

# PolyLX – the MATLAB™ toolbox for quantitative analyses of geometrical and topological characteristics of microstructures

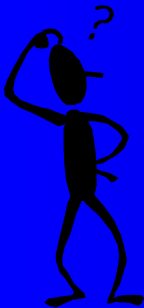
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**LEXA Ondrej**

Institute of Petrology and Structural Geology  
Charles University, Prague, CZ  
recently at ULP Strasbourg, France

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## Why new toolbox ? What are the other tools available?



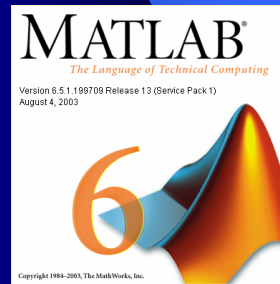
- **Renée Heilbronner**, University of Basel – The **FABRIC** software package - 9 applications for particle and surface orientation including shape analysis, **StripStar**
- Some stand-alone programs for shape analysis, grain-size analysis

Disadvantage: No possibility to modify/create routines for nonprogrammers

# Why MATLAB ?

- Simple scripting language
- Very good graphics capabilities
- Many ready-to-use statistical and numerical routines
- Lot of existing literature
- Accessible on many academic institutions

... but once PolyLX will be transferred to Octave



# What is PolyLX exactly ?

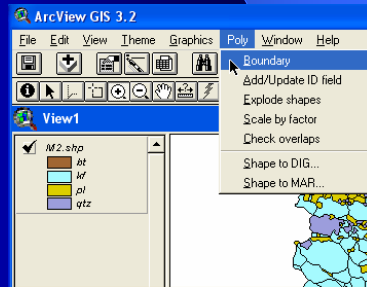
Object-oriented MATLAB™ toolbox i.e. set of routines which cover

- data exchange
  - input from ArcView shapefiles, JML files (Jump GML format), AutoCAD DXF, ELLE files (still in alpha version)
  - export of results in text files, SVG export, CSD export (for Higgins CSDCorrection)
- data storage (native mat-files, MySQL database for advanced management)
- data manipulation (queries, selections...)
- visualization of microstructural statistical data (several predefined graphs)
- analysis of microstructural data (grain size, SPO, GBPO, orientation, strain, topology, spatial characteristics...)
- run on any platform supported by MATLAB™
  - PC, Macintosh, Unix/Linux ...

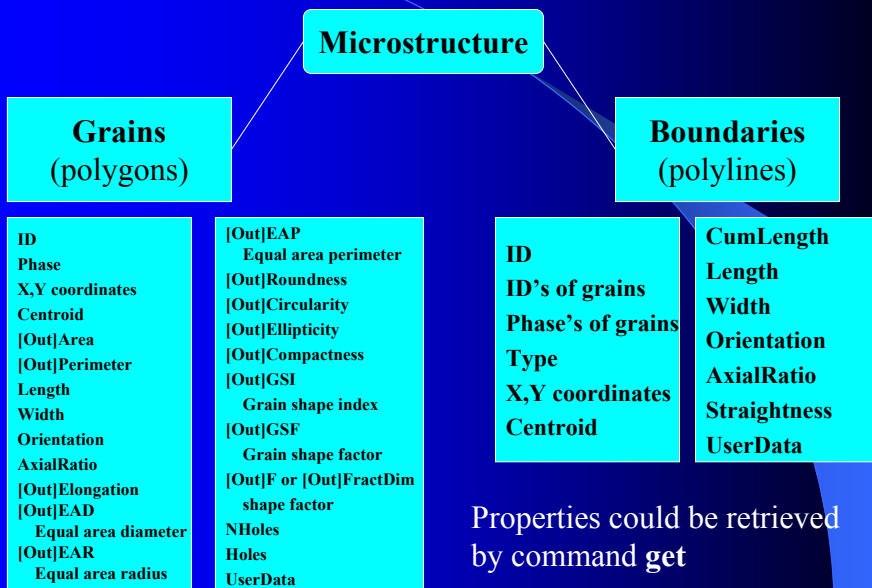
# Data acquisition in GIS environment

- Manual digitizing of outlines from acquired images
- Possibility to mosaic images
- Phase identification
- Automatically controlled topology of grains
  - unavoidable for correct building of boundaries

- We use either ESRI ArcView desktop GIS or public domain JUMP GIS.
- For ArcView we developed extension, which helps preprocessing of digitized grains and automatically build a boundaries.



# Object oriented model



# Geometry

PolyLX use Cartesian coordinate system and angles are measured clockwise from vertical direction.

Units are inherited from imported files and could be freely transformed by **gtrans2d** command.

Storage of data is non-topological and all topology information is created during boundary objects building. Each boundary keep ID's of grains which define individual segment.

Grain objects can have inclusions.



# Grain and grain boundary shape

Shape is extremely difficult property to measure, or even to define in a precise manner. Perhaps this is why there are so many proposed shape measures, none of which has been proved as entirely satisfactory.

A shape measure should possess several desirable properties. Obviously, objects with different shapes should yield different measures, and similarly shapes should yield similar values regardless of the size or orientation of the object. Unfortunately, a shape measure possessing these properties may be a chimera; it has been proven that no single measure can be unique to only one shape.

Therefore, there is a wide spectrum of single value measuring methods available in PolyLX toolbox.

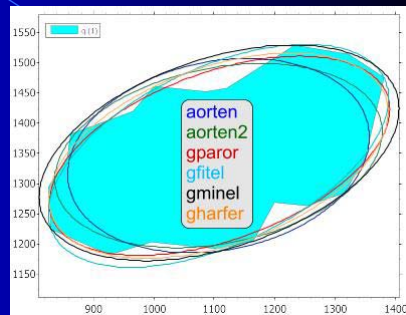
# Grain and grain boundary shape

<b>AxialRatio</b>	$AR = \frac{L}{W}$
<b>Elongation</b>	$E = \frac{\pi L^2}{4A}$
<b>Ferret diameter</b>	$F = 2\sqrt{\frac{A}{\pi}}$
<b>Roundness</b>	$R = \frac{4A}{\pi L^2} = \frac{1}{E}$
<b>Circularity</b>	$C = \frac{4A}{PL}$
<b>Ellipticity</b>	$El = \frac{\pi L^2}{2A}$
<b>Compactness</b>	$Cp = \frac{P^2}{4\pi A}$
<b>Grain shape index</b>	$GSI = \frac{2\pi\sqrt{A/\pi}}{L}$
<b>Grain shape factor</b>	$GSF = \left(\frac{L}{W}\right)^{0.318} \cdot \frac{P}{2\sqrt{A}}$
<b>Straightness</b>	$S = \frac{Ll}{L}$

# Grain and grain boundary preferred orientation

Several techniques implemented in PolyLX

- second order moments based ellipse fitting
- direct least-square ellipse fitting method
- coordinate covariance matrix
- mean matrix of inertia (Harvey & Ferguson (1981))
- minimal volume bounding ellipse
- routines using approach of direction dependent projection of grain or grain boundaries, like PAROR, SURFOR and PARIS of Pannoza (1983) are fully implemented.



# Moments based ellipse fitting

$$a = \iint_R 1 \, dx \, dy \quad \text{zero moment i.e. area}$$

Centralized second order moments

$$\alpha_x = \frac{1}{a} \iint_R x \, dx \, dy$$

first moments ie. centroid of area

$$\alpha_y = \frac{1}{a} \iint_R y \, dx \, dy$$

$$\mu_{xx} = \alpha_{xx} - \alpha_x^2$$

$$\mu_{xy} = \alpha_{xy} - \alpha_x \alpha_y$$

$$\mu_{yy} = \alpha_{yy} - \alpha_y^2$$

Second moments

$$\alpha_{xx} = \frac{1}{a} \iint_R x^2 \, dx \, dy$$

$$\alpha_{xy} = \frac{1}{a} \iint_R xy \, dx \, dy$$

$$\alpha_{yy} = \frac{1}{a} \iint_R y^2 \, dx \, dy$$

We can obtain parameters of ellipse by calculating eigenvalues and eigenvectors of matrix

$$\frac{1}{4(\mu_{xx}\mu_{yy} - \mu_{xy}^2)} \begin{pmatrix} \mu_{yy} & -\mu_{xy} \\ -\mu_{xy} & \mu_{xx} \end{pmatrix}$$

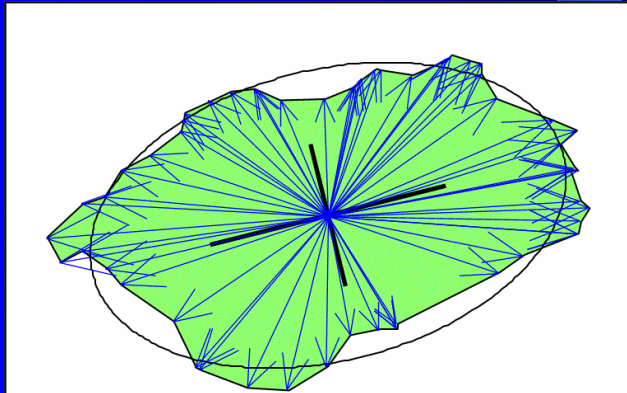
To obtain these integrals, Green's theorem is applied to reduce them to curve integrals over boundary represented as piecewise linear function.

# Coordinate covariance matrix

$$O = \frac{1}{N} \begin{bmatrix} \sum dx^2 & \sum dx dy \\ \sum dx dy & \sum dy^2 \end{bmatrix}$$

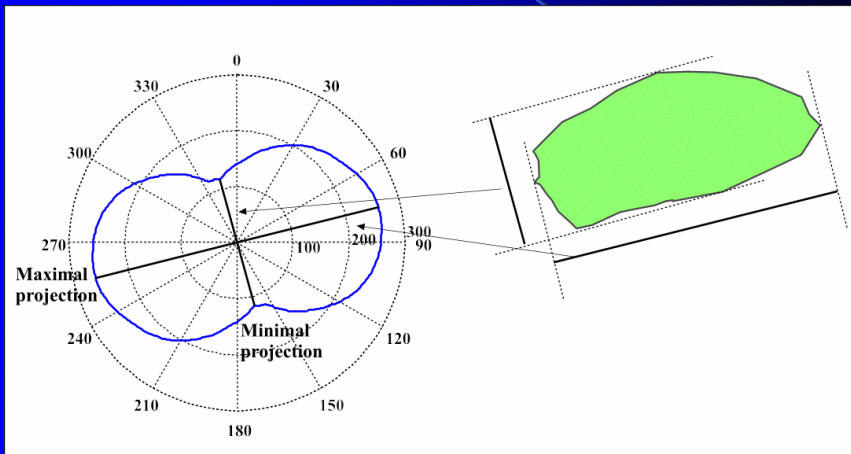
$$dx = x_i - x_c$$

$$dy = y_i - y_c$$



# Projection based methods

PAROR, SURFOR and PARIS



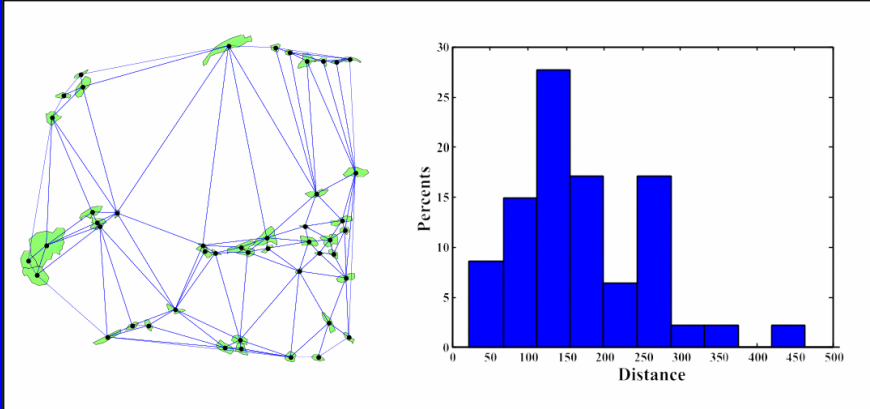
## Spatial statistics

- grain density method - test of randomness is calculated
- nearest neighbour analysis (NNA – spatial pattern index R)
- phase connectivity
- evaluation of deviation from random/expected distribution (Kretz, 1969)
  - Contact frequency method
  - Contact length method
- dihedral angles measurements

# Nearest neighbour analysis

R - nearest-neighbour statistics index

0 - clustered, 1 - random, 2.149 regular



R index: 0.81614 Clustered with standard variation: 2.4114

# Phase connectivity

Method adopted from graph theory (Zhang et. al. 1992)

Bulk connectivity of phase is defined as sum of  $k$ -order connectivity ratios, calculated for each degree of phase partition (degree of partition is equal to number of grain in it).

$$C_k = \sum \frac{b_c}{(b_0 + k)}$$

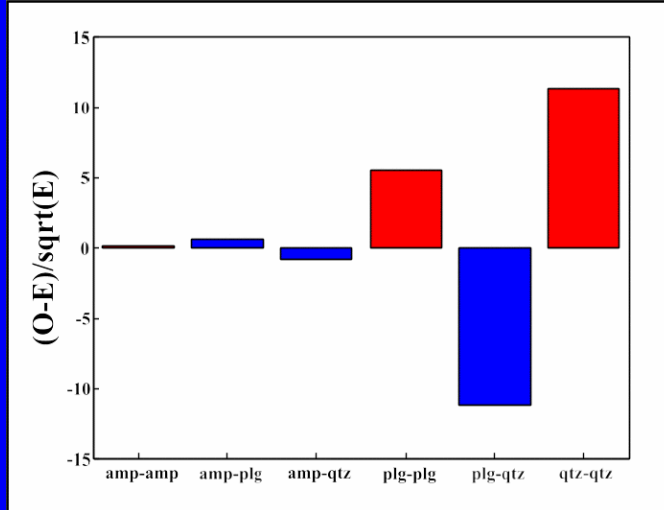
$$C = \sum_{k=2}^n C_k$$

where  $C_k$  is  $k$ -order connectivity  
 $b_c$  is number of grains in partitions with degree  $k$   
 $b_0$  is number of isolated grains

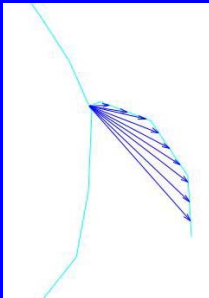
'Phase'	'N'	'isolated'	'Connectivity'
'ac'	[ 31]	[ 24]	[0.2258]
'amp'	[ 534]	[ 187]	[0.6498]
'grt'	[ 9]	[ 9]	[ 0]
'plg'	[1043]	[ 39]	[0.9626]
'qtz'	[1014]	[ 13]	[0.9872]

C for each phase between 0 (all grains are separated) and 1 (all grains are in contact).

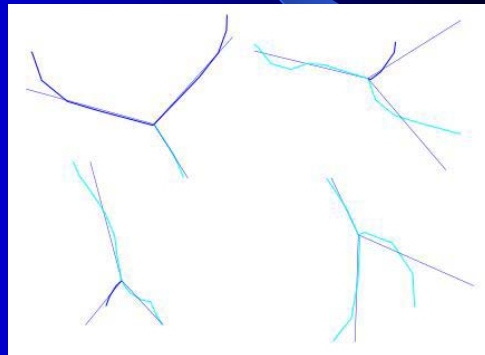
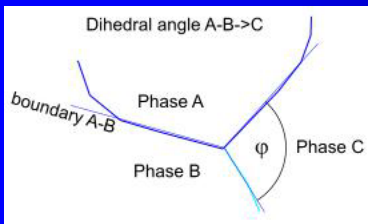
# Contact frequency and length methods of Kretz



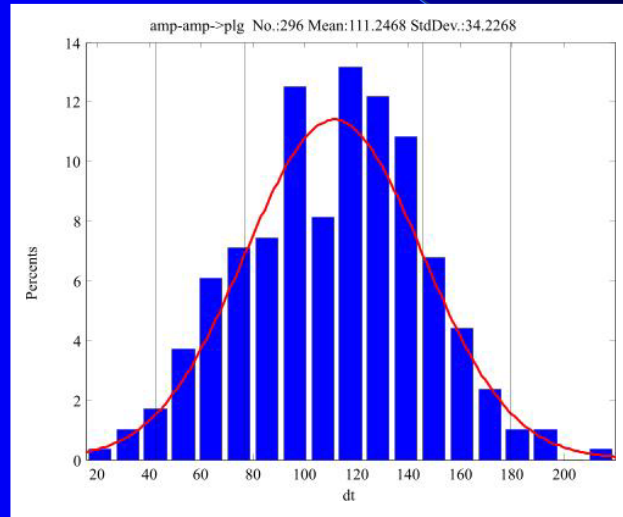
## Dihedral angles



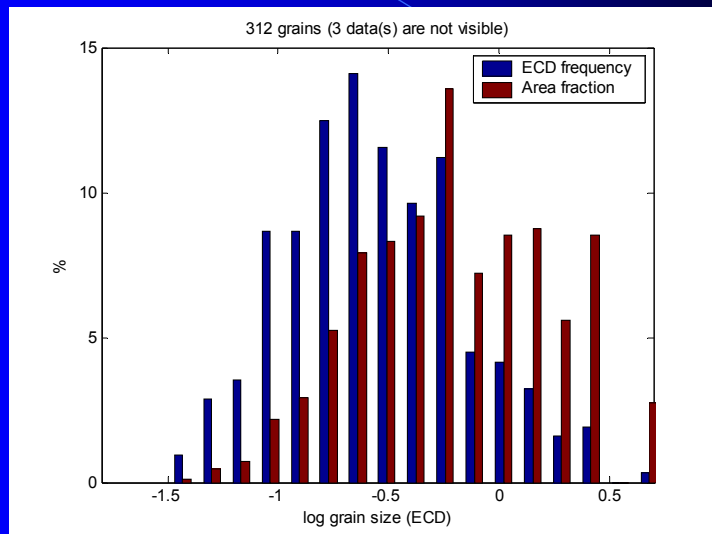
Direction of boundary is approximated as vector sum of vectors weighted by inverse length pointing to evenly spaced points along boundary



# Dihedral angles histogram



# Crystal size



# Crystal size distribution

CSD theory, in principle, determines the number of crystals per size of length,  $L$ , per volume. The total number of crystals is  $N(L_{\max})$  with a cumulative distribution:

$$N(L) = \int_0^L n(L) dL \quad \text{where } n(L) \text{ the number of crystals of given size } L$$

The governing crystal population balance is

$$\frac{\partial(Vn)}{\partial t} + \frac{\partial(GVn)}{\partial L} + Qn = 0$$

For constant volume open system with residence time  $\tau$  ( $=V/Q$ ) and growth rate  $G$  not dependent on size  $L$  population balance equation turn to

$$\frac{dn(L)}{dL} = -\frac{n}{G\tau} \quad \text{After integration this leads to } n = n_0 \cdot e^{-L/G\tau}$$

where  $n_0$  is nucleation density.

Nucleation rate ( $J$ ), however, is defined as

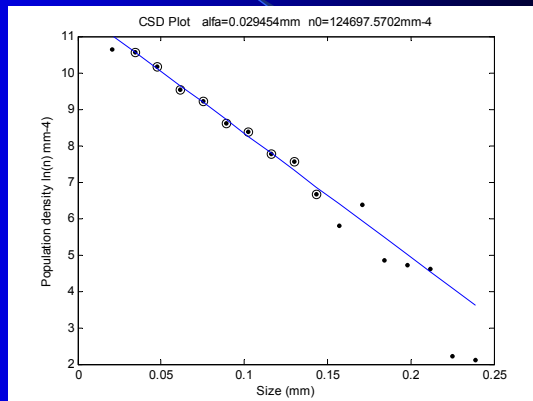
$$J = n_0 \cdot G$$

## CSD plots

To plot 3D CSD curves method of Peterson, 1996 is implemented.

3 factors (experimentally derived) are used to correct raw data, dependent on crystal symmetry and degree of orientation of texture.

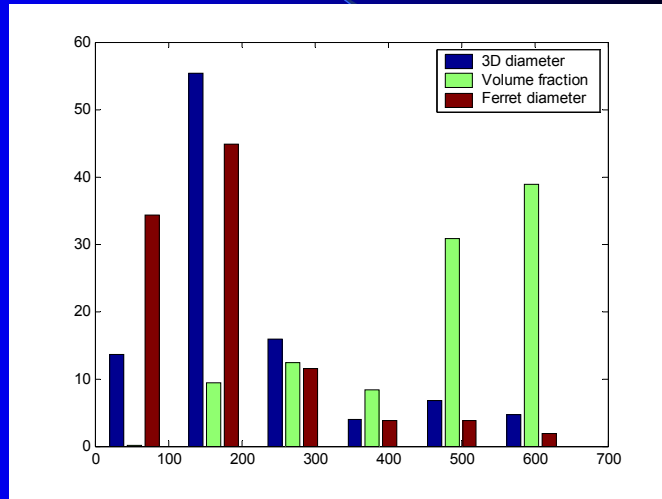
Shape	S	gamma
Sphere	1.269	0.833
Cube (as X11 plate)	0.847	0.515
Dodecahedron	1.425	1.004
Octahedron	1.501	1.139
Tetrahedron	1.022	0.812
Plate 2,1,1	0.927	0.795
Plate 10,1,1	1.063	1.128
Trachytic plate 2,1,1	1.019	0.696
Trachytic plate 10,1,1	1.100	0.780
Cube (as 111 prism)	1.151	0.662
Prism 2,2,1	1.098	0.966
Prism 3,3,1	1.107	1.083
Prism 10,10,1	1.062	1.479
Lineated prism X11	1.106	0.690
Trachytic slab 4,2,1	1.172	0.717
Trachytic slab 6,2,1	1.145	0.724
Trachytic slab 6,3,1	1.136	0.833
Trachytic slab 9,3,1	1.136	0.802



For more sophisticated analysis we can use CSDCorrection software of Higgins. Command **csdwrite** export file with suitable format.

# Conversion from 2D to 3D

Based on sphere sections distribution (StripStar)



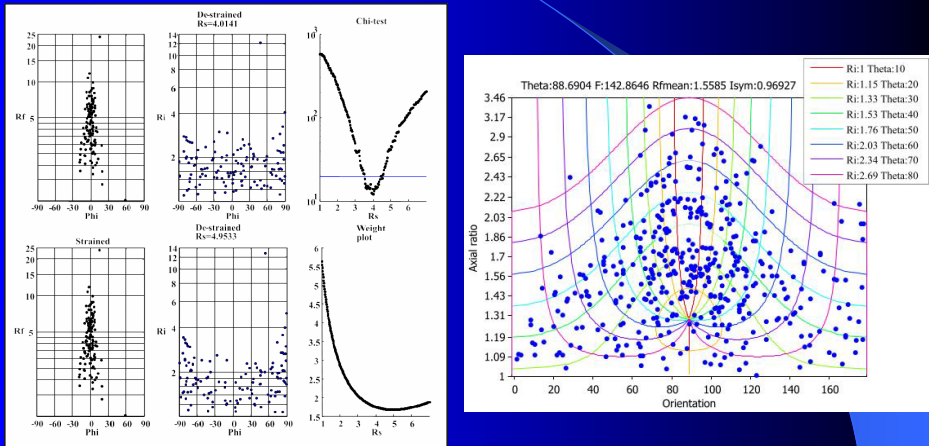
## Strain determination methods

Several techniques to estimate strain are available.

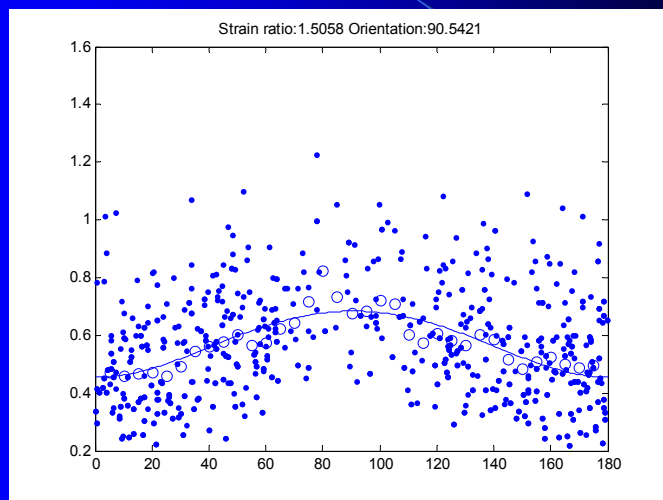
Implemented methods:

- $Rf/\phi$  method
- Centre-to-centre method
- Mean matrix of inertia Harvey & Fergusson (1981)
- Delaunay triangulation nearest-neighbor method
- Area weighted  $Rf/\phi$  method

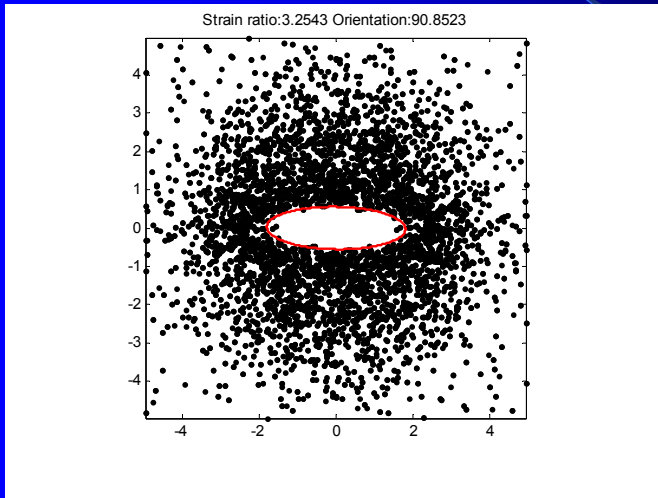
# Rf/ $\phi$ and Area weighted Rf/ $\phi$ method



# Nearest neighbour method



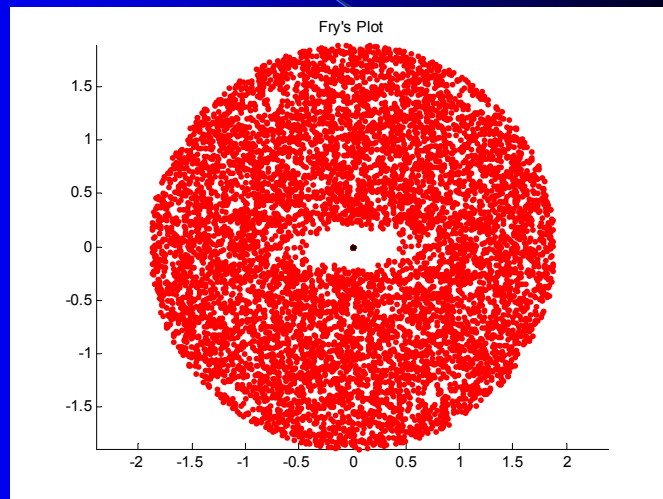
# Delaunay triangulation nearest neighbour method



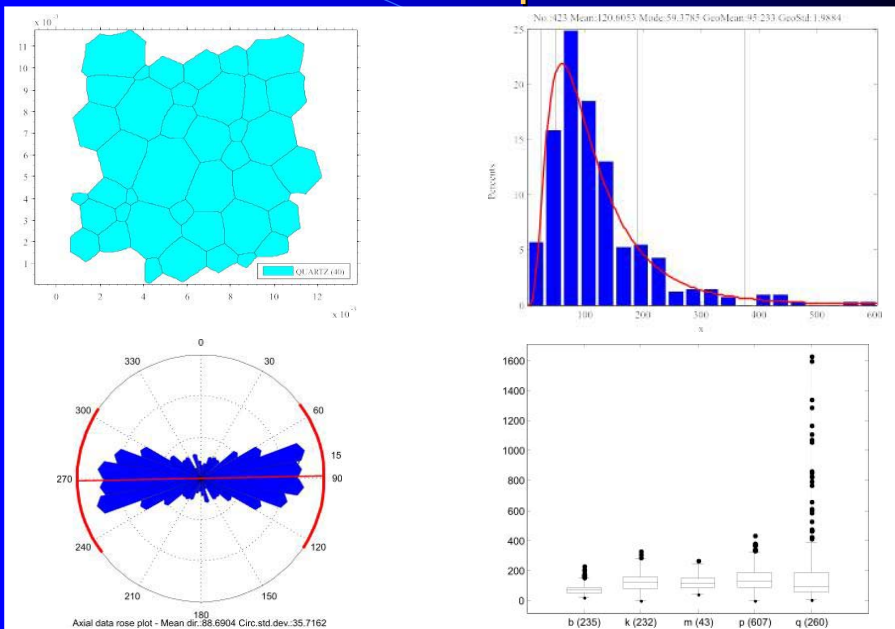
(Mulchrone, 2000)

# Centerpoint distribution method

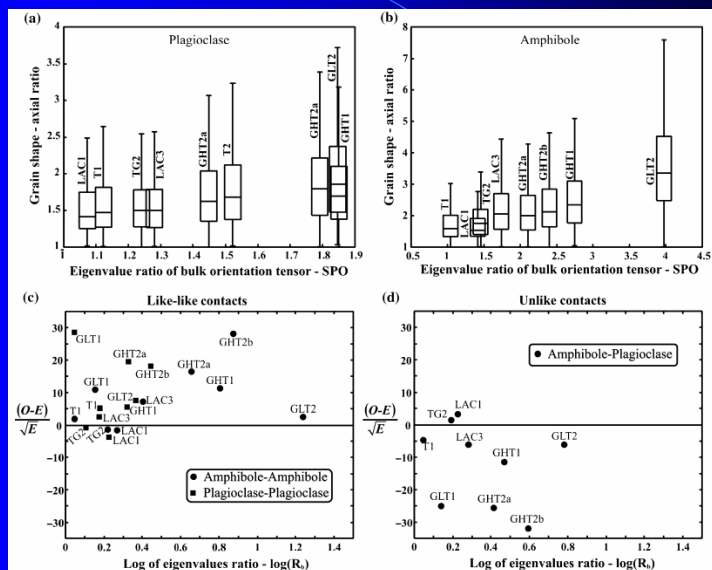
Modified Fry (1979)



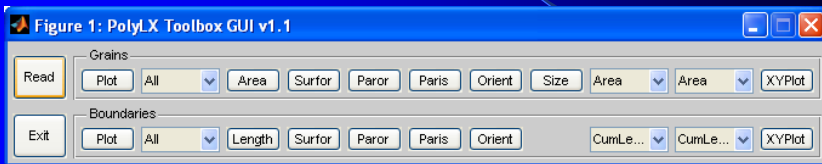
# Common plots



# User-defined graphs



# GUI for PolyLX



very limited, useful for exploration of data

## Command-line interface

- all PolyLX routines are accessible using simple functions
- microstructural data (grain and boundary objects) and results of analyses are stored in MATLAB variables
- users have no limitation to create new scripts (macros) for work automation

```
[output]=function(input);
```

```
>>g=shpread;
```

```
>>[la,sa,la0,sa0]=aorten(g,{opt,plt});
```

```
>>help aorten
```

```
AORTEN - Return results of Ellipse fitting using orientation tensor  
Syntax: [la,sa,la0,sa0]=aorten(g,opt,plt);  
g can be grain and boundary object(s)  
opt 0..use all vertexes 1..use convexhull of vertexes  
Plot option plt 1..plot crosses 2..plot ellipses 3..ellipses and crosses
```

## Grain or boundary selection methods

When we need to analyze only specific objects

**Direct indexing (ID based):**

```
>>a=get(g(12), 'area');  
>>a=get(g(1:100), 'area');
```

**Phase selection**

```
g('qtz');      id=gpsel(g, 'qtz', 'plg');  
>>a=get(g('qtz'), 'area');  
>>a=get(g( gpsel(g, 'qtz', 'plg') ), 'area');
```

## Grain or boundary selection methods II

**Query based selection**

```
>>r=get(g, 'AxialRatio');  
>>g(find( r>2 ));  
>>a=get(g, 'Area');  
>>g(find( r>1.5 & a>100000 ));
```

**Manual mouse-click selection using idplot command**

```
>>a=get(g( getsel ), 'Area');
```

# Where to get it ?

Latest version is available for download on:  
<http://petrol.natur.cuni.cz/~ondro>

polylx:home - Ondrej Lexa Website - Mozilla Firefox

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## PolyLX - the MATLAB™ toolbox for quantitative analysis of microstructures

### Introduction

The textural analysis is a powerful, but underused tool of petrostructural analysis. Except acquisition of common statistical parameters, this technique can significantly improve understanding of processes of grain nucleation and grain growth, can bring insights on the role of surface energies or quantify duration of metamorphic and magmatic cooling events as long as appropriate mineral exist. This technique also allows systematic evaluation of degree of preferred orientation conjunction with their frequencies. This may help to better understand the mobility of grain boundaries in different mineral phases.

We introduce a new open platform, object-oriented MATLAB® toolbox PolyLX providing several core routines for data exchange, visualization and analysis of microstructural data, which can be run on any platform supported by MATLAB®. Detailed descriptions of toolbox routines and methods of implementation of new techniques are given in [PolyLX Reference Manual](#).

The quantitative textural analysis relies on detailed and precise description of grain sizes, grain