$$C_c = \begin{pmatrix} c\psi_1\, c\psi_2 - s\psi_1\, s\psi_2\, c\phi & s\psi_1\, c\psi_2 + c\psi_1\, s\psi_2\, c\phi & s\psi_2\, s\phi \\ -c\psi_1\, s\psi_2 - s\psi_1\, c\psi_2\, c\phi & -s\psi_1\, s\psi_2 + c\psi_1\, c\psi_2\, c\phi & c\psi_2\, s\phi \\ s\psi_1\, s\phi & -c\psi_1\, s\phi & c\phi \end{pmatrix} C_s = g\, C_s$$

- "Zero texture" is interpreted to mean that *g* is a random matrix distributed uniformly in *SO*(3), the set of all 3x3 rotation matrices
- We can show this implies $\{\psi_1, \phi, \psi_2\}$ are mutually independent with marginal PDFs as shown below



$$f_1(\psi_1) = f_2(\psi_2) = \frac{1}{360}$$

$$\psi_1, \psi_2 \in (0, 360)$$

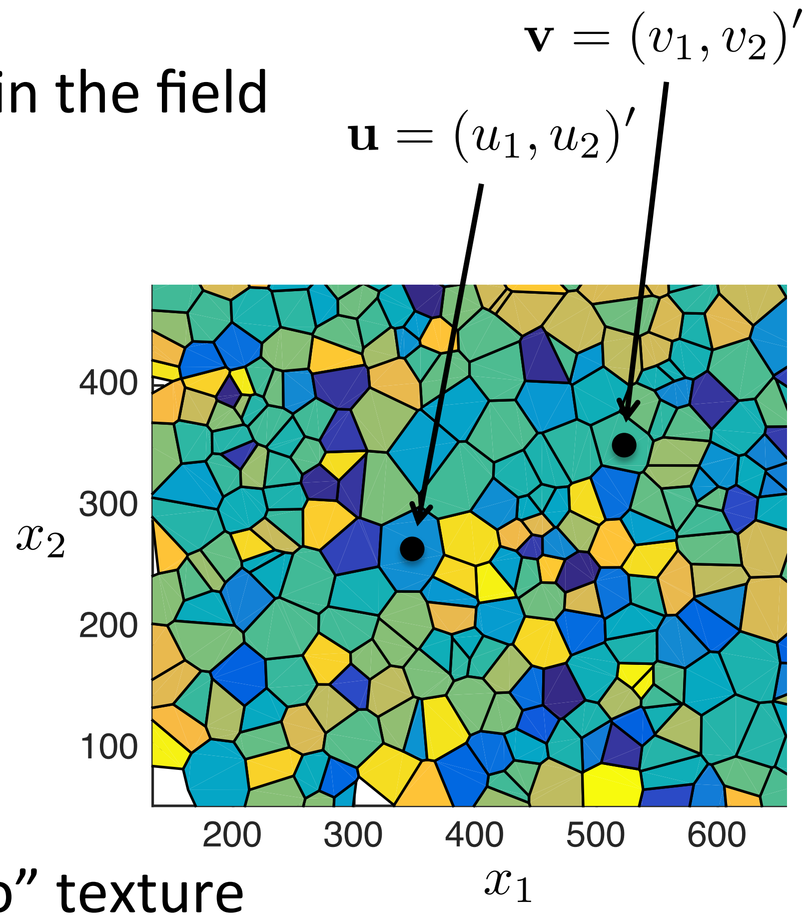


$$f(\phi) = \frac{\pi}{360} \sin\left(\frac{\pi\, \phi}{180}\right)$$

$$\phi \in (0, 180)$$

What is Spatial Correlation?

- A measure of the (average) linear dependence between two points in the field
  - Auto correlation function of ψ_1
    $$\mathrm{E}[\psi_1(\mathbf{u})\,\psi_1(\mathbf{v})]$$
  - Cross correlation between ψ_1 and ϕ
    $$\mathrm{E}[\psi_1(\mathbf{u})\,\phi(\mathbf{v})]$$
- Special cases
  - Statistically homogeneous
    $$\text{Depends on } (\mathbf{u}-\mathbf{v})$$
  - Statistically isotropic
    $$\text{Depends on } \|\mathbf{u}-\mathbf{v}\|$$
- Provides one way to model "micro" texture



Random Field Model – Definition

Sandia National Laboratories

- Let $\mathbf{R}(\mathbf{x}) = (\psi_1(\mathbf{x}), \phi(\mathbf{x}), \psi_2(\mathbf{x}))'$, $\mathbf{x} \in D$, be a vector-valued random field model for the 3 Euler angles
- Model form

$$\mathbf{R}(\mathbf{x}) = \boldsymbol{\mu}(\mathbf{x}) + \mathbf{a}(\mathbf{x})\,\mathbf{Y}(\mathbf{x}) = \begin{pmatrix} \mu_1(\mathbf{x}) \\ \mu_2(\mathbf{x}) \\ \mu_3(\mathbf{x}) \end{pmatrix} + \begin{pmatrix} \sigma_1(\mathbf{x}) & 0 & 0 \\ 0 & \sigma_2(\mathbf{x}) & 0 \\ 0 & 0 & \sigma_3(\mathbf{x}) \end{pmatrix} \begin{pmatrix} Y_1(\mathbf{x}) \\ Y_2(\mathbf{x}) \\ Y_3(\mathbf{x}) \end{pmatrix}$$

$$Y_k(\mathbf{x}) = h_k(G_k(\mathbf{x})) = F_k^{-1} \circ \Phi(G_k(\mathbf{x})), \ \ k = 1, 2, 3$$

$$\mathrm{E}[G_k(\mathbf{u})\, G_l(\mathbf{v})] = \rho_{kl}(\mathbf{u}, \mathbf{v})$$

  - μ_k and σ_k are the mean and standard deviations of R_k
  - F_k is related to the marginal CDF of R_k
  - **G** = (G_1, G_2, G_3)' is a vector-valued Gaussian random field with zero mean, unit variance, and correlation functions { ρ_{kl} }

Random Field Model – Calibration

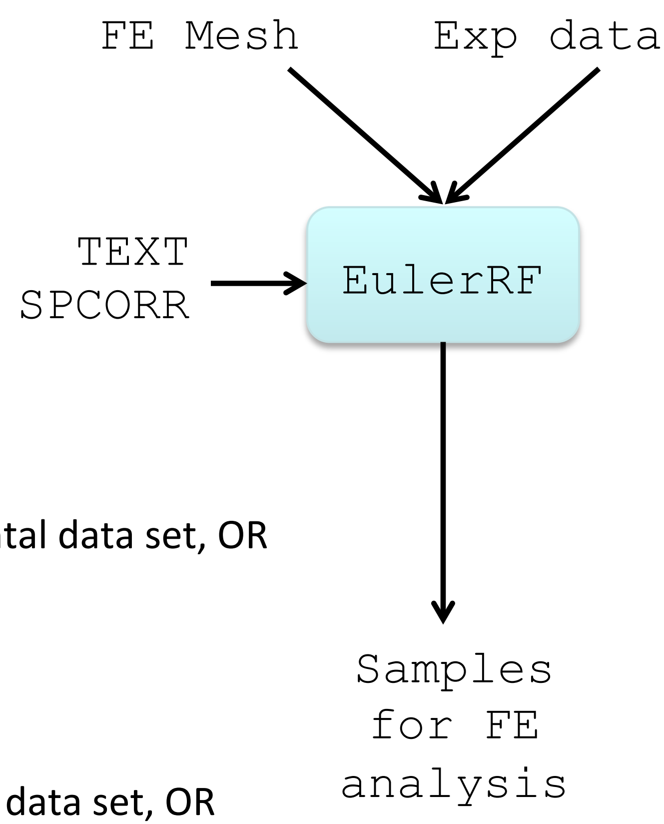
1. Estimate mean and standard deviation functions, μ and **a**
2. Define spatial correlation functions
   - Can map correlation of **G** to correlation of **R**
   - Functional form: exponential or linear decay
     - Homogeneous, isotropic
     - Parameter estimates using least-squares, or user-specified
3. Select marginal distribution functions
   - Choose a functional form
     - Consistent with physics
     - Beta distribution is a good choice
     - Parameter estimates using Method of Maximum Likelihood
   - Empirically-based
     - Requires a medium sized data set

Random Field Model – Discussion

- Why this type of model?
  - Extremely flexible
    - Atmospheric variables, Climate variables, Foam density, Laser weld properties, MEMS dynamics, Soil properties, Turbulence
  - Only three pieces of information are needed
    1. Mean and standard deviation functions
    2. Marginal distribution functions
    3. Spatial correlation function
    - This information is usually directly obtainable from data, making model calibration straightforward; in the absence of data, we make assumptions
  - Consistent with physics
    - Non-Gaussian, spatially correlated fields
  - Simulation is straightforward
    1. Simulate Gaussian random field **G**
    2. Transform each sample of **G** via $\mathbf{R} = \boldsymbol{\mu} + \boldsymbol{a}\, h(\mathbf{G})$

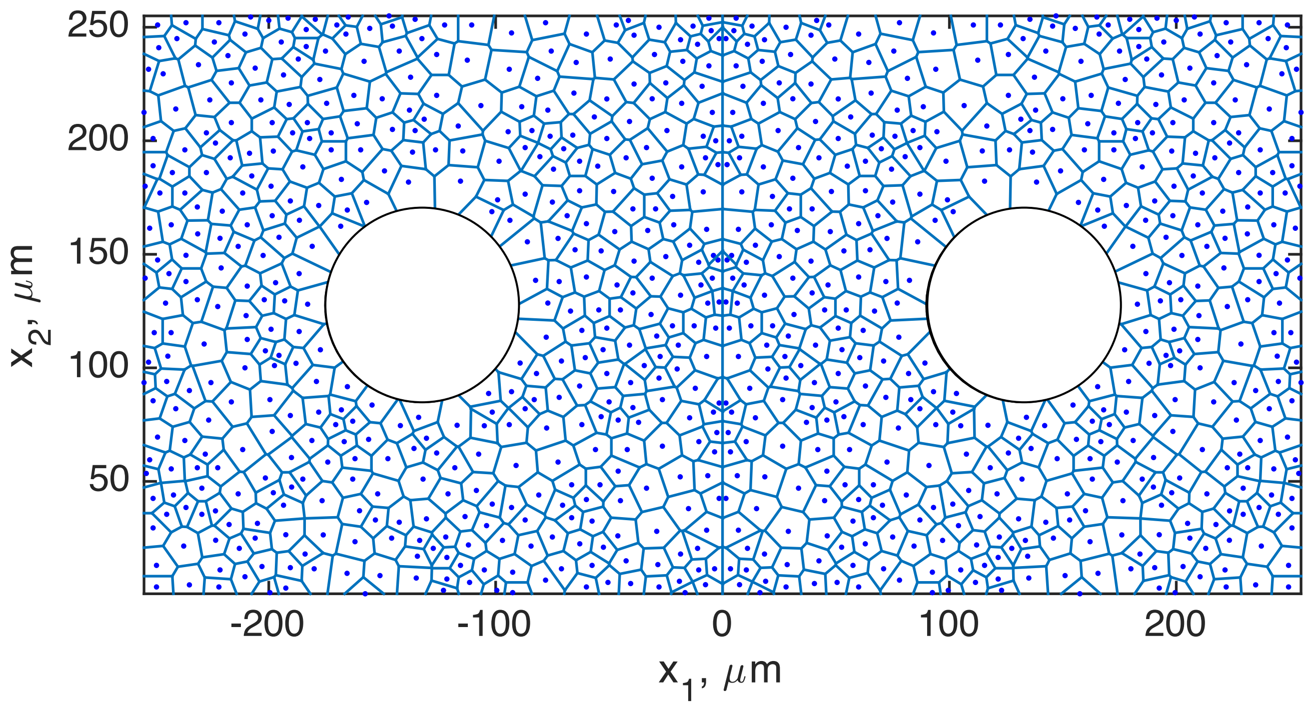
"EulerRF" Code

- Matlab based code to generate samples of Euler angle random field model on FE meshes
- Current assumptions / limitations
  - 2d meshes only (for now)
  - Spatial correlation currently limited
- Options
  - TEXT = "YES" or "NO" (zero texture case)
    - If "YES"
      - Calibrate marginal distributions to experimental data set, OR
      - User-specified distributions
  - SPCORR = "YES" or "NO"
    - If "YES"
      - Calibrate correlation lengths to experimental data set, OR
      - User-specified correlation lengths



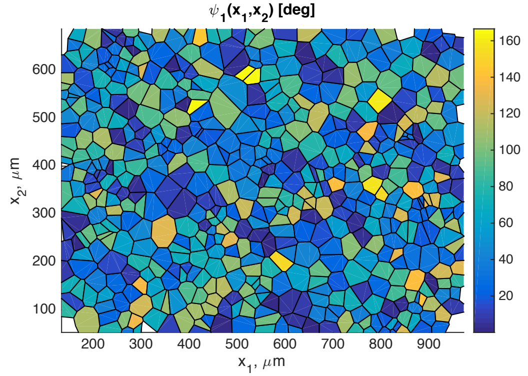
Example

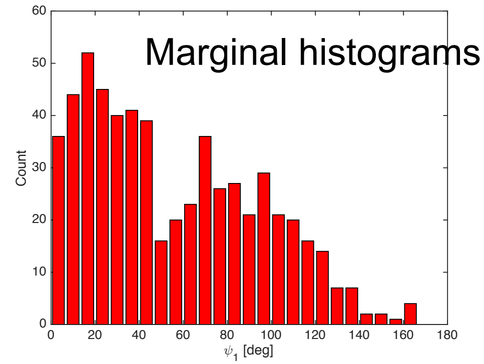
- Given a FE mesh (below)
  1. Calibrate random field model to Ta data set (J. Carroll, 5/17/13)
  2. Produce samples of 3 Euler angles on given FE mesh for later analysis with Sierra mechanics



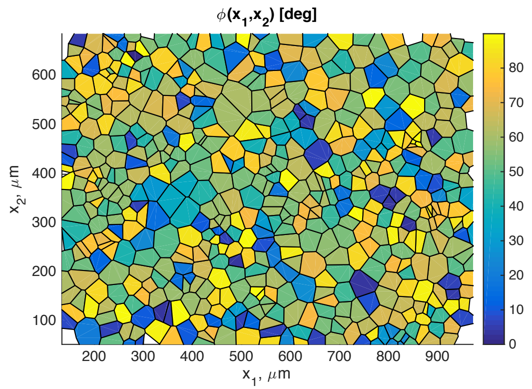
Experimental Data

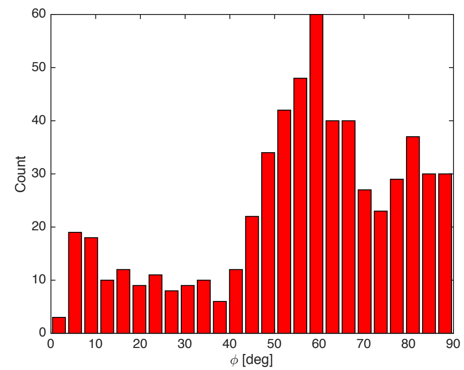
Angle 1: ψ_1



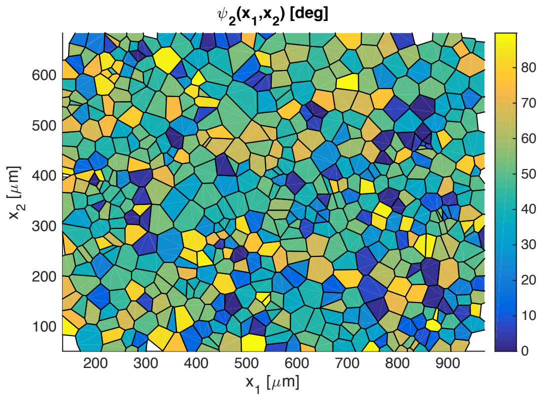


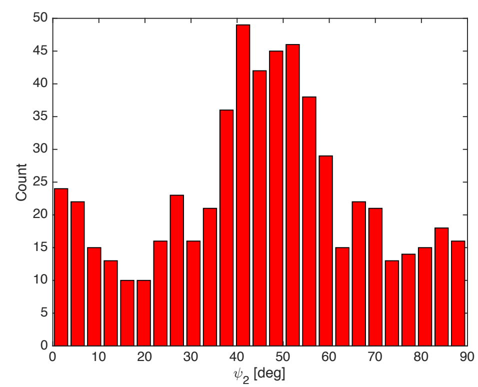
Angle 2: ϕ

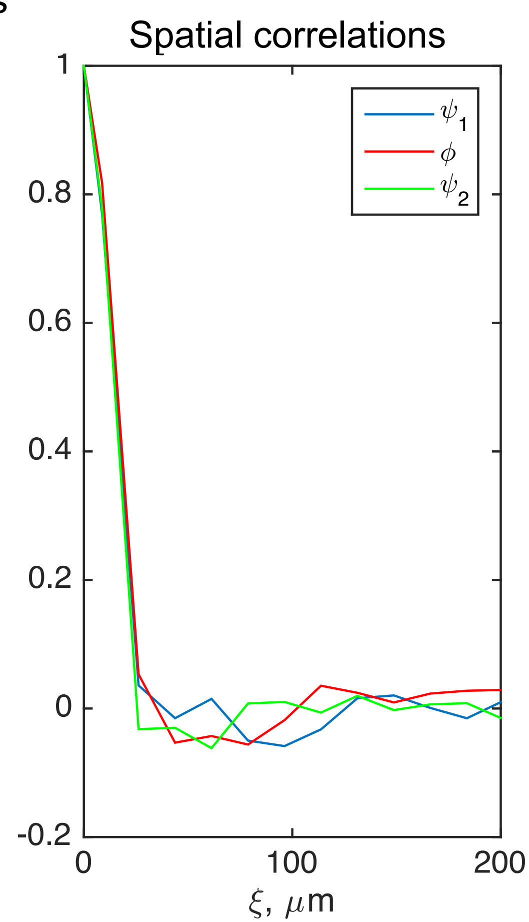




Angle 3: ψ_2

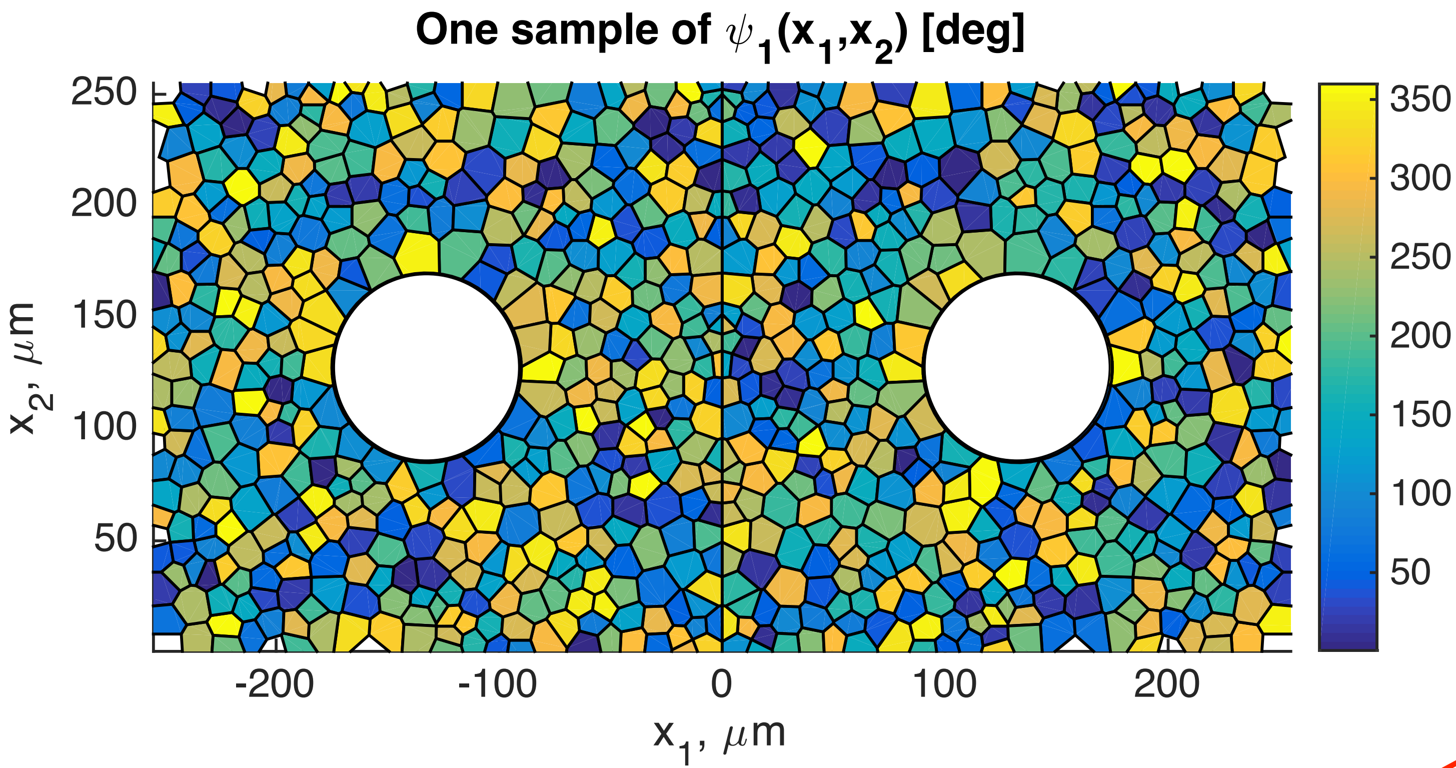


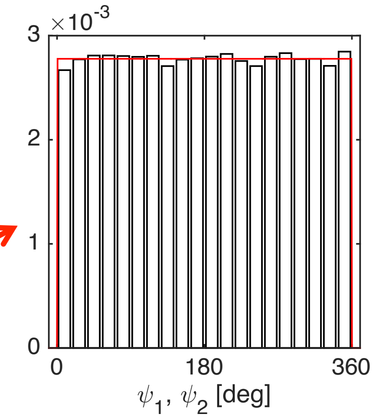




Samples of Random Field

- Zero texture, zero spatial correlation

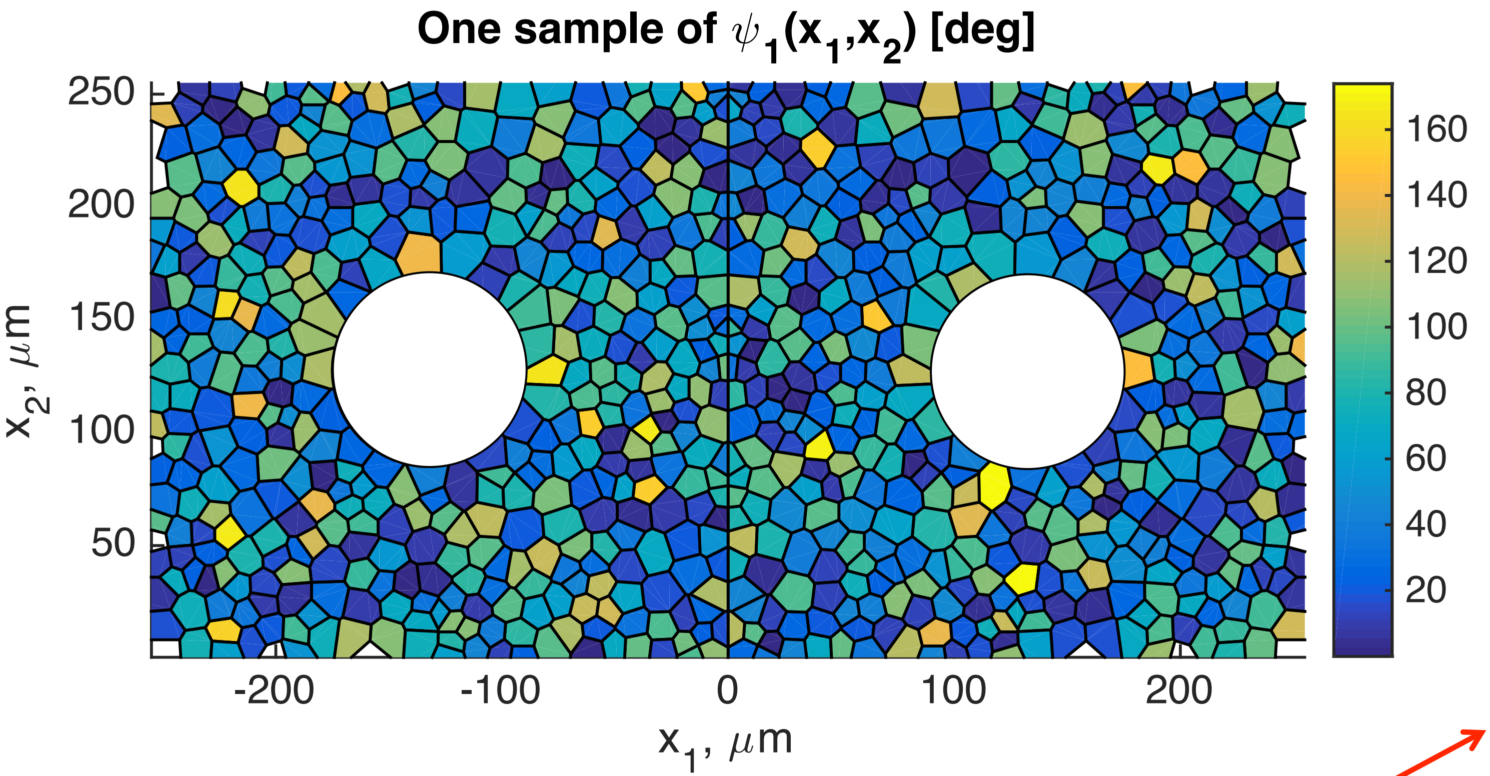


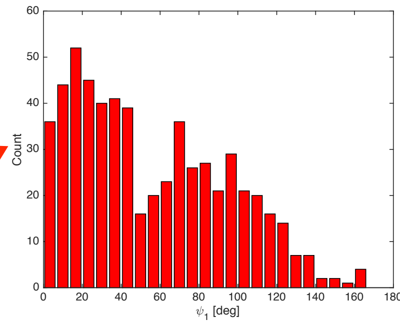


Marginal histogram of ψ_1

Samples of Random Field

- With texture based on data file, zero spatial correlation

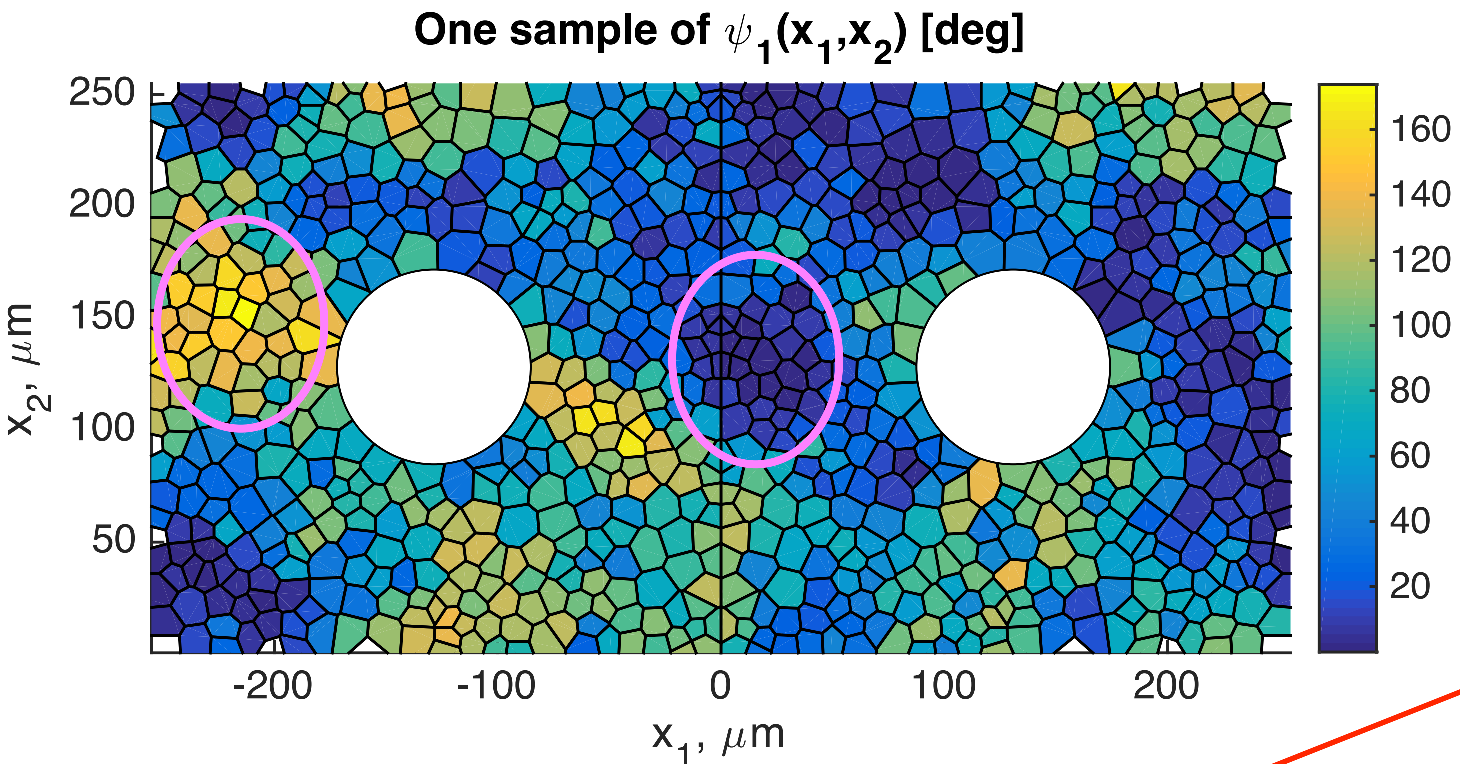




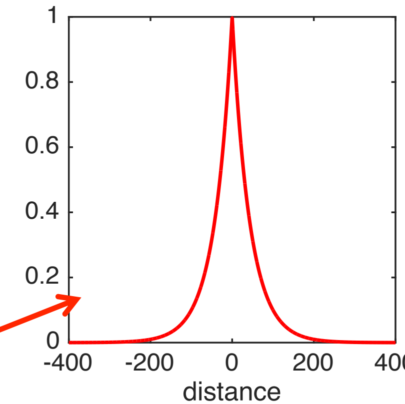
Marginal histogram of ψ_1

Samples of Random Field

- With texture based and spatial correlation
  - Texture based on data file
  - Isotropic (exponential) spatial correlation with correlation length = 200



"Micro"-texture is present



Autocorrelation function of ψ_1

Summary

- Texture can be described by 3 Euler angles
- Texture is random in a material microstructure, so we need a vector-valued random field model to describe the Euler angles
- We have provided such a model
  - Can be calibrated to experimental data
    - Marginal distributions and spatial correlations
  - Address both “micro” and “macro” texture
  - Sample generation for an arbitrary FE mesh is straightforward
- Model is implemented in “EulerRF”
  - Matlab code
  - Intended to be stand alone and used by any interested analysts

Some References

- S. Arwade and M. Grigoriu. Probabilistic model for polycrystalline microstructures with application to intergranular fracture, *Journal of Engineering Mechanics*, 130(9):997–1005, 2004.
- N. Cressie. *Statistics for Spatial Data*, Wiley, 1993.
- O. Engler and V. Randle. *Introduction to Texture Analysis: Macrotexture, Microtexture, and Orientation Mapping*, CRC Press, 2010.
- R. Field, Jr. A translation random field model for the Euler angles describing crystallographic orientation in a material microstructure, *Sandia Technical Memo*, July 8, 2013.
- S. Torquato. *Random Heterogeneous Materials: Microstructure and Macroscopic Properties*, Springer, 2002.

Entropy and "Degree of Texture"

- I have not seen any quantitative measure for the "degree" or "amount" of texture
  - Needed to compare texture of one specimen relative to another
  - Is there interest in this?

- One possible approach is using relative entropy
  - Motivated by the convention that "zero texture" is "fully random"
  - The entropy of Y with pdf g_Y w.r.t. X with pdf f_X

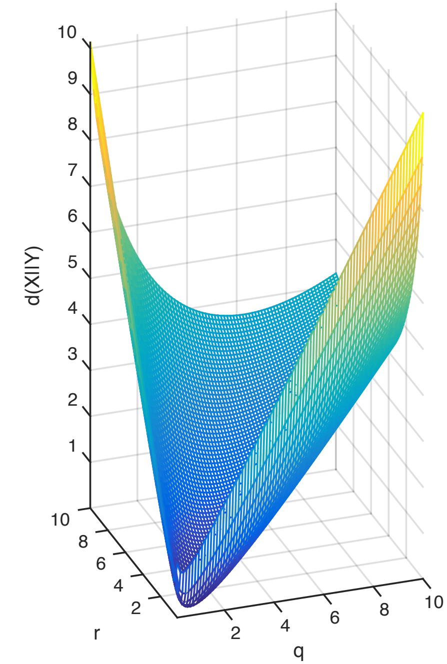
$$d(X||Y) = \int_{\{u:\ f_X(u),\, g_Y(u)>0\}} f_X(u) \log_b \left(\frac{f_X(u)}{g_Y(u)} \right) \mathrm{d}u$$

$$d(X||Y) \geq 0$$

Examples

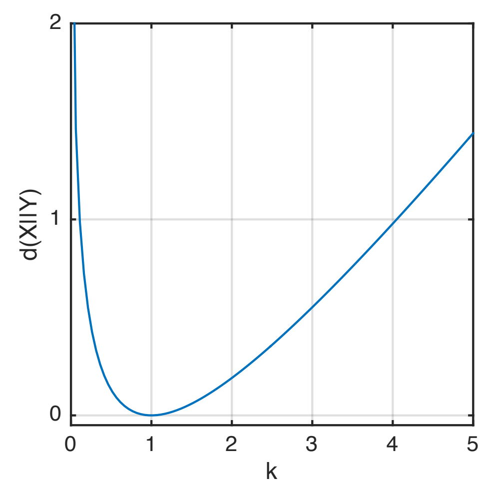
- Entropy of Beta(*q*,*r*) relative to Uniform(0,1)

$$d(X||Y) = \int_0^1 \ln\left(\frac{B(q,r)}{u^{q-1}(1-u)^{r-1}}\right) \mathrm{d}u$$
$$= q + r - 2 + \ln B(q,r)$$



- Entropy of Gamma(*k*,1\λ) relative to Exp(λ)

$$d(X||Y) = \frac{1}{k\,\theta}\int_0^\infty e^{-u/k\,\theta} \ln\left(\frac{\theta^{k-1}\Gamma(k)}{k}\, u^{1-k}\, e^{-u(1-k)/k\,\theta}\right) \mathrm{d}u$$
$$= (1+\gamma)(k-1) - k\,\ln k + \ln\Gamma(k)$$



Apply to Crystallographic Texture

- For our case (crystallographic texture)
  - Reference (*X*) is the "zero texture" case
  - Specimen (*Y*) has texture described by measured Euler angles

$$d(0||(\psi_1,\phi,\psi_2)) = \frac{\pi}{2\,\alpha_1\alpha_2\beta}\int_0^{\alpha_1}\int_0^{\beta}\int_0^{\alpha_2}\sin\left(\frac{\pi\,u_2}{\beta}\right)\ln\left(\frac{\pi\sin\left(\frac{\pi\,u_2}{\beta}\right)}{f(u_1,u_2,u_3)}\right)\mathrm{d}u_1\,\mathrm{d}u_2\,\mathrm{d}u_3$$

$$f(u_1,u_2,u_3) = \text{ joint PDF of } (\psi_1,\phi,\psi_2)$$

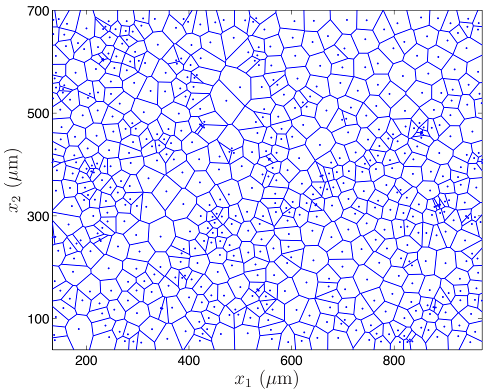
$$d(0||(\psi_1,\phi,\psi_2)) \geq 0$$

- Procedure
  - Estimate *f* from data using, for example, histograms or KDEs
  - Solve for *d* numerically

"Degree of Texture" for Some Data

- I applied the approach to determine degree of texture for two data sets

1. Rolled plate of Ta
   - 589 grains, 640 μm x 750 μm
   - J. Carroll sent to me on 5/17/2013
   - Degree estimate: d = 23.0



2. Ta wire
   - "Drawn in a direction normal to the plane in which measurements were taken"
   - 2,107 grains, 100 μm x 28 μm
   - J. Carroll sent to me on 5/23/2013
   - Degree estimate: d = 20.4