

# VISUALIZATION AND ANALYSIS IN MATERIALS SCIENCE

---

**REU: Brian Sayre (Muskingum University)**

**and Lisa Kam (Baton Rouge Magnet High School)**

**Mentors: Dr. Les Butler (LSU)**

**and Dr. Robert Beaird (LSU)**

# OVERVIEW

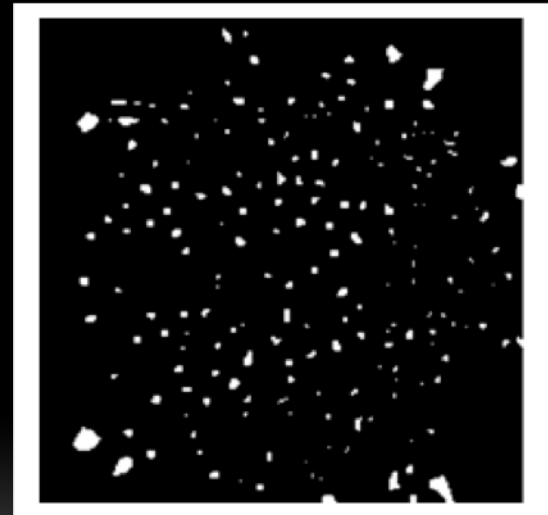
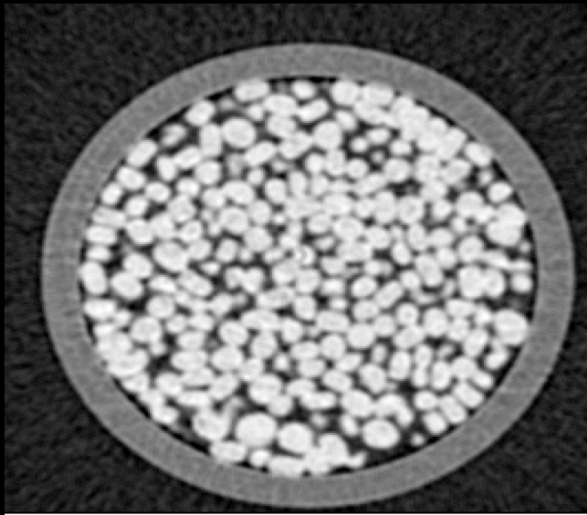
- Image Segmentation & Label Fields
- Spherical Harmonics
- What Our Code Does
- Are we “reinventing the wheel?”

# PROJECT OBJECTIVES

1. Characterize the surface of thousands of 3-D particles.
  - Use image segmentation to generate a label field.
  - Pick a single particle out of the label field.
  - Use spherical harmonics to characterize the surface of the particle.
  - Characterize every particle's surface in a data set.
2. Determine if two particles could be similar in shape and size.
  - Use the moment of inertia tensor, surface area and volume.

# IMAGE SEGMENTATION & LABEL FIELD

- Image segmentation divides an image into multiple parts and creates a label field.
- Technique used: marker-controlled watershed segmentation



# SPHERICAL HARMONICS

- How would you mathematically characterize this plot of data?

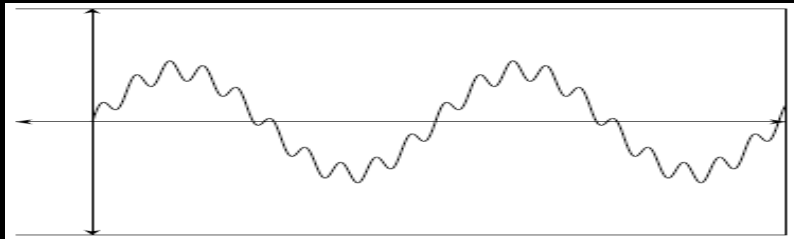
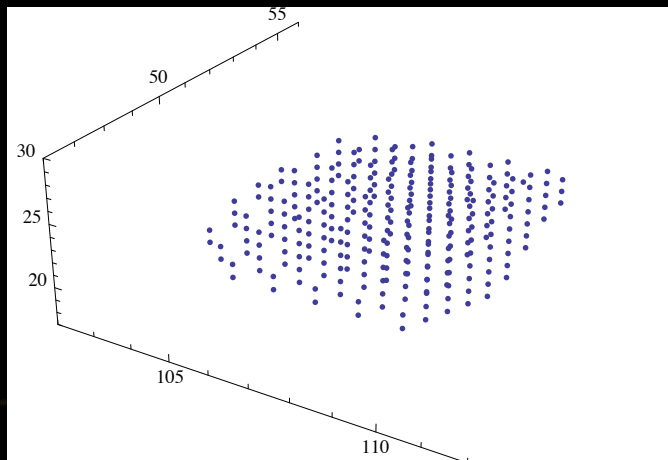


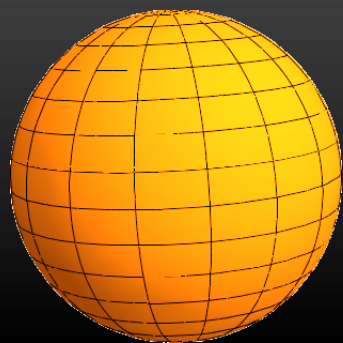
Photo: [www.learner.org](http://www.learner.org)

You would use a set of sine and cosine functions.

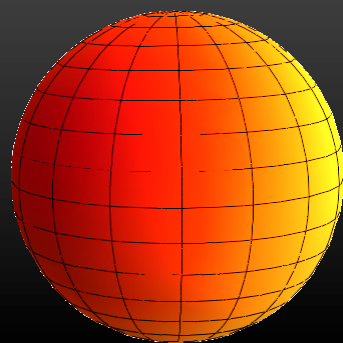
- So, how would you characterize this object?



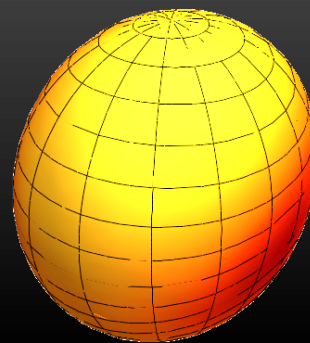
You would use a set of functions called spherical harmonics.



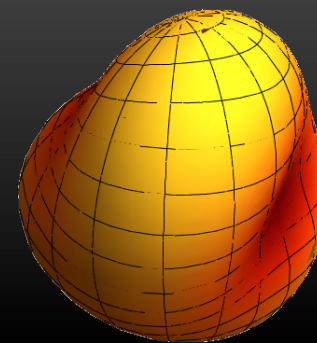
$\ell = 0$



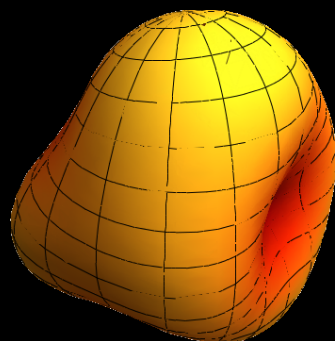
$\ell = 1$



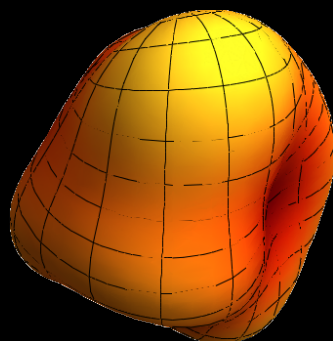
$\ell = 2$



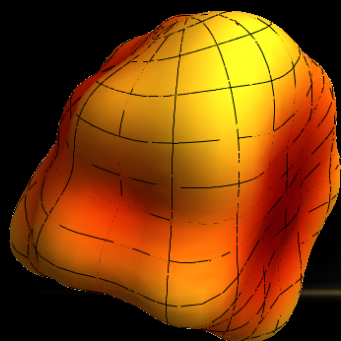
$\ell = 3$



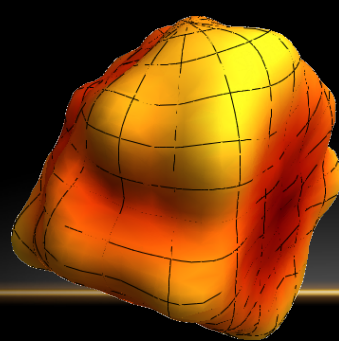
$\ell = 4$



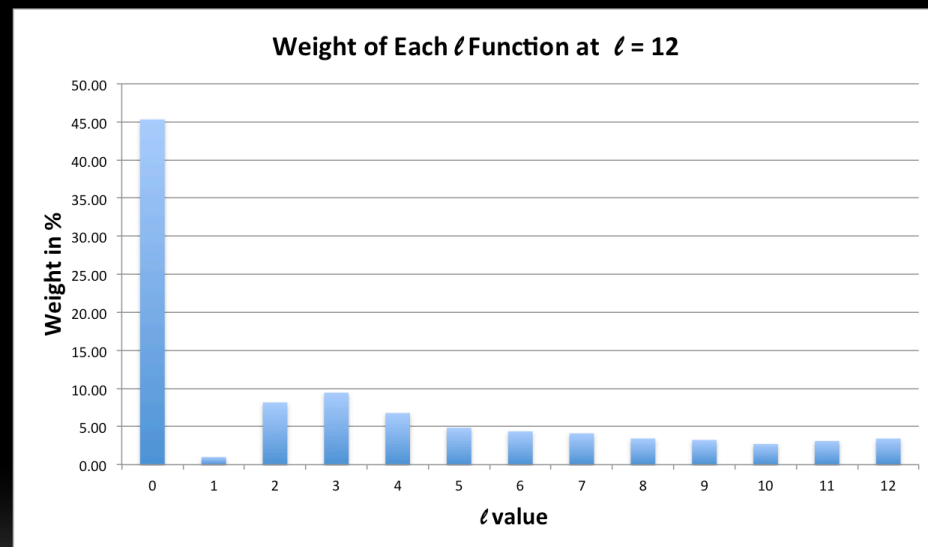
$\ell = 5$



$\ell = 9$

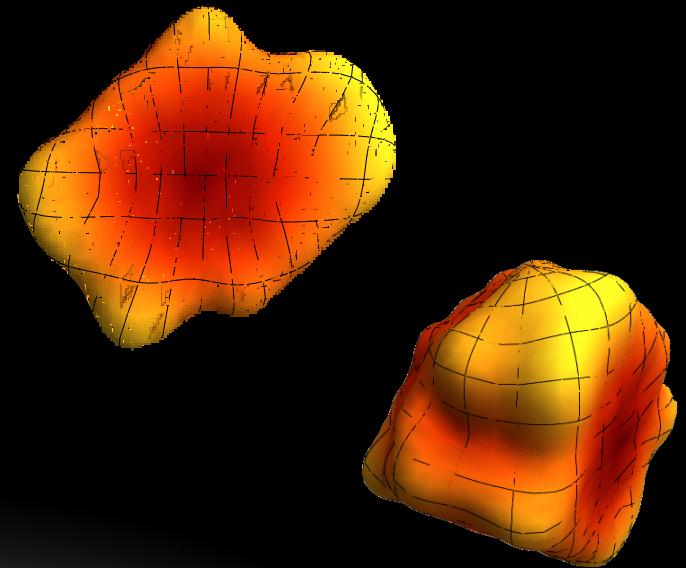
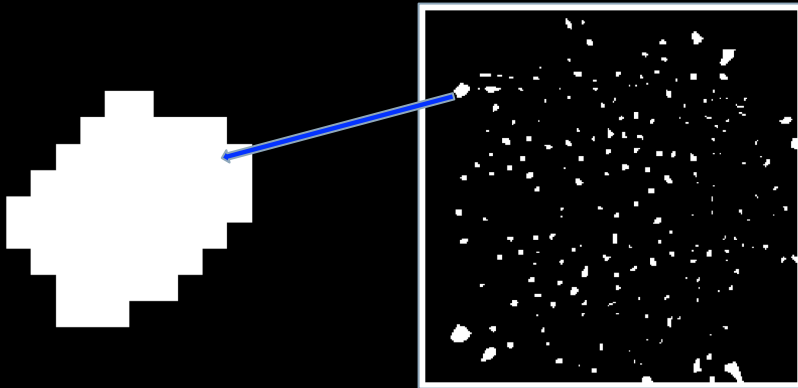


$\ell = 12$



# WHAT OUR CODE DOES

- Takes a 3-D particle out of a label field
- Generates a 3-D model using spherical harmonics. Also calculates moment of inertia tensor and center of mass.



## WHY 'RE-INVENT THE WHEEL?'

- Fortran code is hard to read and is very long.
  - Garboczi's code is 32 pages long.
- *Mathematica*<sup>®</sup> code is:
  - Much easier to read and understand.
  - Much shorter.
  - Much easier to update.



# ACKNOWLEDGEMENTS

- We would like to thank Dr. Les Butler and Dr. Robert Beaird for their help and support throughout the entire project.
- Dr. Ed Garboczi for providing us with his Fortran code that we used as a basis for our code.
- This material is based upon work supported by the National Science Foundation under the NSF EPSCoR Cooperative Agreement No. EPS-1003897 with additional support from the Louisiana Board of Regents. LB thanks the NSF (CHE-0910937 ).

# REFERENCES

- <http://www.physics.arizona.edu/~varnes/Teaching/321Fall2004/Notes/Lecture34.pdf>
- <http://www.wolfram.com/mathematica/>
- <http://rsbweb.nih.gov/ij/>
- <http://www.mathworks.com/products/matlab/>
- <http://mathworld.wolfram.com/SphericalHarmonic.html>
- [www.learner.org](http://www.learner.org)

QUESTIONS/COMMENTS?

# MOMENT OF INERTIA TENSOR

- The moment of inertia tensor is used in this project mainly to align objects.
- Can also be used to determine if objects may be of similar shape and size.
  - Cannot always say if objects are identical, but can often tell when very different.

$$I_{ij} = \int_V \rho(\vec{r}) d^3 r (\delta_{ij} r^2 - x_i x_j)$$

$$I = \begin{bmatrix} I_{11} & I_{12} & I_{13} \\ I_{21} & I_{22} & I_{23} \\ I_{31} & I_{32} & I_{33} \end{bmatrix}$$

$$I = \begin{bmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{bmatrix}$$