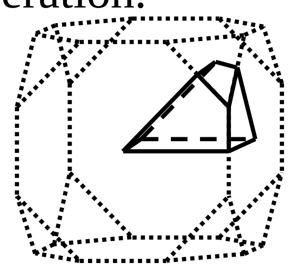
- (Proper) rotations are represented by (special) orthogonal matrices.
- Proper rotations are represented by unit quaternions.

- Rotation/orientation parameterizations:
  - Axis and angle
  - Euler angles
  - Rodrigues parameters
  - Miller indices as orientation descriptors

- Analysis of crystal orientations is influenced by crystal symmetries.
- Orientation *O* is equivalent to *CO*, where *C* is a symmetry operation.
- Asymmetric domains

  Euler angles – OK for low symmetries

  Rodrigues parameterization – Voronoï tessellation



- Reference misorientation angle/axis distributions.

# Geometry of *SO(3)*

# and functions on the orientation space

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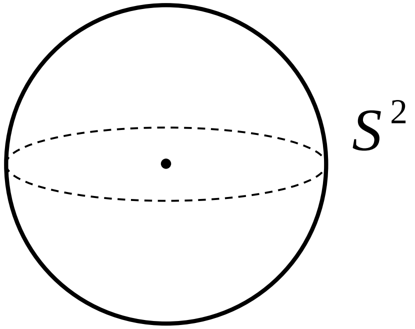
# Outline

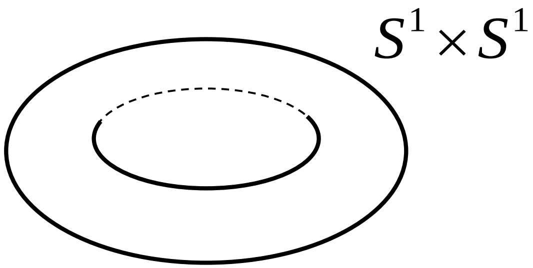
- Topology of SO(3)
- Finite distances
- Infinitesimal distance
- Metric
- Geodesic lines in SO(3)
- Integration on SO(3)

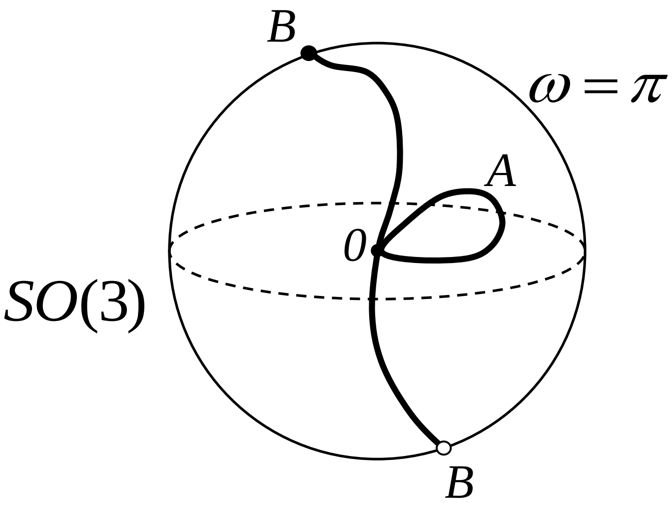
# Topology

<u>Simply connected</u> topological space:

every closed path can be shrunk to a point

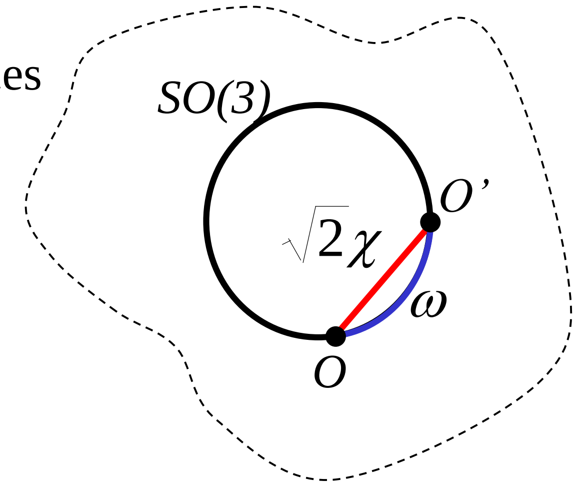



$SO(3)$ is doubly connected

# Finite distance




$$\chi(O,O') = \|O - O'\| / \sqrt{2}$$

$$\omega(O,O') = \arccos\left[\left(tr(O'O^T) - 1\right)/2\right]$$

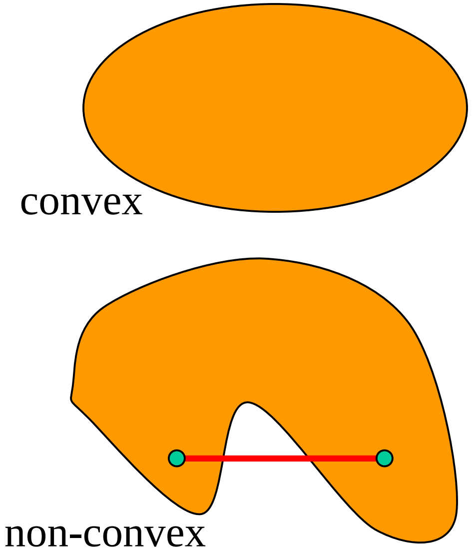
(misorientation angle)

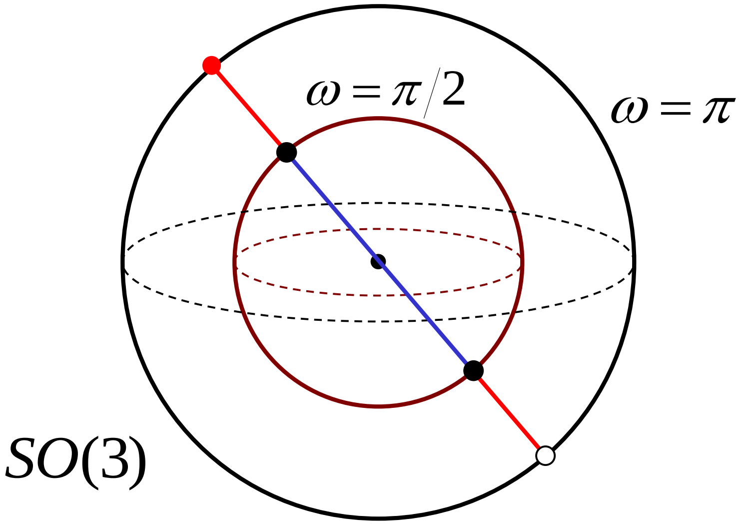
Both distances are **bi-invariant** :

$$\chi(O_L O O_R, O_L O' O_R) = \chi(O,O')$$
$$\omega(O_L O O_R, O_L O' O_R) = \omega(O,O')$$

# Convexity

A subset $\Omega$ is convex if the shortest curve between any two points of $\Omega$ is unique and lies completely within $\Omega$.

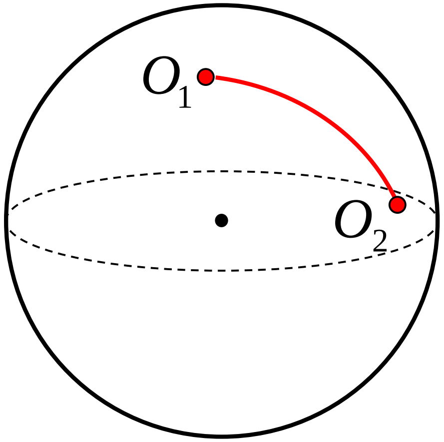


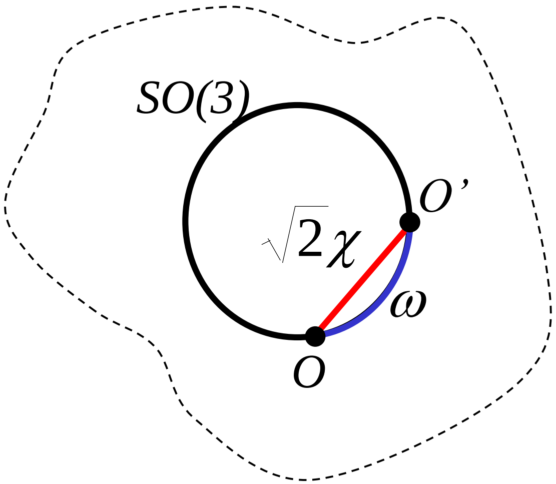

There are non-convex balls in *SO(3)*

# Geodesic lines

- Geodesics in *SO(3)* are the lines representing rotations about fixed axes.
- On sphere of unit quaternions the geodesics are great-circle arcs.
- In the Rodrigues space the geodesics are straight lines.



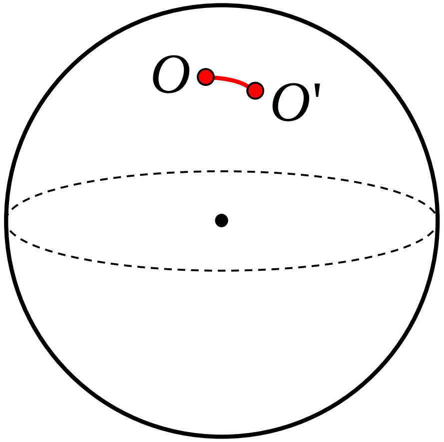
# Infinitesimal distance




$$\chi(O,O') = \|O - O'\| / \sqrt{2}$$

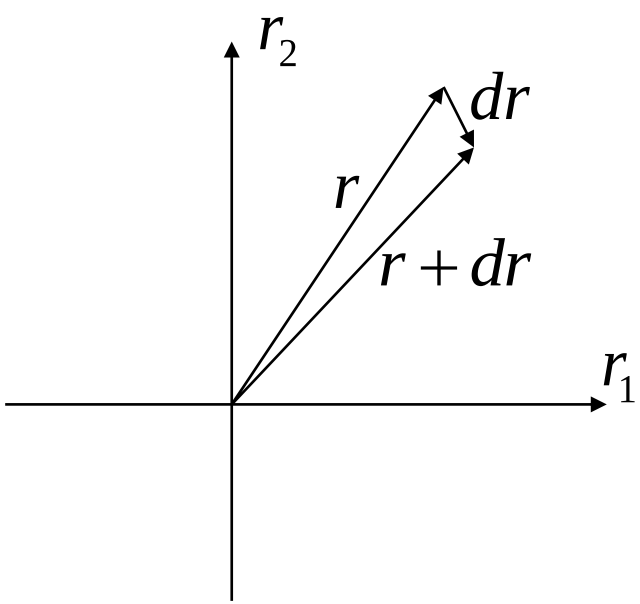
$$\omega(O,O') = \arccos\left[\left(tr(O'O^T) - 1\right)/2\right]$$

For close points: $\chi \approx \omega$



# Infinitesimal distance

Line element: $d\omega^2 = g_{ij} dr_i dr_j$ metric tensor




$$(-r)\circ(r+dr)$$

$$\downarrow$$

$$d\omega^2$$

$$\downarrow$$

$$g$$

# Infinitesimal distance

Line element: $d\omega^2 = g_{ij} dr_i dr_j$ metric tensor

Rodrigues parameters

$$g_{ij} = \frac{1}{\pi^{4/3}} \frac{(1 + r_k r_k)\delta_{ij} - r_i r_j}{(1 + r_l r_l)^2}$$

Euler angles

$$g = \frac{1}{4\pi^{4/3}} \begin{bmatrix} 1 & 0 & \cos\phi \\ 0 & 1 & 0 \\ \cos\phi & 0 & 1 \end{bmatrix}$$

$$(-r) \circ (r + dr)$$

$$\downarrow$$

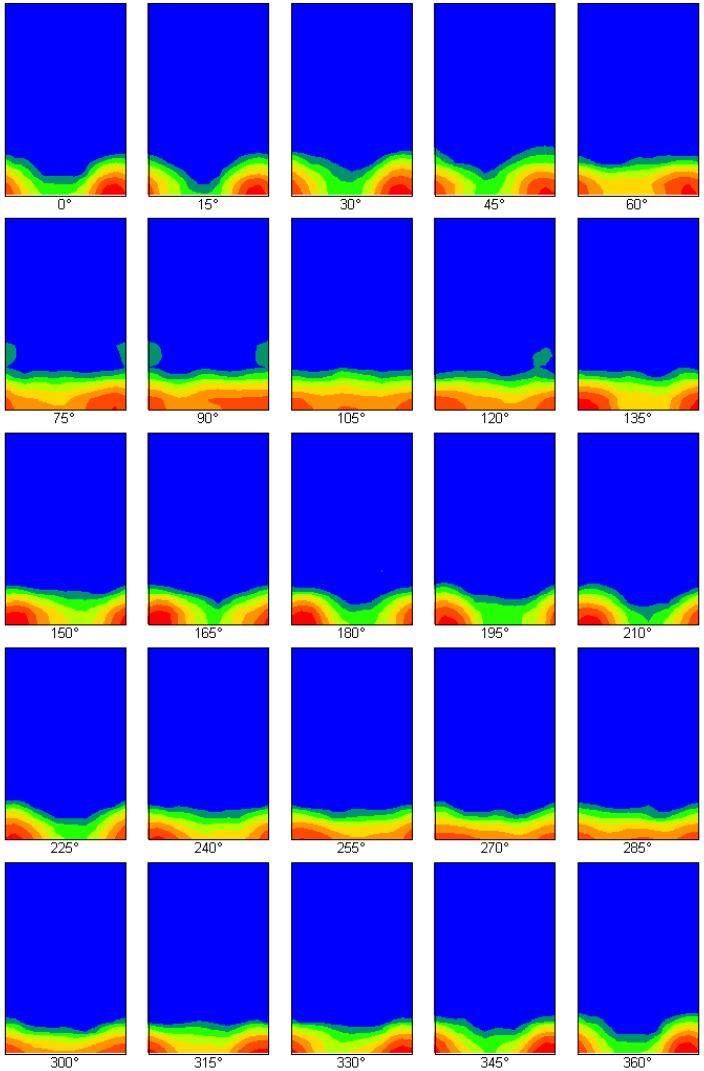
$$d\omega^2$$

$$\downarrow$$

$$g$$

# Integration

„Volume element”




Definition of ODF

$$f(O) = \frac{d(V(O)/V)}{dO}$$

What is the fraction
of orientations
of a given kind?

# Integration

Integration on a manifold makes sense only if it is independent of coordinates (parameterization).

This is also true for integration in $R^n$

$$I = \int_{\Omega_x} f(x_i) dx_1 dx_2 \ldots dx_n$$

Change of variables $x_i = x_i(x'_j)$

$$dx_1 dx_2 \ldots dx_n = \left|\det J\right| \, dx'_1 dx'_2 \ldots dx'_n \qquad J_{ij} = \partial x_i / \partial x'_j$$

$$I = \int_{\Omega_{x'}} f(x'_j) \left|\det J\right| \, dx'_1 dx'_2 \ldots dx'_n$$

# Integration on $SO(3)$

Requirement : invariance

With metric $g$, invariant volume element is $\propto \sqrt{\det g}$

---

Rodrigues parameters $\sqrt{\det g} = \dfrac{1}{\pi^2 \left(1 + r_k r_k\right)^2}$

Euler angles $\sqrt{\det g} = \dfrac{1}{8\pi^2} \sin\phi$

isochoric parameters $\sqrt{\det g} = 1$

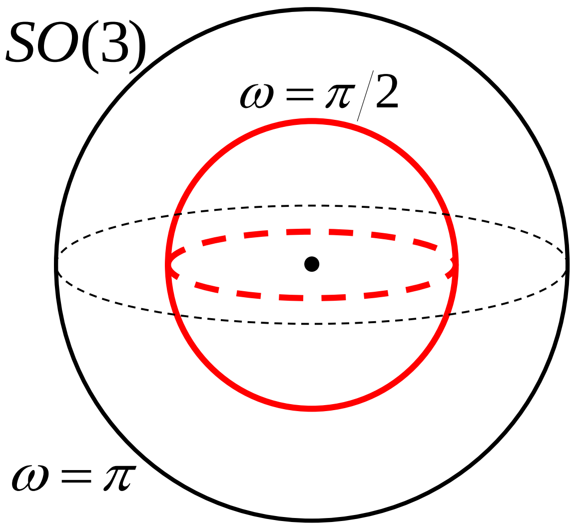
# Integration on $SO(3)$

## Volume of a ball of radius $\omega_0$

Rodrigues parameters

$$V(ball) = \int_{ball} dO = \int_{ball} \sqrt{\det g}\; dr_1 dr_2 dr_3$$

$$V(ball) = \int_0^{\rho_0} 4\pi\rho^2 \sqrt{\det g}\; d\rho = \int_0^{\rho_0} \frac{4\pi\rho^2}{\pi^2\left(1+\rho^2\right)^2} d\rho = \frac{2}{\pi}\left( ArcTan(\rho_0) - \frac{\rho_0}{1+\rho_0^2} \right)$$




$$\sqrt{\det g} = \frac{1}{\pi^2\left(1+r_k r_k\right)^2} \qquad r_k r_k = \rho^2$$

$$V(\omega_0) = \left(\omega_0 - \sin\omega_0\right)/\pi$$

$$V(\pi/2) = 1/2 - 1/\pi \approx 0.18$$

$$V(132.3^\circ) \approx 0.5$$

# Summary

*SO*(3) is doubly connected

Geodesics – the lines of rotations about fixed axes.

Two ‘natural’ finite distances are in use

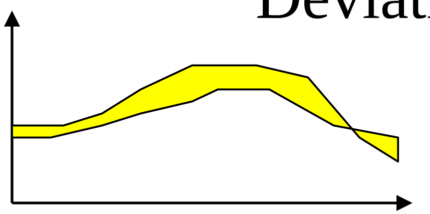
Invariant volume element on *SO*(3)

# Functions on the orientation space

- Comparison of distributions
- Sampling the rotation space
- Model distributions on *SO(3)*

# Comparison of (well-behaved) ODFs

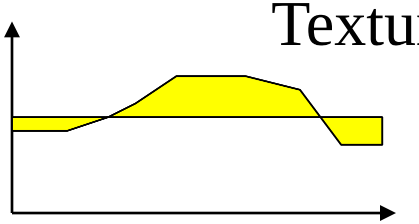
Deviation between distributions $f_1$ and $f_2$



$$\frac{1}{2}\oint \left| f_1(O) - f_2(O) \right| \, dO$$

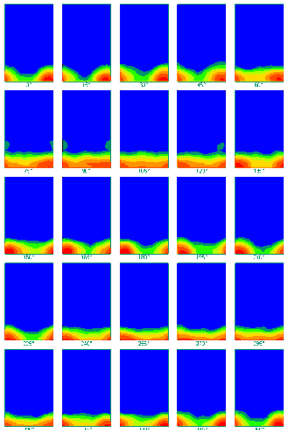
range [0,1]

Texture sharpness – compare $f$ with random distribution



$$\frac{1}{2}\oint \left| f(O) - 1 \right| \, dO$$

Texture sharpness – texture index



$$\oint f(O)^2 dO$$

$[1, \infty)$

Texture sharpness – statistical entropy

$$-\oint f(O) \ln\left( f(O) \right) dO$$

$(-\infty, 0]$

# Generation of random orientations

Euler angles

$$\sqrt{\det g} = \frac{1}{8\pi^2}\sin\phi$$

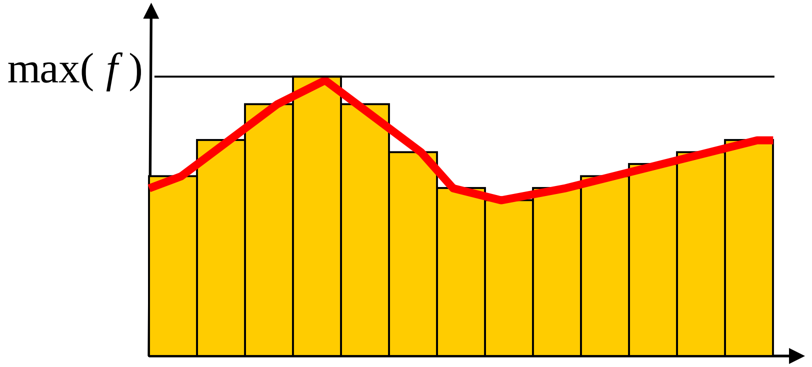
$$dO \propto (\sin\phi)d\varphi_1 d\phi\, d\varphi_2 \propto d\varphi_1 d(\cos\phi)d\varphi_2$$

Algorithm:

1. Generate three random numbers $x_1, x_2, x_3 \in [0,1]$
2. Take $\varphi_1 = 2\pi x_1$ $\quad \varphi_2 = 2\pi x_2$
3. Take $\phi = \arccos\left(2x_3 - 1\right)$
4. Go to point 1

# Generation of orientations

$f$ - non-uniform orientation distribution

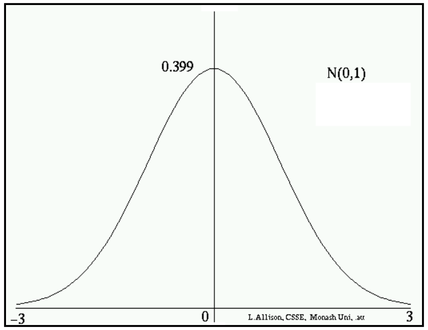



(Rejection) algorithm:

1. Generate a random number $x \in [0,1]$
2. Generate a random orientation $O$
3. If $x \max(f) > f(O)$ discard $O$
4. Go to point 1

# Model distributions on *SO(3)*

$R^n$ – there is a distinguished distribution,
the normal (Gauss) distribution




- central limit theorem
- maximum entropy
- Brownian motion
- diffusion equation

On *SO(3)*, there is no unique distribution with all these characteristics.

# Model distributions on *SO(3)*

Von Mises – Fisher distribution

$$f_{vMF}(O) \propto \exp\left( \; tr(FO^T) \; \right)$$

Valid for
$p$ - dim object in $N$ - dim space
$O - p \times N$ matrix

$F = KP$ $\quad$ $K$ – symmetric $\quad$ $P$ – special orthogonal

$F=0$ – uniform distribution

$K$ – positive (negative) definite – maximum (minimum) at $P$

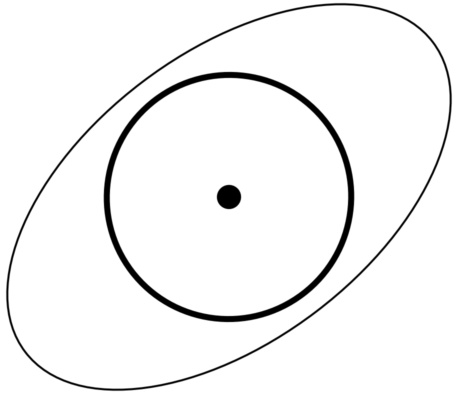
$K = \alpha I$ $\qquad$ $f_{vMF}(O) \propto \exp\left(tr(\alpha P O^T)\right) \propto \exp\left(2\alpha \cos\omega\right)$

$\omega$ – misorientation angle between $O$ and $P$

'Gauss shaped standard function'

# Model distributions on *SO(3)*

Centro-symmetric distribution
on the quaternion sphere



Bingham distribution

$$f_B(q) \propto \exp\left(q^T S q\right)$$

$S$ – symmetric matrix, $q$ – unit quaternion (as vector)

Bingham distribution = von Mises – Fisher distribution

# Model distributions on *SO(3)*

$$f_{Brown}(\omega) = \sum_{k=0}^{\infty} (2k+1) \exp(-k(k+1)t) \frac{\sin((2k+1)\omega/2)}{\sin(\omega/2)}$$

- a version of central limit theorem
- a form of Brownian motion
- diffusion equation

T.I.Savyolova

'Lorentz shaped standard function'

$$f_L(\omega) = (1-t^2) \frac{(1+t^2)^2 + 4t^2 \cos^2(\omega/2)}{((1+t^2)^2 - 4t^2 \cos^2(\omega/2))^2}$$

# Effective elastic properties of polycrystals

# Crystal elasticity - basics

$\varepsilon_{ij}$ strain tensor

$2U = c_{ijkl}\varepsilon_{ij}\varepsilon_{kl} = \varepsilon c \varepsilon$ $U$ – elastic energy

$\sigma_{ij} = c_{ijkl}\varepsilon_{kl}$ $\sigma = c\varepsilon$ $c$ – stiffness tensor

$\varepsilon_{ij} = s_{ijkl}\sigma_{kl}$ $s$ – compliance tensor

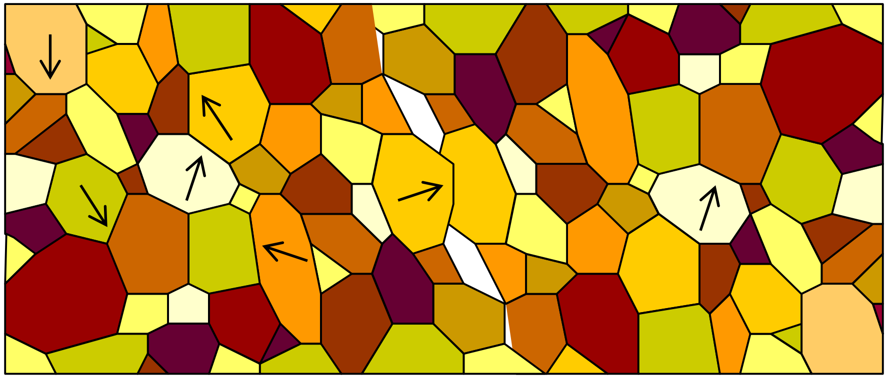
$c_{ijkl}s_{klmn} = \left(\delta_{im}\delta_{jn} + \delta_{in}\delta_{jm}\right)/2 = I_{ijmn}$ $cs = I$

$\partial_j \sigma_{ij} + f_i = 0$ equilibrium conditions

# Effective constants

$$\varepsilon = \varepsilon(x) \quad \sigma = \sigma(x) \qquad c = c(x) \quad s = s(x)$$

Anisotropic crystallites deformed as parts of an aggregate.
The stress and strain in each crystallite are distinct.



The problem: calculate the elastic constants of a polycrystal based on single crystal data ($c$, $s$) and on the texture and microstructure of the material.

# Effective constants

$$\varepsilon = \varepsilon(x) \quad \sigma = \sigma(x) \qquad c = c(x) \quad s = s(x)$$

$$<\varepsilon>, \ <\sigma> \ \text{– averages}$$

Constant tensors $c^*$ and $s^*$ describing the overall elastic properties.

$$c^* <\varepsilon> = <\sigma> \qquad <\varepsilon> c^* <\varepsilon> = <\varepsilon c \varepsilon>$$

$$s^* <\sigma> = <\varepsilon> \qquad <\sigma> s^* <\sigma> = <\sigma s \sigma>$$

$$c^* s^* = I$$

# Averages

Ensemble average

$$<\varepsilon> = \frac{1}{V}\int_V \varepsilon(x)\ \ d_3x$$ volume average

# Voigt-Reuss bounds

Voigt method:

$$\varepsilon = const = <\varepsilon>$$

$$<\sigma> = <c\varepsilon> = <c><\varepsilon>$$

$$c^{*} = c^{V} = <c>$$

Reuss method:

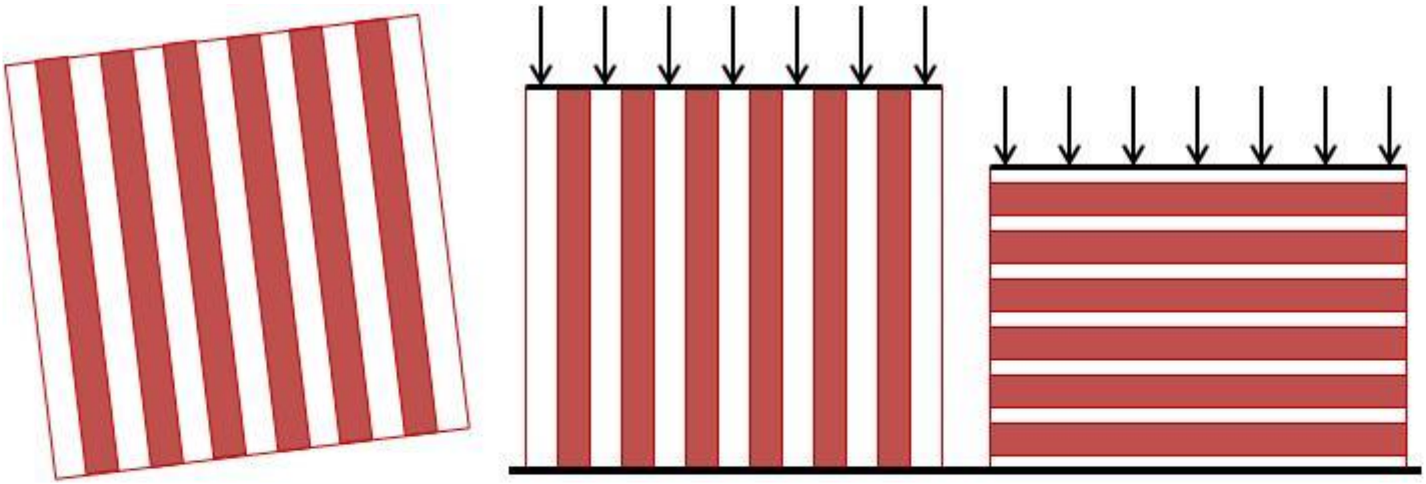
$$\sigma = const = <\sigma>$$

$$<\varepsilon> = <s\sigma> = <s><\sigma>$$

$$s^{*} = s^{R} = <s>$$

$$c^{R} = (s^{R})^{-1} = <s>^{-1} = <c^{-1}>^{-1}$$

# Voigt-Reuss bounds



$$c^R \neq c^V$$

# Voigt-Reuss bounds

$$c^R \le c^* \le c^V$$

Hill average

$$c^* = (c^R + c^V)/2 \qquad s^* = (s^R + s^V)/2$$

+ iteration

Geometric average

$$c^* = \exp < \log(c) >$$

$$\exp x = \sum_{n=0}^{\infty} x^n / n!$$

$$\log x = -\sum_{n=1}^{\infty} (I - x)^n / n$$

# Averages

$$< c > = \frac{1}{V} \int_V c(x)\ d_3 x$$

volume average

$$< c > = \int_{SO(3)} f(O)\ c(O)\ dO$$

orientation average

$$c_{ijkl}^{sample}(O) = O_{mi} O_{nj} O_{pk} O_{ql}\ c_{mnpq}^{crystal}$$

$$< c >_{ijkl} = \int_{SO(3)} f(O)\ O_{mi} O_{nj} O_{pk} O_{ql}\ dO\ c_{mnpq}^{crystal}$$

# Perturbation methods

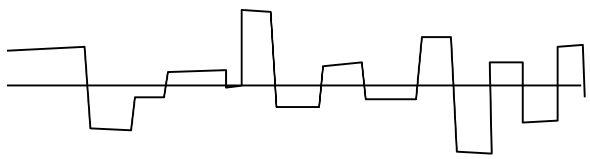
$$\partial_j \left( c_{ijkl} \varepsilon_{kl} \right) + f_i = 0$$

equilibrium conditions

+ boundary conditions

$$\varepsilon(x) = \int G(x, x') \;\; f \, dx' + \varepsilon^0(x)$$

$$\partial_j \left( c_{ijkl} \varepsilon_{kl} \right) = 0 \qquad c(x) = c^0 + c'(x)$$



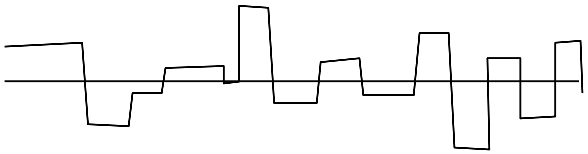
$$\partial_j \left( c^0_{ijkl} \varepsilon_{kl} \right) = -\partial_j \left( c'_{ijkl} \, \varepsilon_{kl} \right)$$

$$\varepsilon = \mathbf{G} c' \varepsilon + \varepsilon^0 \qquad \mathbf{G} = \mathbf{G}(c^0)$$

# Perturbation methods

$$\varepsilon = \varepsilon^0 + \mathbf{G} c' \varepsilon$$

$$\langle \varepsilon \rangle = \varepsilon^0 + \mathbf{G} \langle c' \varepsilon \rangle$$



$$\varepsilon = \langle \varepsilon \rangle + \mathbf{G}\left(c' \varepsilon - \langle c' \varepsilon \rangle\right)$$

(0) $$\varepsilon = \langle \varepsilon \rangle$$

(1) $$\varepsilon = \langle \varepsilon \rangle + \mathbf{G}\left(c' - \langle c' \rangle\right) \langle \varepsilon \rangle$$

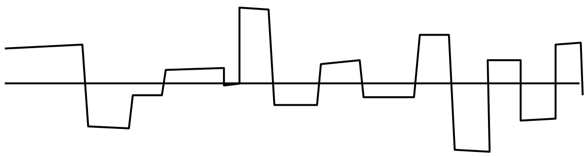
(2) $$\varepsilon = \langle \varepsilon \rangle + \mathbf{G}\left(c' - \langle c' \rangle\right) \langle \varepsilon \rangle + \ldots$$

$$\varepsilon = A \langle \varepsilon \rangle$$

$$c^* \langle \varepsilon \rangle = \langle \sigma \rangle = \langle c \varepsilon \rangle = \langle cA \rangle \langle \varepsilon \rangle$$

$$c^* = \langle cA \rangle$$

# Self-consistent approach



$$c^* = \langle cA \rangle$$

$$A = A(c^0)$$

$$c^* = \langle cA(c^0) \rangle$$

$$c^* = \langle cA(c^*) \rangle$$

# Summary

Distances in the orientation space.

Geodesic lines in the orientation space.

Invariant volume element in the orientation space.

Comparison of orientation distributions.

Sampling the orientation space.

Some model distributions in the orientation space.

# Summary

Effective properties of polycrystals.

- Averages over orientations.
- Voigt and Reuss bounds.
- Arithmetic (Hill) average and geometric average.
- Perturbation methods.
- Self-consistent approach.