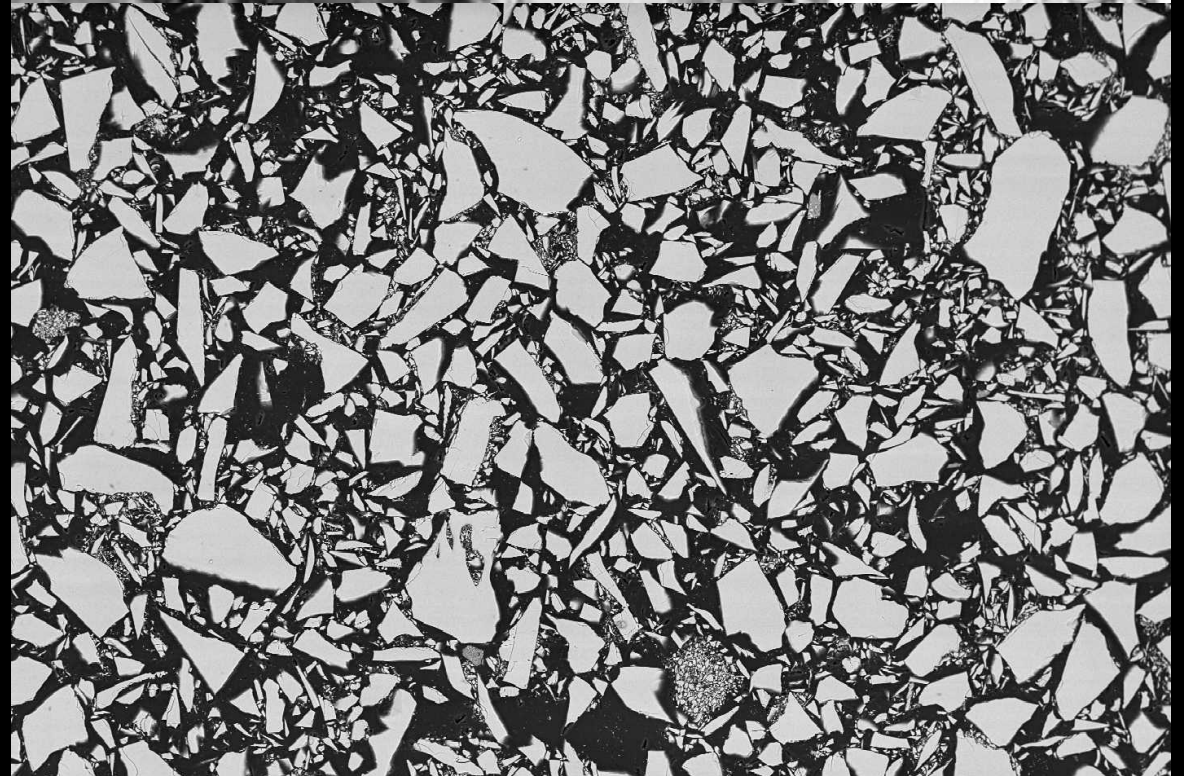
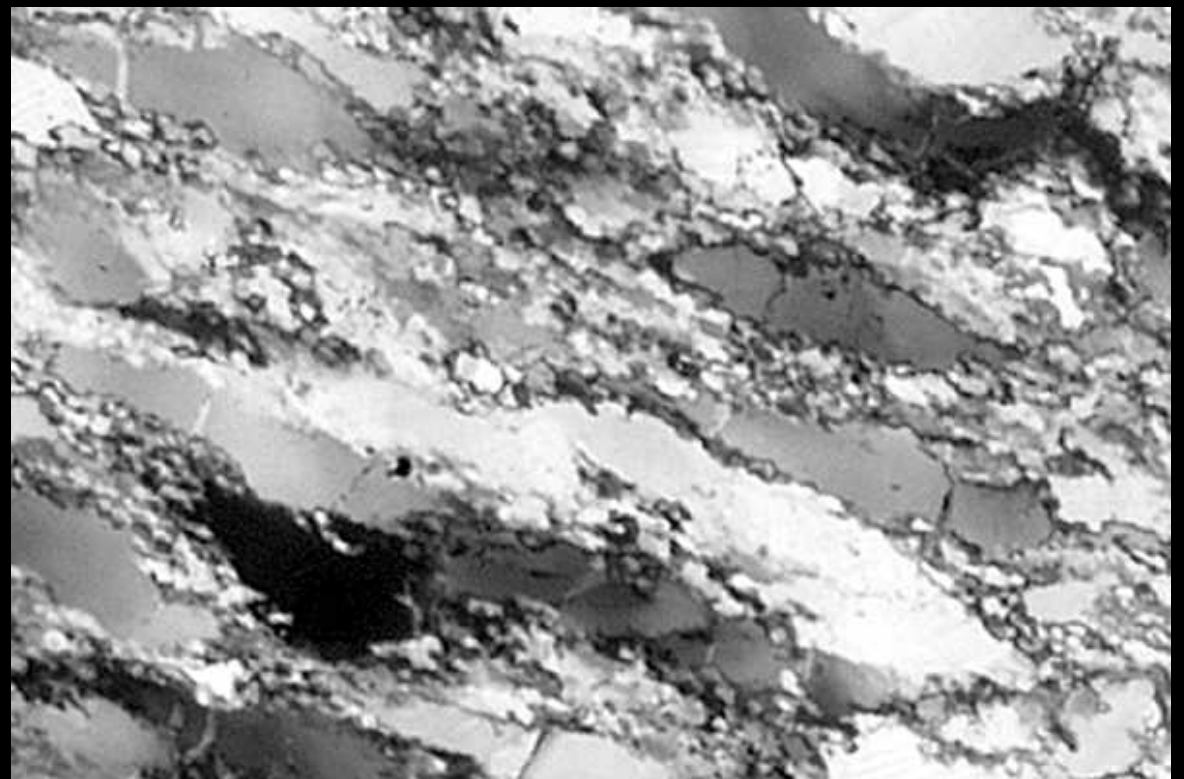


# grain size – the good, the bad ... and the ugly

Renée Heilbronner

[renee.heilbronner@unibas.ch](mailto:renee.heilbronner@unibas.ch)

Martin-Luther-Universität  
Halle, 23. Januar 2023



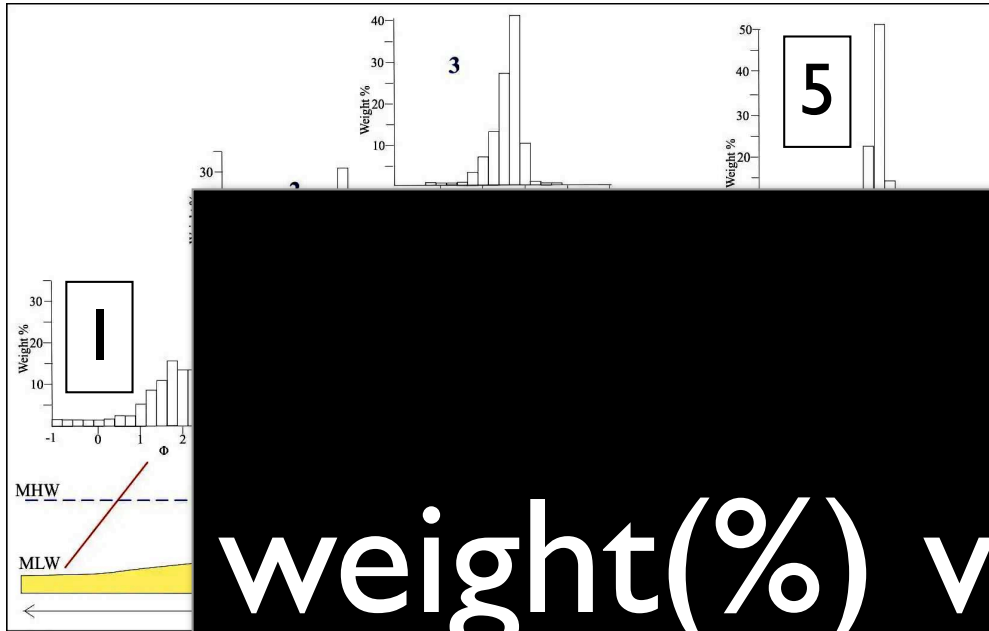
In this talk, we will follow a fictitious rock through an imagined geological cycle:

- sedimentation
- cementation
- grain growth
- dynamic recrystallization
- fragmentation
- healing



...and observe the associated "grain size"

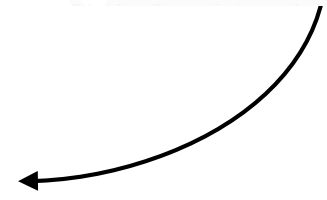
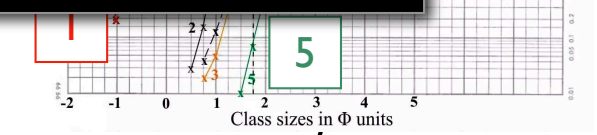
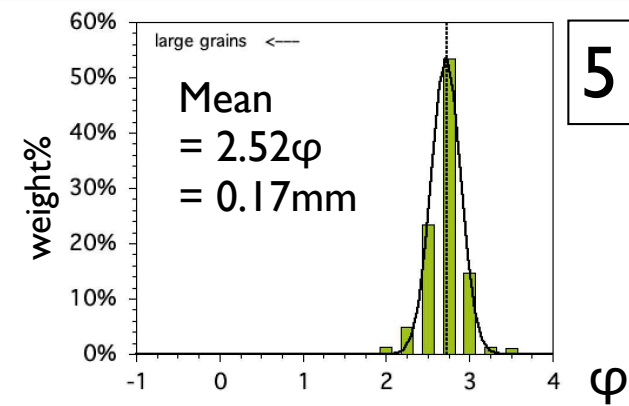
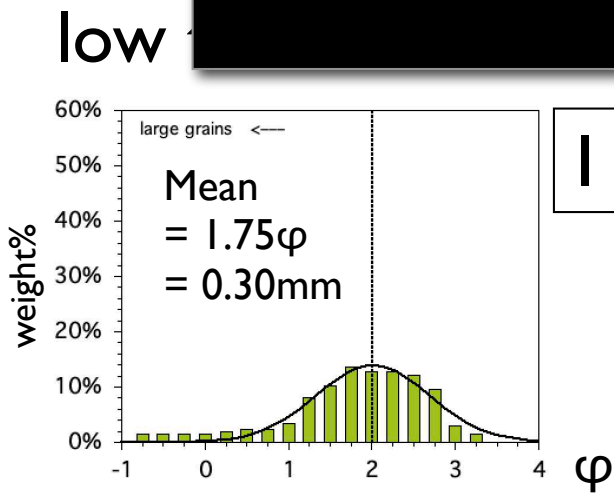
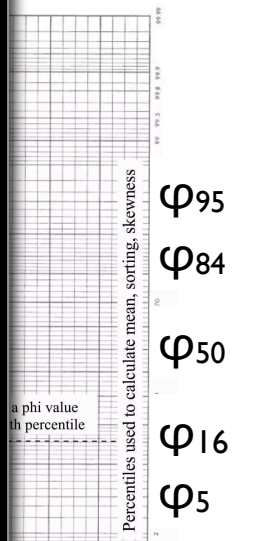
# "grain size" I – sieving



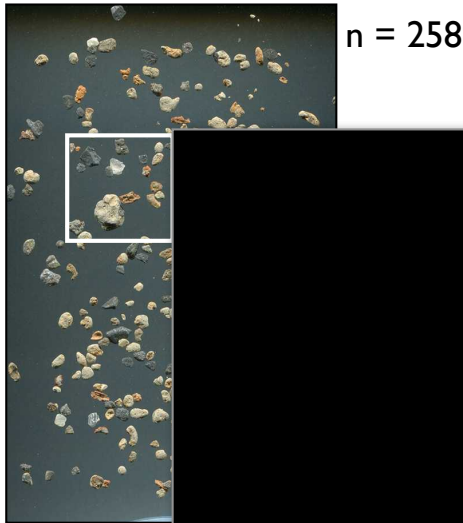
"Grain size":  
 Mean  $M\phi = (\phi_{16} + \phi_{50} + \phi_{84})/3$   
 Sorting  $\sigma\phi = (\phi_{84} - \phi_{16})/4 + (\phi_{95} - \phi_5)/6.6$   
 (number)

weight(%) vs.  $\phi$ -values

Great Exhibition  
<https://www.ge...>

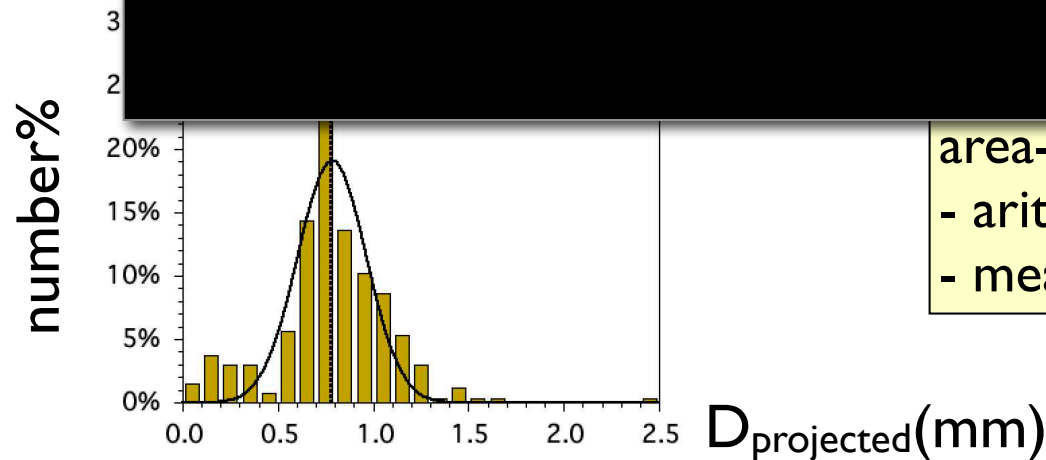


# "grain size" 2 – strewn samples



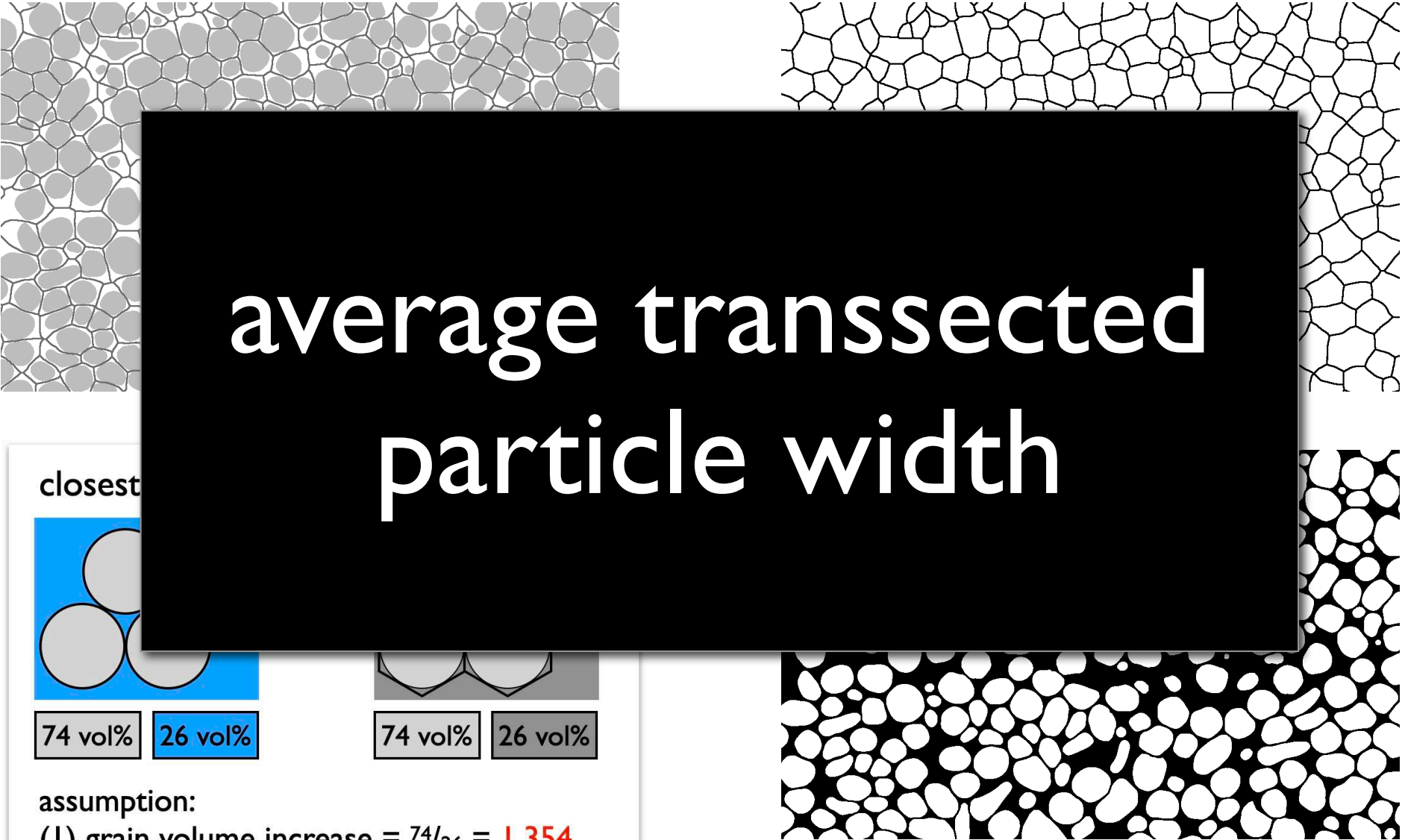
number(%) vs.  
projected diameter

Solheim, A.:  
marine chronology  
– 0 cal years BP.



of  
area-equivalent circles of projected areas  
- arithmetic mean  
- mean/mode of Gaussian curve fit

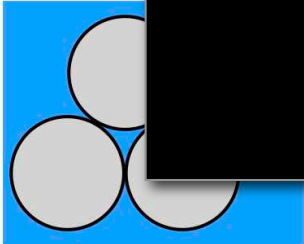
# "grain size" 3 – intercept length



The image features a central black box with white text. Surrounding this box are four micrographs of grain structures. The top-left and bottom-right micrographs show a network of grain boundaries. The top-right and bottom-left micrographs show a similar network but with a different grain size distribution. The bottom-left micrograph is a schematic diagram with labels for volume fractions and an assumption.

average transsected  
particle width

closest



74 vol% 26 vol%



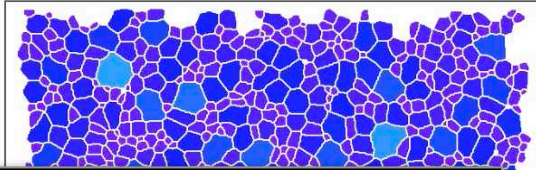
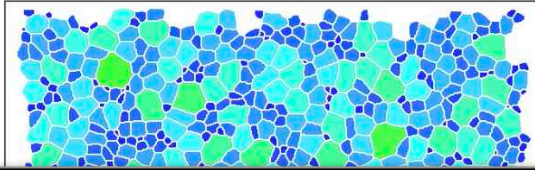
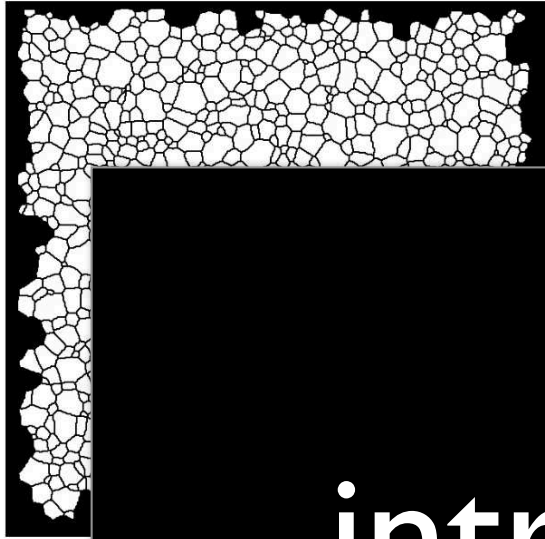
74 vol% 26 vol%

assumption:

(1) grain volume increase =  $\frac{74}{26} = 1.354$

(2)  $d_{\text{cemented}} : d_{\text{original}} = \sqrt[3]{1.354} = 1.106$

# "grain size" 4 – numerical simulation



intrinsic 2D size

grain gr

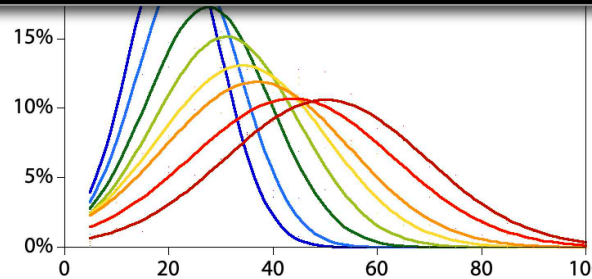
Chen LQ, Yang W  
Computer-simula  
quenched system  
order parameter

Phys Rev B 50: 15752--15756

[https://www.youtube.com/watch?v=p0rY2r0E\\_2k](https://www.youtube.com/watch?v=p0rY2r0E_2k)

"Grain size":

- arithmetic mean of 2D diameter
- mean/mode of curve fit



in terms of normal distribution:

→ increasing mean ( $\mu$ )

→ increasing standard deviation ( $\sigma$ )

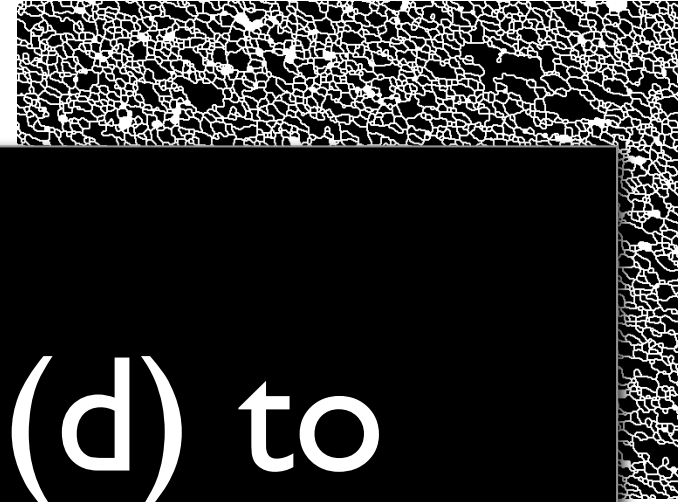
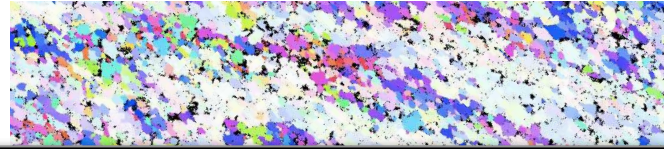
⇒ distribution matters

00 sqpx

average size

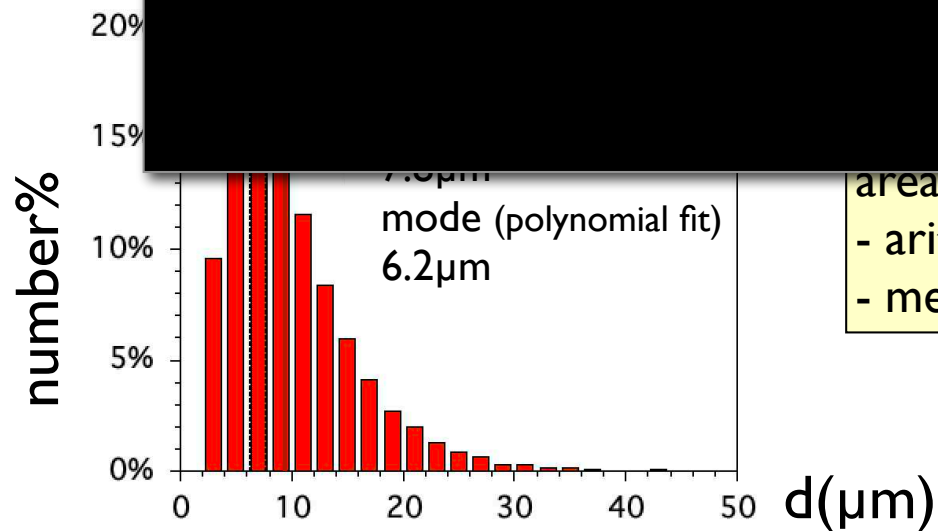
increasing spread

# "grain size" 5 – thin sections



Regime 3

from 2D  $h(d)$  to  
3D  $\text{vol}\%(D)$



area-equivalent circles or sectional shapes  
- arithmetic mean  $\mu$   
- mean/mode of curve fits

# "grain size" 6 – particle analyzer



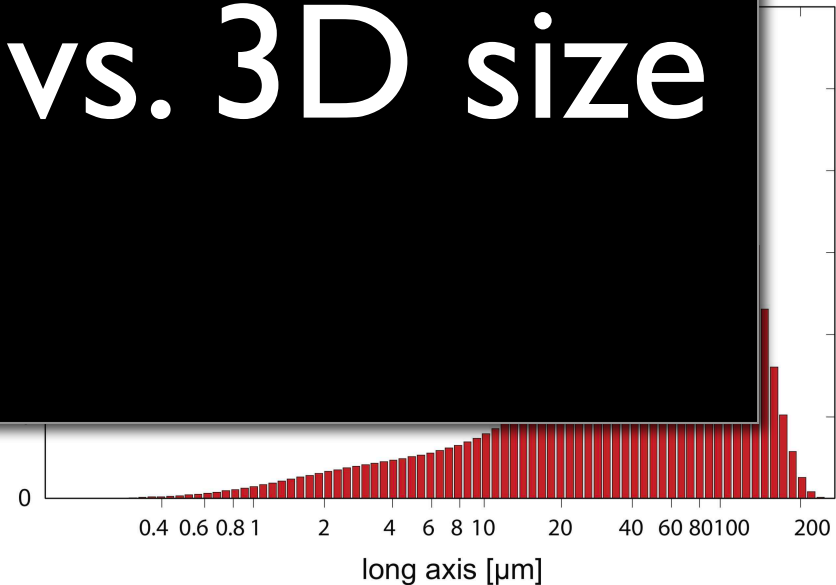
volume(%) vs. 3D size

Range  
Mean  
Mode

"Grain size":

mean or mode of log (3D size)  
(e.g., long axes of particles)

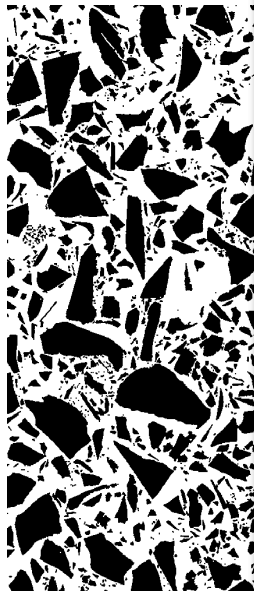
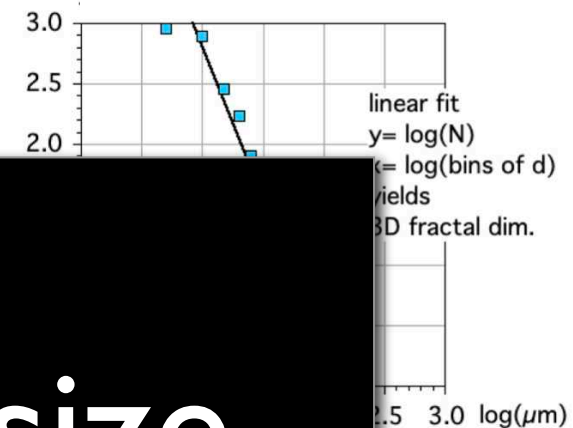
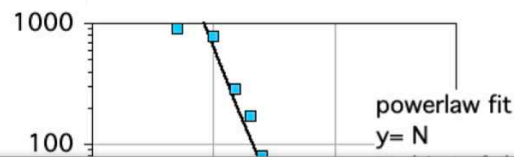
- arithmetic mean
- mean/mode of curve fits



Richter, B., 2017, *The brittle-to-viscous transition in experimentally deformed quartz gouge*. Dissertation, Basel University. <https://edoc.unibas.ch/57805/>



# "grain size" 7 – multi-scale analysis



00143336

number vs. 3D size  
 $\log(N)$  vs.  $\log(D_{\text{equ}})$

fractal dimension for 2 or 3 dimensions

$$D_{2d} = D_{3d} - 1$$

Fractal size distributions should span at least 3 orders of magnitude

when we talk about  
grain size ...

# why look at grain size ?

grain size data carries information

sediments, sands, silts

→ environment of deposition

statically recrystallized rocks

→ time and conditions of grain growth

dynamically recrystallized rocks

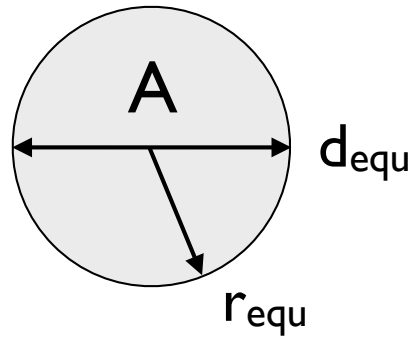
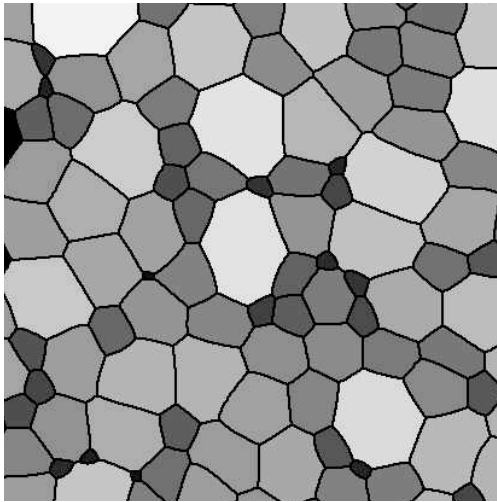
→ level of flow stress

crushed rocks, powders

→ types of fragmentation processes

... etc.

# the size of a grain – a scalar

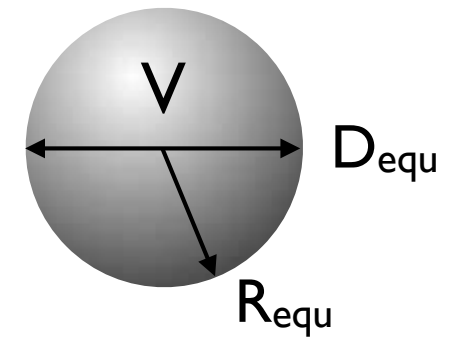
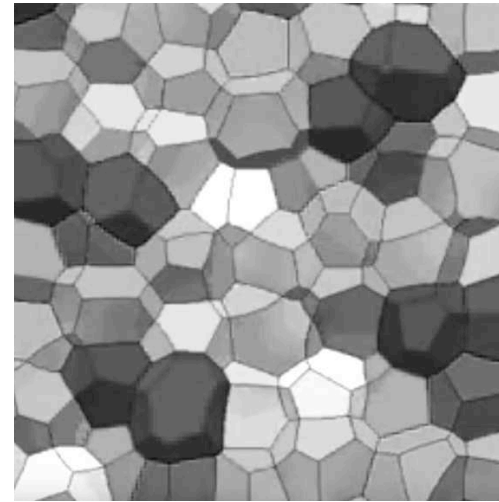


thin sections:  
size = diameter,  $d$ , of area

area of circle:  $A = \pi \cdot r^2$

$$\Rightarrow d = 2 \cdot \sqrt{A/\pi}$$

$$d = 2r \text{ (lower case)}$$



loose grains, particles:  
size = diameter,  $D$ , of volume

volume of sphere:  $V = 4\pi/3 \cdot R^3$

$$\Rightarrow D = 2 \cdot \sqrt[3]{3V/(4\pi)}$$

$$D = 2R \text{ (upper case)}$$

# the (in)famous 'mean grain size'

arithmetic mean	$\bar{X}$	$=$	$1/n \cdot \sum x_i$
geometric mean	$G$	$=$	$n\sqrt{\prod x_i}$
harmonic mean	$H$	$=$	$1 / ( 1/n \cdot \sum 1/x_i )$ $=$ $n / \sum 1/x_i$
root-mean-square	$RMS$	$=$	$\sqrt{ ( 1/n \cdot \sum x_i^2 ) }$

$\Sigma$  = sum

$\Pi$  = product

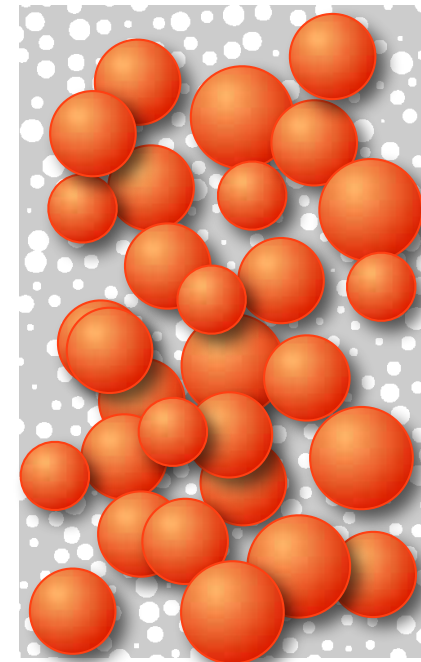
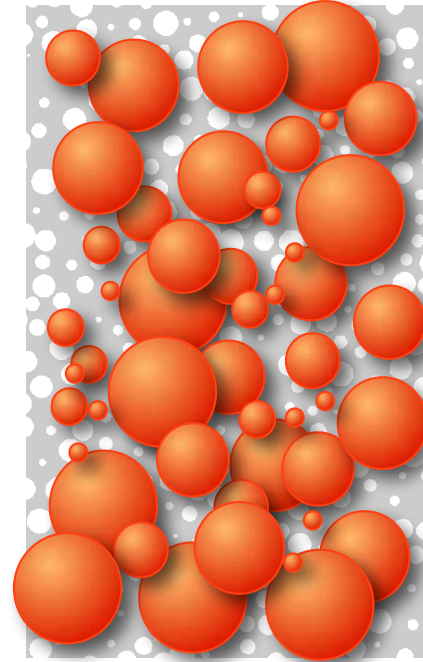
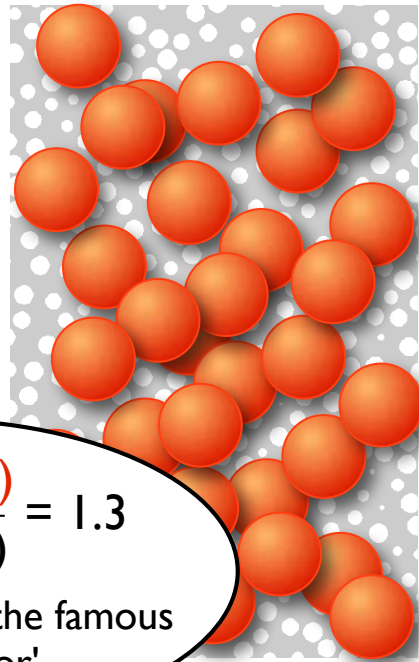
$i = 1, \dots, n$

$$RMS > \bar{X} \geq G \geq H$$

median	$=$	$x_{(n+1)/2}$	if $n =$ odd
	$=$	$(x_{n/2} + x_{n/2+1}) /$	if $n =$ even
mode	$=$	most frequent value	

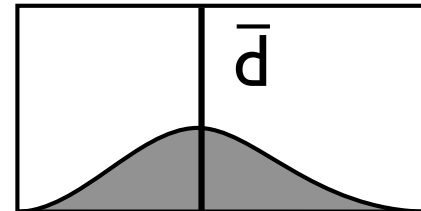
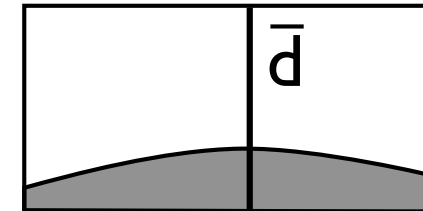
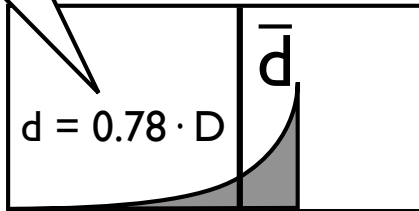
# why 3D ?!

... that's why !

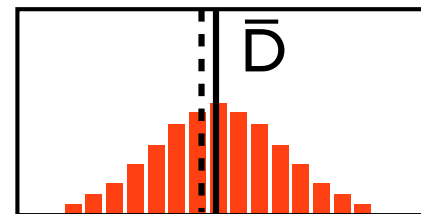
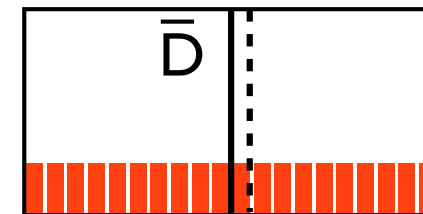
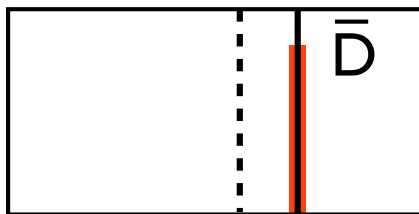


$\frac{\text{mean of } h(D)}{\text{mean of } h(d)} = 1.3$   
... the origin of the famous 'correction factor' ...

h(%) sections



h(%) spheres

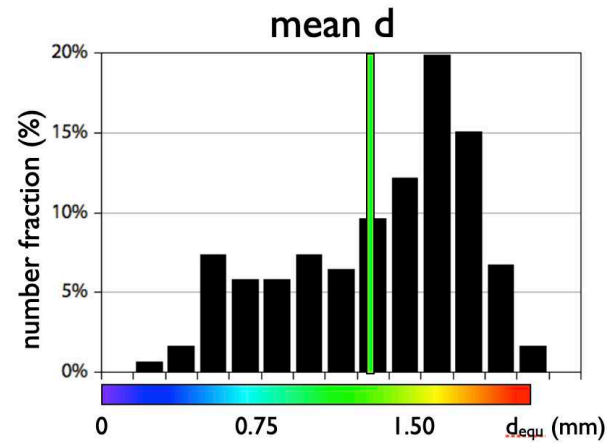
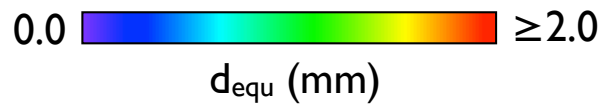
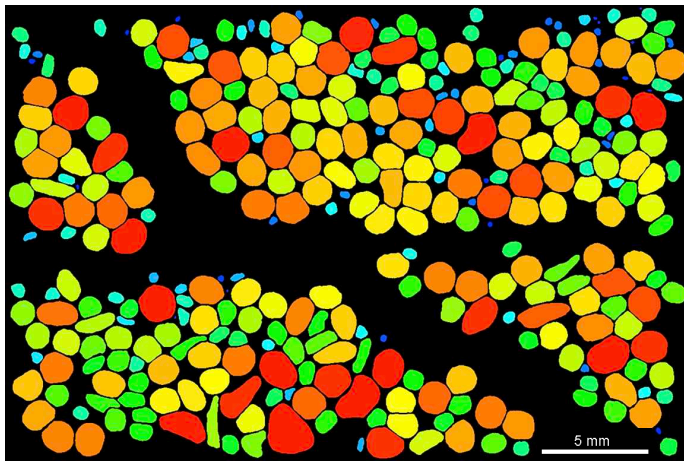


diameter

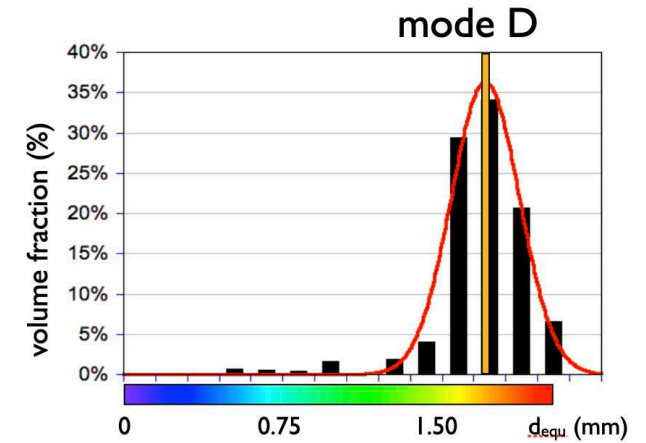
diameter

diameter

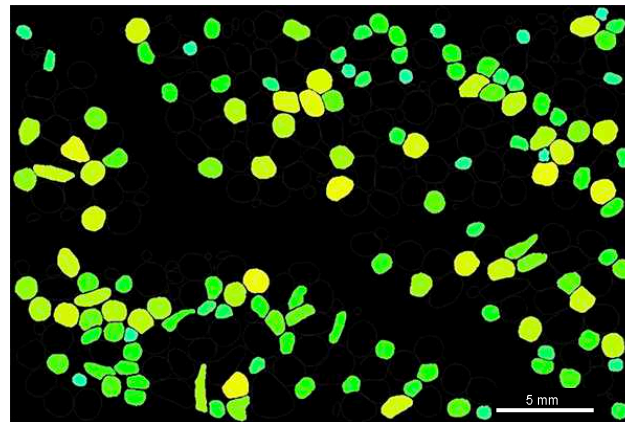
# we 'see' 3D, not 2D, modal grain size



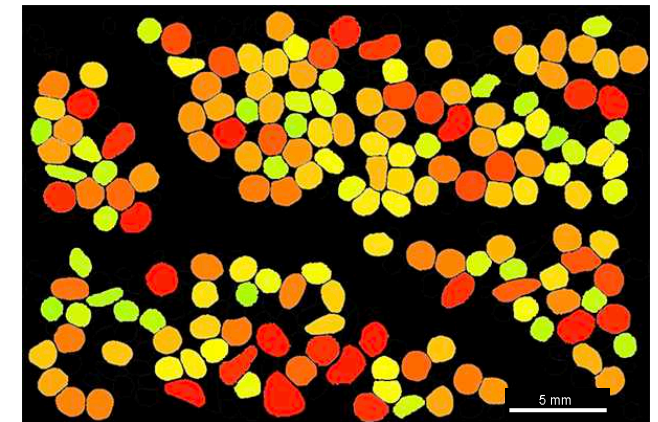
number-weighted  
2D mean 1.31  
2D st.dev. 0.43



volume-weighted  
3D mode 1.70  
3D st.dev. 0.11

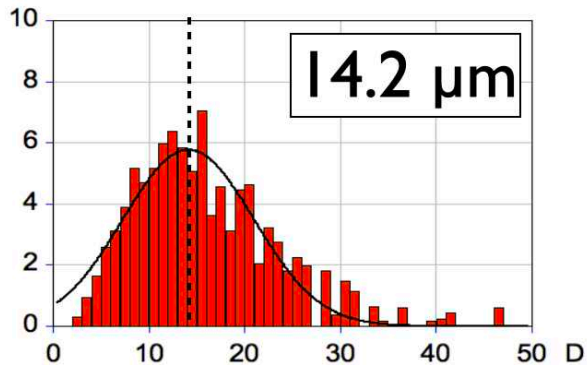


$\neq$  visual impression



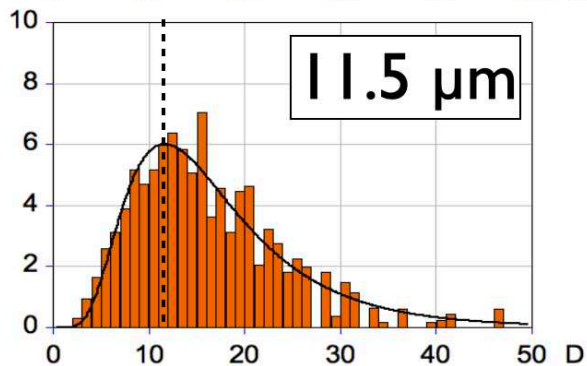
$=$  visual impression

# finding the mode by curve fitting



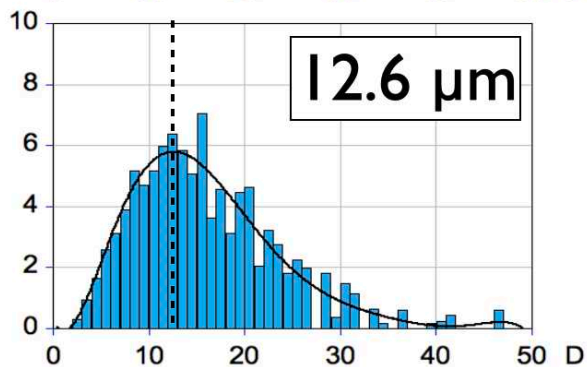
Normal curve fit

$$\frac{1}{\sqrt{2\pi\sigma^2}} \cdot \exp\left(-\frac{(\mu - x)^2}{2\sigma^2}\right)$$



Lognormal curve fit

$$\frac{1}{x\sqrt{2\pi\sigma^2}} \cdot \exp\left(-\frac{(\ln(x)-\mu)^2}{2\sigma^2}\right)$$



Polynomial curve fit

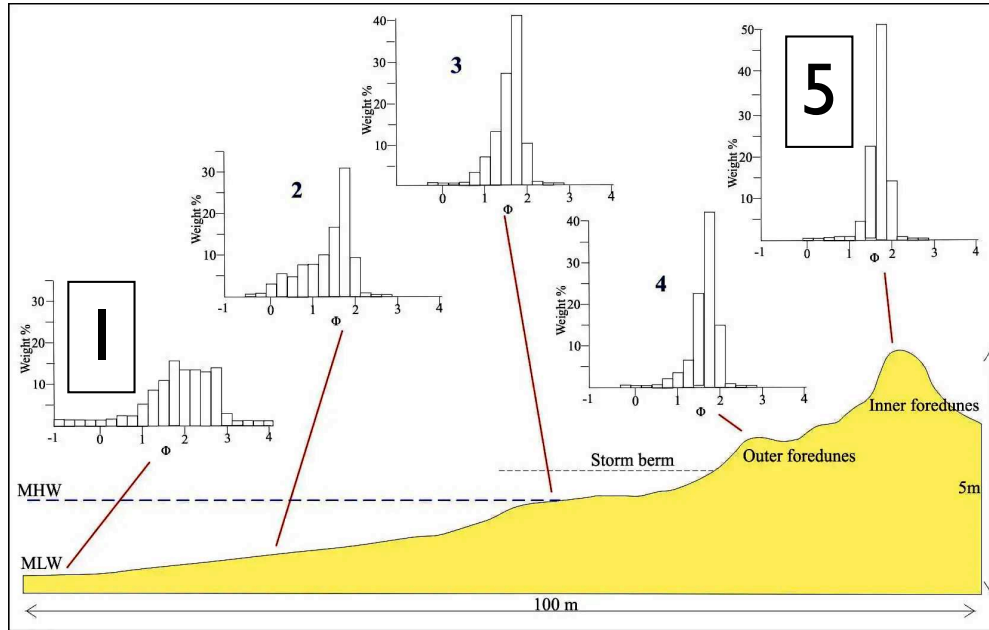
$$m_0 + m_1x + m_2x^2 + m_3x^3 + \dots$$

in all cases: fit through center of bin !



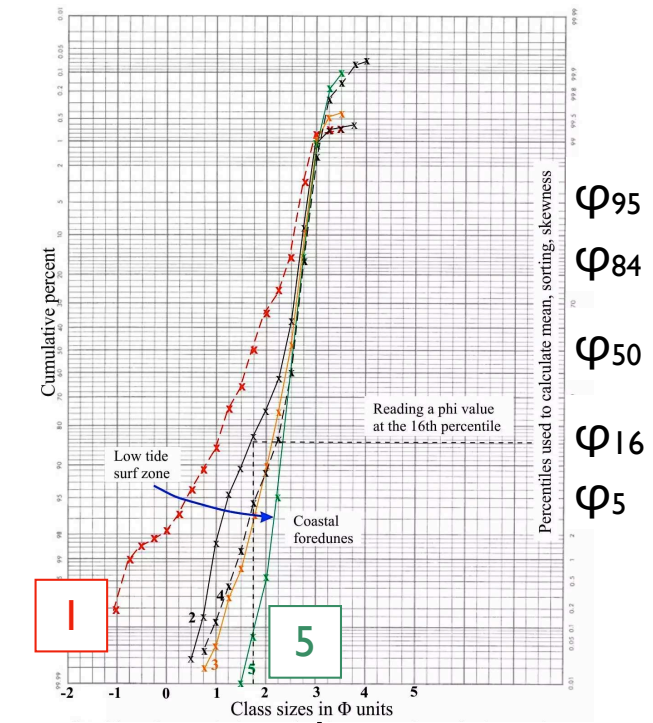
"grain size" |  
sedimentation  
sieving

# "grain size" I: beach sand

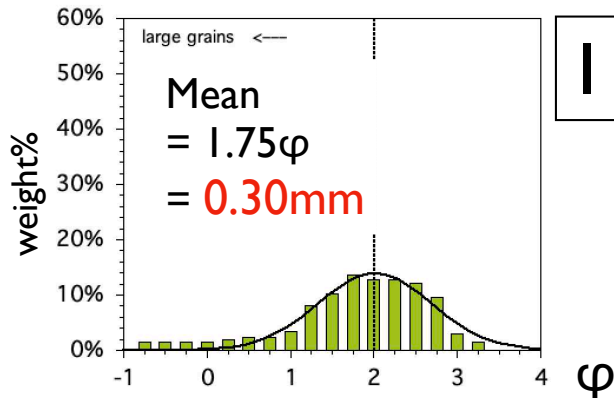


Great Exhibition Bay, NZ  
<https://www.geological-digressions.com/analysis-of-sediment-grain-size-distributions/>

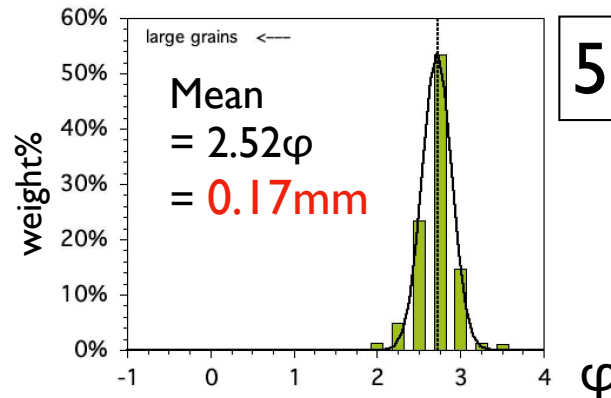
"Grain size":  
 Mean  $M\phi = (\phi_{16} + \phi_{50} + \phi_{84})/3$   
 Sorting  $\sigma\phi = (\phi_{84} - \phi_{16})/4 + (\phi_{95} - \phi_5)/6.6$   
 $\phi$  equivalent to  $\log(3D \text{ diameter})$



## low tide surf zone

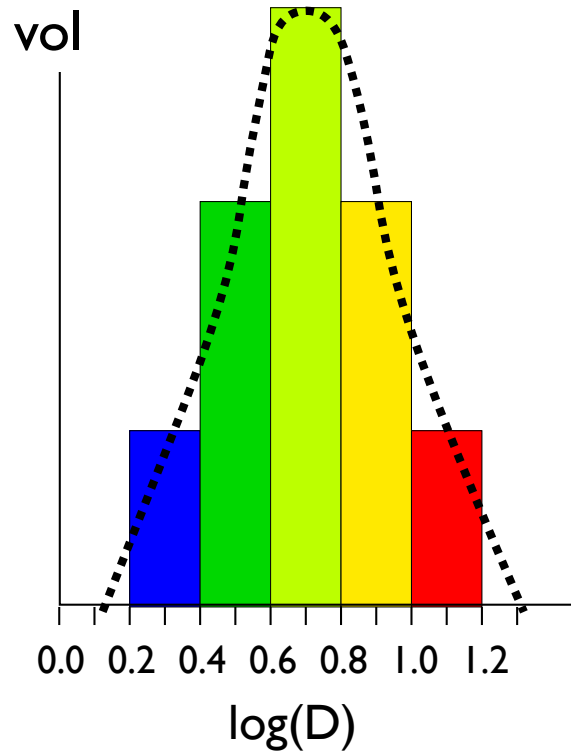


## coastal foredunes



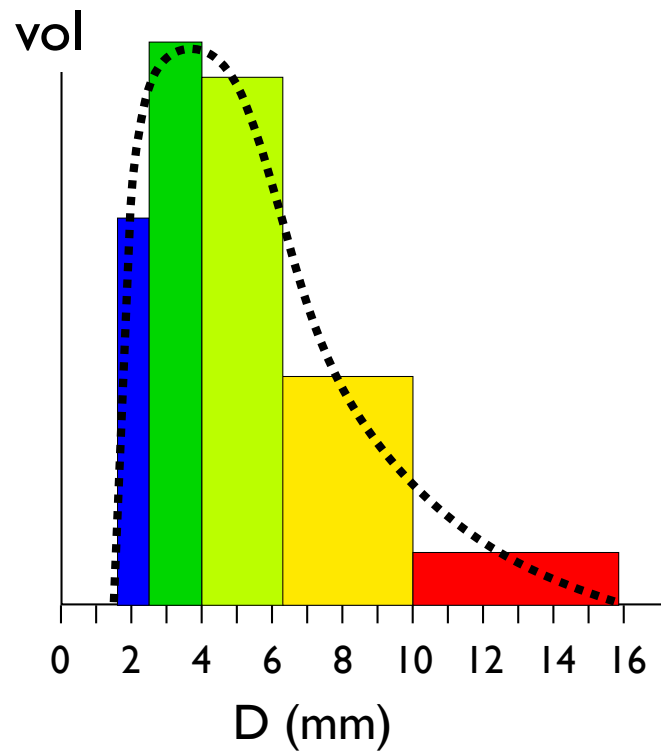
# from logarithmic to linear

$\text{vol}(\log(D)) \neq$   
density function



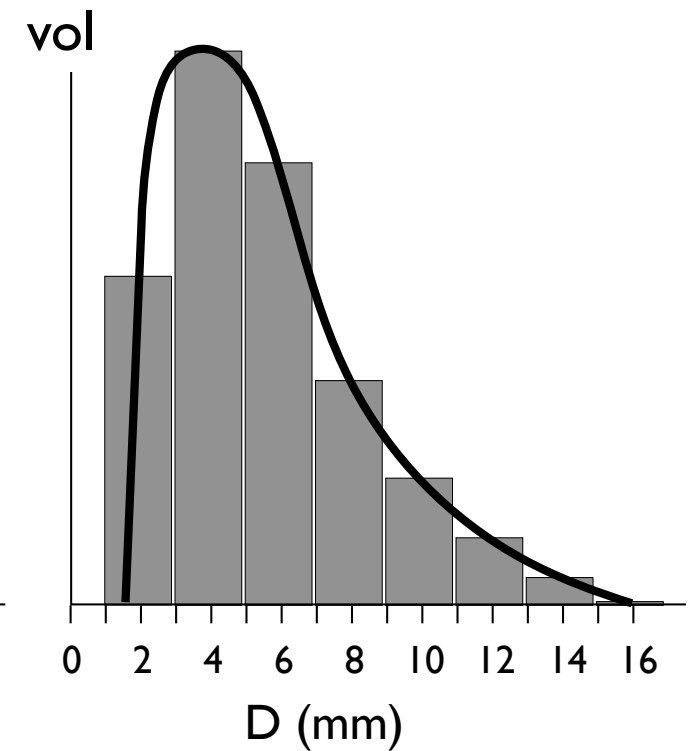
$\Delta \log(D) = \text{constant}$   
 $\Delta D \neq \text{constant}$

$\text{vol}(D) =$   
density function



$\text{vol} / \Delta D = \text{density}$   
blue, green, ... etc. area on  
 $\log(D)$ -plot = blue, green, ...  
etc. area on  $D$ -plot

$\text{vol}(D) =$   
density function

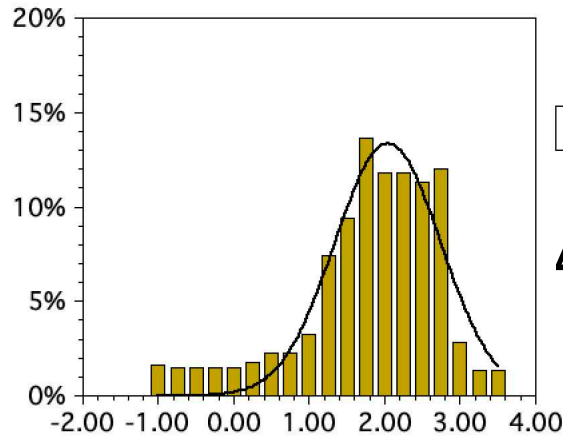


$\Delta D = \text{constant}$

$\Sigma$  area of histogram bars = area under curve = constant

# $\varphi$ -values... – double trouble

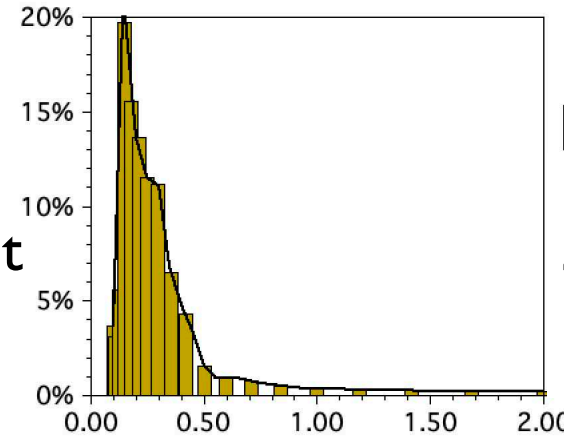
surf zone



w% histo

$\Delta \log(D) = \text{const}$

weight% vs.  $\varphi$  Gaussian normal fit  
 $M\varphi = 2.05 \Rightarrow D_{\text{mean}} = 0.241 \text{ mm}$

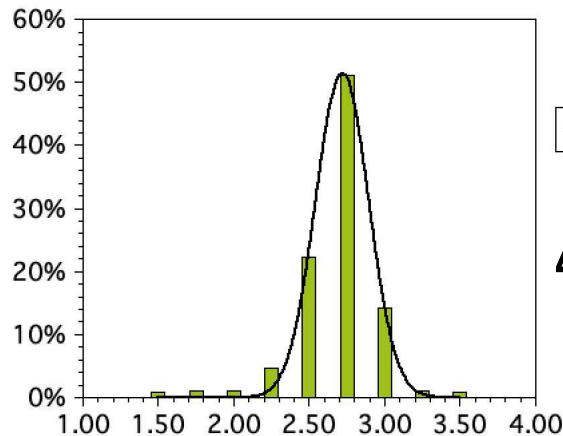


w-dens=w%/bin (%)

$\Delta D \neq \text{const}$

weight% vs.  $D$ (mm) w% binwidth corrected  
overlay = cubic spline fit (39pts)

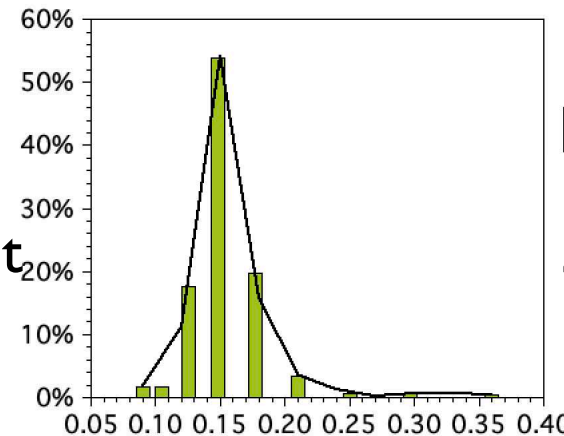
foredune



w% histo

$\Delta \log(D) = \text{const}$

weight% vs.  $\varphi$  Gaussian normal fit  
 $M\varphi = 2.72 \Rightarrow D_{\text{mean}} = 0.152 \text{ mm}$



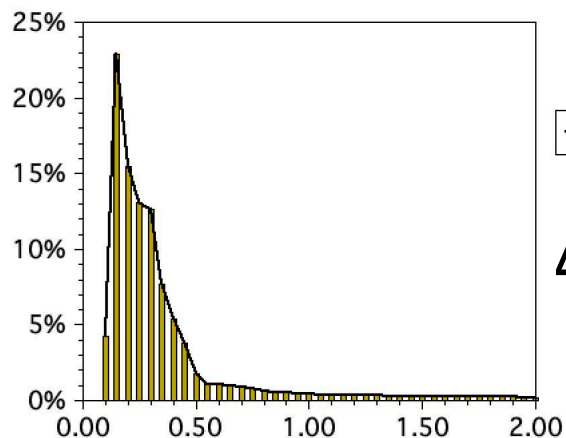
w%/bin (%)

$\Delta D \neq \text{const}$

weight% vs.  $D$ (mm) w% binwidth corrected  
overlay = cubic spline fit (10pts)

# converting the data

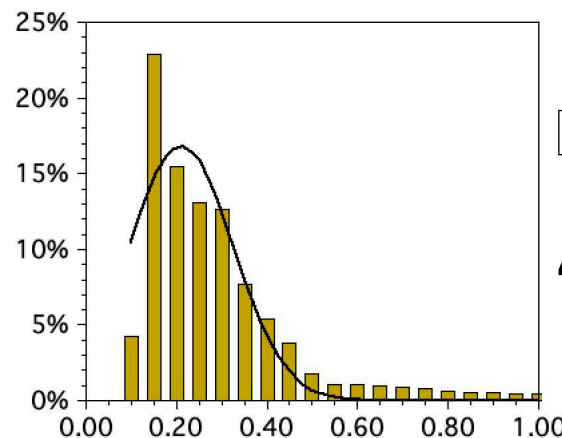
surf zone



fit w-dens (%)

$\Delta D = \text{const}$

weight% vs. D(mm) d from cubic spline fit  
overlay = cubic spline fit (39pts)

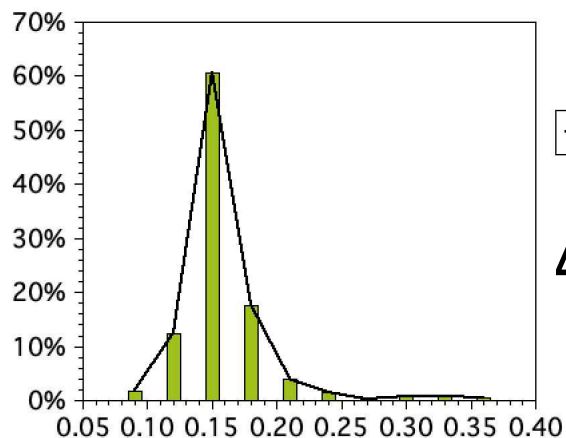


fit w-dens (%)

$\Delta D = \text{const}$

weight% vs. D(mm) Gaussian normal fit  
 $D_{\text{mean}} = 0.212\text{mm}$  ( $\sigma = 0.130\text{mm}$ )

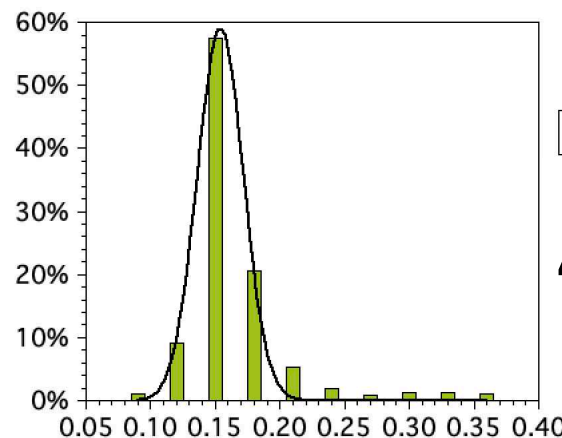
foredune



fit w-dens (%)

$\Delta D = \text{const}$

weight% vs. D(mm) d from cubic spline fit  
overlay = cubic spline fit (10pts)



fit w%

$\Delta D = \text{const}$

weight% vs. D(mm) Gaussian normal fit  
 $D_{\text{mean}} = 0.154\text{mm}$  ( $\sigma = 0.020\text{mm}$ )

# $\varphi$ -derived versus converted

$M\varphi = 2.05$

$D_{\text{mean}} = 0.24\text{mm}$

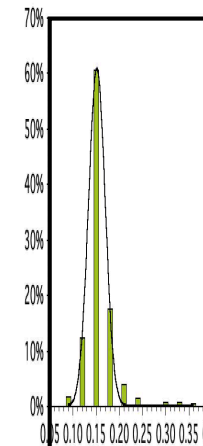
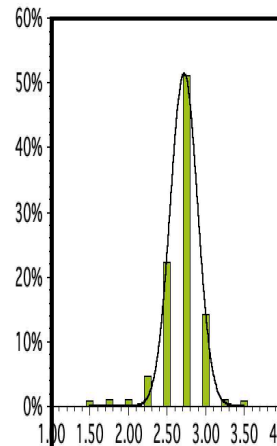
weight%.vs. $\varphi$

$\Rightarrow D_{\text{mean}} = 0.15\text{mm}$

weight%.vs.D(mm)

$D_{\text{mean}} = 0.15\text{mm}$

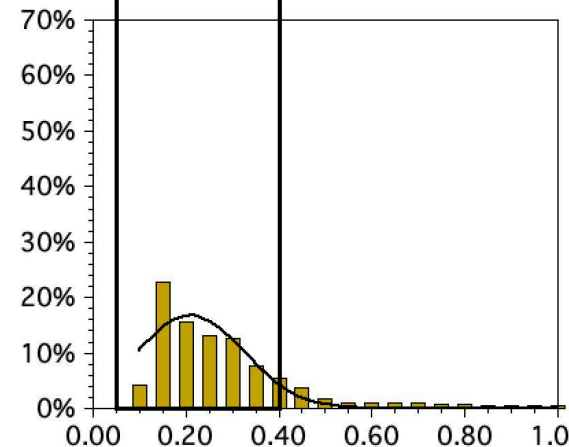
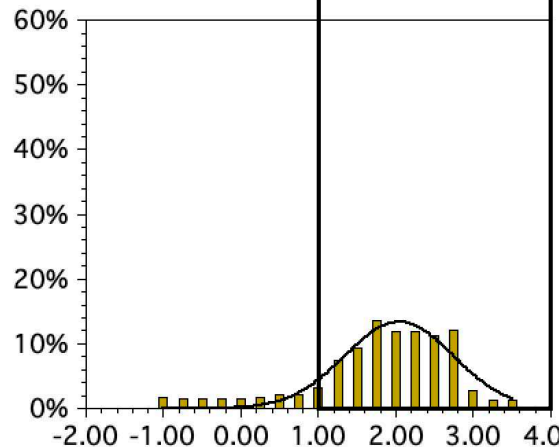
foredune



$D_{\text{mean}}$  from  $\varphi$   
depends on width  
of distribution

$D_{\text{mean}} = \text{mode of vol\%(D)}$

surf zone



$M\varphi = 2.72$

$D_{\text{mean}} = 0.30\text{mm}$

weight%.vs. $\varphi$

$\Rightarrow D_{\text{mean}} = 0.24\text{mm}$

weight%.vs.D(mm)

$D_{\text{mean}} = 0.21\text{mm}$

# what have we learned ?

Results from sieving are difficult to interpret  
(... unless you are a sedimentologist ...)

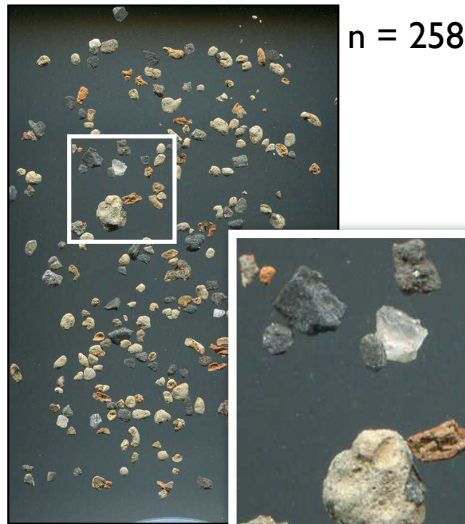
To derive a meaningful mean grain size,  $\varphi$ -values are best converted to vol% vs. linear size.

Derived  $D_{\text{mean}}$  - values depend on standard deviation.

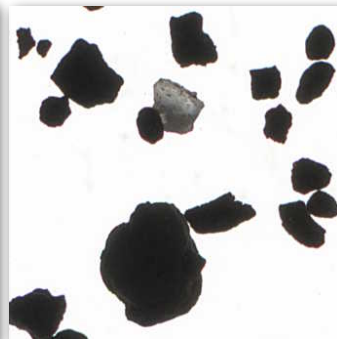
"grain size" 2  
glacial transport  
strewn samples



# "grain size" 2: glacigenic sediments



incident light



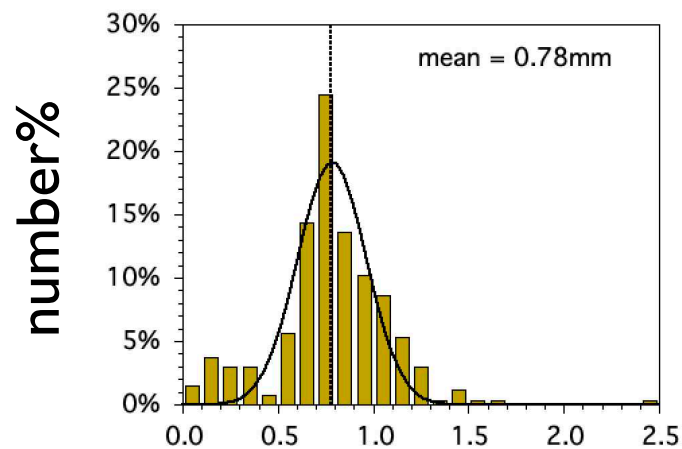
transmission



bitmap

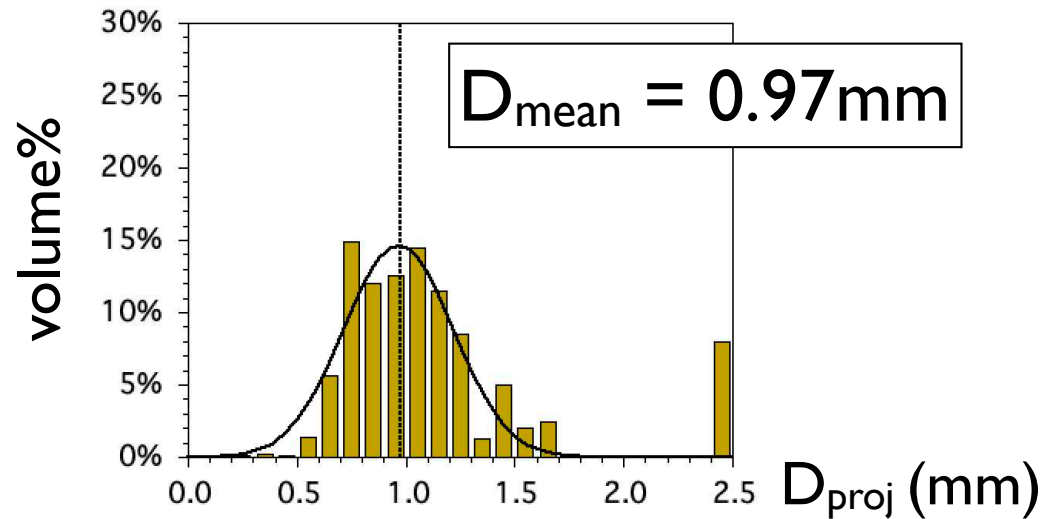
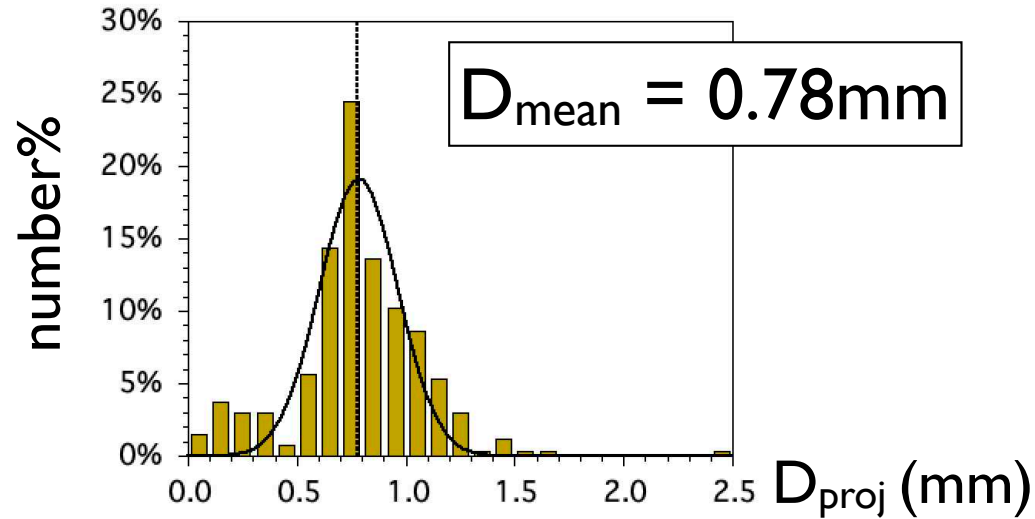


Jessen, S.P., Rasmussen, T.L., Nielsen, T., Solheim, A.:  
A new Late Weichselian and Holocene marine chronology  
for the western Svalbard slope 30,000 – 0 cal years BP.  
Quaternary Science Reviews,  
doi:10.1016/j.quascirev.2010.02.020



"Grain size":  
mean or mode of 3D diameters of  
area-equivalent circles of projected areas  
- arithmetic mean  
- mean/mode of Gaussian curve fit

# volume weighting



number%

converting  
 $\text{vol}(D) = h(D) \cdot D^3$

volume%

$D_{\text{mean}}$  from  $\text{vol}\%(D)$   
 $\neq D_{\text{mean}}$  from  $h(D)$

Note:  $D_{\text{projected}} =$  diameter of area-equivalent circle of projected area

# what have we learned ?

Sands and powders are easily analyzed using a scanner.

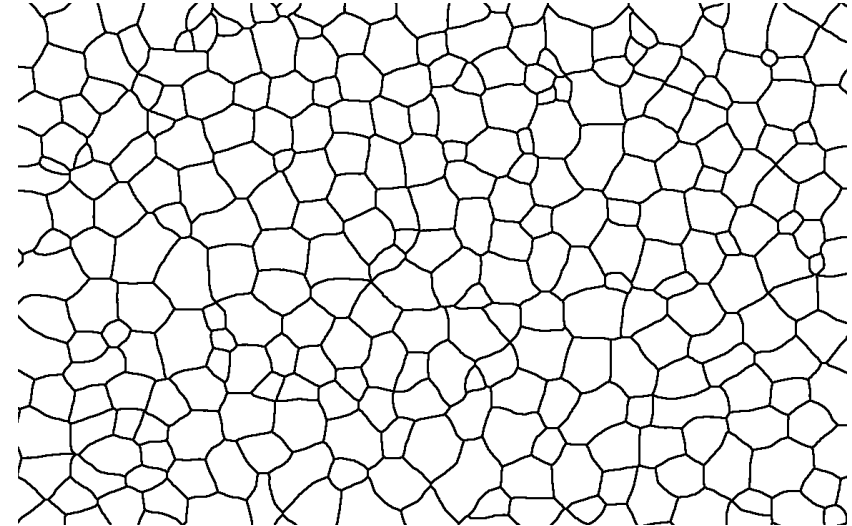
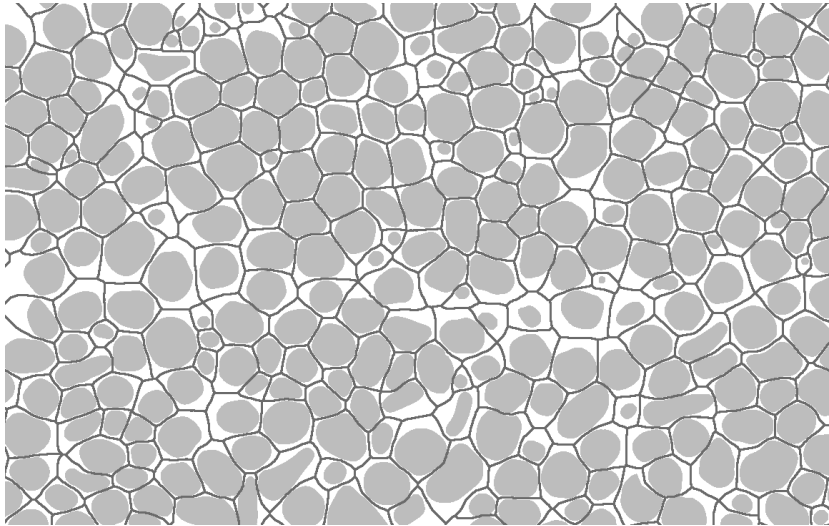
In this case, the area-equivalent diameters  $d_{\text{equ}} = D_{\text{equ}}$  represent the diameters of the volume-equivalent spheres  $D_{\text{equ}}$ .

No conversion from 2D to 3D is necessary

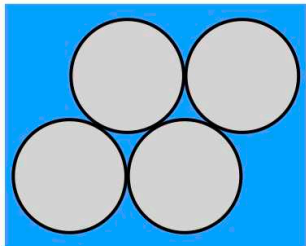
The conversion from  $h(D)$  to  $\text{vol}(D)$  is trivial:  
 $\text{vol}(D) = h(D) \cdot D^3$

"grain size" 3  
cementation  
intercept method

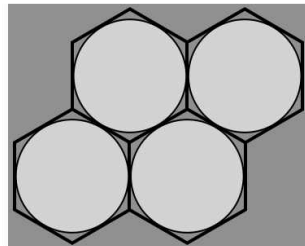
# "grain size" 3: cemented sandstone



closest packing = 74 vol%



74 vol% 26 vol%

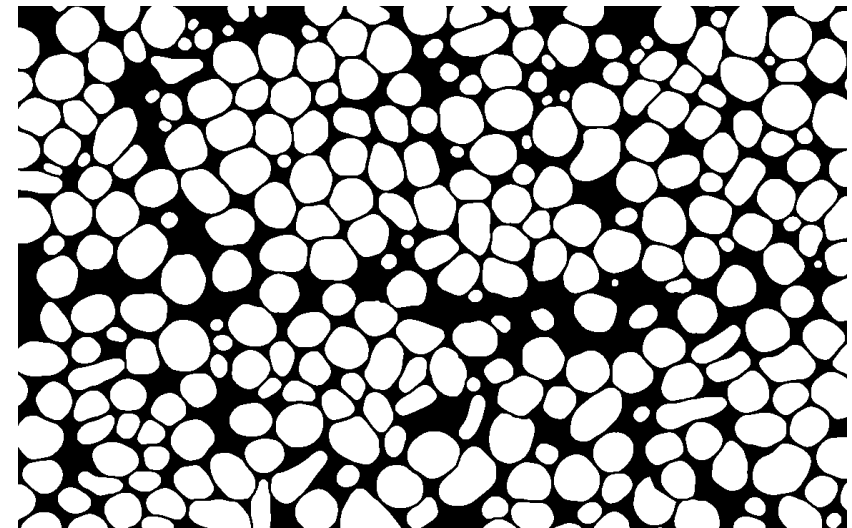


74 vol% 26 vol%

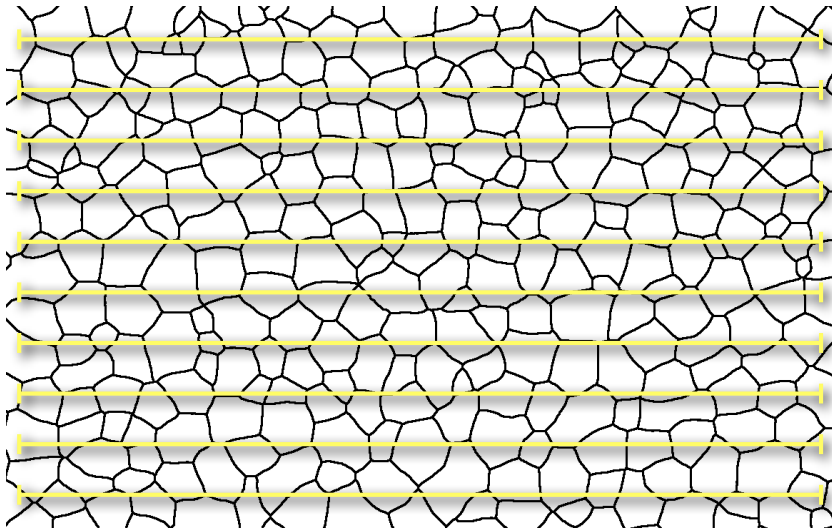
assumption:

(1) grain volume increase =  $\frac{74}{26} = 1.354$

(2)  $d_{\text{cemented}} : d_{\text{original}} = \sqrt[3]{1.354} = 1.106$



# intercept method – limitations

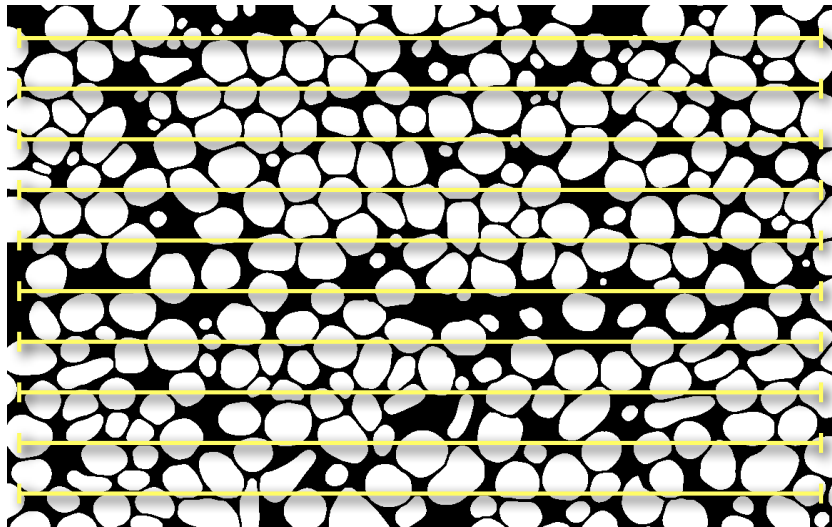


$$\text{grainsize} = \frac{\text{length of test line (L)}}{\text{number of transected grains (N)}}$$

from grain boundaries:

$$L = 23100 \mu\text{m}, N = 221$$

$$\text{size of (grains+cement)} = L / N = 105 \mu\text{m}$$



for uncemented grains:

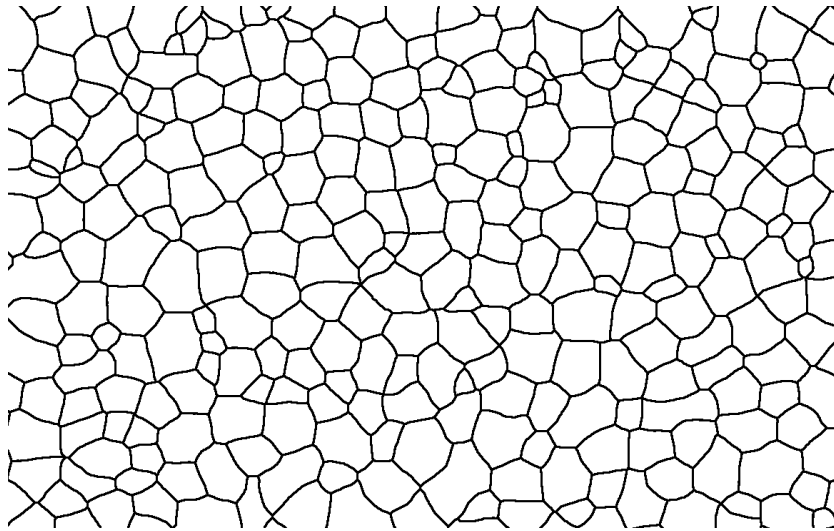
??

"Grain size":

mean of intercept lengths  
(= 2D size, no distribution)

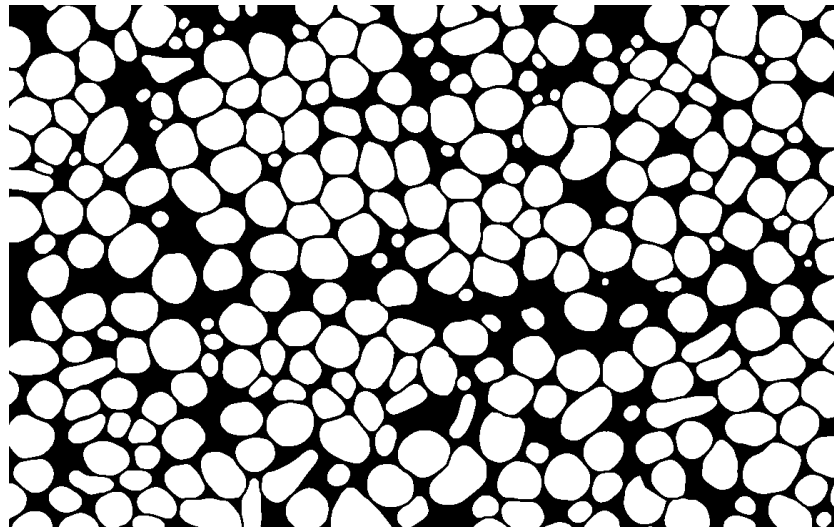
does not work for grains in matrix

# check against digital image analysis



check (1) diameters (long axis fit ellipse)

grains from intercept	105 $\mu\text{m}$
grains from ellipse fit	110 $\mu\text{m}$



check (2) ratios

long axes of fit ellipse:

grains	110 $\mu\text{m}$
(grains+cement)	130 $\mu\text{m}$

(grains+cement) : grains = 1.22  $\neq$  1.11



area%

grains	72.9 vol%
(grains+cement)	100.0 vol%

(grains+cement) : grains = 1.37  $\approx$  1.35



# what have we learned ?

The intercept method is practical and fast – can be done at the microscope – or on un-segmented micrographs, ... but ...

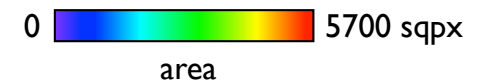
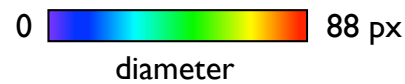
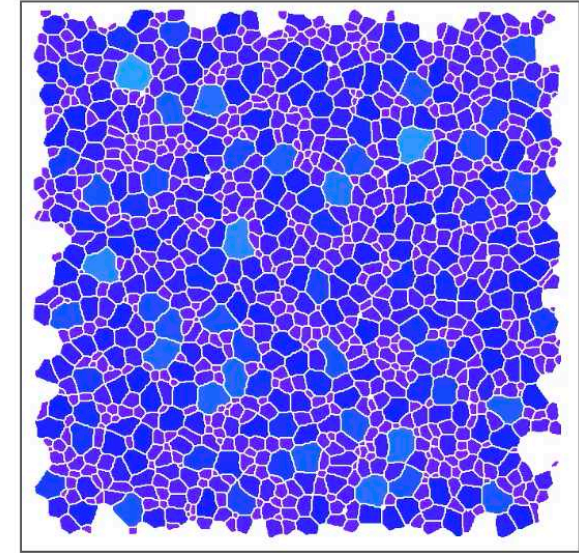
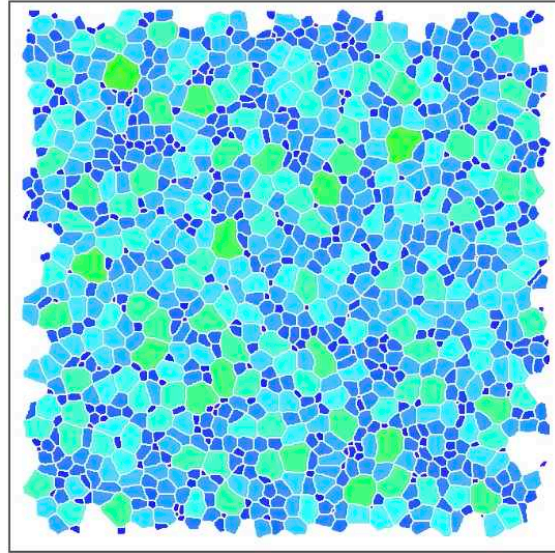
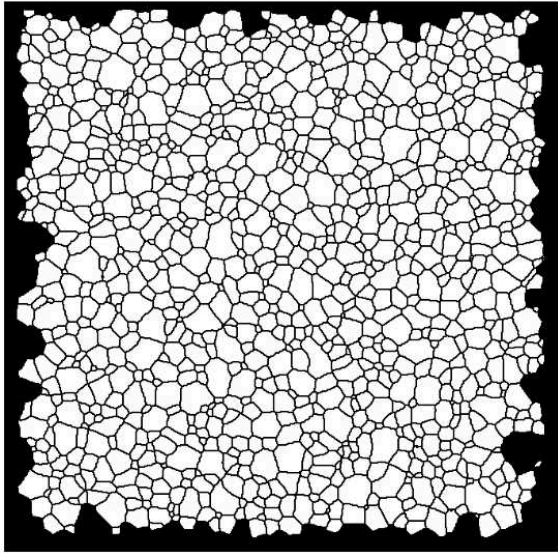
Only mean the arithmetic 2D mean can be calculated.

Cannot be used for grains in matrix.



"grain size" 4  
grain growth  
2D experiment

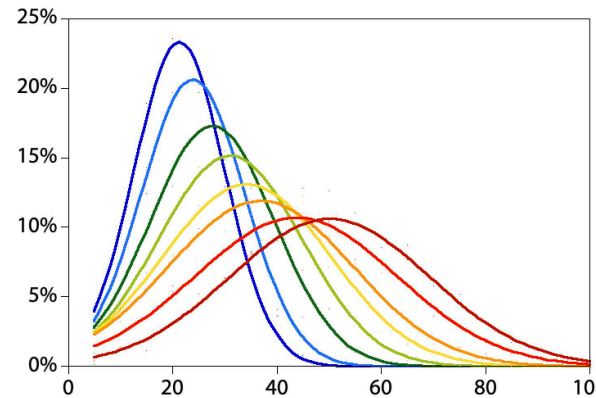
# "grain size" 4: Ostwald ripening



## grain growth kinetics

Chen LQ, Yang W (1994)  
Computer-simulation of the domain dynamics of a quenched system with a large number of nonconserved order parameters—the grain-growth kinetics.  
Phys Rev B 50: 15752--15756  
[https://www.youtube.com/watch?v=p0rY2r0E\\_2k](https://www.youtube.com/watch?v=p0rY2r0E_2k)

"Grain size":  
- arithmetic mean of 2D diameter  
- mean/mode of curve fit



## grain growth

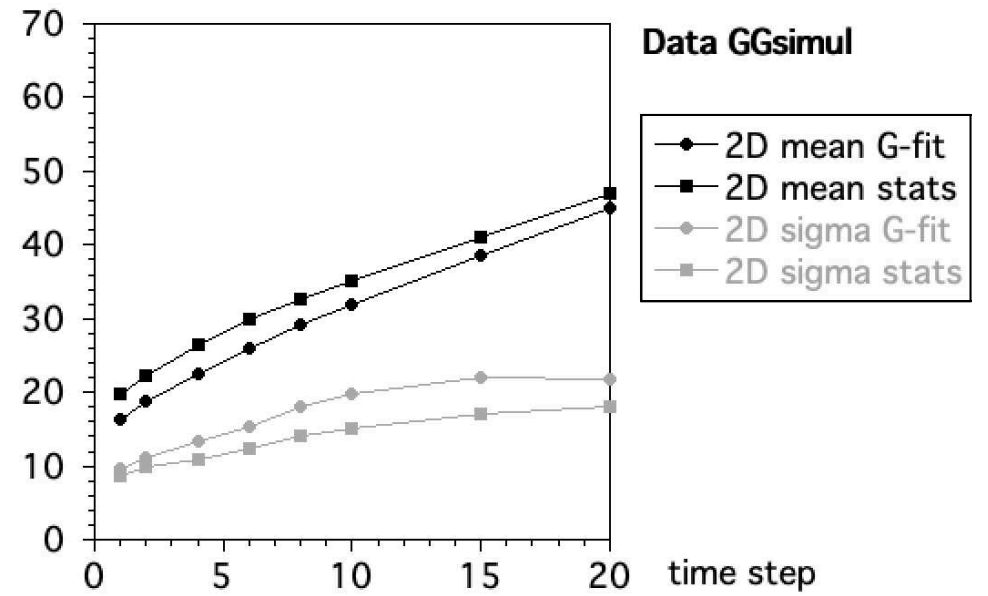
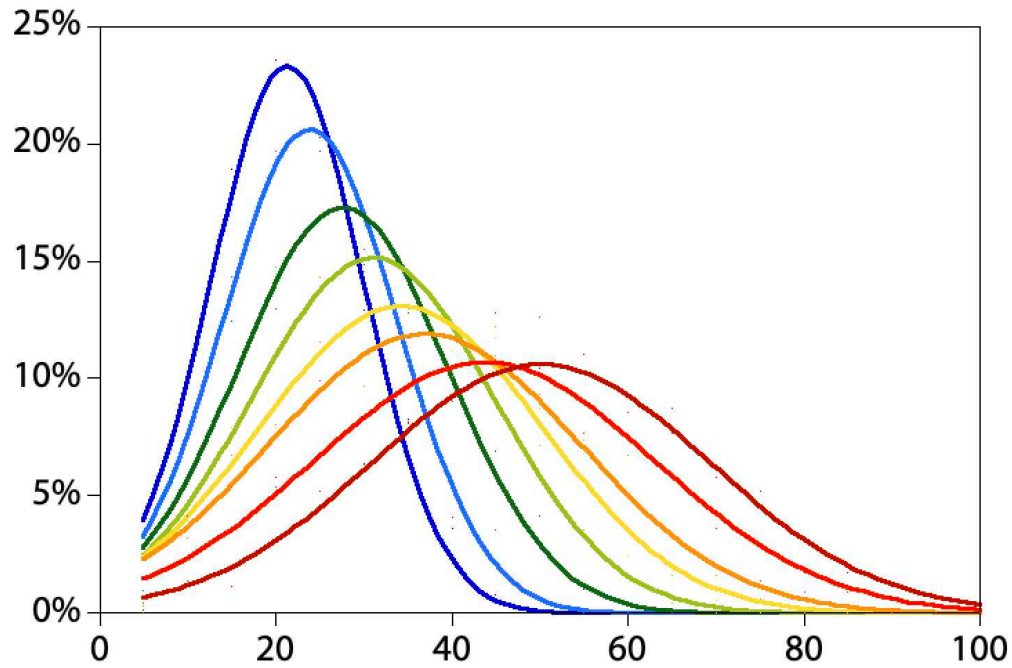
- increasing average size
- increasing spread

in terms of normal distribution:

- increasing mean ( $\mu$ )
- increasing standard deviation ( $\sigma$ )

⇒ distribution matters

# 2D simulation



### G-fit = curve fitting

d-01.out		
	Value	Error
m1	18.896	0.38953
m2	44.579	1.7004
m3	12.732	0.57973
Chisq	20.75	NA
R	0.99525	NA

### stats = arithmetic mean

---

statistics for output file d-01.out.txt  
(data not saved - need to copy from screen):

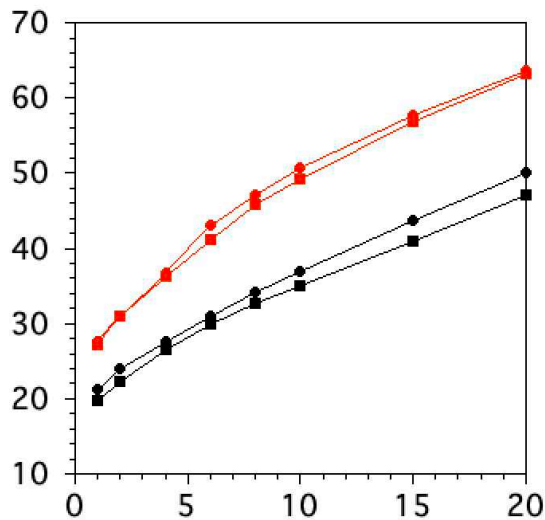
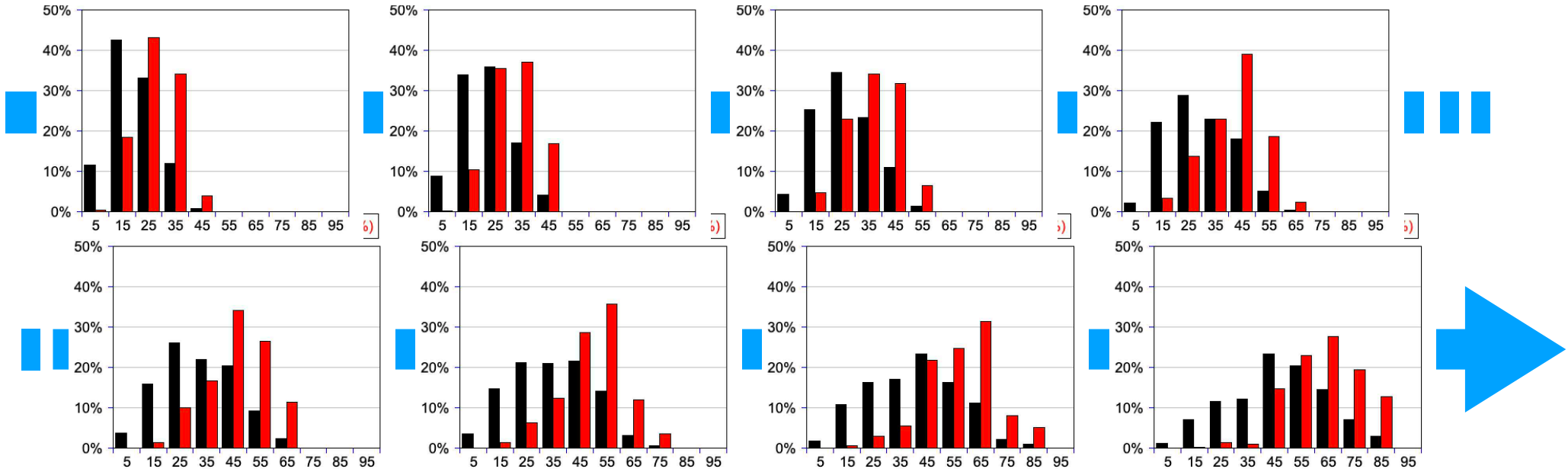
	mean	st.dev.
statistics of d	19.76689	8.74732
statistics of D	19.70738	8.28300
statistics of V	27.25517	8.04039
statistics of D*	19.70738	8.28300
statistics of V*	27.25517	8.04039

---

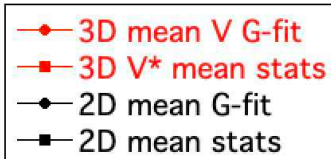
# should we convert to 3D...?

$h(d)$  frequency of 2D size

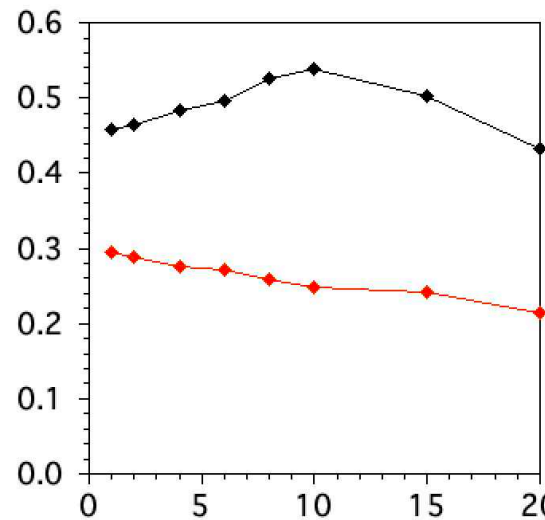
$v(D)$  volume% of 3D size



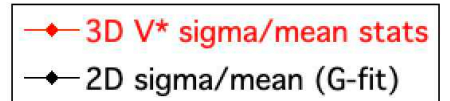
diameter(t)



timestep



(stdev/mean)(t)



timestep

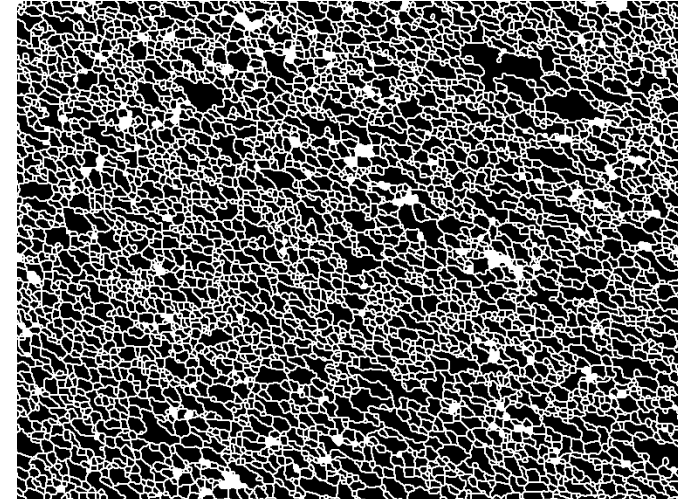
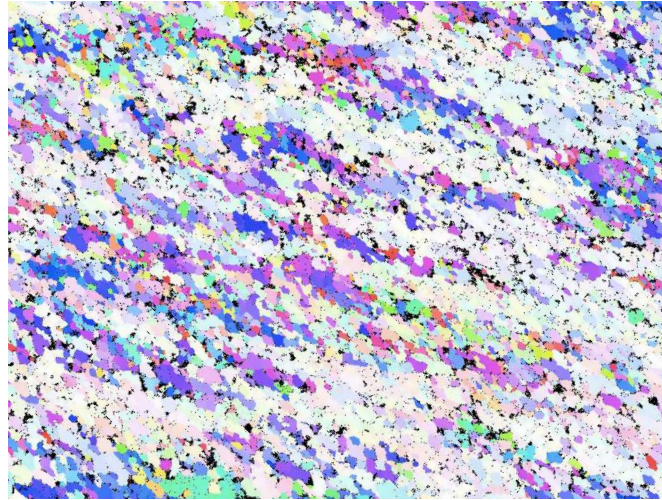
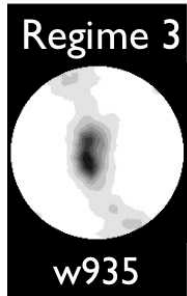
# what have we learned ?

In a fully cemented / fully crystallized rock grain growth has to be volume conserving.

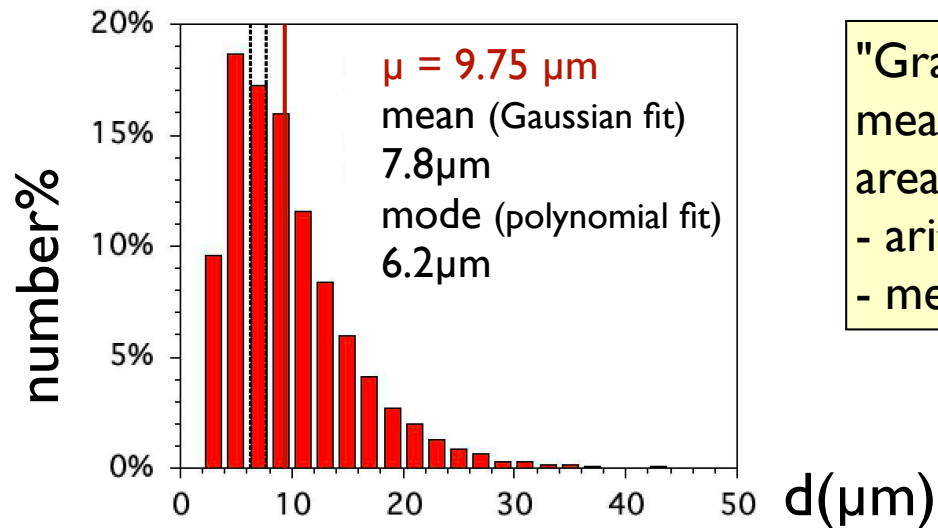
Ostwald ripening is a valid model for such a process: starting with a normally distributed grain size, both the mean and the standard deviation increase with time.

"grain size" 5  
dynamic  
recrystallization  
from 2D to 3D

# "grain size" 5: sheared quartzite

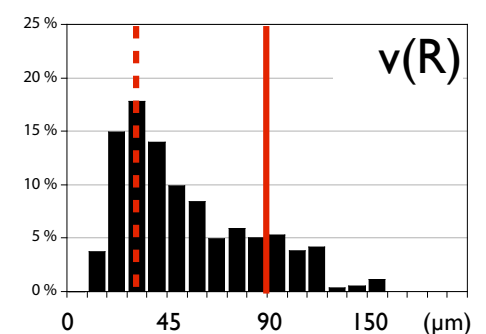
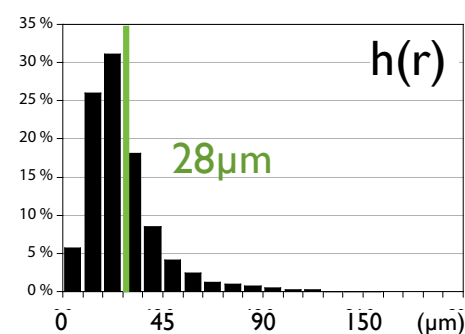
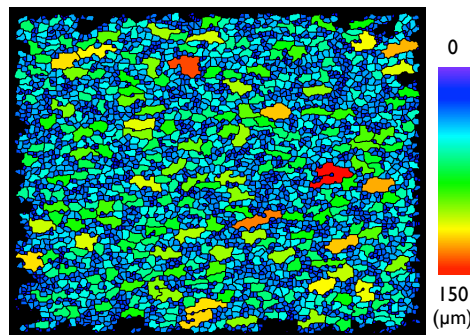
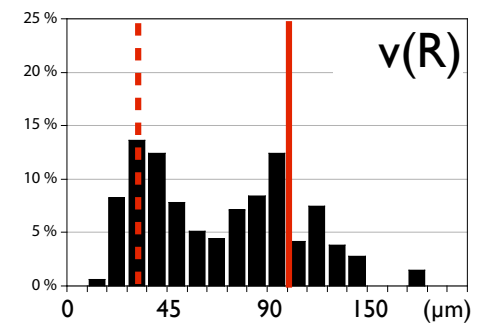
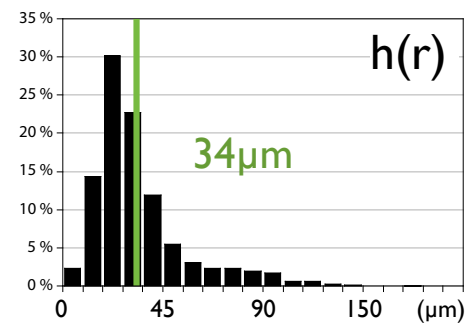
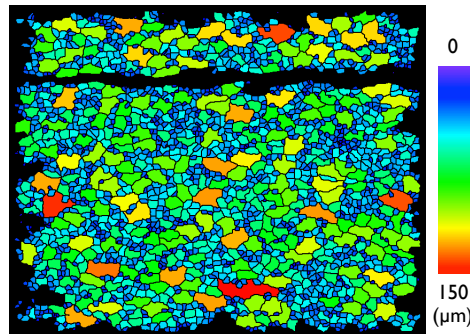
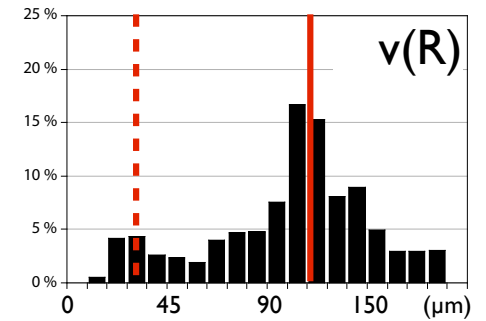
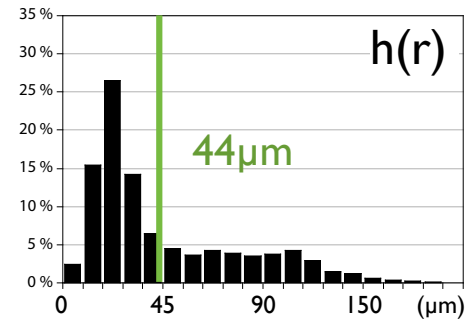
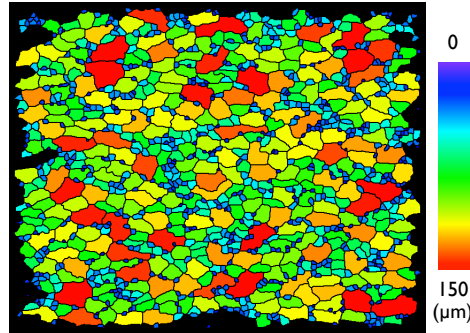
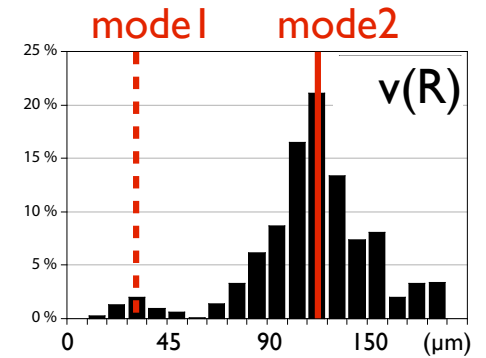
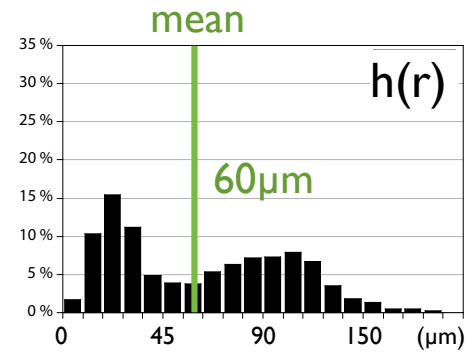
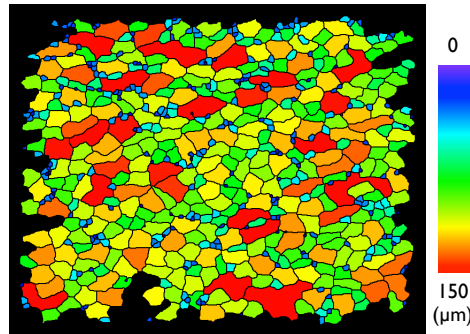
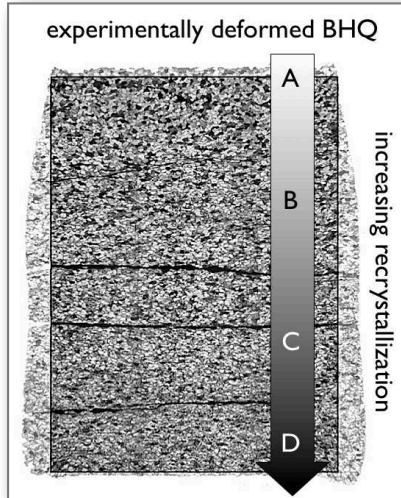


Heilbronner, R. & Kilian, R. (2017). The grain size(s) of Black Hills Quartzite deformed in the dislocation creep regime. *Solid Earth*, 8, 1071–1093, 2017, doi.org/10.5194/se-8-1071-2017.



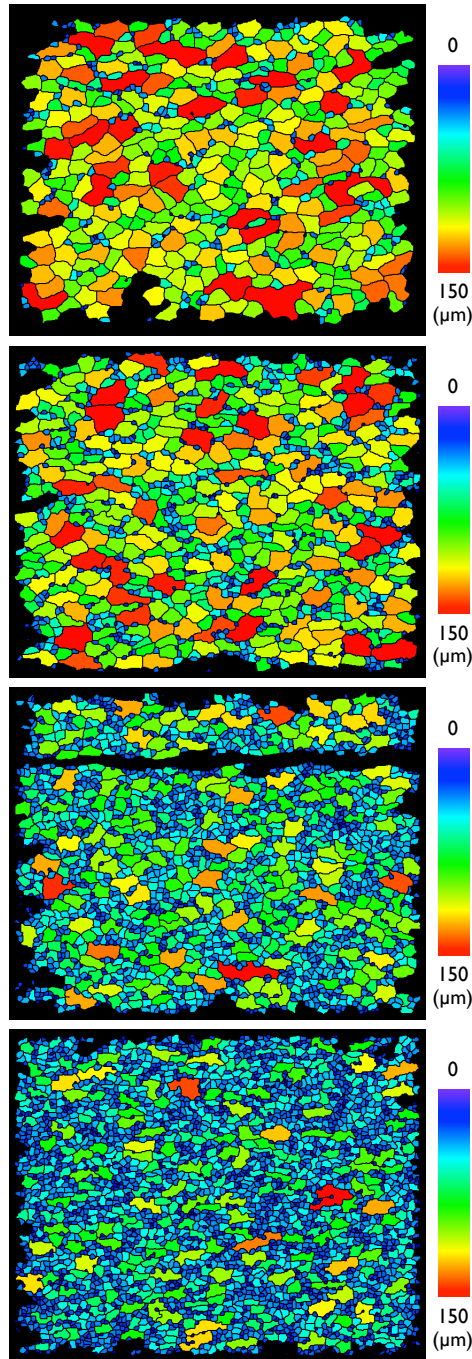
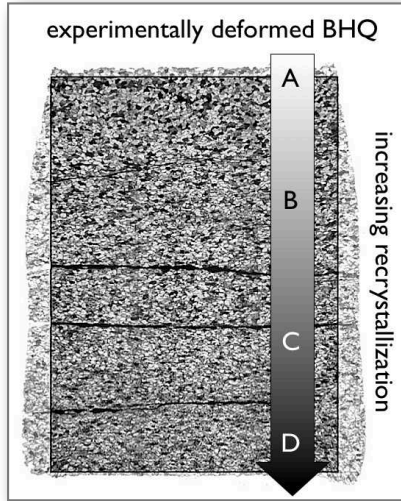
"Grain size":  
mean or mode of 2D diameters of  
area-equivalent circles of sectional shapes  
- arithmetic mean  $\mu$   
- mean/mode of curve fits

# 2D versus 3D – mean versus mode



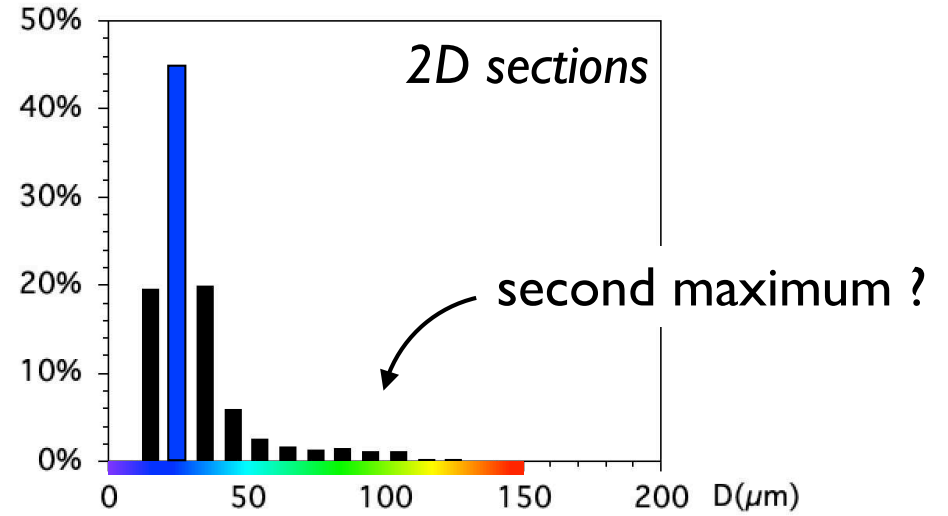


# detect second maximum



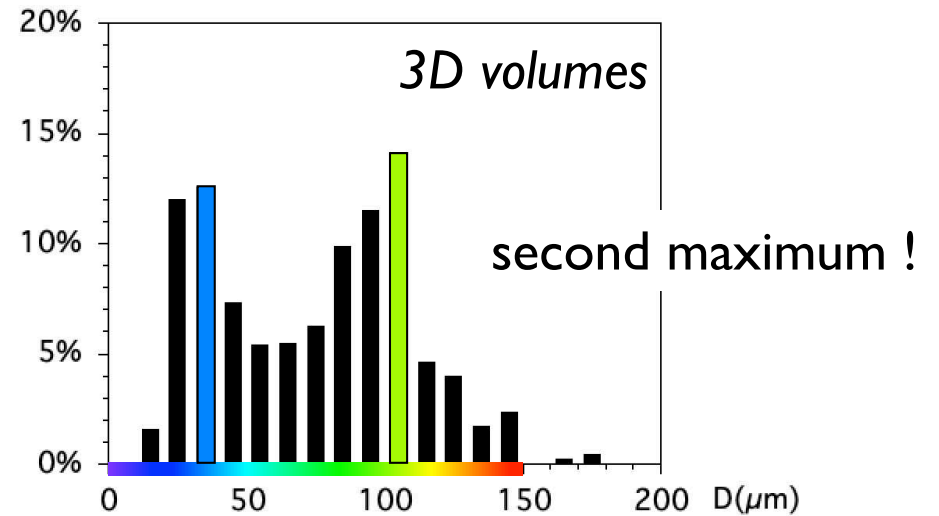
A+B+C+D

■  $h(D)(\%)$



A+B+C+D

■  $v(D)(\%)$



# what have we learned ?

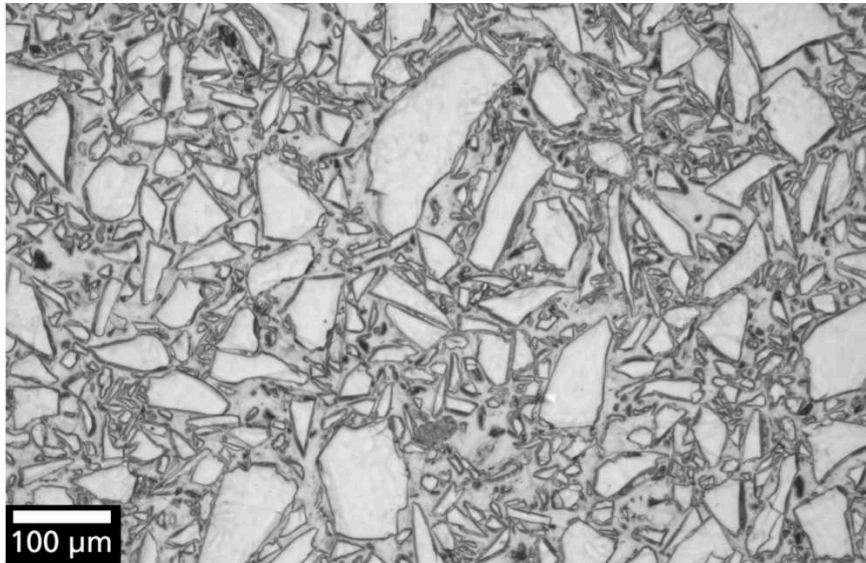
Converting 2D grain size data to 3D is highly recommended!

Volume weighted 3D histograms should be used – they are free from sectioning artefacts!

Modal 3D grain size identifies the physically most relevant grain size(s).

"grain size" 6  
powder  
particle analyzer

# "grain size" 6: crushed quartz

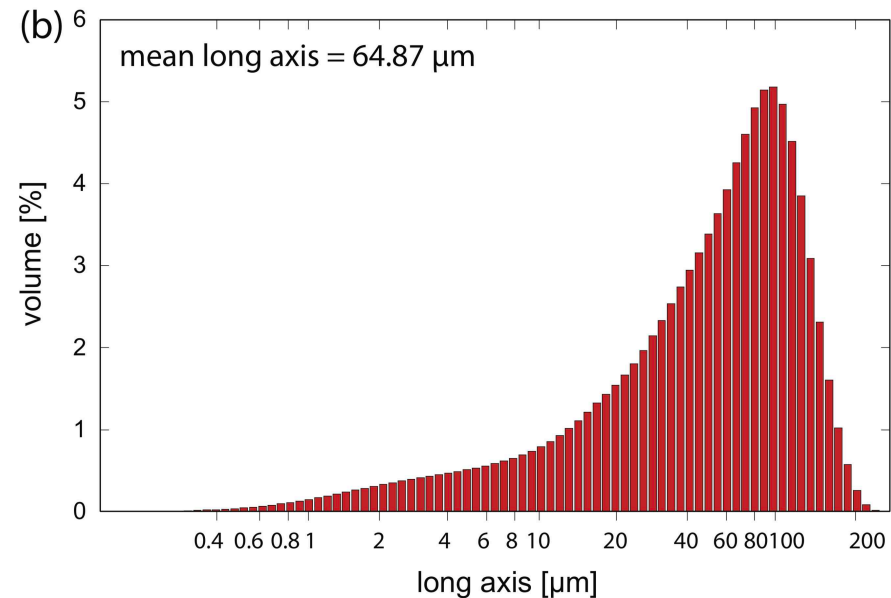


Range from 0.2  $\mu\text{m}$  up to 300  $\mu\text{m}$   
Mean length is about 65  $\mu\text{m}$  and  
Mode between 90 and 95  $\mu\text{m}$ .

"Grain size":

mean or mode of log (3D size)  
(e.g., long axes of particles)

- arithmetic mean
- mean/mode of curve fits



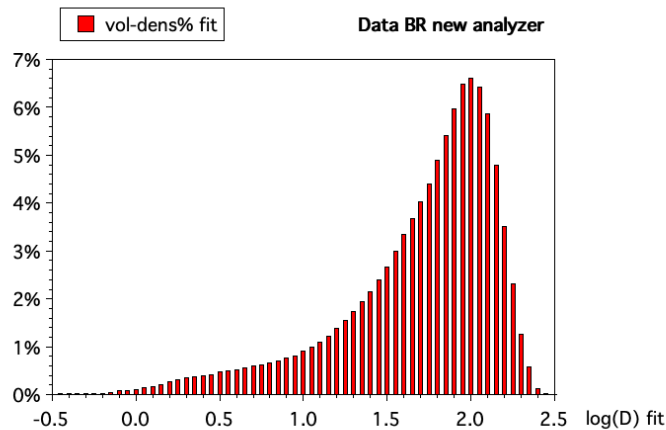
Richter, B., 2017, *The brittle-to-viscous transition in experimentally deformed quartz gouge*. Dissertation, Basel University. <https://edoc.unibas.ch/57805/>

# to get the mean grain size ...

... proceed like this:

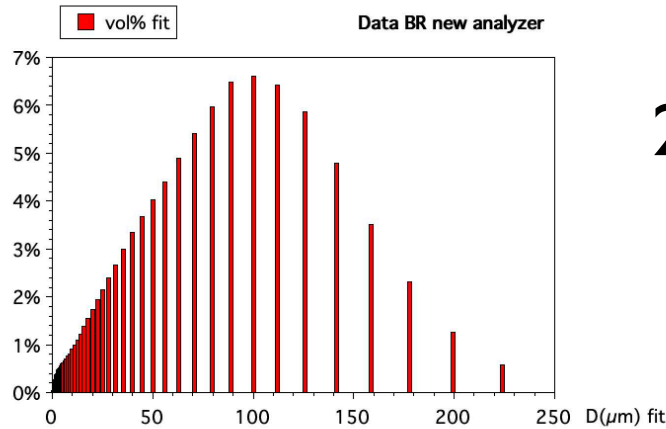
1. Clean original data:  
Plot = vol% vs. log(D)

1



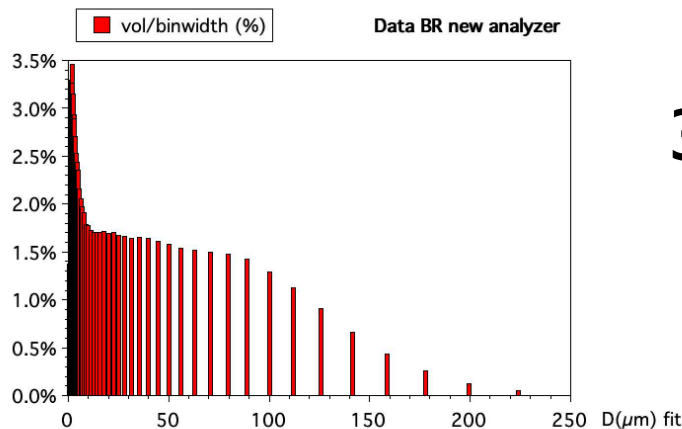
2. Convert to linear D:  
 $d = 10^{\log(d)}$   
Plot = vol% vs. D( $\mu\text{m}$ )

2

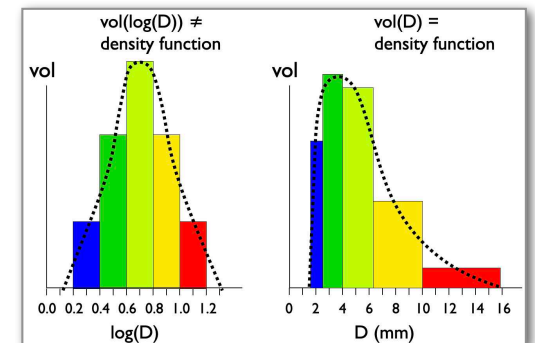


3. Correct for bin width:  
 $\text{vol}_{\text{corr}} = \text{vol} / \text{bin width}^*$

3

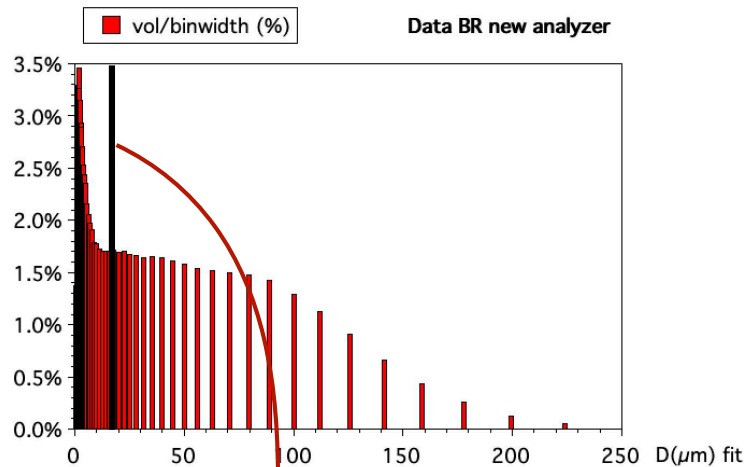


*pro memoria:*

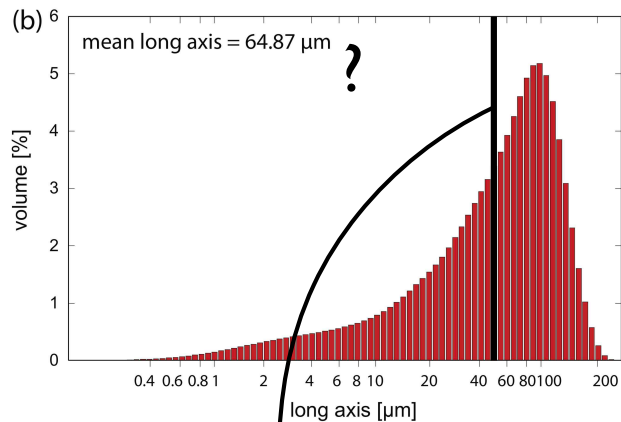


*\*) if  $\Delta \log(d) = \text{constant}$   
 $\Rightarrow \Delta d \neq \text{constant}$*

# ... $\neq$ the mean of log histograms !



mean long axis =  
 $D_{\text{mean}} = 17.5 \mu\text{m} !!$



"mean" long axis =  $49 \mu\text{m}$

evaluated from linear data

$$\Rightarrow D_{\text{mean}} = 17.5 \mu\text{m}$$

*depends on upper and lower bound,  
 only true for  $(-0.5 \leq \log(D) \leq 2.3)$   
 i.e., for  $(3 \mu\text{m} \leq D \leq 200 \mu\text{m}) !!!$*

evaluated from log data

mean value of  $\log(D) = 1.69$

$$\Rightarrow D_{\text{mean}} = 10^{1.69} = 49 \mu\text{m}$$

modal value of  $\log(D) = 1.95$

$$\Rightarrow D_{\text{mean}} = 10^{1.95} = 90 \mu\text{m}$$

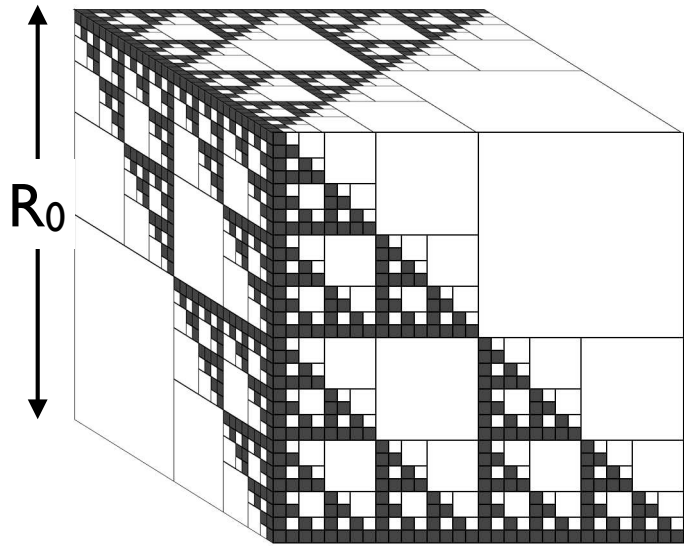
Range from  $0.2 \mu\text{m}$  up to  $300 \mu\text{m}$

Mean length is about  $65 \mu\text{m}$  and

Mode between  $90$  and  $95 \mu\text{m}$ .

Richter, B., 2017, *The brittle-to-viscous transition in experimentally deformed quartz gouge*. Dissertation, Basel University.  
<https://edoc.unibas.ch/57805/>

# intermezzo: fractal size distributions



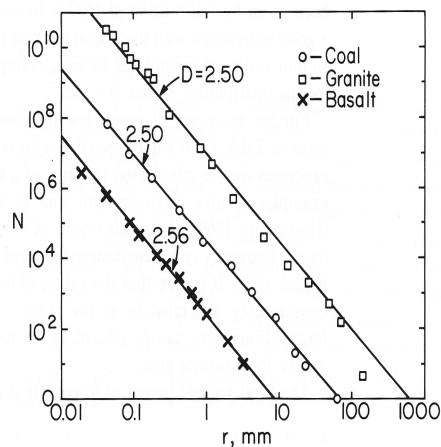
$F$  number of fragments created  
 $C$  number of fragments being fragmented  
 $f = C/F$  fragmentation fraction  
 $R_i$  size (diameter) of fragment  
 $N_i$  number of cracked fragments

Fractal dimension

$$D = \frac{\log (N_{i+1} / N_i)}{\log (R_i / R_{i+1})}$$

## published example:

The number  $N$  of fragments with **cube root of volume** greater than  $r$  is given as a function of  $r$  for broken coal (Bennett, 1936), broken granite from a 61 kt underground nuclear detonation (Schoutens, 1979), and impact ejecta due to a  $2.6 \text{ km s}^{-1}$  polycarbonate projectile impacting on basalt (Fujiwara *et al.*, 1977). The best-fit fractal distribution from (2.6) is shown for each data set.



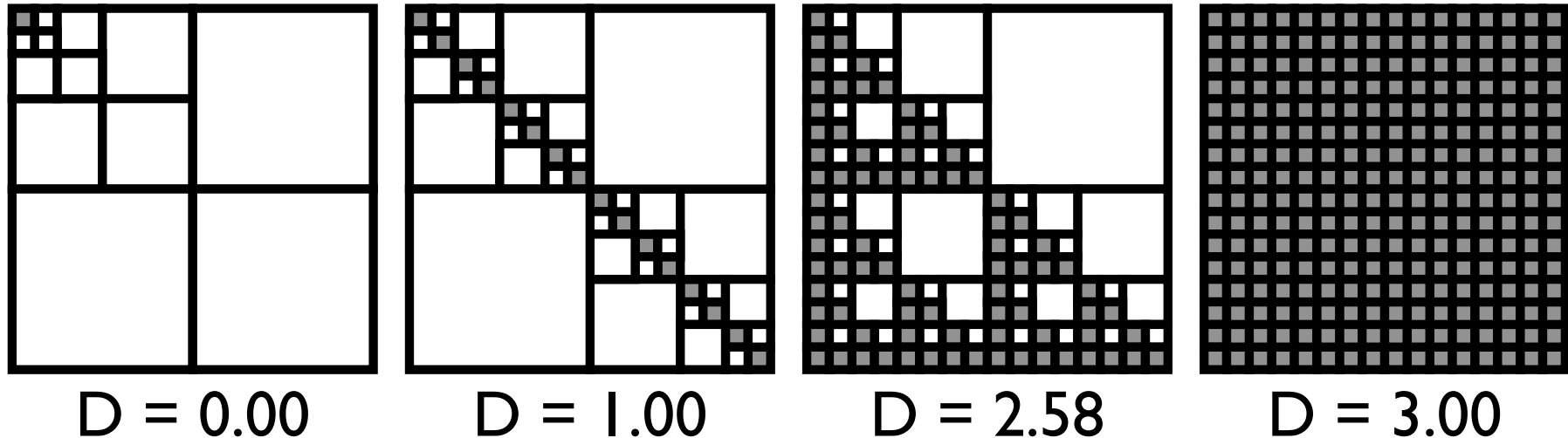
Example:

$$\begin{array}{lll}
 F & = & 8 \\
 C & = & 6 \\
 f & = & 6 / 8
 \end{array}
 \quad
 \begin{array}{lll}
 R_1 & = & R_0 / 2 \\
 R_2 & = & R_0 / 4
 \end{array}
 \quad
 \begin{array}{lll}
 N_1 & = & 6 \\
 N_2 & = & 36
 \end{array}$$

$$D = \frac{\log (N_2 / N_1)}{\log (R_1 / R_2)} = \frac{\log (6)}{\log (2)} = 2.585$$

# maximum value for $D = 3.00$ – why ?

map views of cube:



The fractal distribution  $N_i(R_i)$  is characterised by a constant ratio  $D = \frac{\log (N_{i+1} / N_i)}{\log (R_i / R_{i+1})}$  ( $0 \leq D \leq 3.00$ )

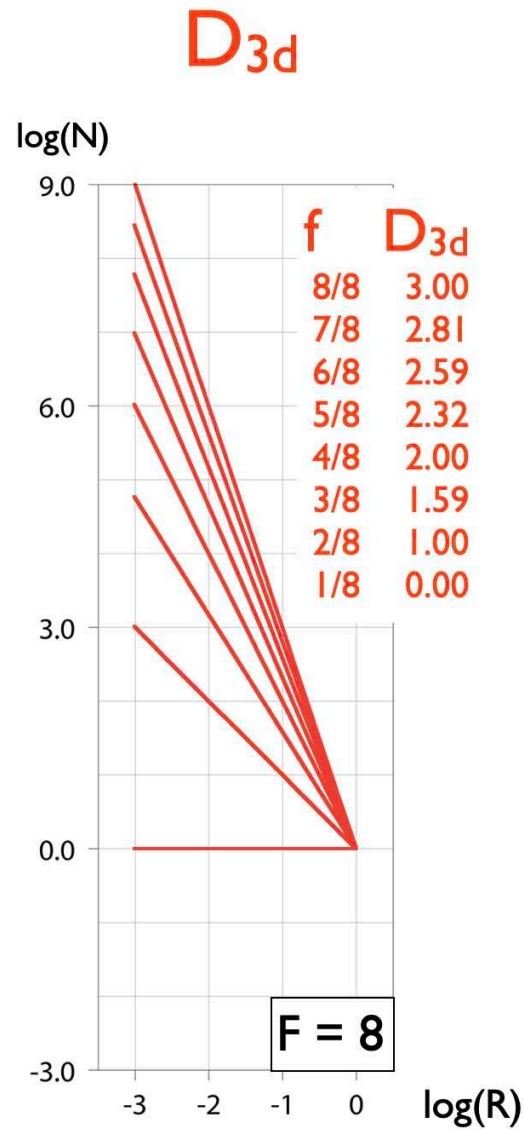
$N_{i+1} / N_i$  = frequency ratio of smaller to larger grain size

$R_i / R_{i+1}$  = size ratio of larger to smaller grain size

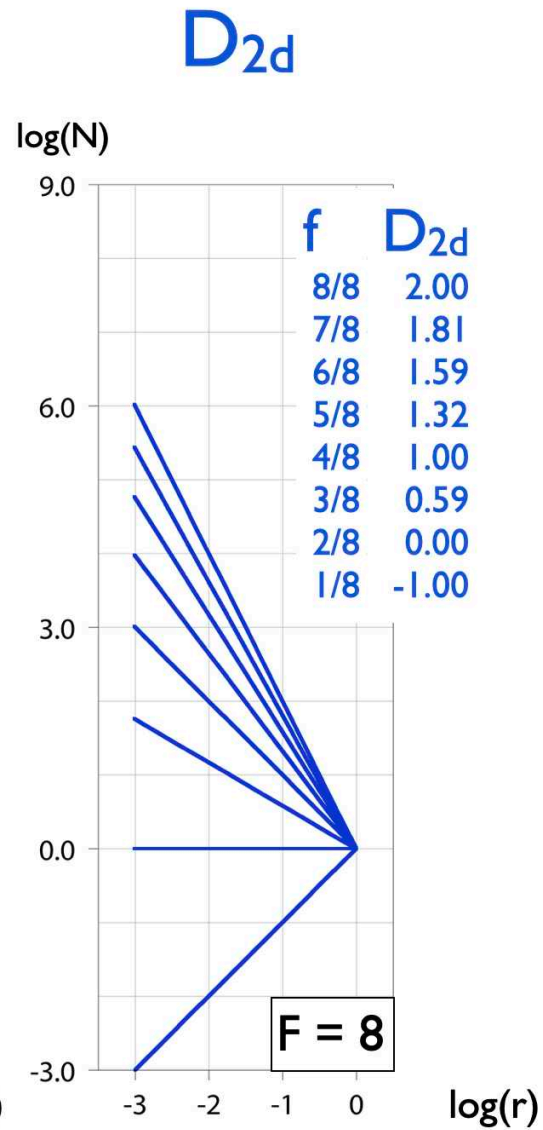
At the maximum value of  $D = 3.0$ , the 2-dimensional fracture surface (grain boundary surface) is completely room-filling, and thus itself a 3-d volume. A higher value than  $D = 3$  cannot be attained by this process of fragmentation



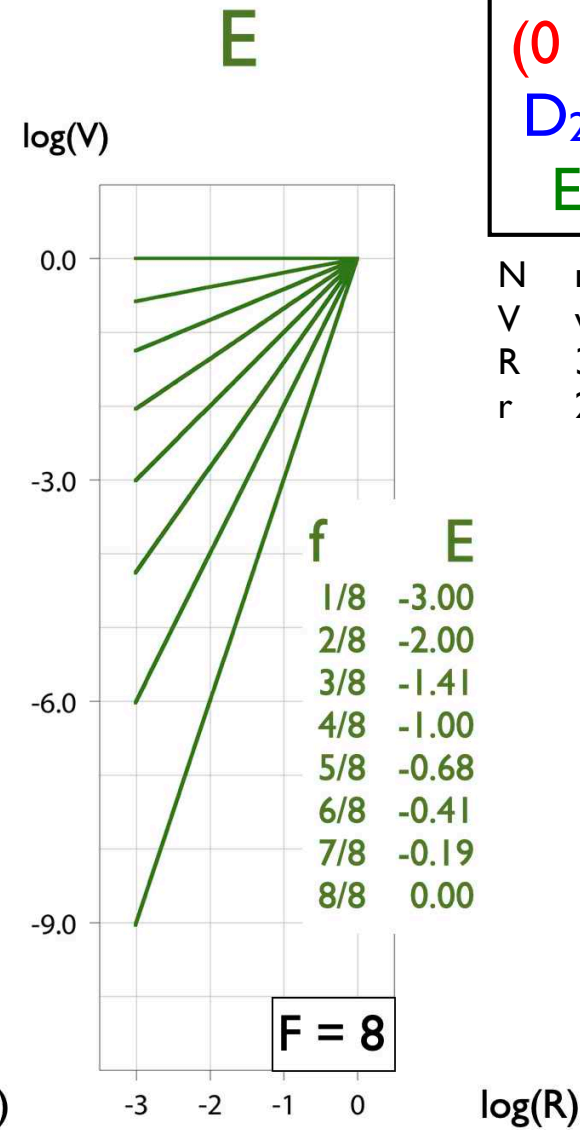
# more from the fractal world



fractal dimension  
(number of 3D grains)



fractal dimension  
(number of 2D sections)



volume fraction  
(volume % of 3D grains)

$(0 \leq D_{3d} \leq 3)$   
 $D_{2d} = D_{3d} - 1$   
 $E = 3 - D_{3d}$

N number of fragments  
V volume of fragments  
R 3D diameter of fragments  
r 2D section diameter

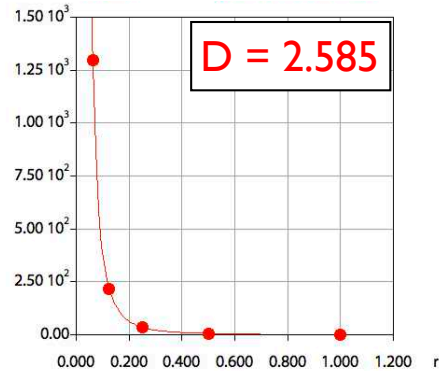
# $D_{2d}, D_{3d}, E$ from $N/R$ or $\log(N)/\log(R)$

powerlaw fit to linear data

exponent =  $D$

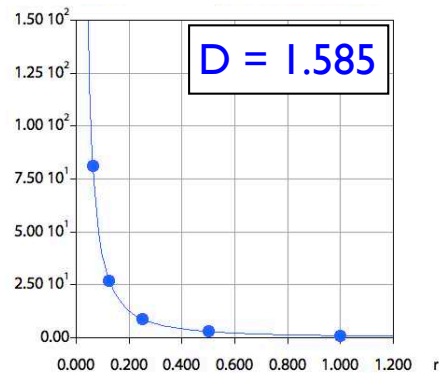
$D_{3d}$

$$N = R^{-D_{3d}}$$



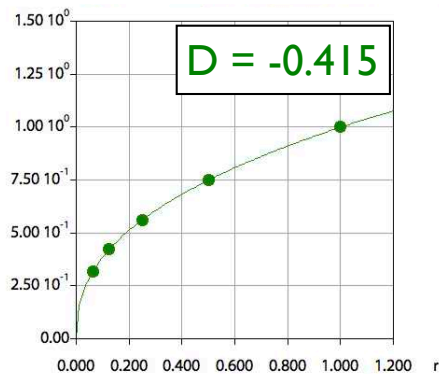
$D_{2d} = D_{3d} - 1$

$$N = R^{-D_{2d}}$$



$E = 3 - D_{3d}$

$$N = R^E$$

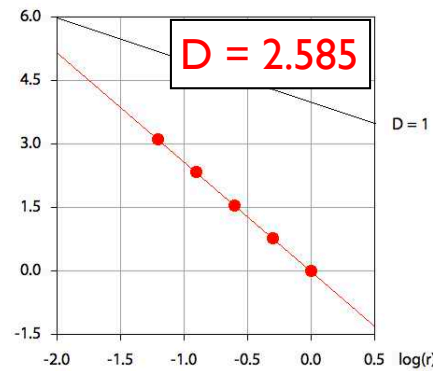


linear fit to log data

slope =  $D$

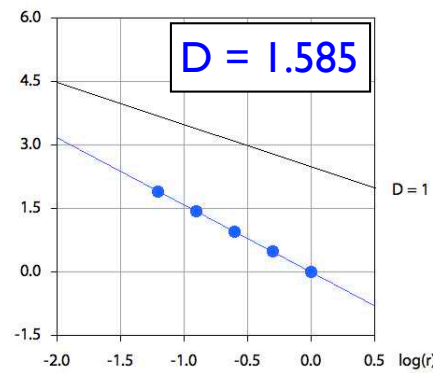
$D_{3d}$

$$\log N = -D_{3d} \cdot \log R$$



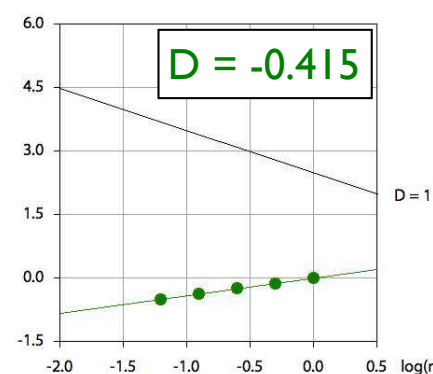
$D_{2d} = D_{3d} - 1$

$$\log N = -D_{2d} \cdot \log R$$

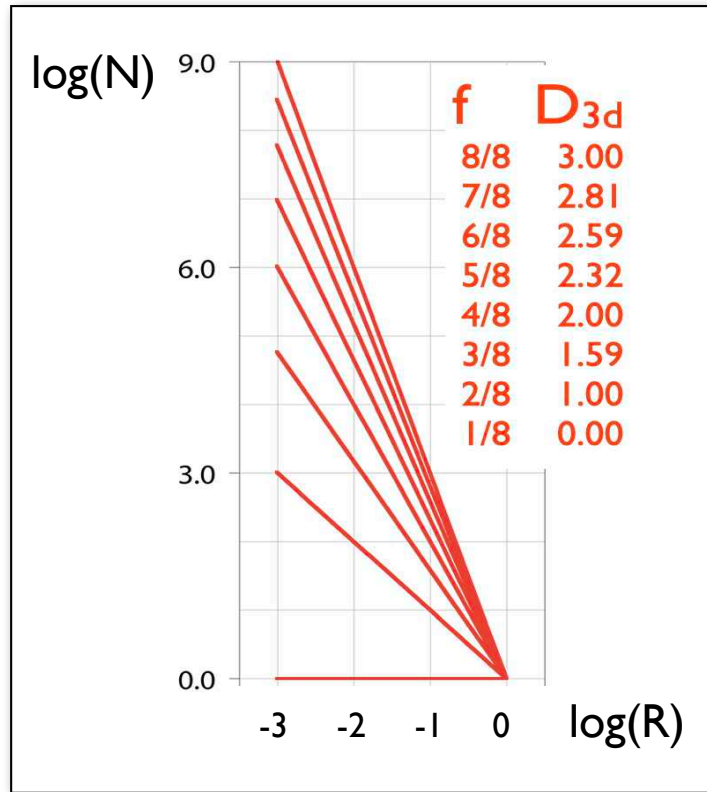


$E = 3 - D_{3d}$

$$\log N = E \cdot \log R$$

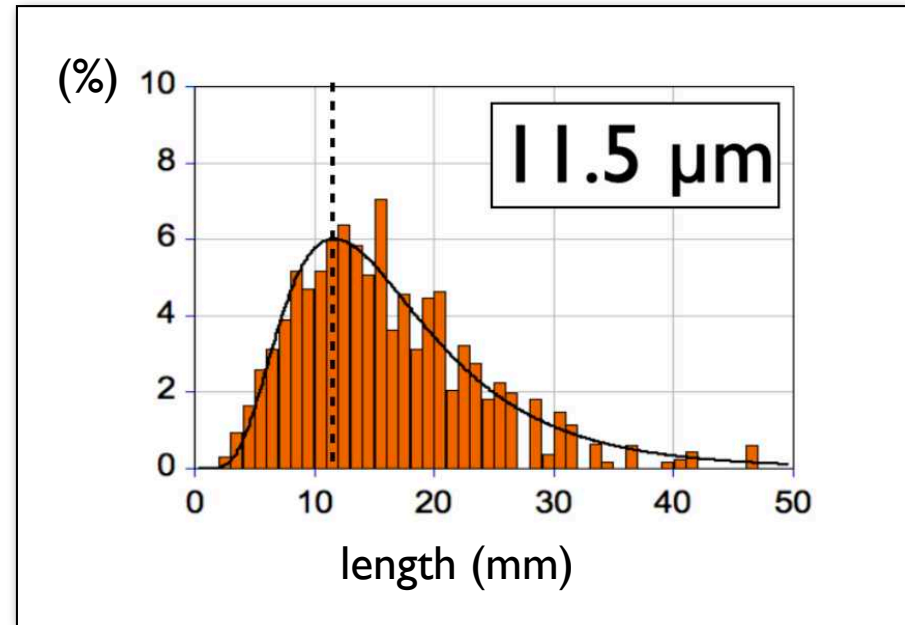


# beware: fractal $\neq$ modal distribution



characteristics:

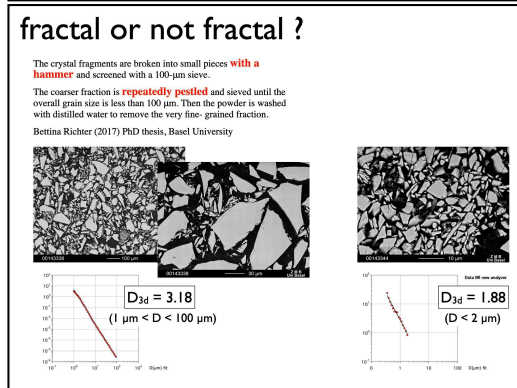
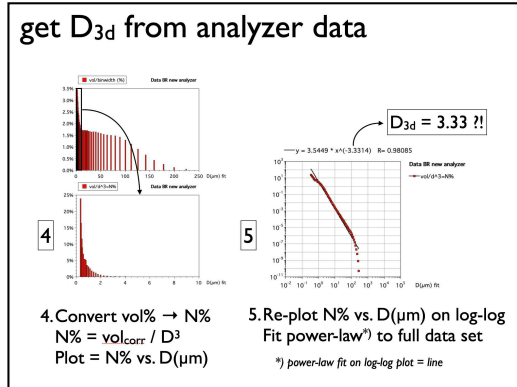
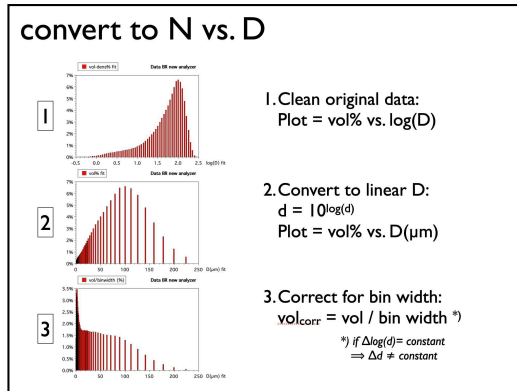
- fractal dimension  $D$   
= grain size ratio
- unbounded:
- no minimum, no maximum
- no mean or mode



characteristics:

- moment of central tendency  
= most significant grain size
- mean or mode of distribution
- bounded:
- total (area under curve) = 100%

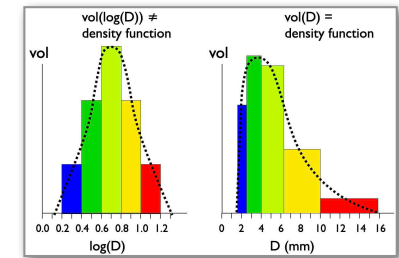
# ... returning to the talk



what was said in the talk:

- you should correct analyzer vol% to account for increasing bin width with size:  $\text{vol}_{\text{corr}} = \text{vol\%} / \text{bin width}$
- after calculating N% from  $\text{vol}_{\text{corr}}$ , N% was plotted versus D( $\mu\text{m}$ ) and the powerlaw fit yielded  $D_{3d} > 3.0$

keeping this in mind:



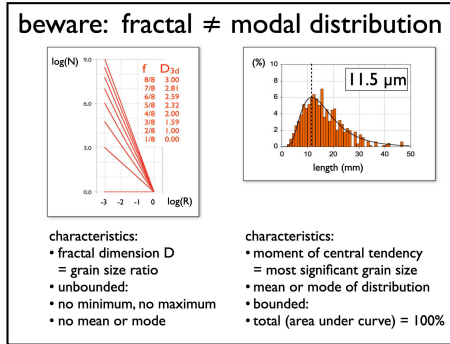
how this was explained in the talk:

- the processes of hammering and pestling do not correspond to fractal fragmentation

unfortunately, that was rubbish !!

# ...doing it right

now we know:



Therefore

1. Clean original data:  
Plot = vol% vs. log(d)

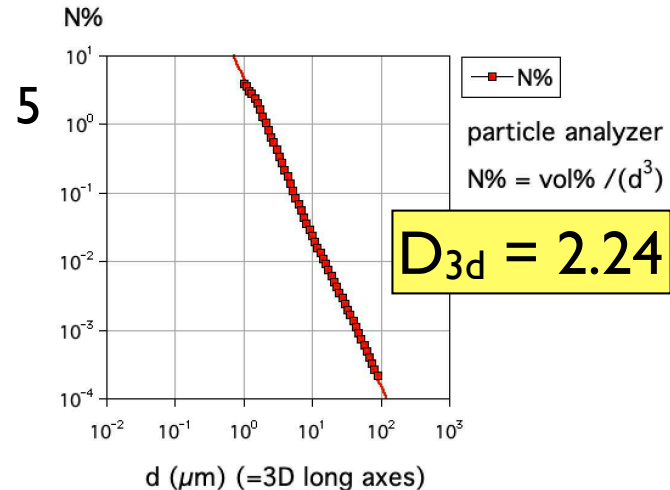
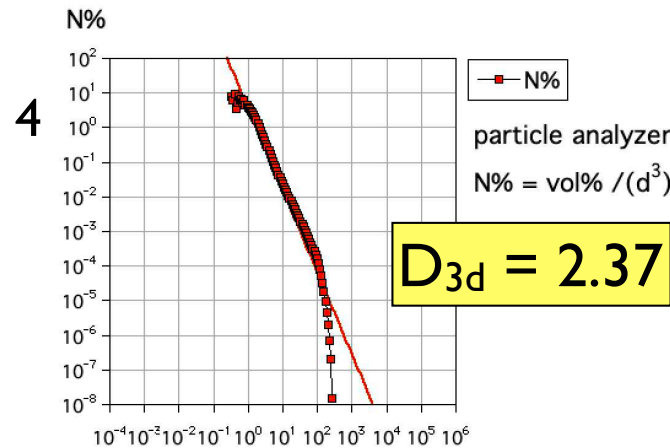
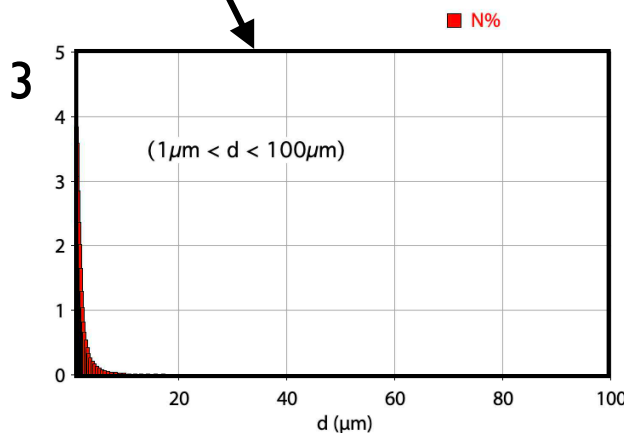
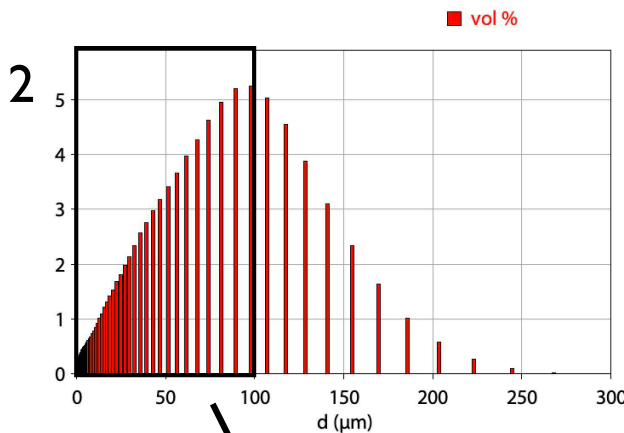
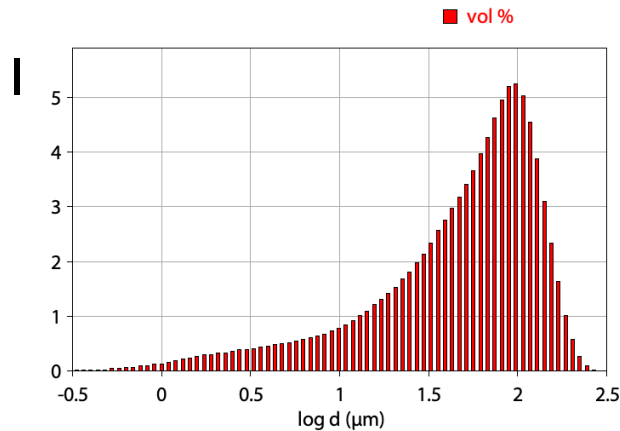
2. Convert to linear bin size:  
 $d = 10^{\log(d)}$   
Plot = vol% vs. d( $\mu\text{m}$ )

~~3. Correct bin width:  
vol<sub>corr</sub> = vol / bin width \*~~

3. **Directly**  
convert vol%  $\rightarrow$  N%  
 $\text{no}\% = \text{vol}\% / d^3$   
Plot = N% vs. d( $\mu\text{m}$ )

4. Plot N% vs. d( $\mu\text{m}$ ) on log-log  
Fit power-law to full data

5. Fit power-law to cropped  
( $1\mu\text{m} \leq d \leq 100\mu\text{m}$ )

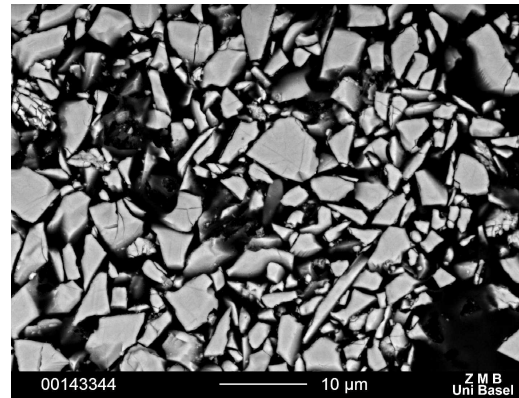
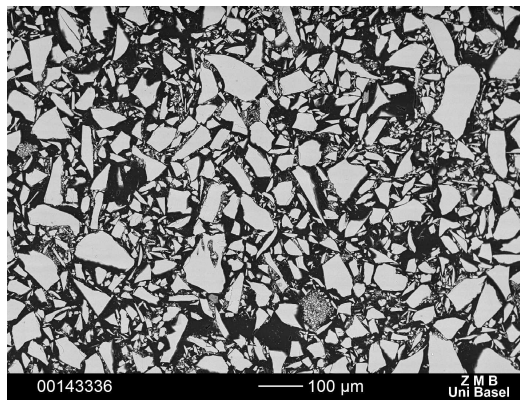


# what does $D_{3d}$ mean ?

The crystal fragments are broken into small pieces **with a hammer** and screened with a 100- $\mu\text{m}$  sieve.

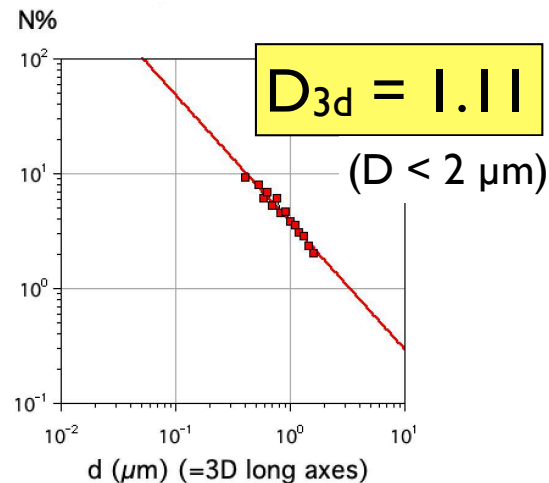
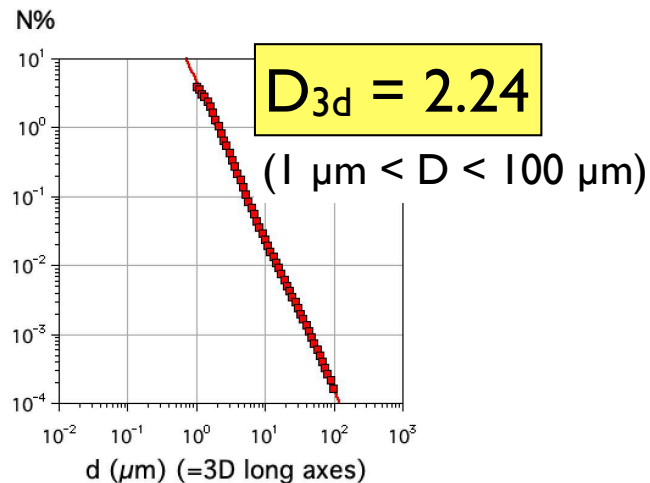
The coarser fraction is **repeatedly pestled** and sieved until the overall grain size is less than 100  $\mu\text{m}$ .

Bettina Richter (2017) PhD thesis, Basel University



how this is explained:

- the processes of hammering and pestling generate grain size distributions with  $D_{3d} < 3.00$  i.e., compatible with fractal fragmentation processes
- $D_{3d} = 2.24$  (fragmentation fraction  $\approx 5/8$ ) for grains  $> 1 \mu\text{m}$
- $D_{3d} = 1.11$  (fragmentation fraction  $\approx 2/8$ ) for grains  $< 2 \mu\text{m}$  (below grinding limit)



# what have we learned ?

Data from particle analyzers are particularly prone to misinterpretation.

The mean of a fractal distribution is quite meaningless.

Rather, convert analyzer data to linear histograms of volume density versus linear size...

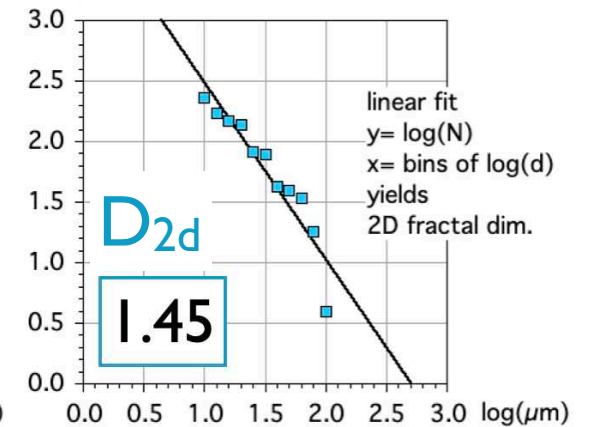
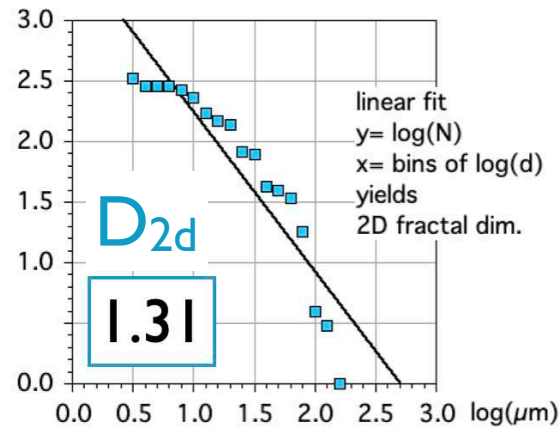
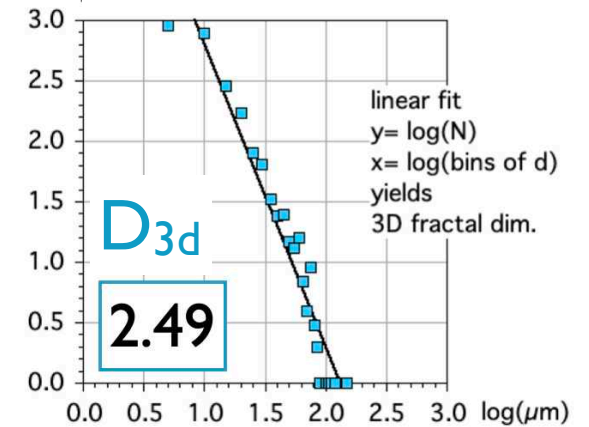
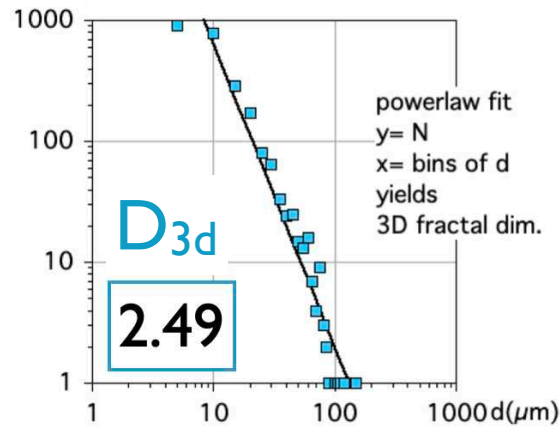
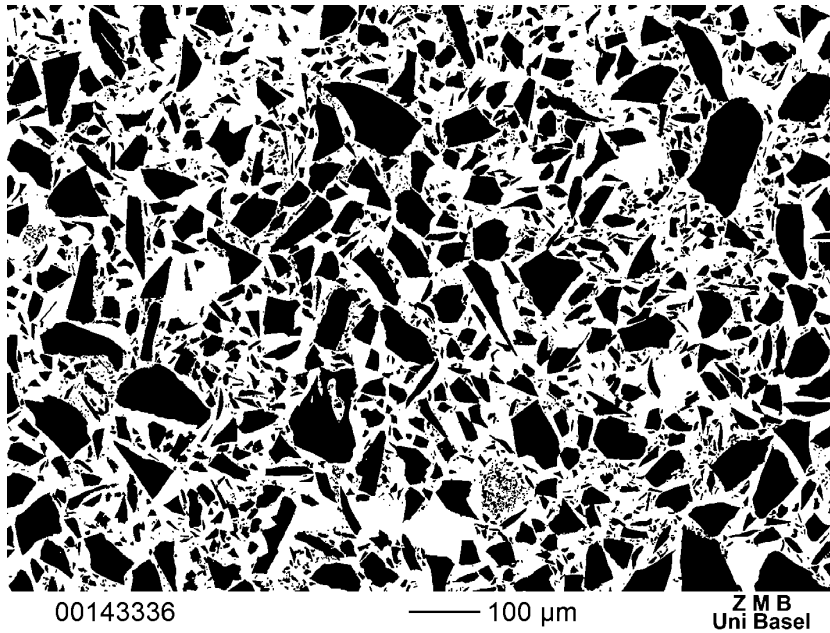
... and check on a log-log plot of N.vs.size:

if the slope,  $D$ , of the powerlaw fit is a straight line, and if  $(0 \leq -D \leq 3)$ , the distribution may be due to fractal fragmentation.

"grain size"  $\gamma$   
friction & healing  
fractal dimension



# "grain size" 7: brittle fault rocks

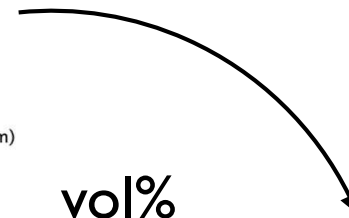
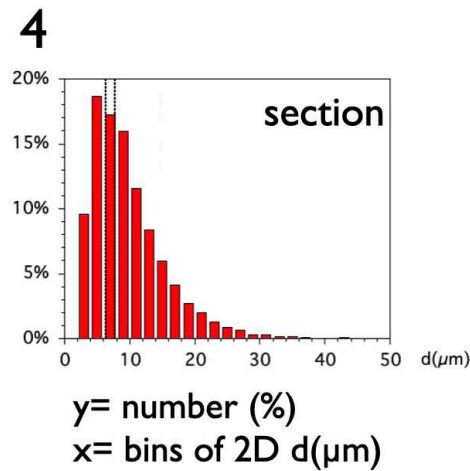
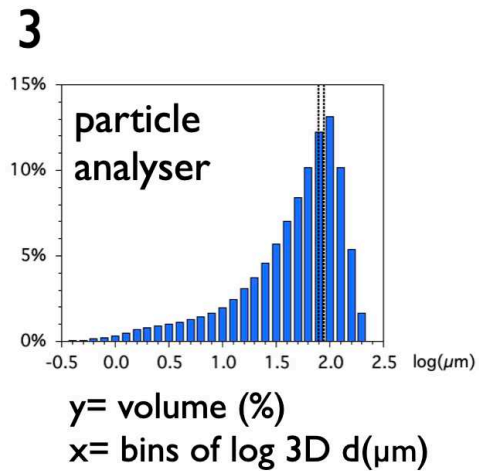
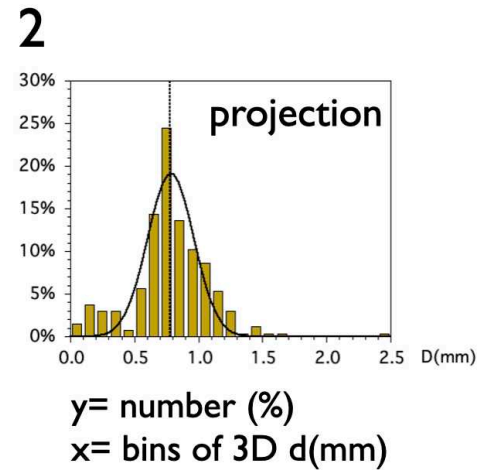
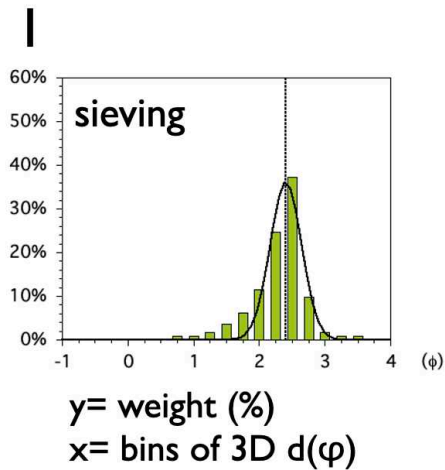


fractal dimension for 2 or 3 dimensions

$$D_{2d} = D_{3d} - 1$$

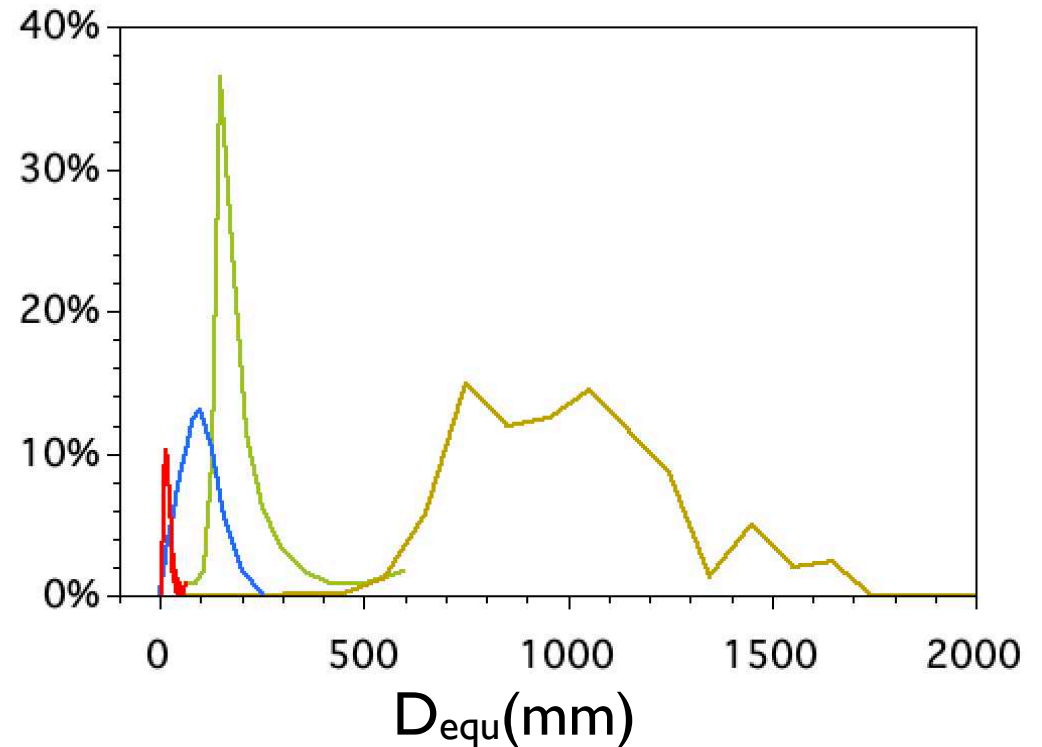
... but fractal size distributions should span at least 3 orders of magnitude

# comparing grain size distributions

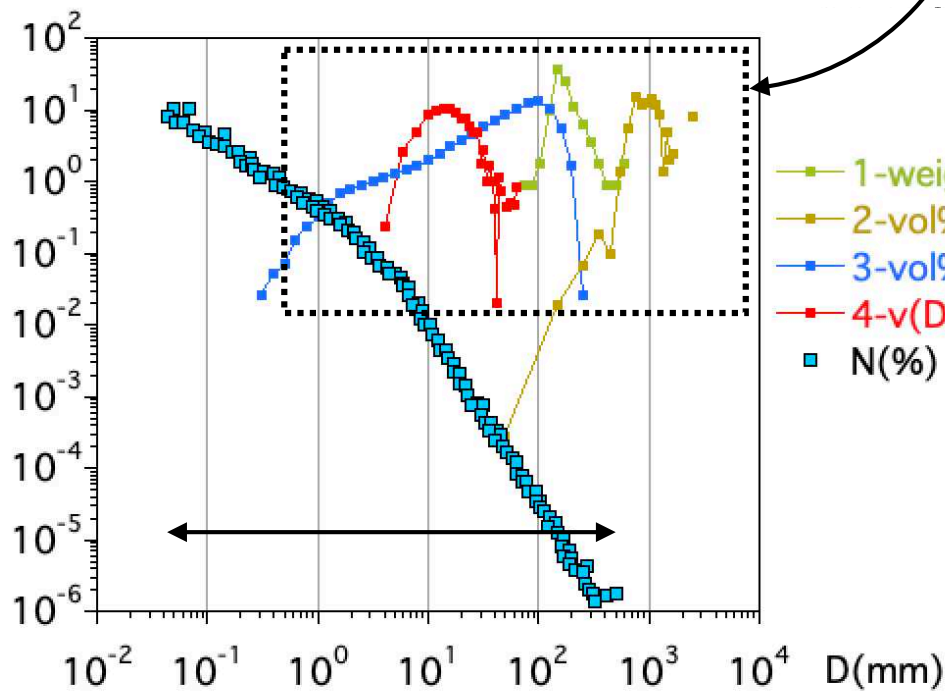
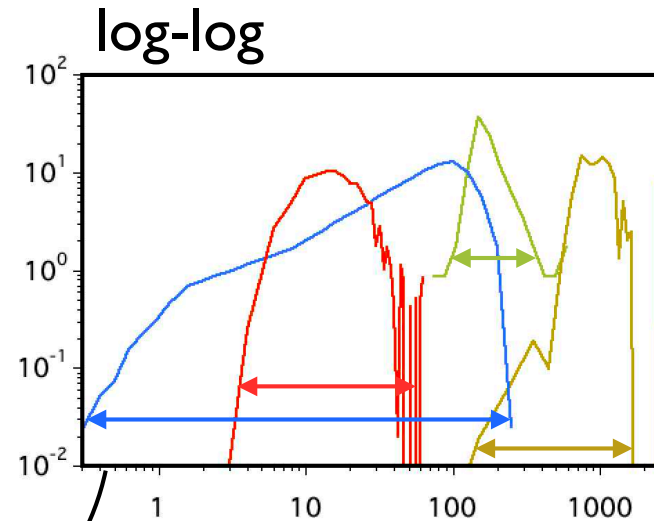
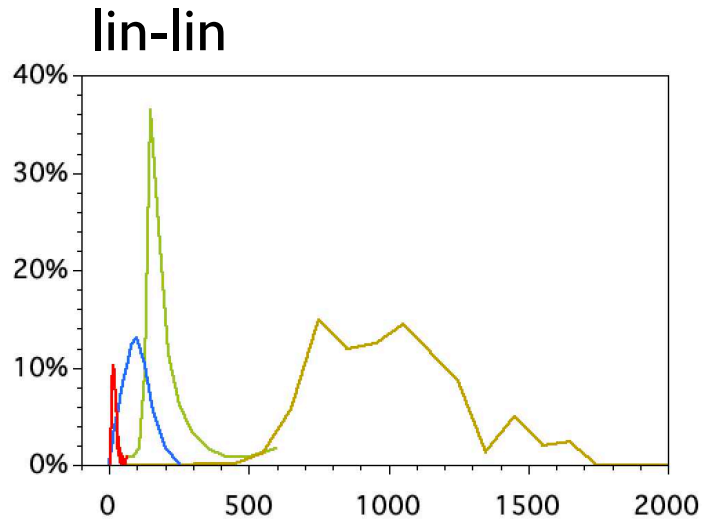


all plotted as  
vol% vs. linear D

vol%



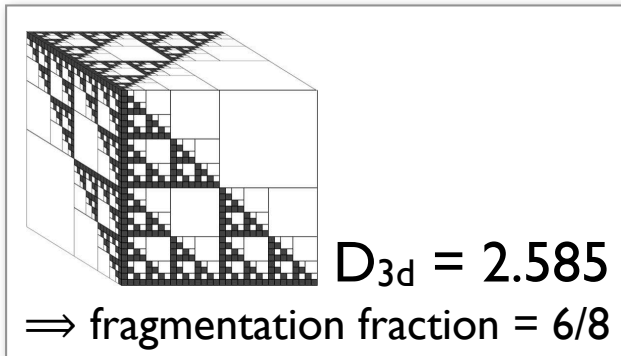
# typical data ranges



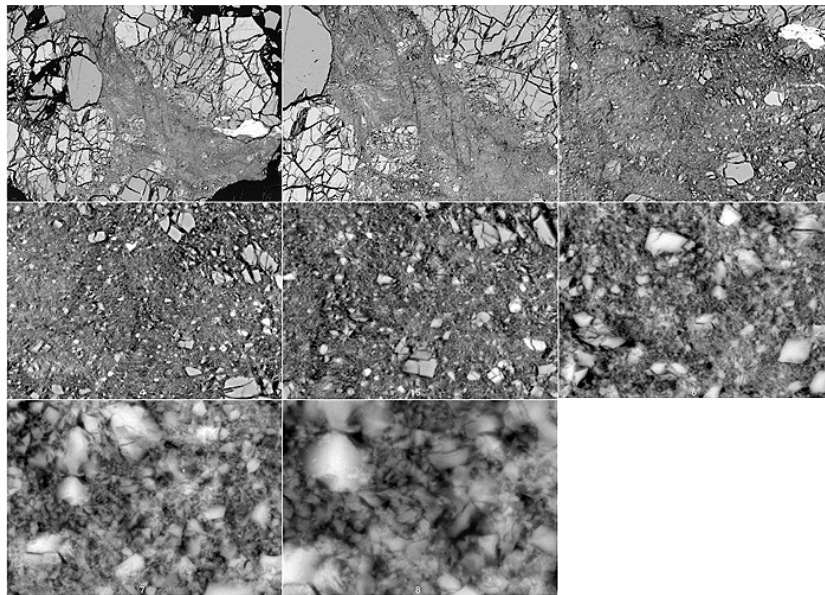
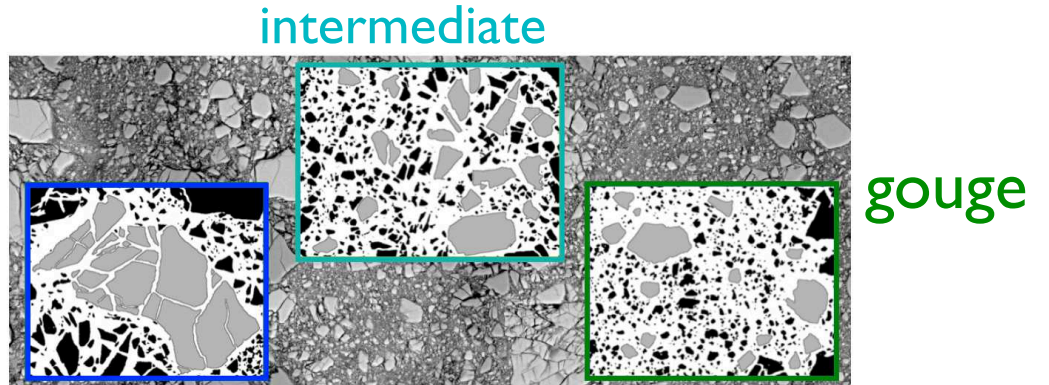
- data range  
(orders of magnitude)
- 1-weight(%) sieved beach sand 0.6
  - 2-vol%(D) scanned glacig. 0.8
  - 3-vol%meas part.analyzer crushed ~3
  - 4-v(D)(%) thin section rexl.qtz 0.9
  - N(%) polyscale NK ~4

Keulen, N., Heilbronner, R., Stünitz, H., Boullier, A.-M. and Ito, H. (2007). Grain size distributions of fault rocks: a comparison between experimentally and naturally deformed granitoids, *J. Struct. Geol.*, 29, 1282-1300, doi: 10.1016/j.jsg.2007.04.003.

# the 'universal' fractal dimension

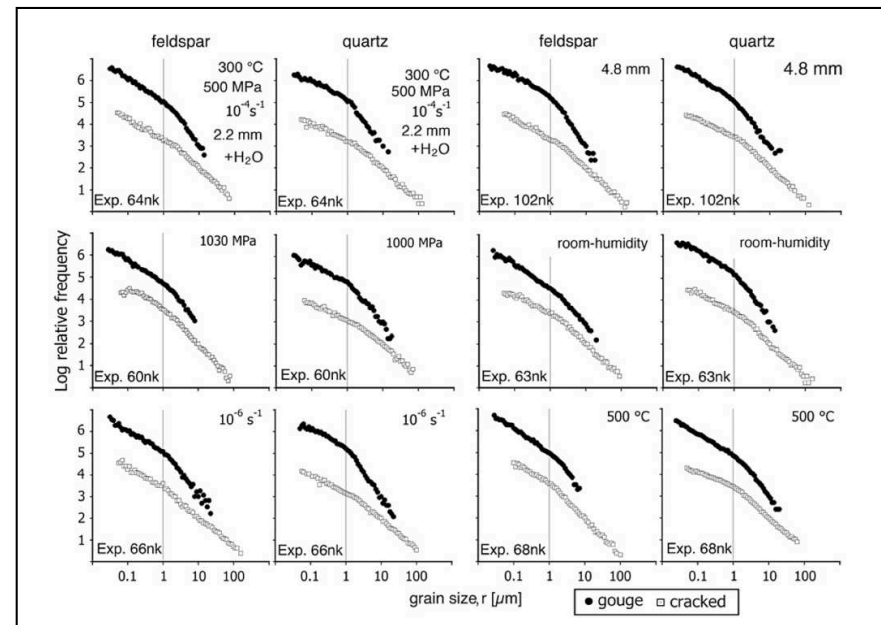


cracked



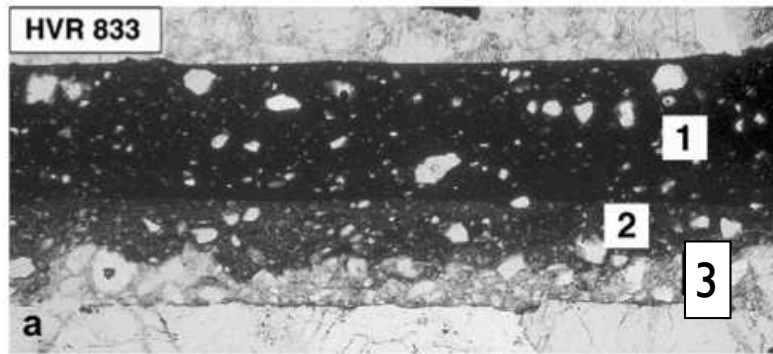
$D_{3d}$  cracked = ~2.5  
 $D_{3d}$  gouge = 3.0 - 3.2 !!  
 $D_{<grinding\ limit}$  = 1.8 - 2.0

Keulen, N., Heilbronner, R., Stünitz, H., Boullier, A.-M., Ito, H. (2007). Grain size distributions of fault rocks: a comparison between experimentally and naturally deformed granitoids, *Journal of Structural Geology*, 29, 1282-1300, doi:10.1016/j.jsg.2007.04.003.

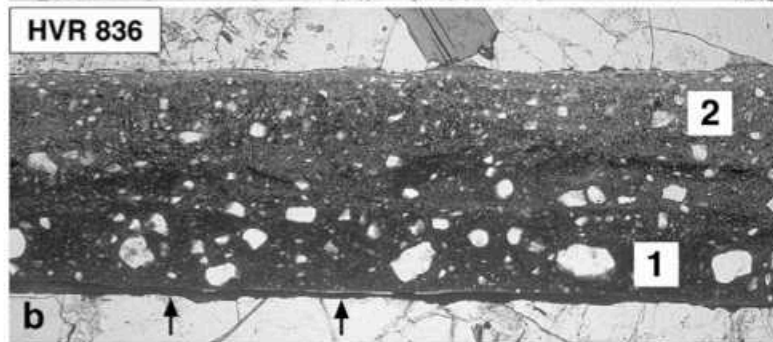


# $D_{3d}$ gouge $\neq f(\text{displacement})$

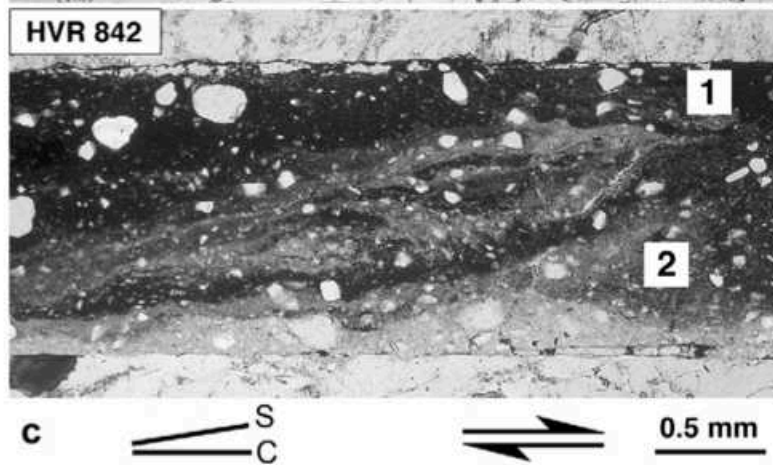
$d = 24\text{m}$



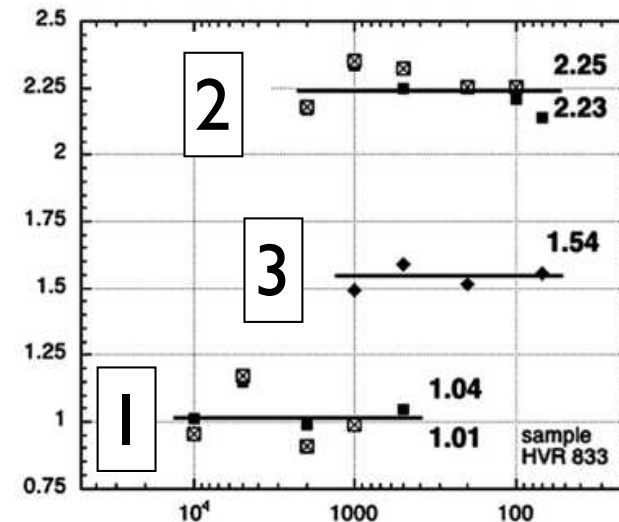
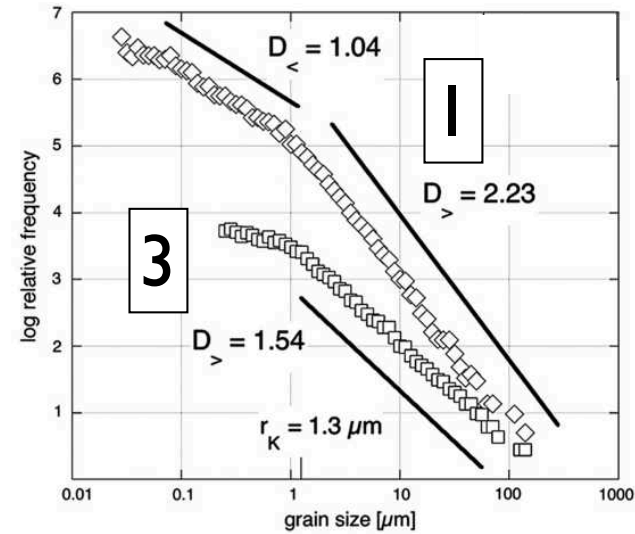
$20\text{m}$



$40\text{m}$



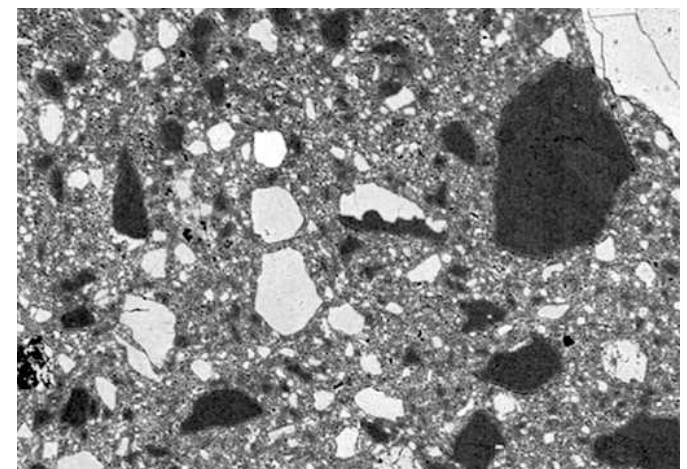
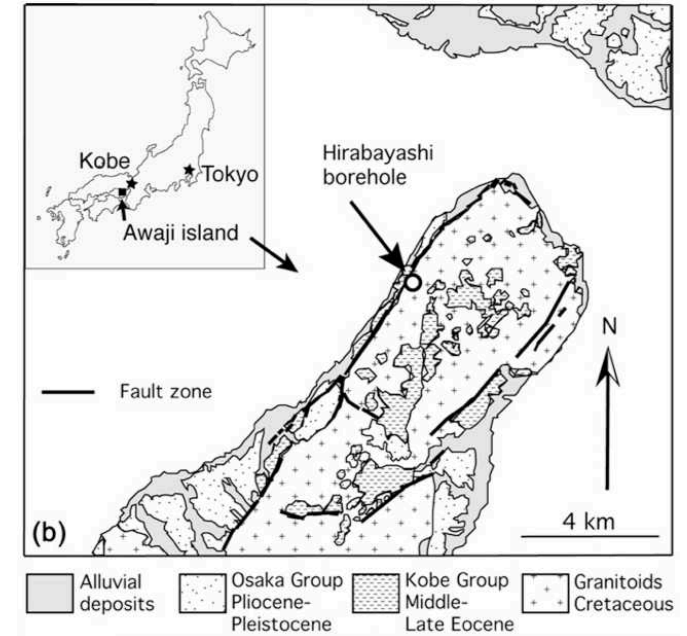
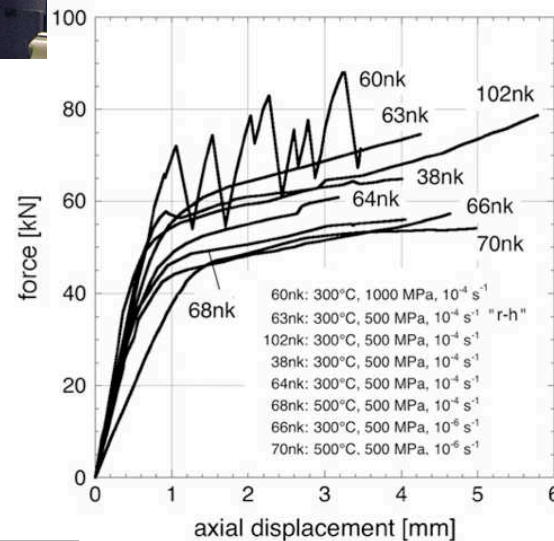
high velocity friction experiments  
(rotary shear apparatus)



Stünitz, H., Keulen, N., Hirose, T., Heilbronner, R. (2010). Grain size distribution and microstructures of experimentally sheared granitoid gouge at coseismic slip rates – criteria to distinguish seismic and aseismic faults? *J. Structural Geology*, 32, 59-69, doi:10.1016/j.jsg.2009.08.002

# experimental and natural fault rocks

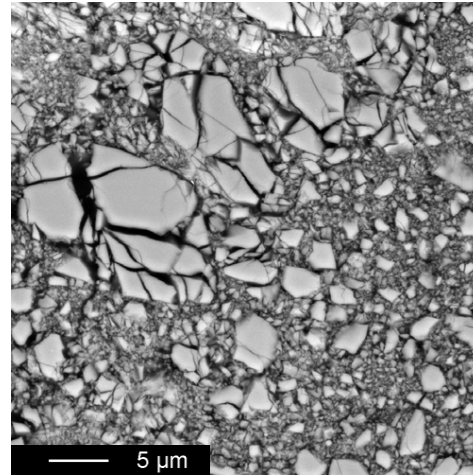
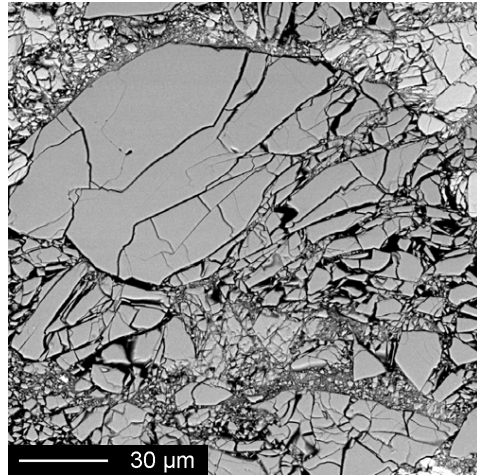
experimentally produced fault rock  $\longleftrightarrow$  naturally produced fault rock



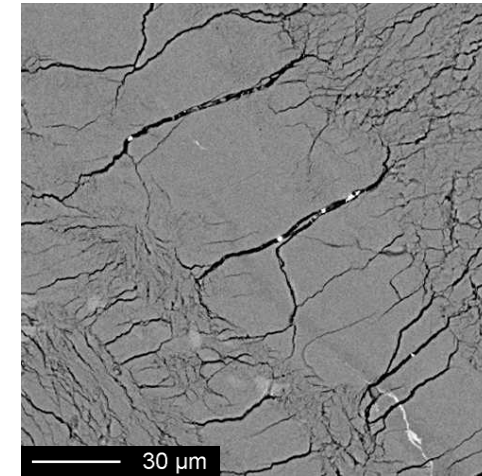
Keulen, N., Heilbronner, R., Stünitz, H., Boullier, A.-M., Ito, H. (2007). Grain size distributions of fault rocks: a comparison between experimentally and naturally deformed granitoids, *Journal of Structural Geology*, 29, 1282-1300, doi:10.1016/j.jsg.2007.04.003.

# rupture – faulting – healing

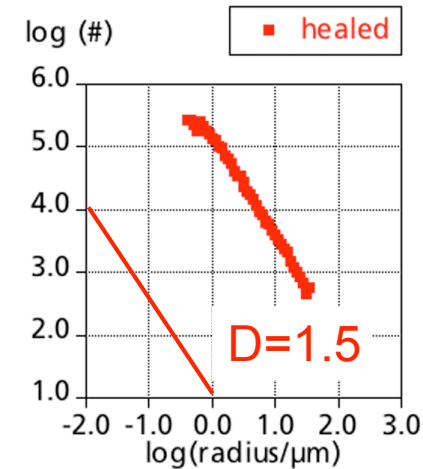
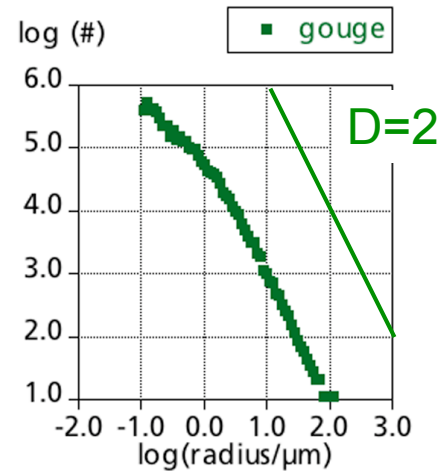
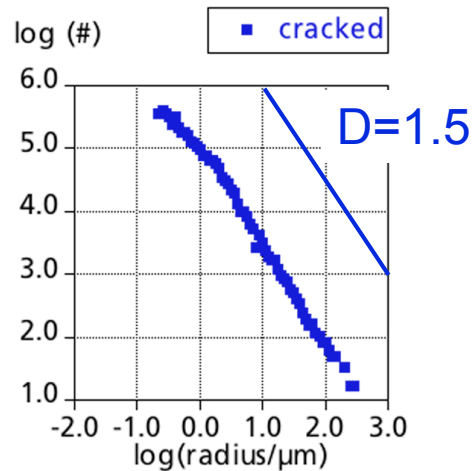
## deformation and healing experiments



fresh



healed



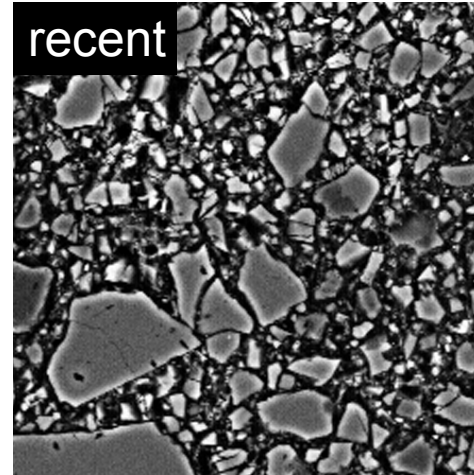
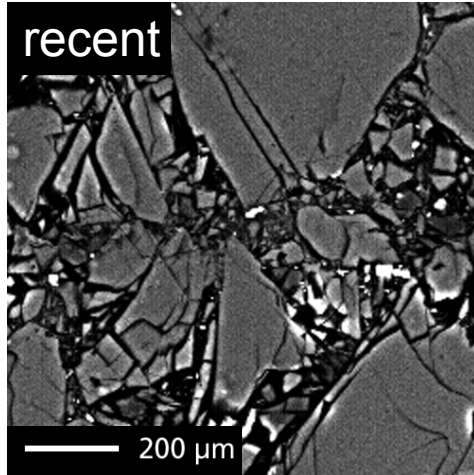
Keulen, N., Stünitz, H., and Heilbronner, R. (2008). Healing microstructures of experimental and natural fault gouge. *Journal of Geophysical Research-Solid Earth* 113.



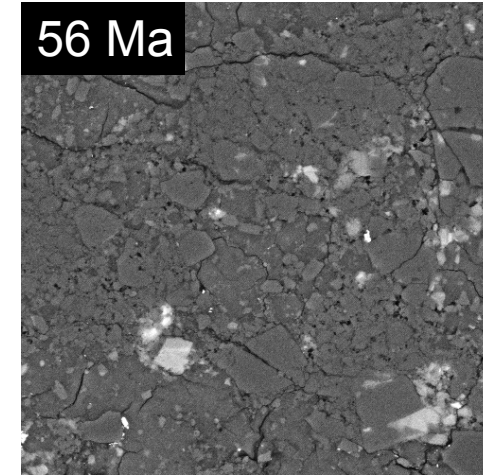
"A hydrostatic healing law for qtz and fs:  
 $\Delta D(t) = D(t) - D_f = A \cdot e^{(-\lambda t)}$ ,  
 $\Rightarrow$  Healing of monomineralic gouge:  
in  $\sim 1$  year at  $T = 100^\circ - 200^\circ\text{C}$ ."

# Nojima Fault

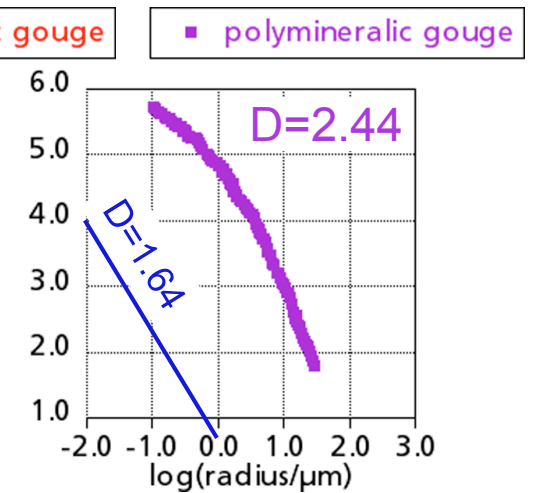
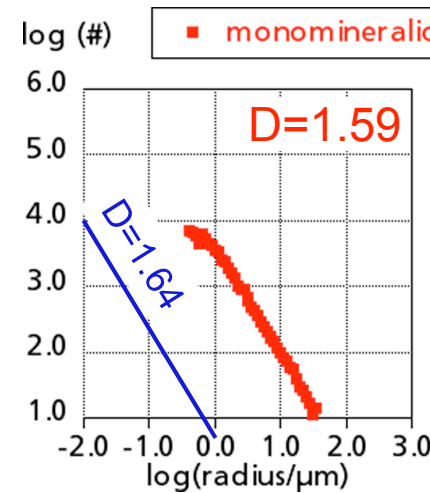
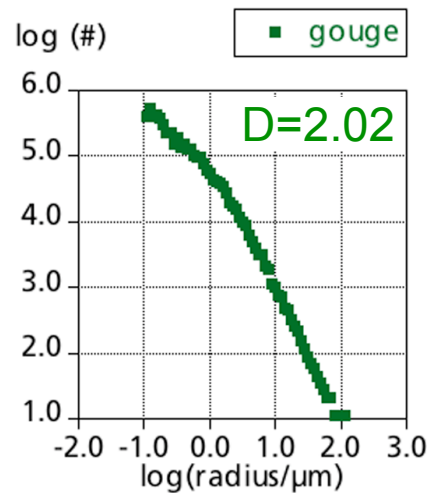
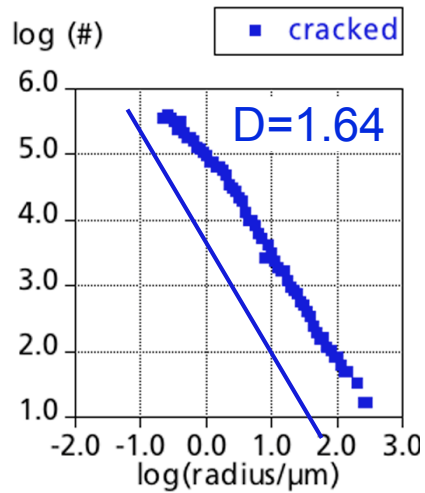
natural fault rocks



fresh



healed



Keulen, N., Stünitz, H., and Heilbronner, R. (2008). Healing microstructures of experimental and natural fault gouge. *Journal of Geophysical Research-Solid Earth* 113.



# what have we learned ?

The fractal dimension of freshly fragmented rocks seems to be a 'universal':  $D_{3d} = 2.58$ .

Mature gouge is 'supra-fractal' with a saturation values of  $D_{3d} > 3.00$ , indicating the contribution of non-fractal processes (spalling, abrasion), and is independent of the amount of displacement.

Healing of monomineralic fault rocks (gouge) yields  $D_{3d} = 2.58$ ; healing is very fast (on the order of years); for polymineralic rocks  $D_{3d}$  remains  $>3$ .

# in summary ...

## we have considered ...

1. what  $\varphi$ -values mean in the physical (linear) world
2. the usefulness of a flatbed scanner
3. the fast and easy intercept method
4. if  $d_{\text{mean}}$  from 2D simulations can be extrapolated to 3D
5. how to convert  $d_{\text{mean}}$  from 2D sections to  $D_{\text{mean}}$  in 3D
6. how to derive fractal dimensions from particle analyzers
7. that fractal grain size distributions have no mean

... and we found that ...

for any given distribution of grains ...

the arithmetic mean of  $h(d_{\text{equ}})$   
 $\neq$  mean of  $h(D_{\text{equ}})$   
 $\neq$  mode of  $\text{vol}\%(D_{\text{equ}})$   
 $\neq M\varphi$   
 $\neq$  mean of  $\text{vol}\%(\log(D_{\text{equ}}))$   
 $\neq$  ... etc.

*see data from:*  
*image analysis*  
*scanner*  
*stripstar*  
*sieving*  
*particle analyzer*

**$\Rightarrow$  ask yourself:**

**which "grain size" you need to know**

grain size –  
3D,  
2D ...  
and fractal

Renée Heilbronner  
renee.heilbronner@unibas.ch

Martin-Luther-Universität  
Halle, 23. Januar 2023

