Carnegie Mellon University

Shape Descriptors for the Quantification of Microstructures

Aerospace Materials for Extreme Environments, Program Review
February 11-15, 2013

Marc De Graef, PI

AFOSR-FA9550-12-1-0475

Outline

- Motivation
- Shape descriptors: why use them?
- Moment invariants and such…
  - 2D
  - 3D
- Alternative moment approaches
- Conclusions & Future work

Motivation

- Microstructure and properties modeling requires availability of reliable and accurate descriptions of grain and particle shapes.
  - make a library of real shapes and reuse them
  - quantify shapes and sample distributions of shape descriptors to generate new shapes with similar characteristics
  - generate shapes using physics-based modeling (requires objective comparison between digital and real shapes)

Motivation

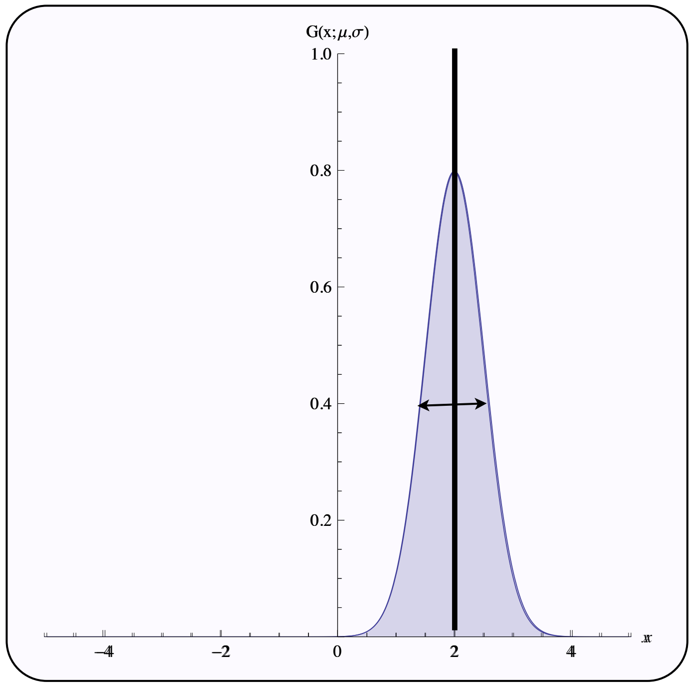
- Shapes are typically described
  - verbally (mostly shape classes, conveys limited quantitative information)
  - mathematically (implicit or explicit equation, exact description)
  - digitally (voxel grid, characteristic or shape function, approximate)
  - graphically (triangles or higher order polygons covering the surface, approximate)
- The human brain is VERY good at identifying shapes;
- To mimic this in a computer program is VERY difficult.

Current Practice

- When comparing experimentally observed shapes with theoretical predictions/simulations or reconstructions, one often uses/hears phrases like
  - “that looks good!” or
  - “they look pretty much the same”
- Our long-term goal is to replace these statements by quantitative ones…

A familiar concept: 1-D moments

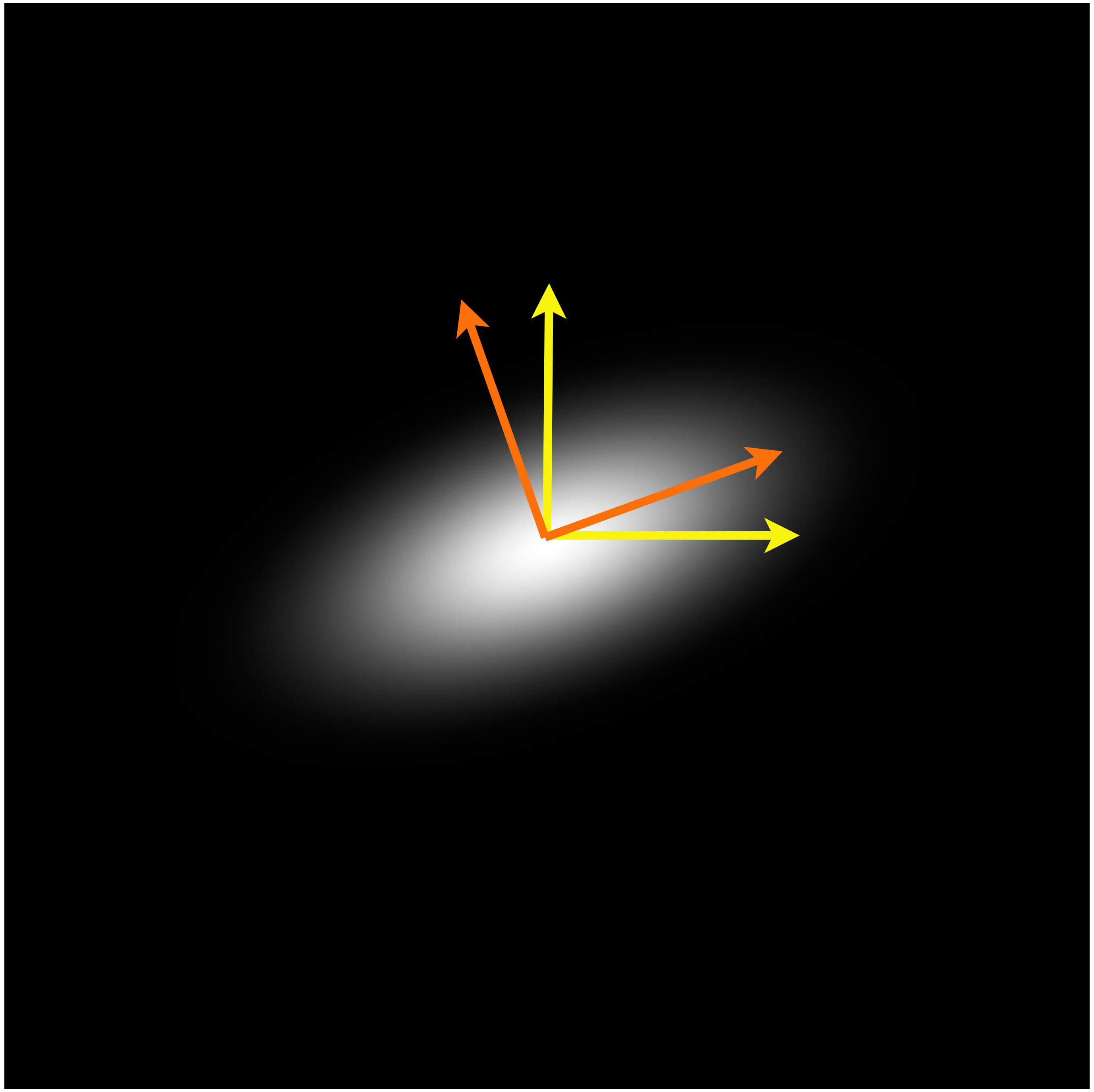
Gaussian $G(x;\mu,\sigma) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$



Moments

Order 0	$\int_{-\infty}^{+\infty} \mathrm{d}x\, G(x;\mu,\sigma)$	Area	1
Order 1	$\int_{-\infty}^{+\infty} \mathrm{d}x\, xG(x;\mu,\sigma)$	Mean	μ
Order 2	$\int_{-\infty}^{+\infty} \mathrm{d}x\, x^2G(x;\mu,\sigma)$	Width	$\mu^2+\sigma^2$
Order 3	$\int_{-\infty}^{+\infty} \mathrm{d}x\, x^3G(x;\mu,\sigma)$	Skewness	"asymmetry"
Order 4	$\int_{-\infty}^{+\infty} \mathrm{d}x\, x^4G(x;\mu,\sigma)$	Kurtosis	"peakedness"

What about 2-D ?

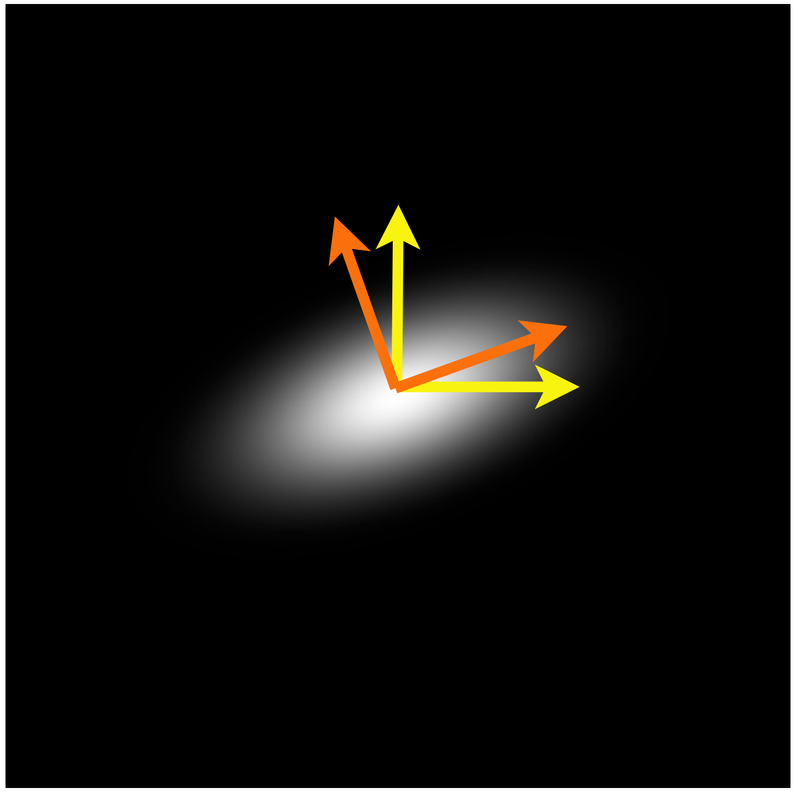


What about 2-D ?

- Multiple reference frames are possible
- One is special ("eigen" frame, in orange)
- Moments depend on the reference frame...

$$\mu_{pq} = \iint_D \mathrm{d}x\mathrm{d}y\, x^p y^q$$

- A coordinate-independent moment description is highly desirable



2-D moment invariants

$$\mu_{00} = A \text{ (area)}$$

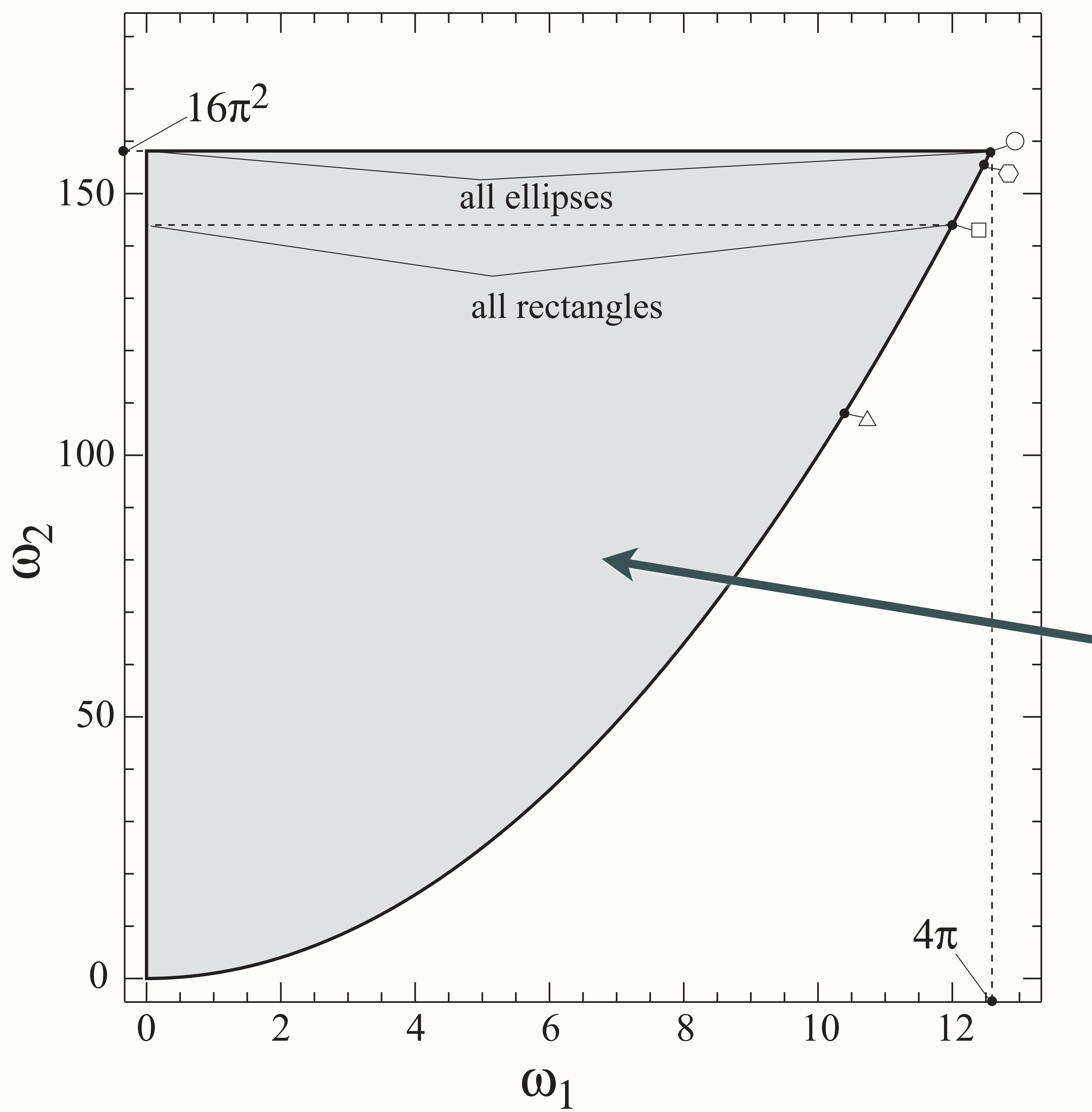
$$(\mu_{10}, \mu_{01}) = \text{ center-of-mass}$$

$$(\mu_{20}, \mu_{02}, \mu_{11}) = \text{ moments-of-inertia}$$

There are two dimensionless combinations of moments that are invariant under similarity or affine coordinate transformations:

$$\omega_1 = \frac{2A^2}{\mu_{20} + \mu_{02}} \quad \text{and} \quad \omega_2 = \frac{A^4}{\mu_{20}\mu_{02} - \mu_{11}^2}$$

There are the moment invariants (MIs) of second order.



SOMIM

Second Order
Moment Invariant Map

All 2D shapes lie inside this grey area !

3-D moment invariants

- Consider the shape function of an object:

$$D(\mathbf{r}) = \begin{cases} 1 & \mathbf{r} \text{ inside} \\ 0 & \mathbf{r} \text{ outside} \end{cases}$$

- The cartesian shape moments are defined as:

$$s_{pqr} = \int_{\text{all space}} \mathrm{d}^3\mathbf{r}\, x^p y^q z^r D(\mathbf{r}) = \int_V \mathrm{d}^3\mathbf{r}\, x^p y^q z^r$$

- These can be computed efficiently

see Novotni & Klein, *Shape retrieval using 3D Zernike descriptors*. Computer-Aided Design, 36:1047–1062, 2004

- Certain algebraic combinations of moments are invariant with respect to coordinate transformations

3-D moment invariants

- The second order moment invariants are:

$$\Omega_1 = \frac{3V^{5/3}}{\bar{\mu}_{200} + \bar{\mu}_{020} + \bar{\mu}_{002}} = \frac{3V^{5/3}}{I_1};$$

$$\Omega_2 = \frac{3V^{10/3}}{\bar{\mu}_{200}\bar{\mu}_{020} + \bar{\mu}_{200}\bar{\mu}_{002} + \bar{\mu}_{020}\bar{\mu}_{002}} = \frac{9V^{10/3}}{I_2};$$

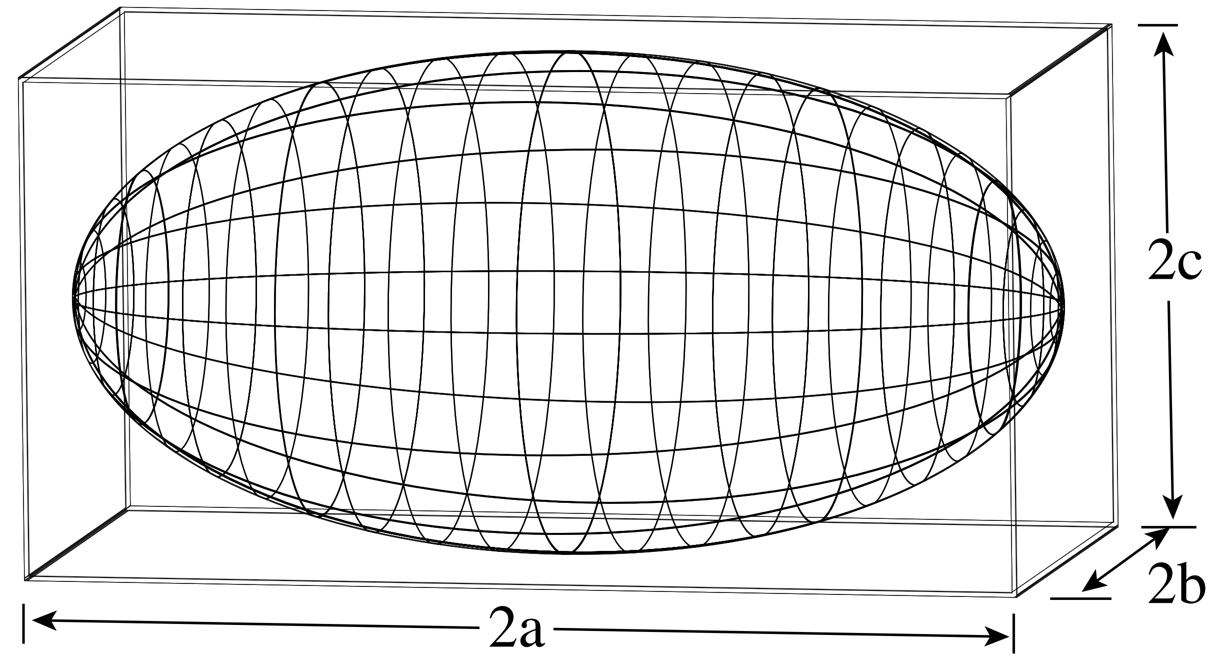
$$\Omega_3 = \frac{V^5}{\bar{\mu}_{200}\bar{\mu}_{020}\bar{\mu}_{002}} = \frac{3^3 V^5}{I_3}$$

- Typically, we normalize these numbers by the sphere numbers, to get invariants in the interval [0,1]

Example: Ellipsoid

$$\tau_1 = b/a$$

$$\tau_2 = c/a$$



$$\Omega_1 = \left(\frac{2000\pi^2}{9}\right)^{1/3} \frac{3\tau_1{\tau_2}^{2/3}}{1+\tau_1^2+\tau_2^2}$$

$$\Omega_2 = \left(\frac{2000\pi^2}{9}\right)^{2/3} \frac{3\tau_1{\tau_2}^{4/3}}{\tau_1^2\tau_2^2+\tau_1^2+\tau_2^2}$$

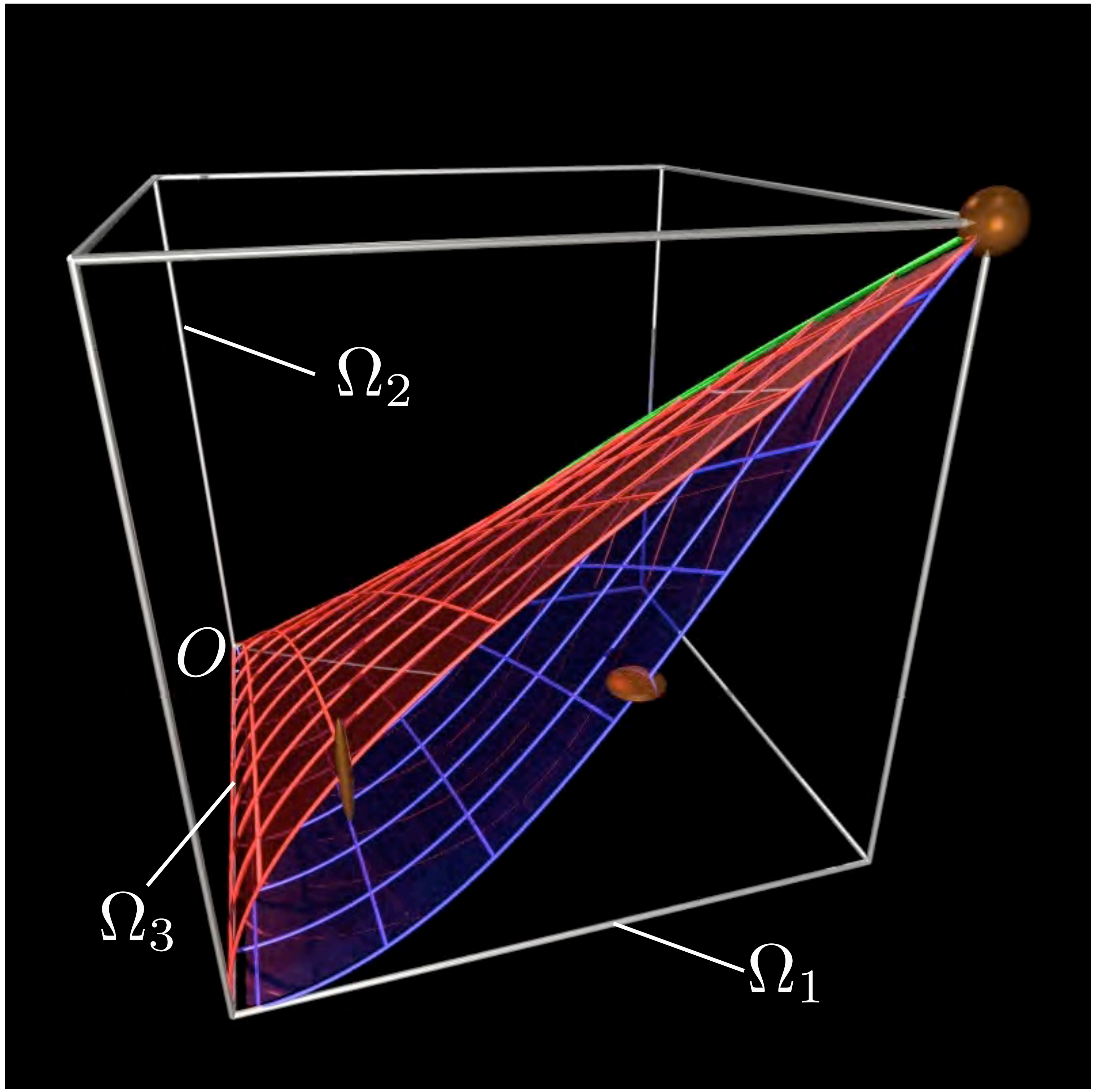
$$\Omega_3 = \frac{2000\pi^2}{9}$$

$$\Omega_1^{\text{Sphere}} = \left(\frac{2000\pi^2}{9}\right)^{1/3}$$

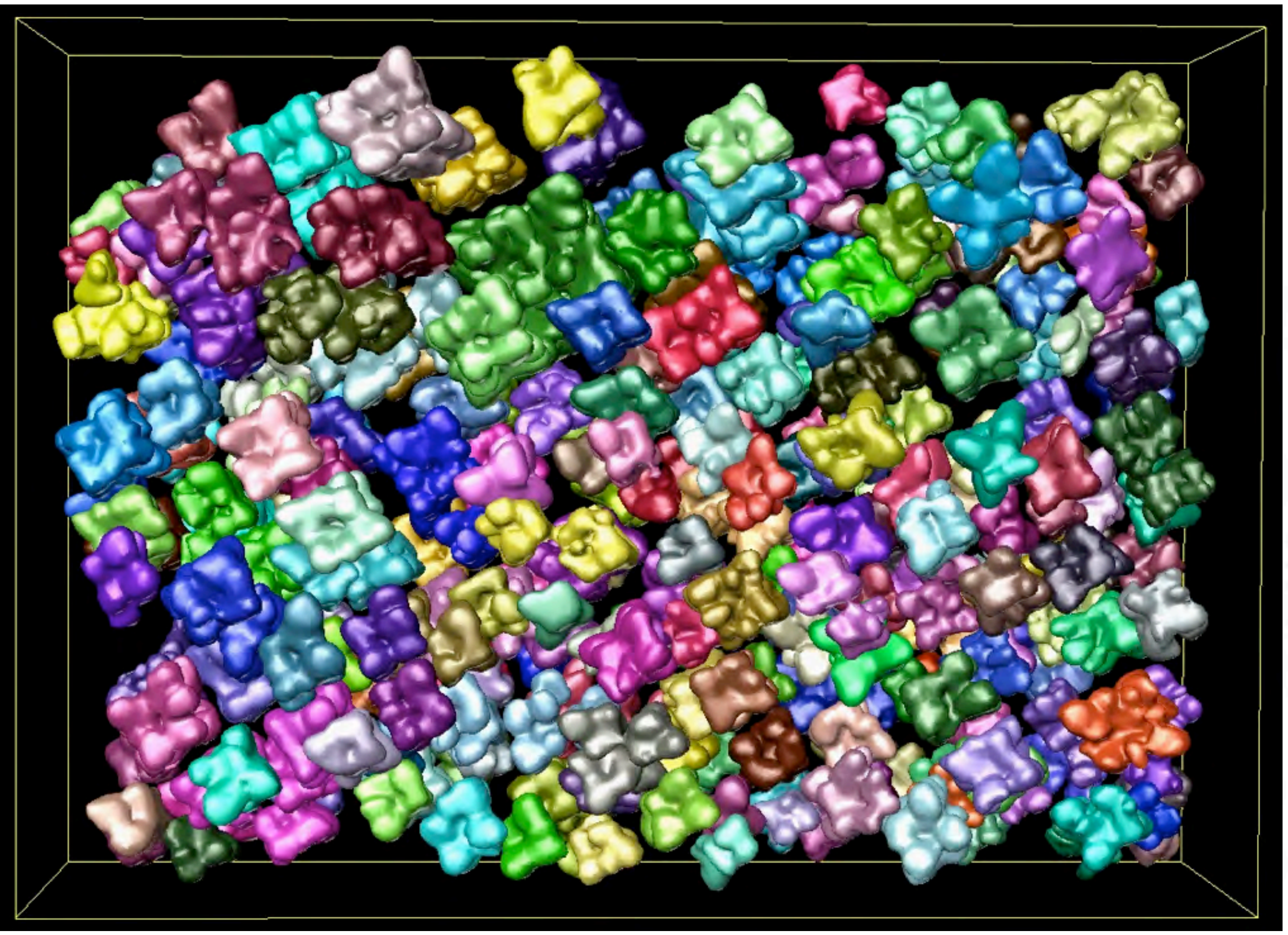
$$\Omega_2^{\text{Sphere}} = \left(\frac{2000\pi^2}{9}\right)^{2/3}$$

$$\Omega_3^{\text{Sphere}} = \frac{2000\pi^2}{9}$$

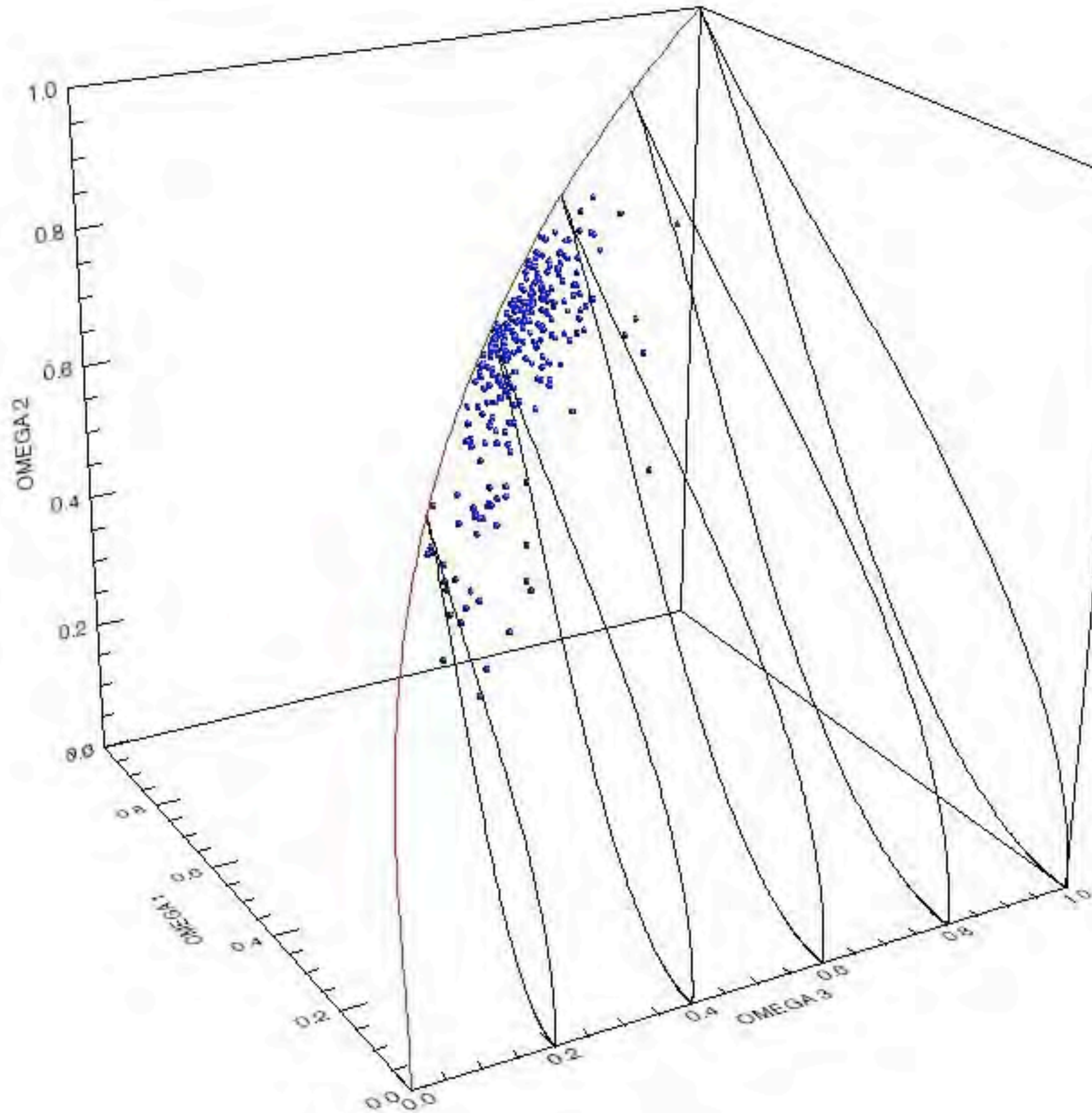
Moment Invariant Space



Moment Invariant Space



Rene88-DT



2-D vs. 3-D

- Modern tools allow for nearly automated 3-D characterization of microstructures; however, the experiments are time-consuming, the equipment is expensive and data analysis is not straightforward.
- Traditional metallography is widely used, relatively cheap and fast, so if we had the ability to determine 3-D shapes based on 2-D sections only, that would be an important improvement.
- Is it possible to have a computer algorithm decide what the most likely 3-D shape is that corresponds to a 2-D image of, say, precipitates in a material?

2-D higher-order moments

Let us consider only 2nd and 4th order invariants...

$$\omega_1 \equiv \frac{A^2}{2\pi(\bar{\mu}_{20} + \bar{\mu}_{02})};$$

$$\omega_2 \equiv \frac{A^4}{16\pi^2(\bar{\mu}_{20}\bar{\mu}_{02} - \bar{\mu}_{11}^2)}.$$

$$\tau_1 = \frac{A^3}{3\pi^2}\left(\bar{\mu}_{40} + 2\bar{\mu}_{22} + \bar{\mu}_{04}\right)^{-1};$$

$$\tau_2^a = \frac{A^6}{48\pi^4}\left(\bar{\mu}_{40}\bar{\mu}_{04} - 4\bar{\mu}_{31}\bar{\mu}_{13} + 3\bar{\mu}_{22}^2\right)^{-1};$$

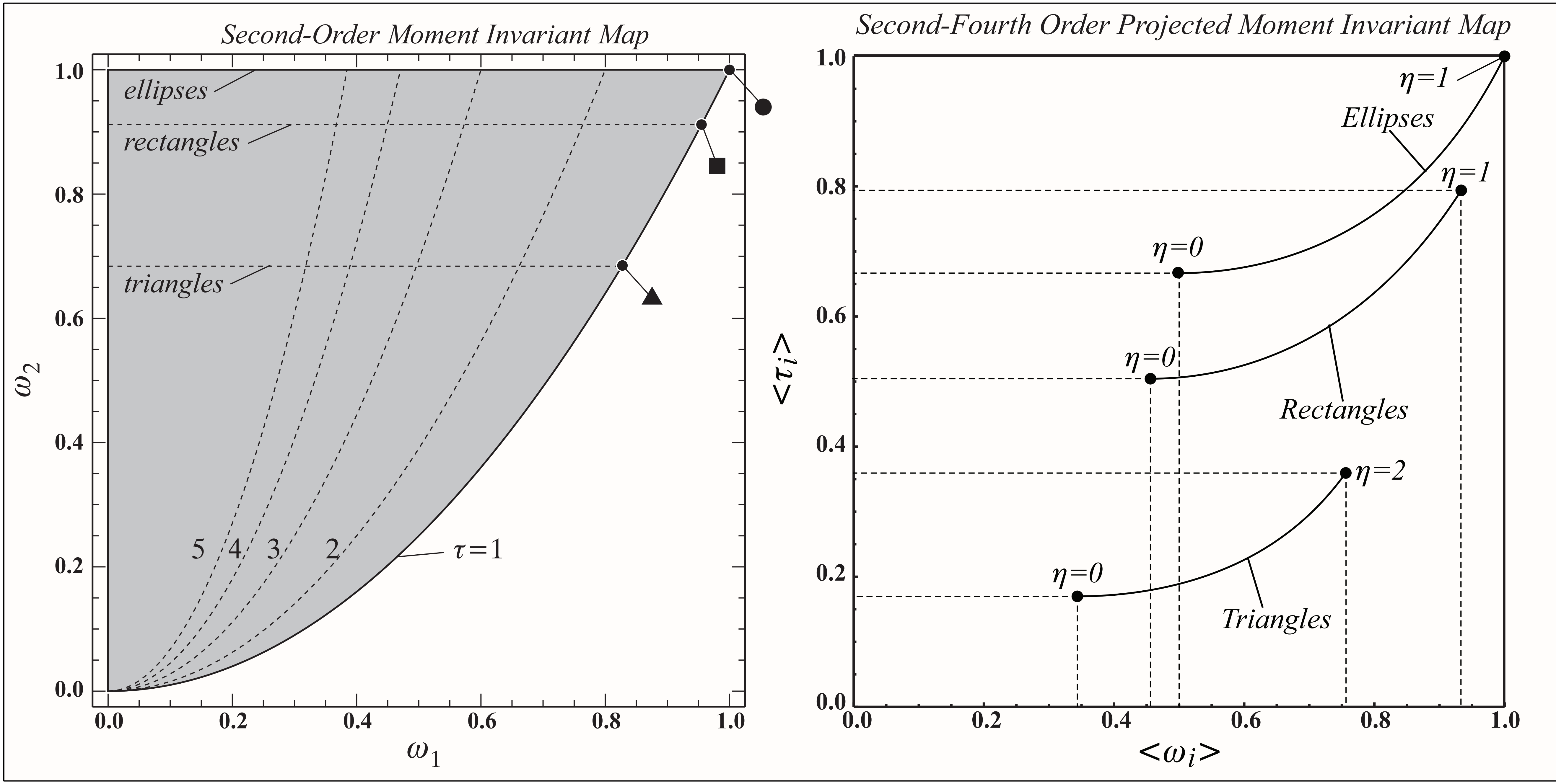
$$\tau_3^a = \frac{A^9}{1728\pi^6}\left(\bar{\mu}_{40}\bar{\mu}_{22}\bar{\mu}_{04} - \bar{\mu}_{40}\bar{\mu}_{13}^2 - \bar{\mu}_{04}\bar{\mu}_{31}^2 + 2\bar{\mu}_{31}\bar{\mu}_{13}\bar{\mu}_{22} - \bar{\mu}_{22}^3\right)^{-1}.$$

This is already a 5-D space ...

5-D: simplification to 2-D

- We'll take the average of the 2nd order and the average of the 4th order invariants, which corresponds to projecting the invariants onto the diagonals of the respective invariant spaces.
- This allows us to create a Projected Moment Invariant Map or PMIM, in addition to the SOMIM that we introduced before.

Moment invariant density maps



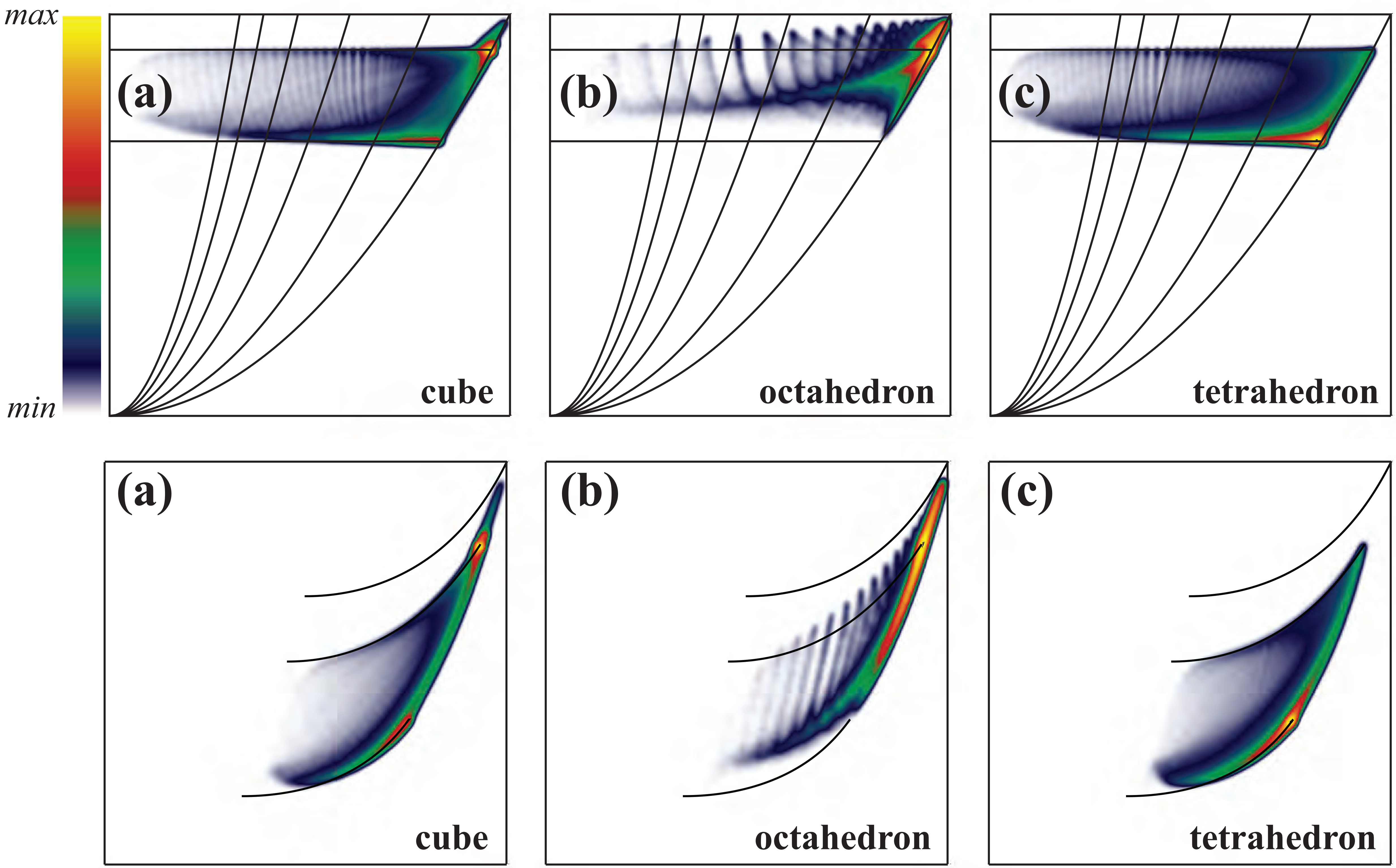
Let's consider two applications of these density maps ...

Carnegie Mellon University

Shape Density Map Library

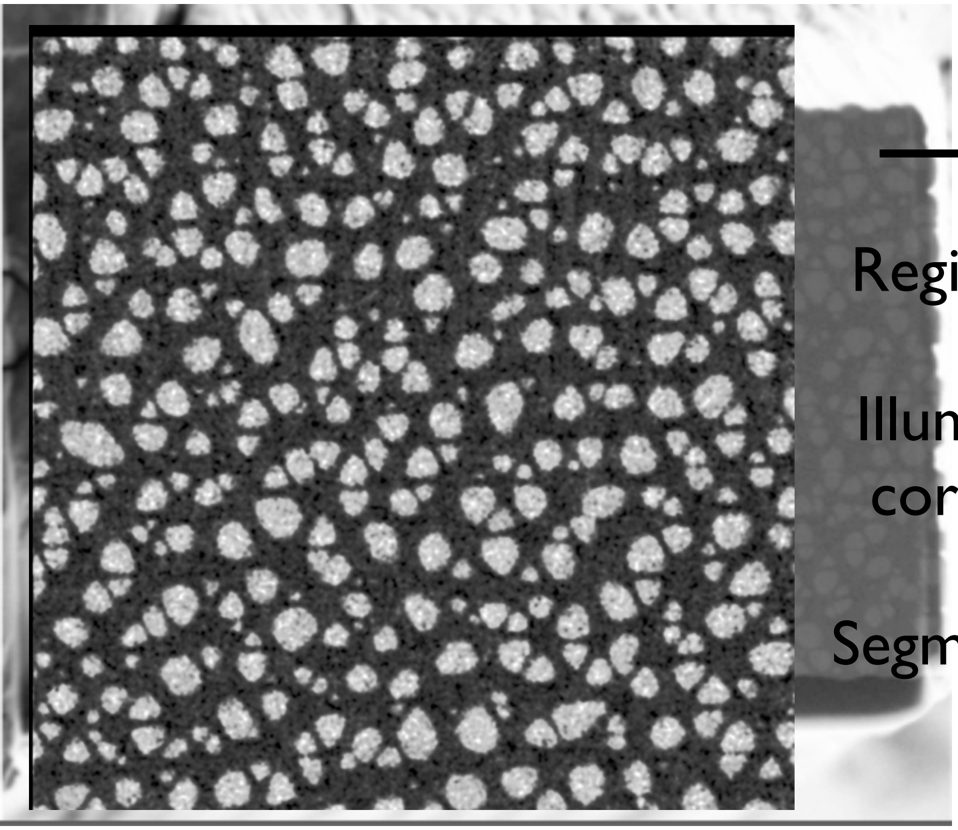
- Pick a 3D shape class, and represent several representative members in a binary array of voxels;
- Slice through these arrays in many random orientations, and for each section, compute the 2^{nd} and 4^{th} order moment invariants;
- This produces, for each section, a single point in the SOMIM and PMIM maps;
- Accumulate many points for thousands of random sections and plot the SOMIM and PMIM maps as density maps; the value in a given point is then proportional to the probability that a random section through the object will produce the corresponding values of the moment invariants.
- Do this for a series of shape class members to create a density map library.

Examples


max
min
(a)
cube
(b)
octahedron
(c)
tetrahedron
(a)
cube
(b)
octahedron
(c)
tetrahedron

Experimental alloy UMF-19

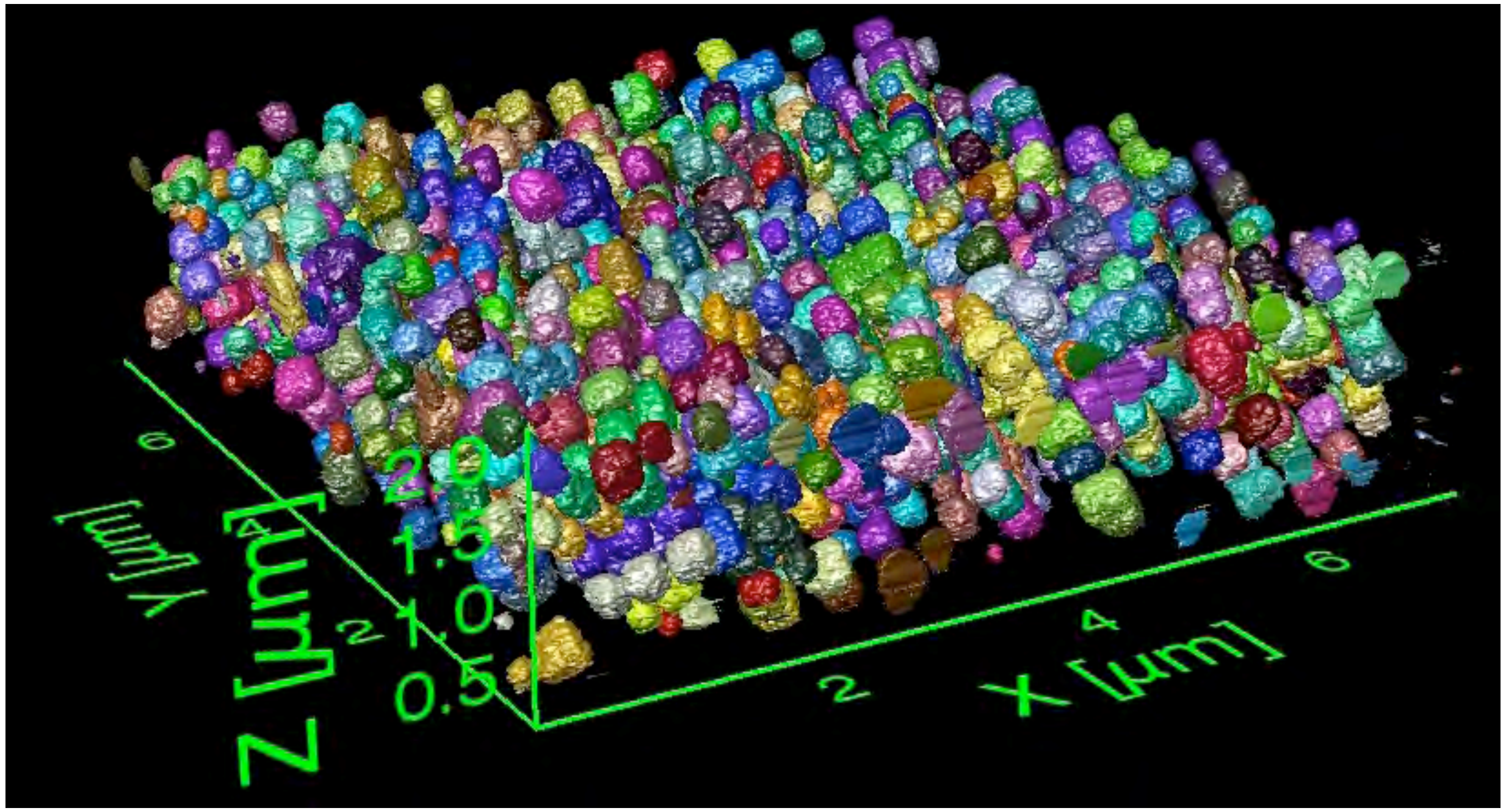
Ni-6.0Al-7.2Co-6.7Cr-4.5Re-8.1Ta-3.0W-5.7Ru
Alloy courtesy of T. Pollock, UCSB



Registration

Illumination correction

Segmentation



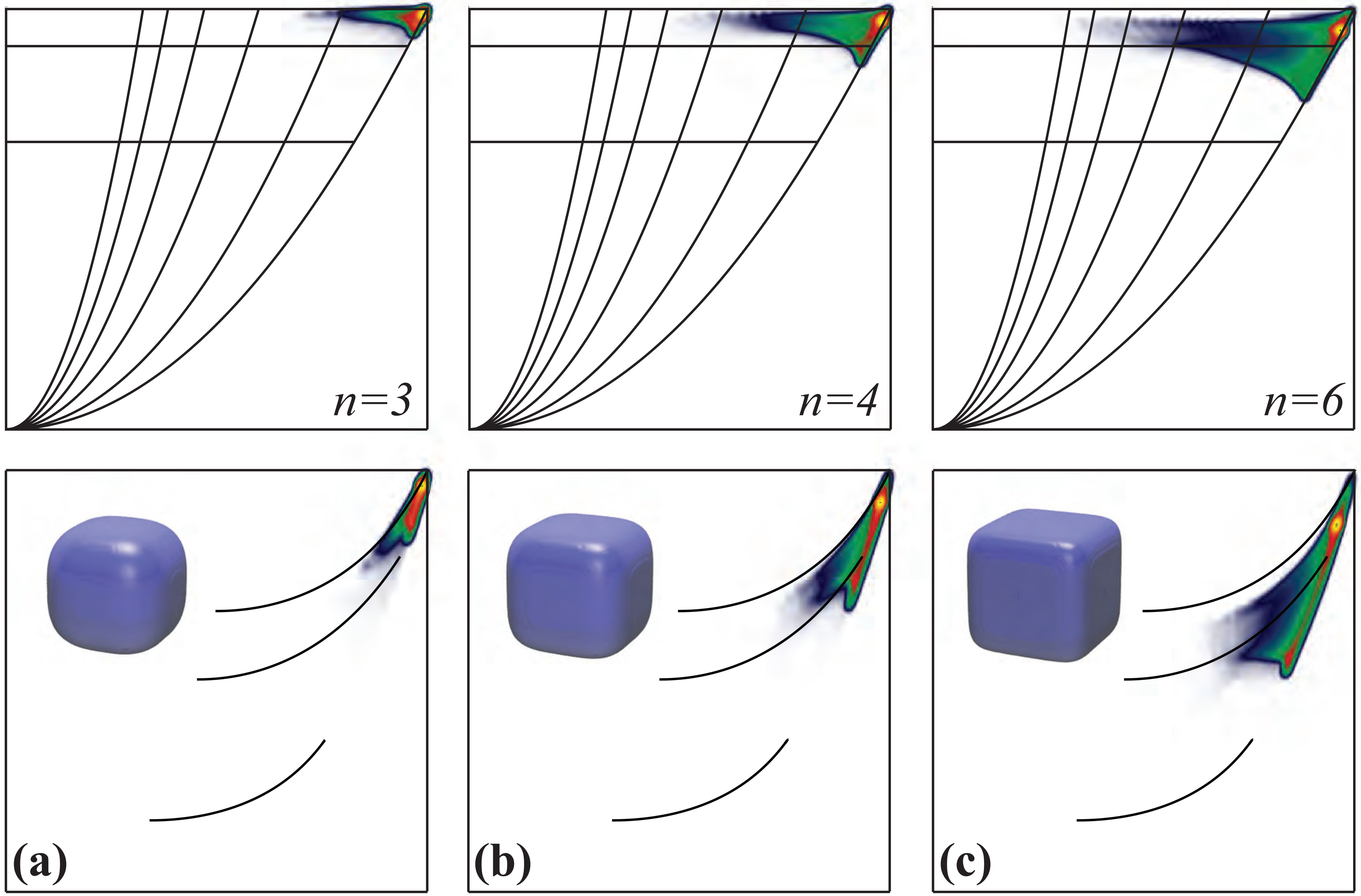
Focused Ion Beam Serial Sectioning

140 slices near [111]
7x7 microns, 20 nm slices

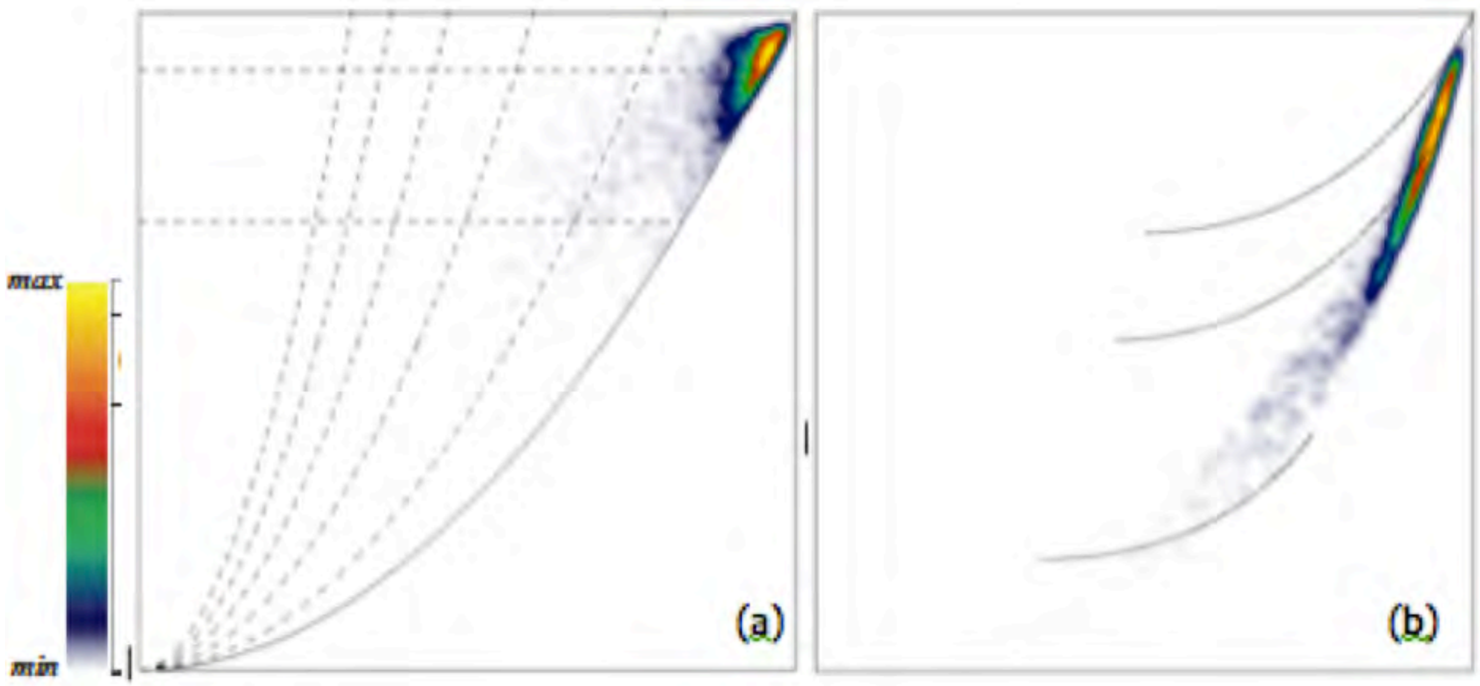
These precipitates are described to have a cuboidal shape. Can we be more precise and quantify these shapes, given a shape class? And, can we do this if we consider only the 2-D shapes?

Cuboidal shapes: superellipsoid

Shape class: $$\left|\frac{x}{a}\right|^n + \left|\frac{y}{b}\right|^n + \left|\frac{z}{c}\right|^n = 1$$

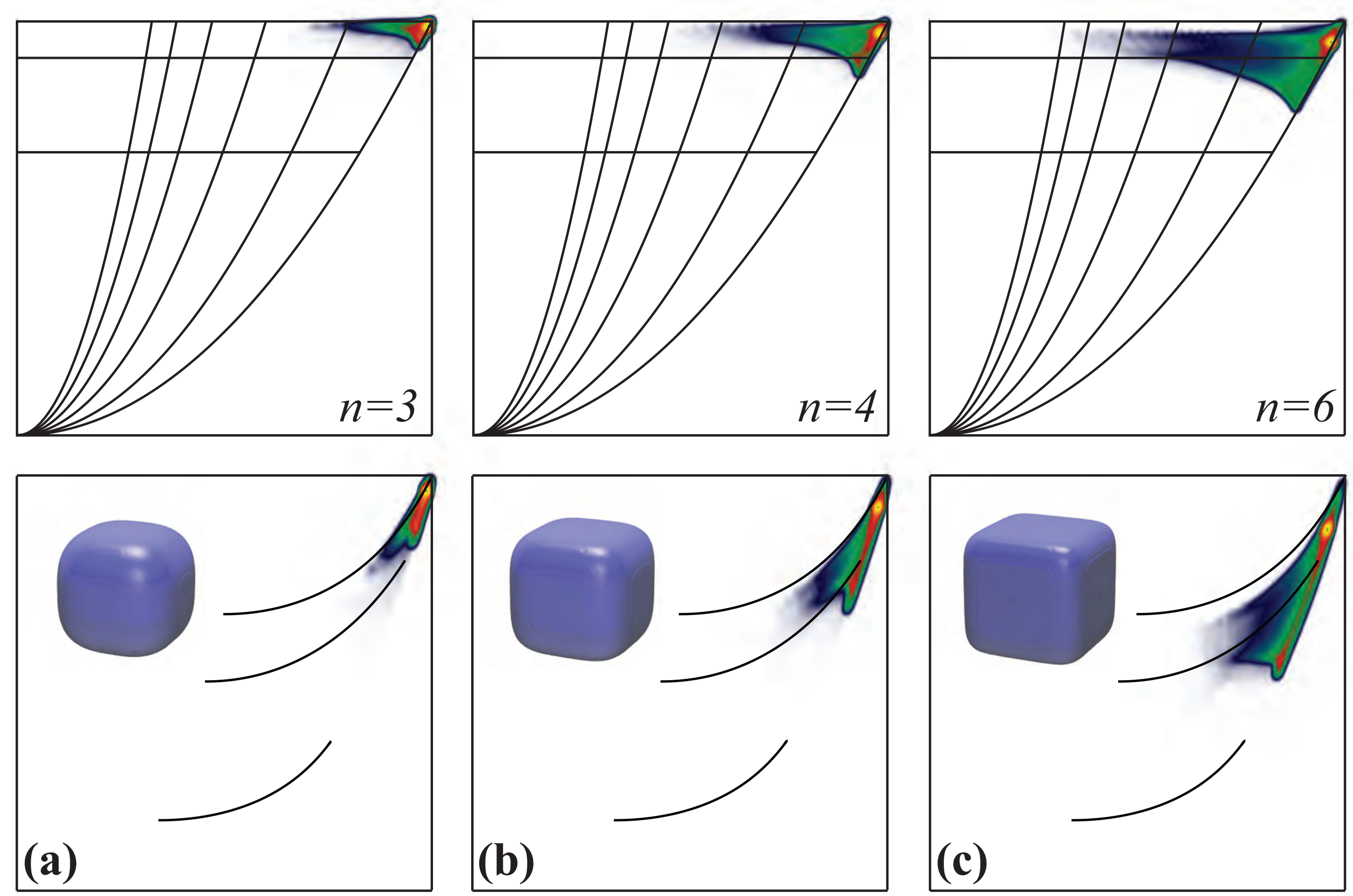


UMF-19 2-D sections



Experimental data

Superellipsoid library maps



Comparison of maps

The modified *Bhattacharyya coefficient* $H(p,q)$, also known as the Hellinger distance, was found to provide a good balance between ease of use, speed of computation and the ability to distinguish between two different density maps p and q. The regular Bhattacharyya coefficient $\beta(p,q)$ is a measure of the similarity between two normalized distributions and can be written in discrete form as :

$$\beta(p,q) = \sum_{i=1}^{N} \sqrt{p(i)q(i)}, \qquad \left(\text{with} \sum_{i=1}^{N} p(i) = \sum_{i=1}^{N} q(i) = 1\right) \tag{1}$$

where the summation runs over all of the N bins of the SOMIM or PMIM density maps. The larger the value of β, the more similar the two distributions are. The Hellinger distance $H(p,q)$ is defined by

$$H(p,q) = \sqrt{1 - \beta(p,q)}, \tag{2}$$

and can be shown to satisfy all the requirements to be a true metric ($\beta(p,q)$ itself is not a metric since it does not satisfy the triangle inequality); the similarity between two distributions p and q is higher for smaller values of $H(p,q)$.

Comparison of maps

Shape	H(SOMIM)	H(PMIM)	weighted
n=6	0.433	0.405	0.420
n=5	0.471	0.444	0.458
n=4	0.570	0.552	0.561

Analysis of 2-D sections (near [111]) suggests a 3-D shape with an exponent between $n=5$ and $n=6$.

Use full 3-D analysis to verify whether or not this is reasonable...

UMF-19 3-D analysis (preliminary)

3-D affine invariant for the superellipsoid:

$$\Omega_3 = \left(\frac{6}{\pi}\right)^2 \frac{\Gamma[1+\frac{1}{n}]^9\Gamma[\frac{5}{n}]^3}{\Gamma[\frac{3}{n}]^3\Gamma[1+\frac{3}{n}]^5}$$

From histogram of experimental values:

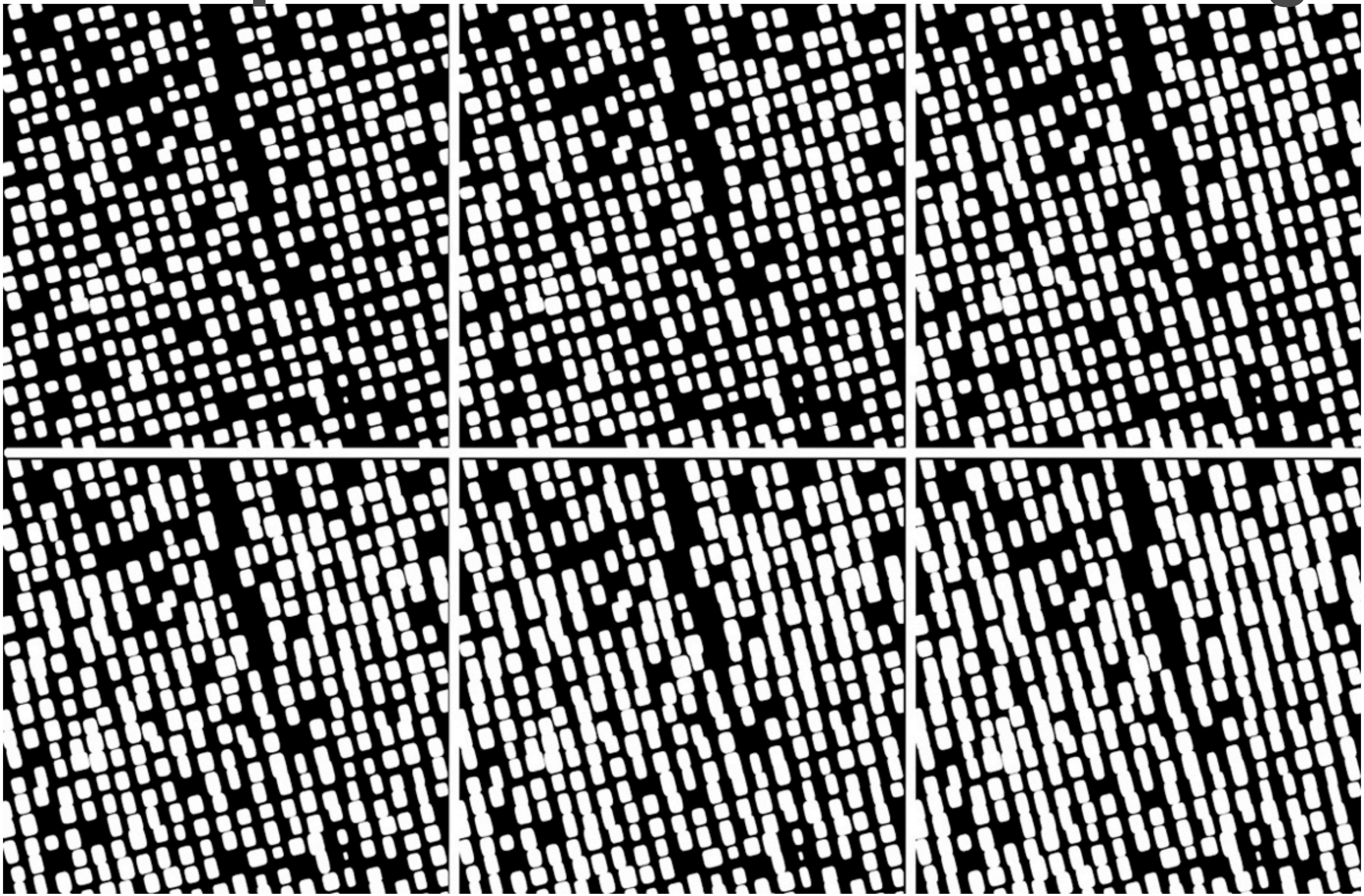
$$\Omega_3 = 0.89$$

Solve for *n*:

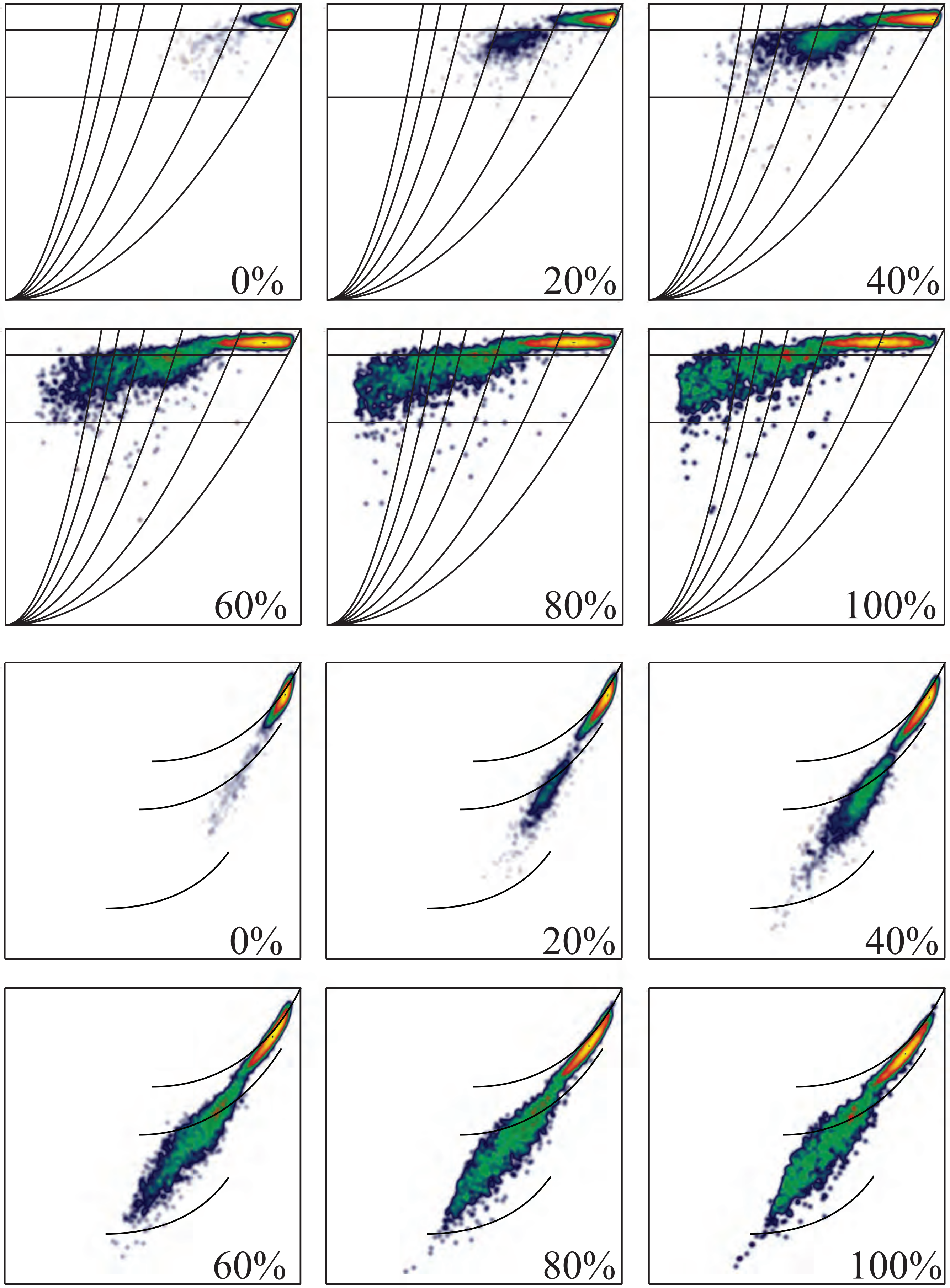
$$n = 5.4$$

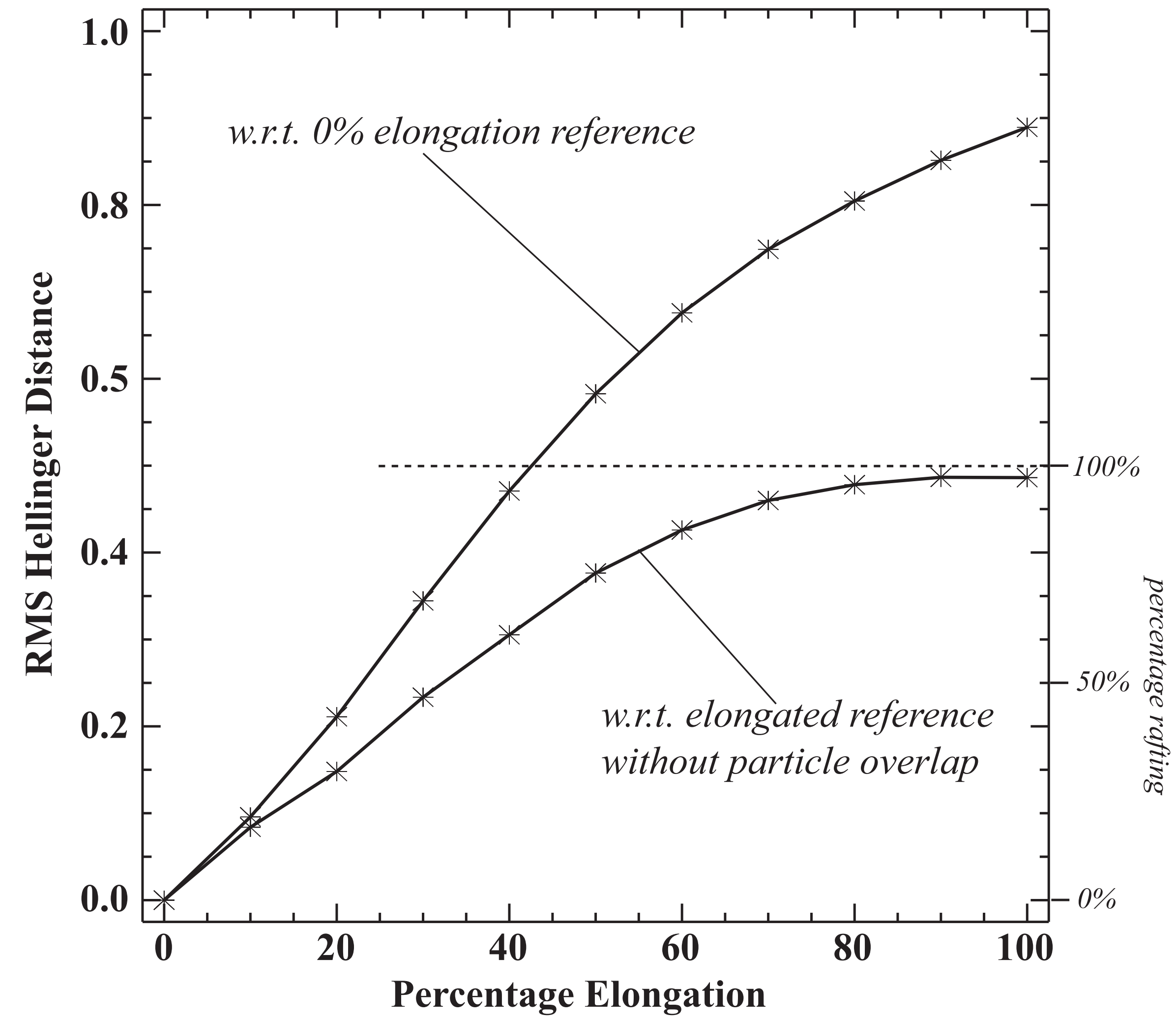
3-D result is consistent with 2-D finding, lending some confidence to the moment invariant density map characterization of shapes from 2-D experimental sections.

Example 2: detection of rafting



Carnegie Mellon University





This is an encouraging result; further analysis on more realistic microstructures (including experimental data) is underway.

Conclusions

- Moment invariants are useful shape descriptors; 2nd order may not be sufficient for the wide range of shapes present in modern materials.
- Quantitative and objective comparison between experimental and reconstructed shapes requires the use of easily computable shape descriptors.
  - In particular, moment invariants allow for a quantitative description of γ' precipitate shapes
- SOMIM and PMIM density maps appear to be a good approach for 3-D shape identification from 2-D sections
- Inclusion of higher order moments both in 2-D and 3-D will be necessary for more complex shapes.