

# BeatMark Software to reduce the cost of x-ray mirrors (Stochastic Analysis of Surface Metrology data)

11-06-2018

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*Valeriy Yashchuk* (LBNL)

*Supported by NASA SBIR-II NNX16CM09C*



Second Star Algonumerix: <http://www.secondstaralgonumerix.com>

# Overview

1. Our team and collaborators
2. Challenges in X-Ray mirror fabrication for Lynx X-Ray surveyor
3. What does the method solve?
4. Stochastic processes and InTILF analysis method
5. BeatMark software
6. 2D analysis method and 2D profile generation
7. Application to Polishing Optimization
8. Conclusions

# Our Team has over 160 years combined experience in developing new mathematical methods into software

## Research and Math



Anastasia Tyurina  
CEO and CTO



Prof. Yury Tyurin  
head of math development

## Software team

Dr. Sergey Panov (Lead/physics)

Doug Paris (GUI)

Peter Panov (GUI/IT/ Platforms)



## Business Development



Michael McComas  
(Proposals )



Chris Ilsley  
(Strategy)

## IP and licensing



Michelle Freno  
(licensing) (IP)



Anna Ganelina

## Interns



Jonathan Borowsky (WASHU )



Daniella Ganelin (MIT)



Jacob Panov (NHS)



Second Star SBIR-II NNX16CM09C

# Second Star works with amazing collaborators



Polishing and metrology tools manufacturer



Dave Mohring (SBIR) Mike Bechtold (CEO)



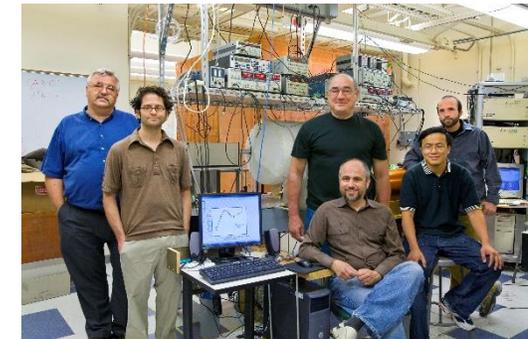
Ed Fess (R&D head)



The best Metrology Lab in US



Dr Valeriy Yashchuk



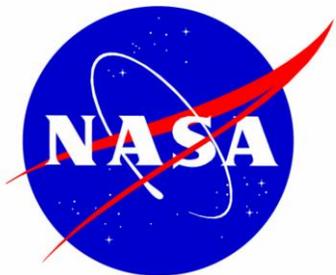
Our collaborators think that if our technology works it will bring a revolution in polishing



Second Star Algonumerix

# Misha Gubarev

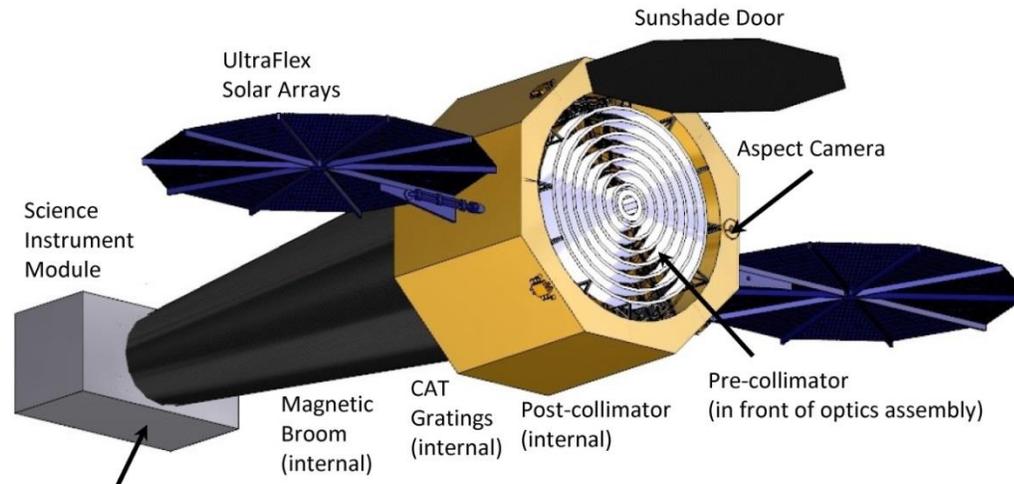
The project would not be where it is now without his expertise and support



<https://www.gofundme.com/mikhail-v-gubarevs-memorial>

# Objective of the project: *To reduce fabrication cost of x-ray mirrors*

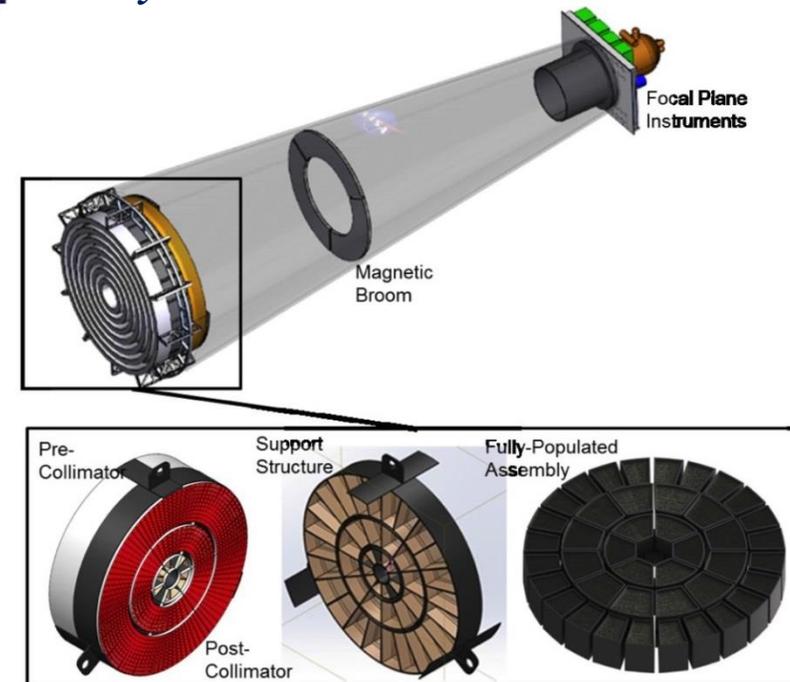
## Lynx - X-ray Surveyor Mission Concept\*



X-ray Microcalorimeter Imaging Spectrometer (XMIS)  
High Definition X-ray Imager (HDXI)  
CAT X-ray Grating Spectrometer (XGS) Readout

- *292-segmented shells nested into 42 individual mirror modules with overall size of 3 m outer diam.;*
- *~ 0.2 arcsec root-mean-square (rms) slope error;*
- *\$600-1000 M estimated total cost of the mirrors*

*The X-ray Surveyor requires X-ray mirrors to achieve large throughput with high angular resolution (0.5 arcsec) in order to avoid X-ray source confusion and background contamination. High angular resolution is critical for providing unique identifications of faint X-ray sources.*



*X-ray Surveyor Telescope*

\* J. A. Gaskin, M. C. Weisskopf, A. Vikhlinin, et. al., "The X-ray Surveyor Mission: A Concept Study," Proc. SPIE 9601, UV, X-Ray, and Gamma-Ray Space Instrumentation for Astronomy XIX, 96010J (August 24, 2015); doi:10.1117/12.2190837

# What can our InTILF method do for X-ray mirror fabrication?

Yashchuk, V. V., Tyurin, Y. N., and Tyurina, A. Y., “Application of time-invariant linear filter approximation to parameterization of one- and two-dimensional surface metrology with high quality x-ray optics,” Proc. SPIE 8848, 88480H-1-13 (2013).

## Decrease Fabrication Cost

- Faster and easier fabrication through simplified and standardized quality control
- Polishing optimization
- Enable medium size mirror manufacturers to join the X-ray mirror market

## Increase Fabrication Speed

- Less metrology
- Less re-polishing

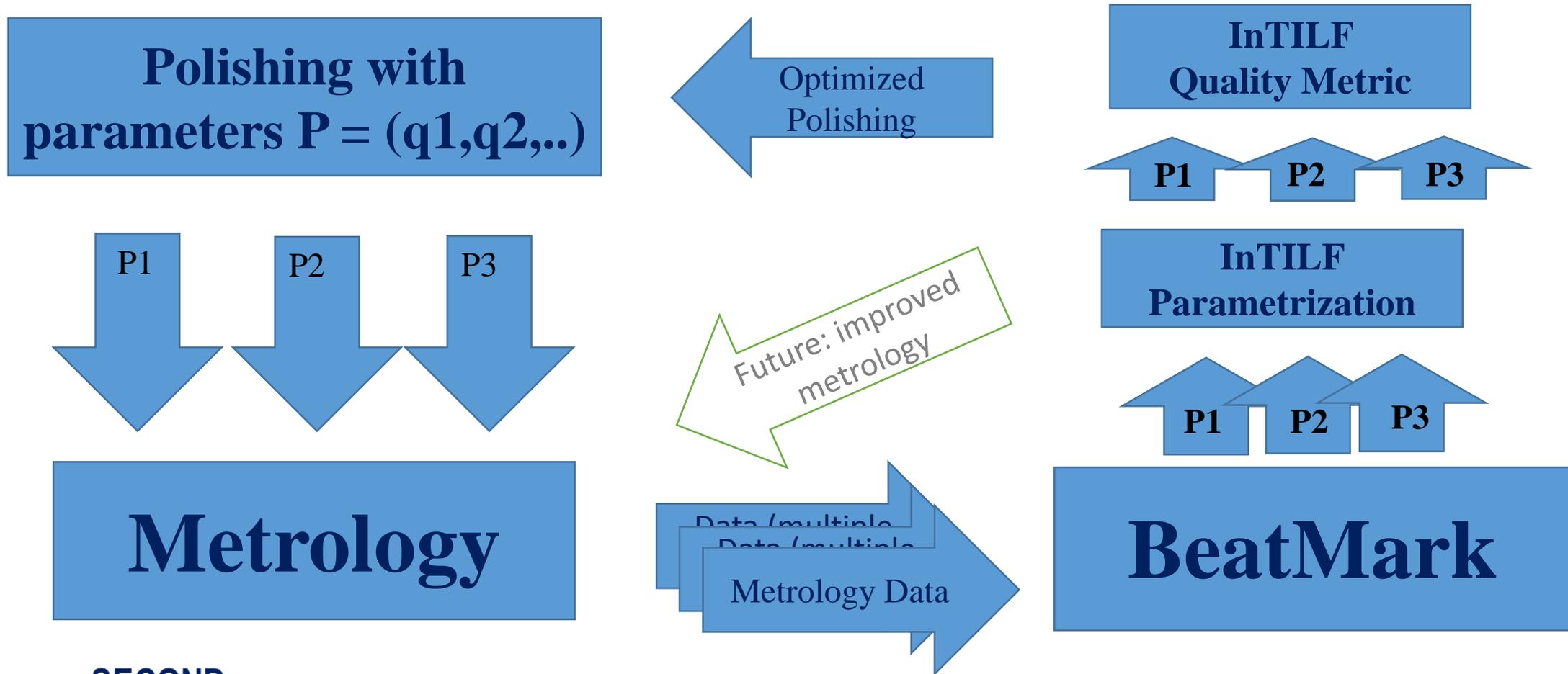
## Increase Fabrication Predictability

- Metrics of quality and comparison of mirrors
- Generation of statistically equivalent metrology data
- Simulation of the X-ray mirror behavior within an X-ray optical system

see Opt Eng 54(2) 025108, Specification of x-ray mirrors in terms of system performance (Yashchuk, Samoylova, Kozhevnikov)



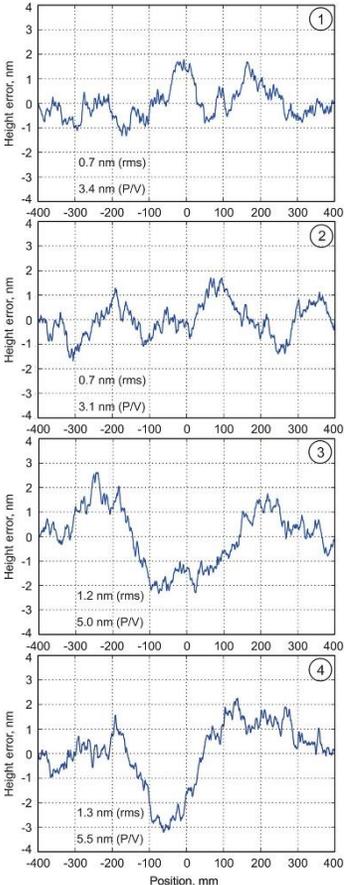
# BeatMark concept step 2: Optimization of polishing and metrology process



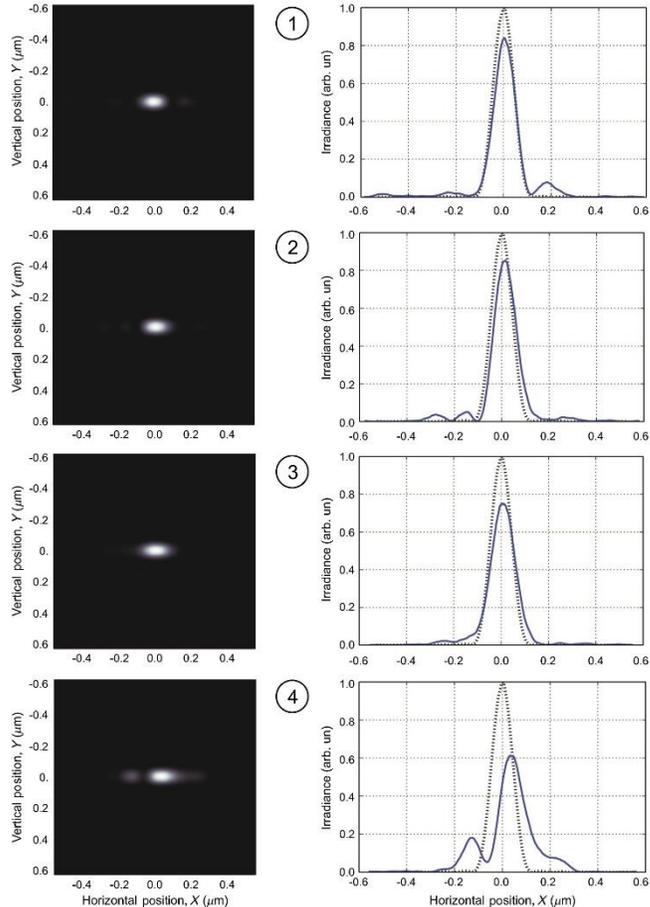
# Patterns left on the mirror by polishing process are bad for imaging

Yashchuk, Samoylova, and Kozhevnikov: Specification of x-ray mirrors in terms of system performance (Opt Eng. 54-2-025108-2015)

Simulated x-ray mirror profiles of the same surface height error rms



Simulated x-ray mirror imaging of a single point source (left) and its cross sections (right)



It is not just rms!

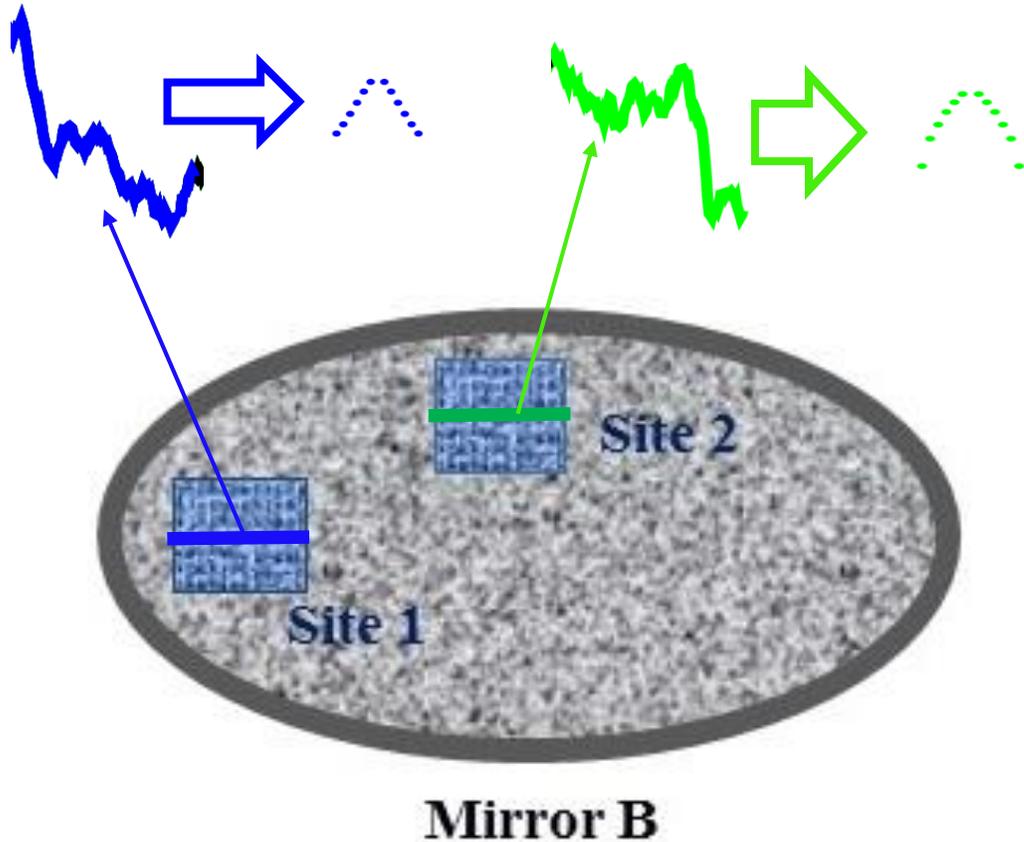
# Logic of the project

- Periodic process – spectral characteristics (aka correlations) are surmised by Fourier transform
- Stochastic process – spectral characteristics (aka correlations) are surmised with statistical tools
- We think we can optimize the polishing and metrology process because we learned to characterize stochastic surface data with **Invertible Time Invariant Linear Filters (InTILF)**

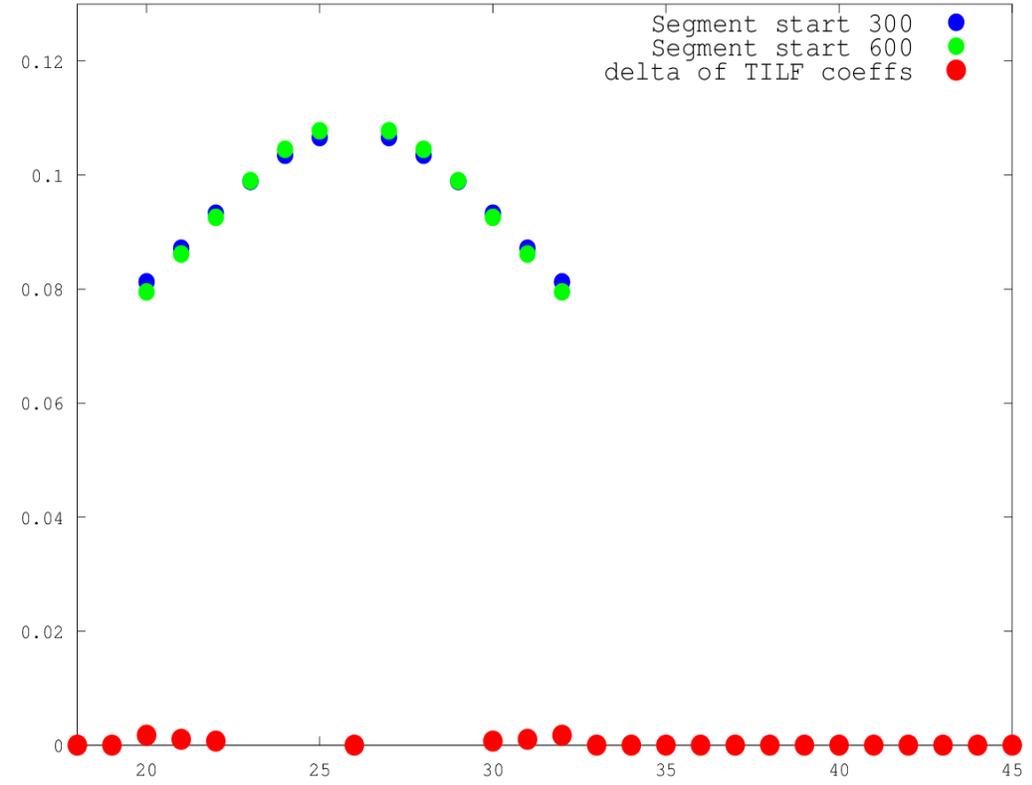
# InTILF method provides characterization of the surface based on small metrology samples

Segments length = 300

Segments length = 300

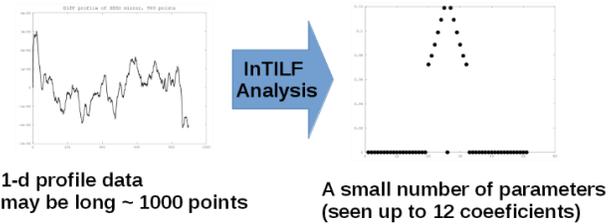


TILF coefficients for segments

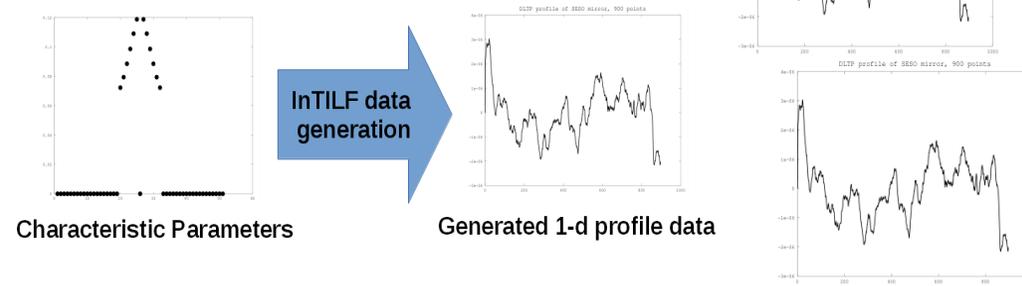


# BeatMark prototype software

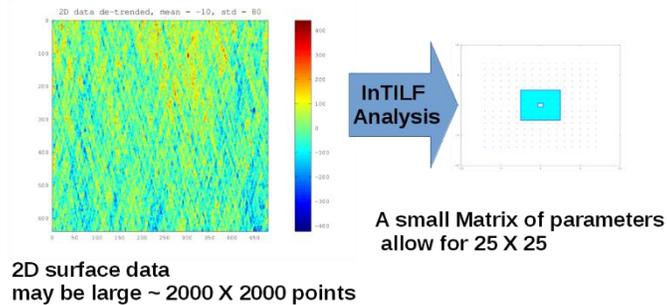
UseCase1: 1d data to parameters  
(InTILF coefficient)



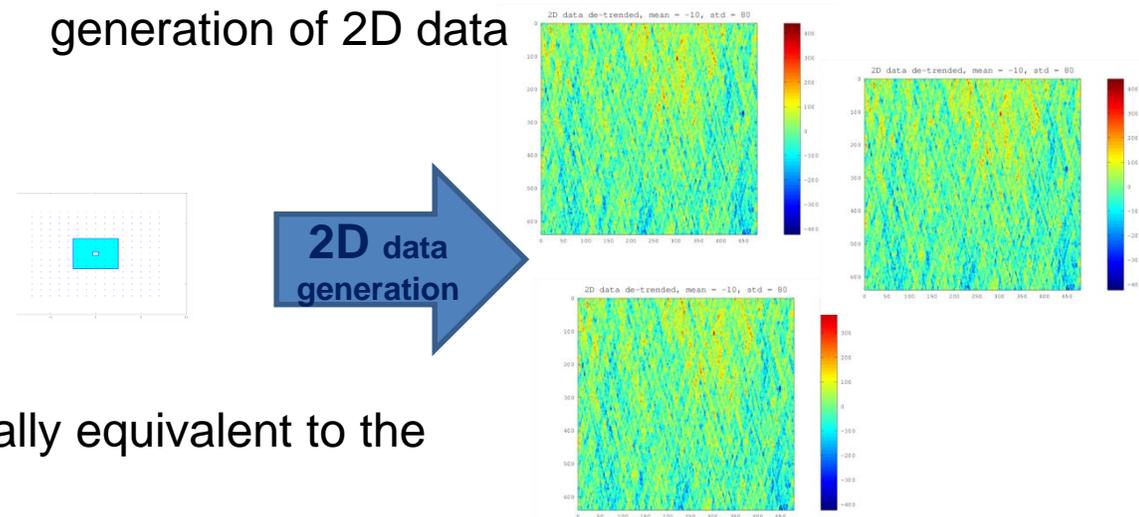
Use case 2



UseCase3: 2D data to parameter Matrix



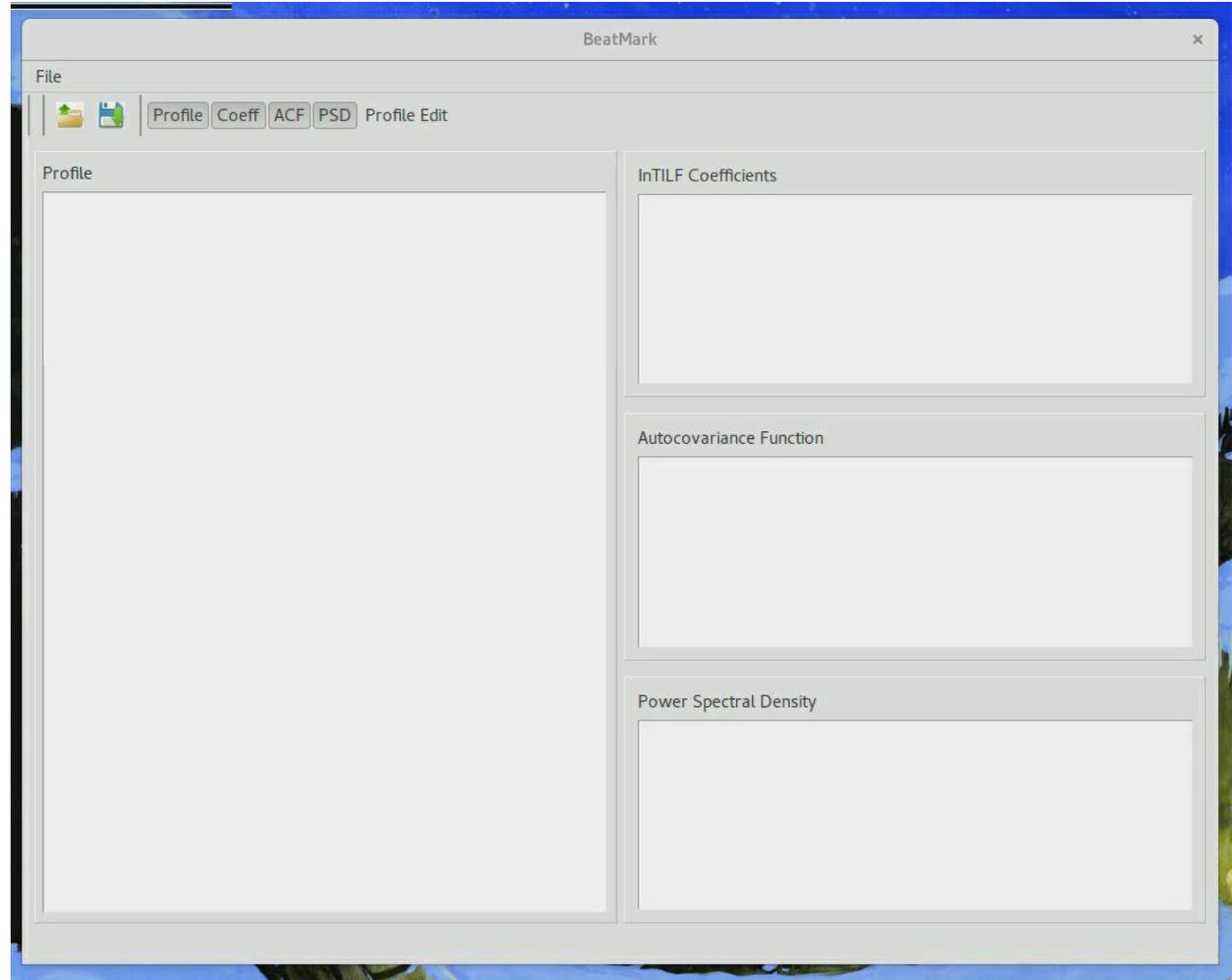
UseCase4:  
generation of 2D data



Generated Data is statistically equivalent to the original data



# BeatMark prototype demo



# BeatMark software is the first to provide:

- statistical analysis of 2D metrology profiles (surface)
- generates 2D profiles statistically equivalent to a given 2D profile

# Projects status

## 1) Software development

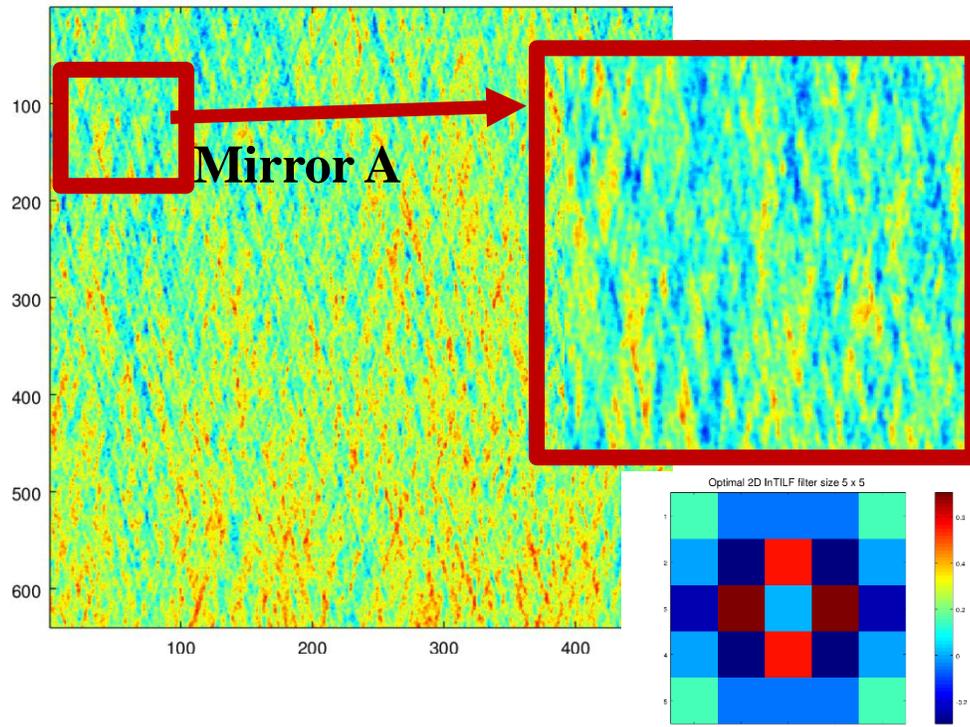
- 1D application – commercial prototype is ready
- 2D application developed for finding InTILF models
- 2D surfaces generation
- Format readers, a few developed, ongoing

## 2) Application to polishing

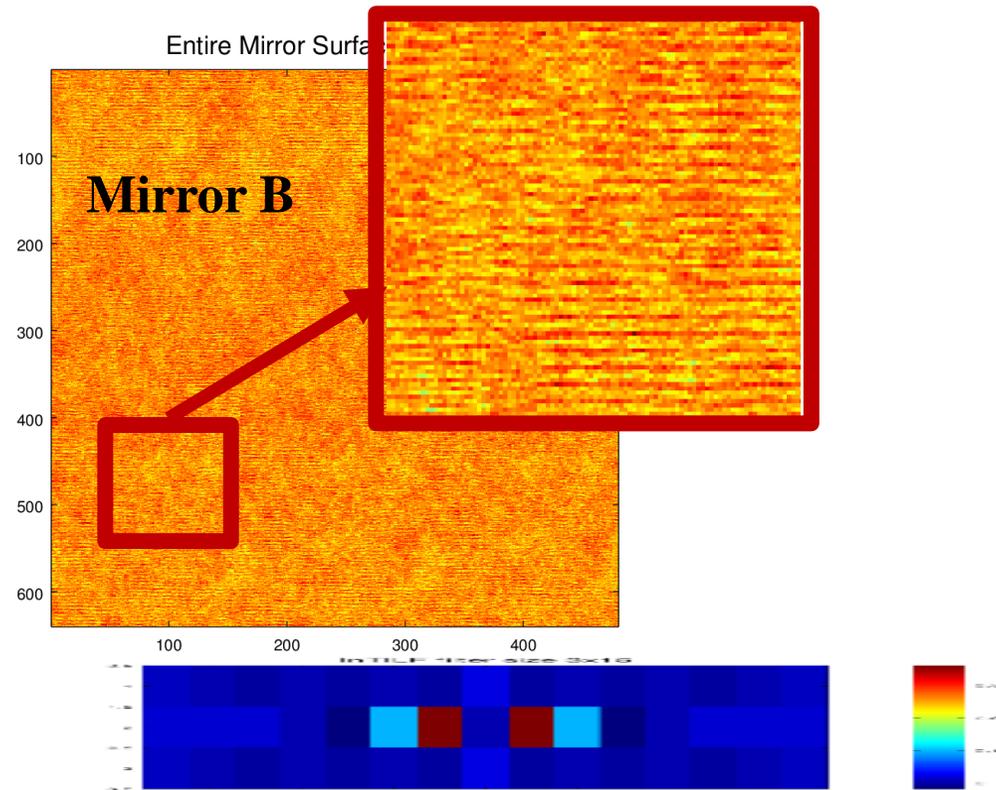
- OptiPro completed two polishing data collections
- LBNL received re-measured one set of samples is re-measuring the other
- Second Star is analyzed the first data collection the results will be presented
- The team is discussing the analysis of the second data collect



# BeatMark-2D analysis



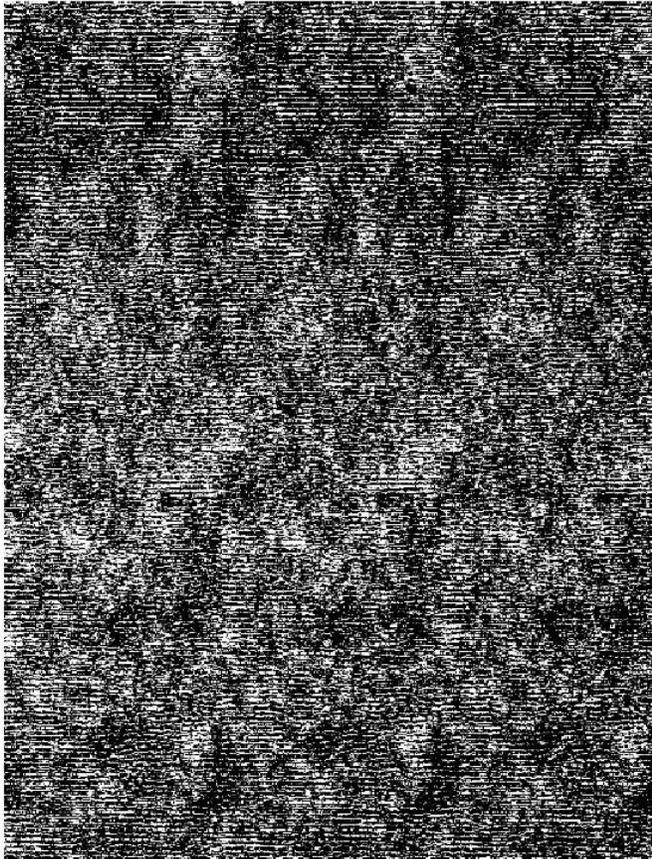
**BeatMark assessment of Mirror A:**  
**InTILF 5x5 matrix**  
**Residual < 1 %**



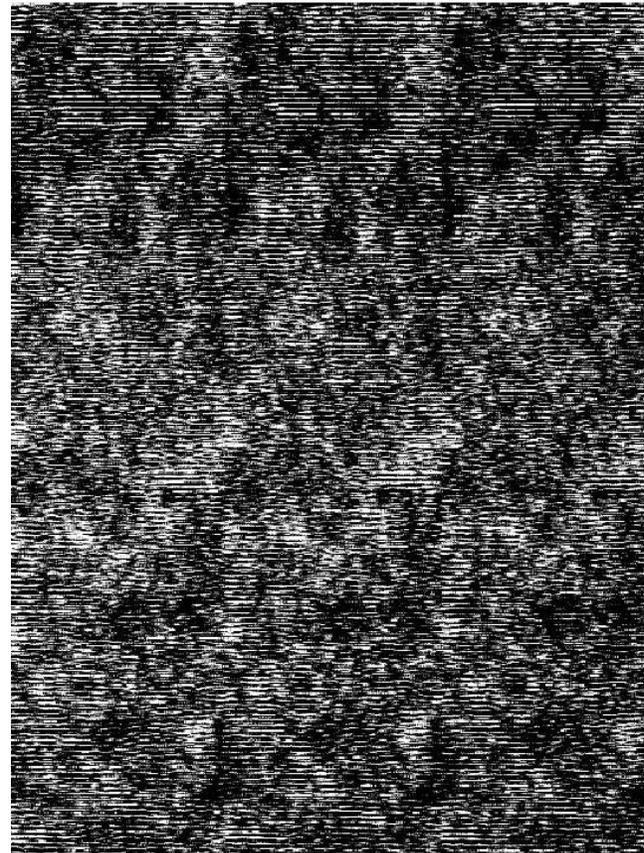
**BeatMark assessment of Mirror B:**  
**InTILF = 3 x 15 matrix**  
**Residual = 23%**

# 2D InTILF analysis of Mirror B

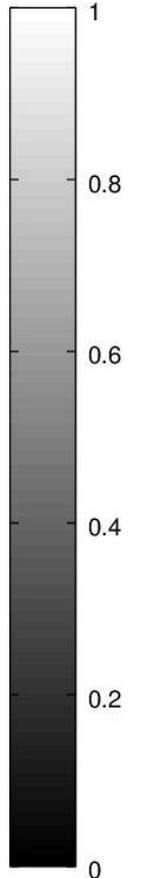
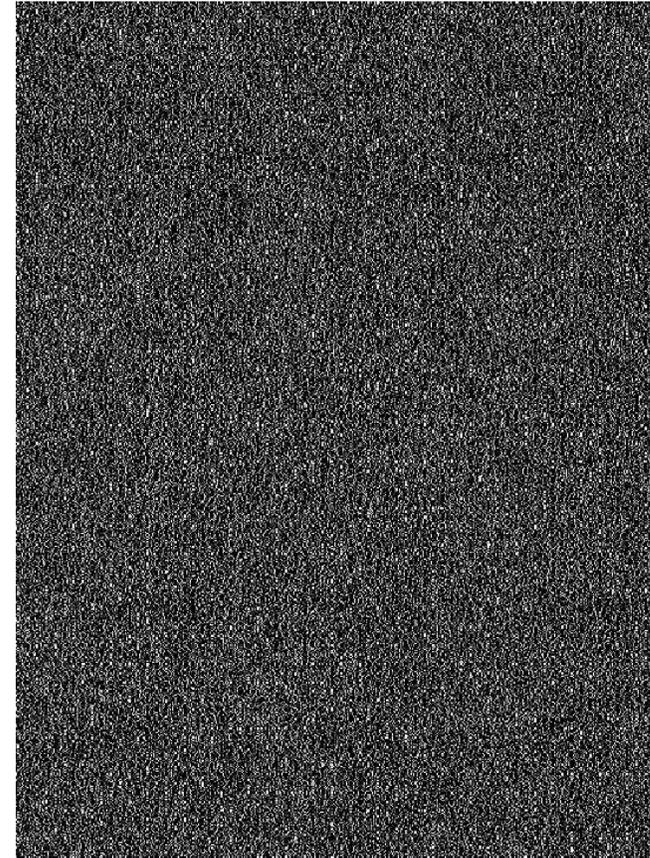
Original data (mirror B)



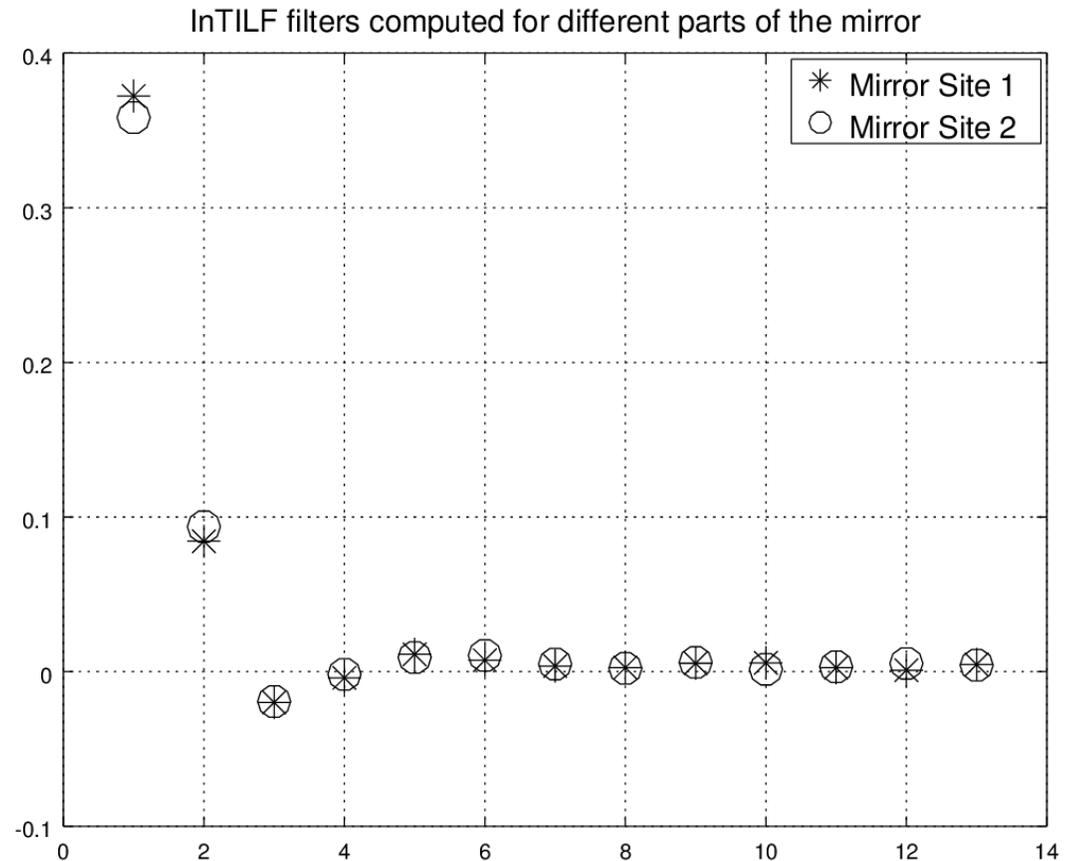
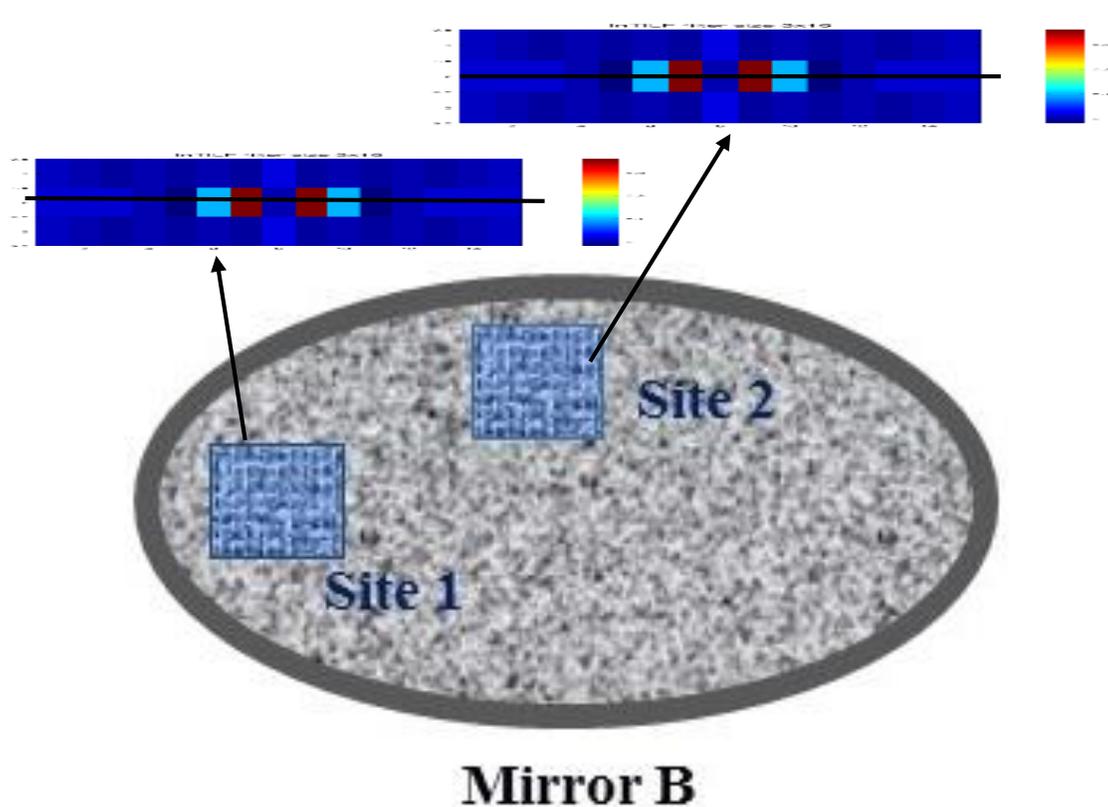
Filtered data = InTILF Model



**Residual is White noise like**

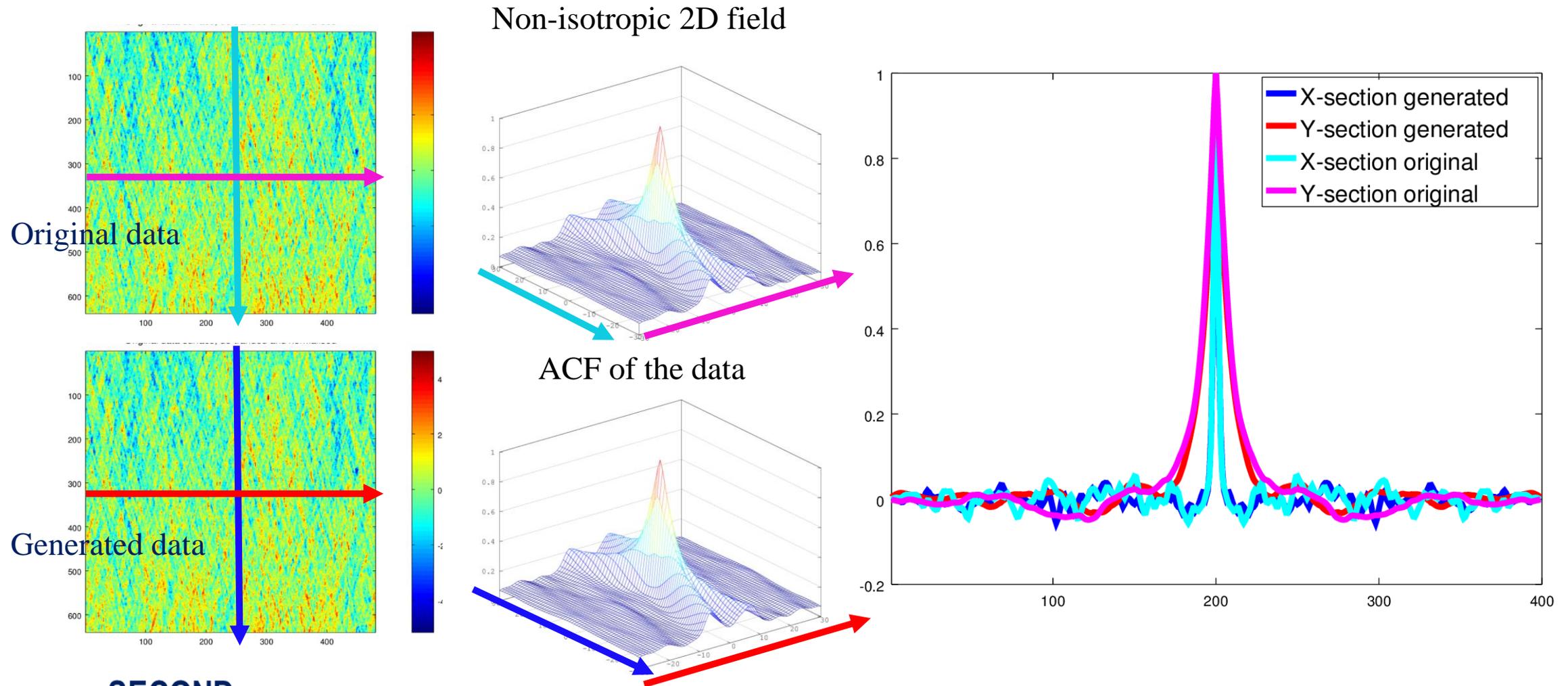


# 2D InTILF analysis is stable along the mirror



Good agreement of InTILF coefficients along the mid-row of InTILF matrices computed for metrology data from Site 1 and Site 2. The difference is  $< 3.5\%$  value

# Generation of 2D InTILF model (use case 4)



**Simulations demonstrate high spectral fidelity**

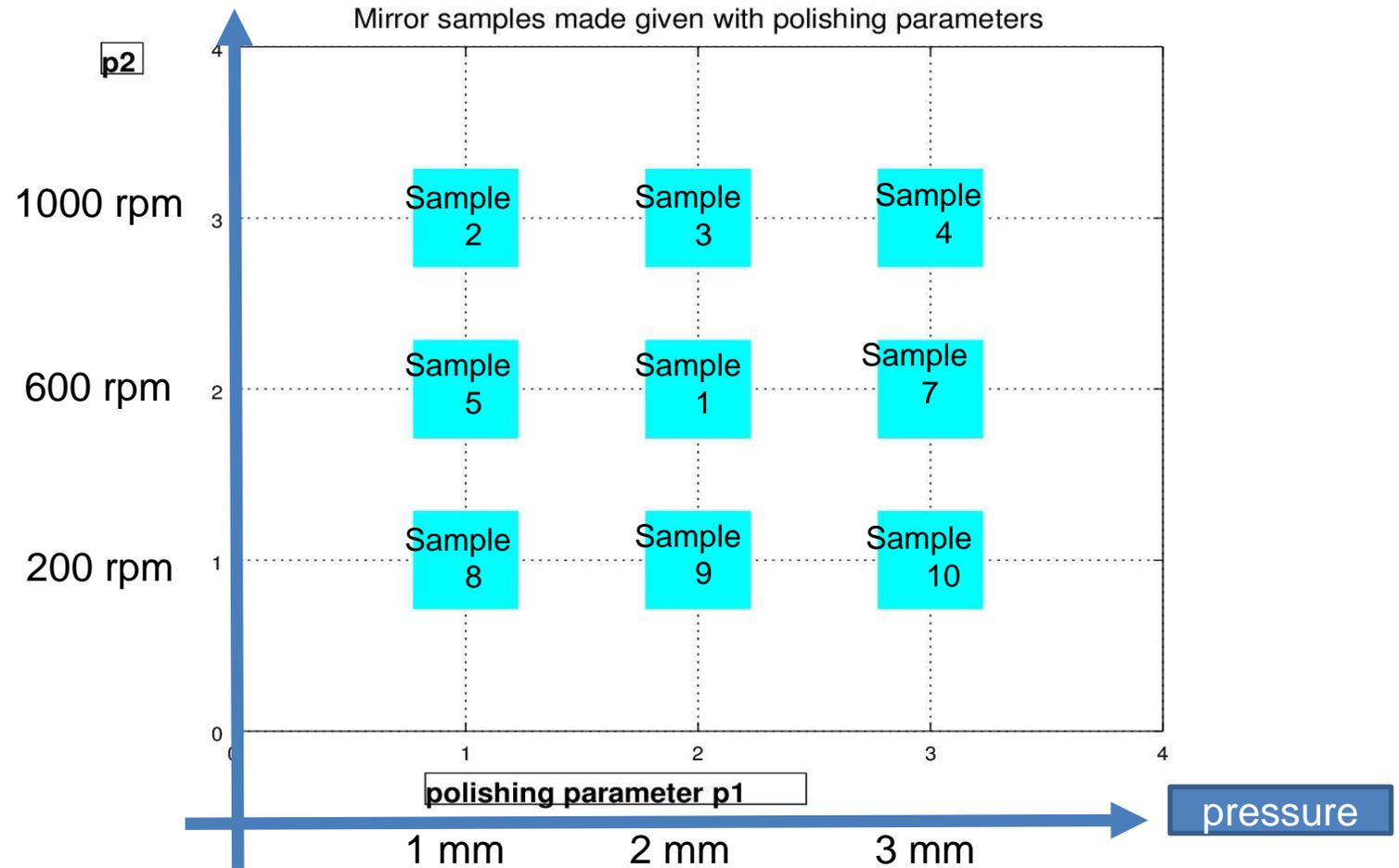
# Application of BeatMark to Polishing Optimization (BeatMark step 2, slide 9)

Data Collection 1:

10 Samples Polished with different polishing parameters

Two polishing parameters:

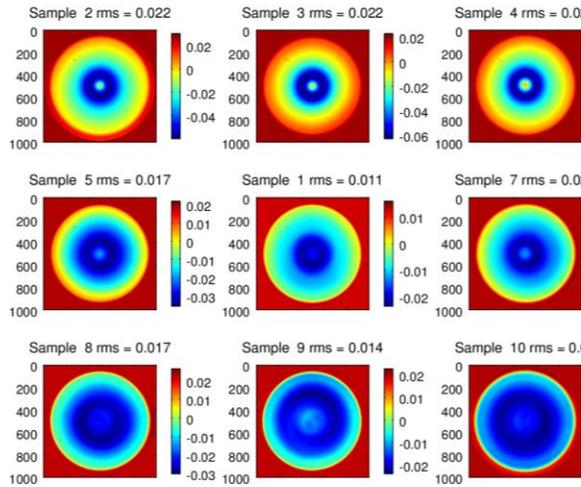
- **speed** (in rpm) and
- **pressure** (in mm) were varied around perceived optimal values of
  - **600 rpm**
  - **2 mm.**



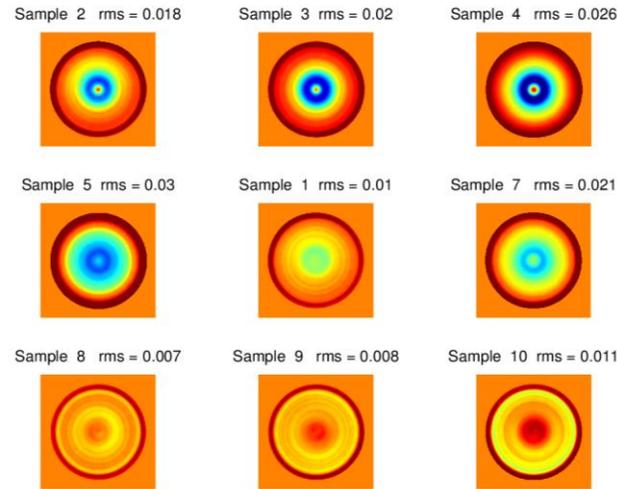
# Samples were measured with different instruments

Instrument	Measured by	Dimension – 1D or 2D
Interferometer	OptiPro	2
UltraSurf	OptiPro	2
Profilometer	OptiPro	1
New View	OptiPro	2 (at higher resolution)
Interferometer	LBNL	2

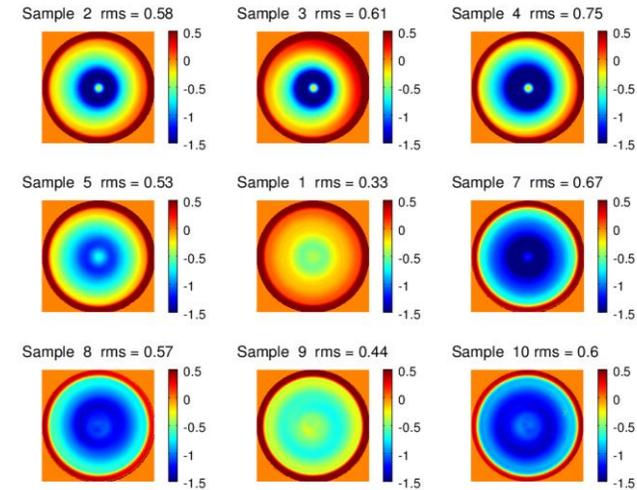
# Samples measured by different Instruments



OptiPro Interferometer

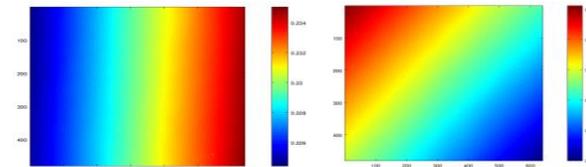


OptiPro UltraSurf



LBNL Interferometer

For the rough analysis that we did in this first experiment we saw no material differences in analysis results. This will have to be monitored when we progress toward finer experiments.

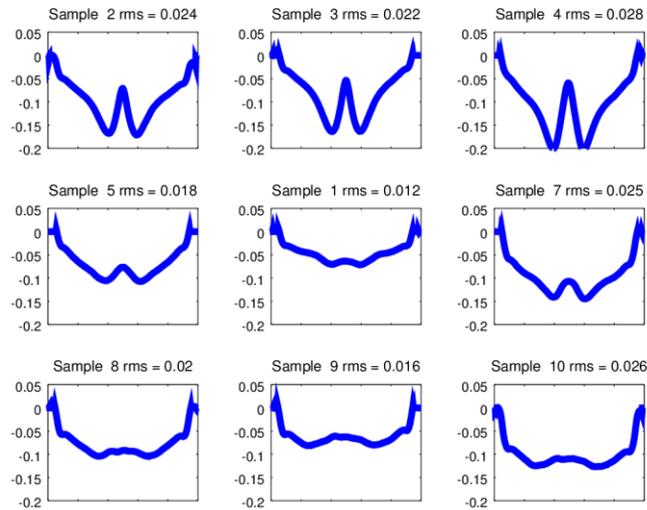


OptiPro NewView

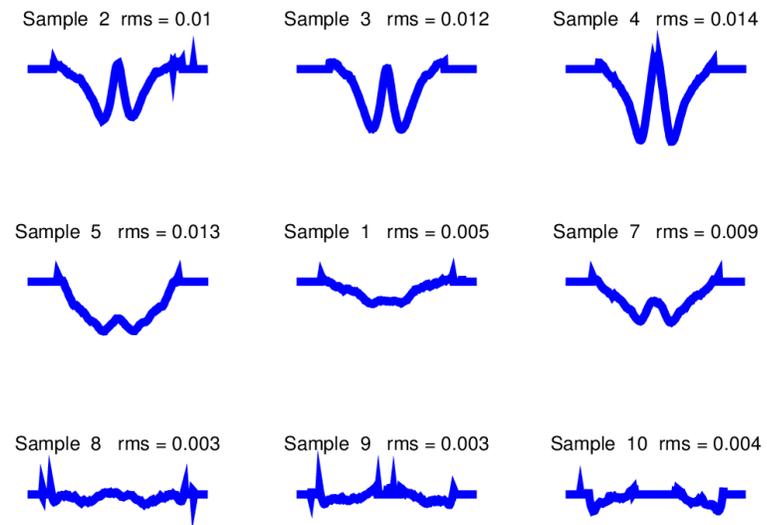


# 1D profiles for all instruments

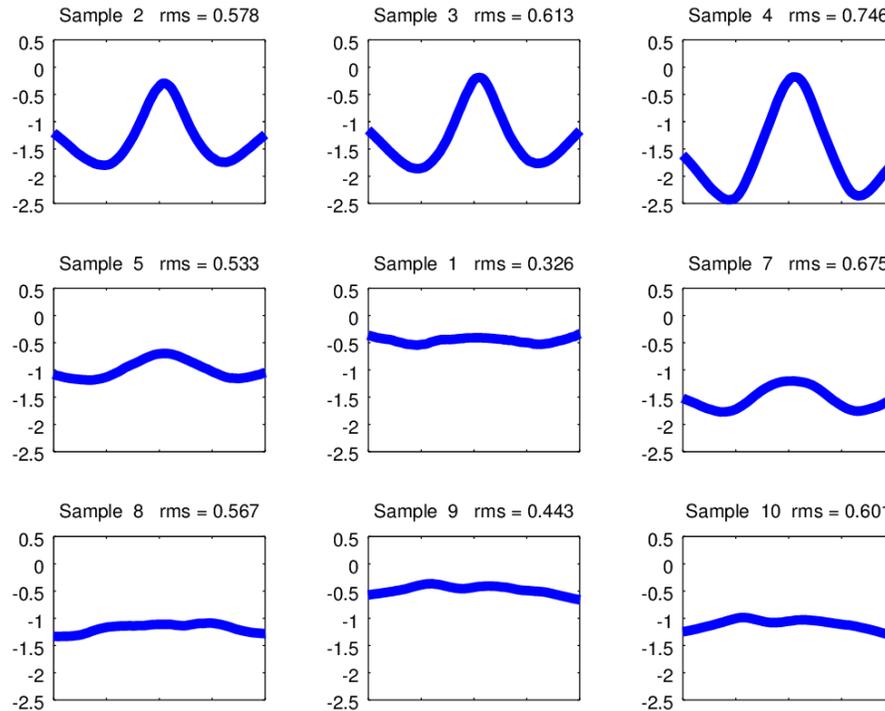
OptiPro Interferometer



OptiPro UltraSurf



# All Sections as measured by LBNL



Mirror Height

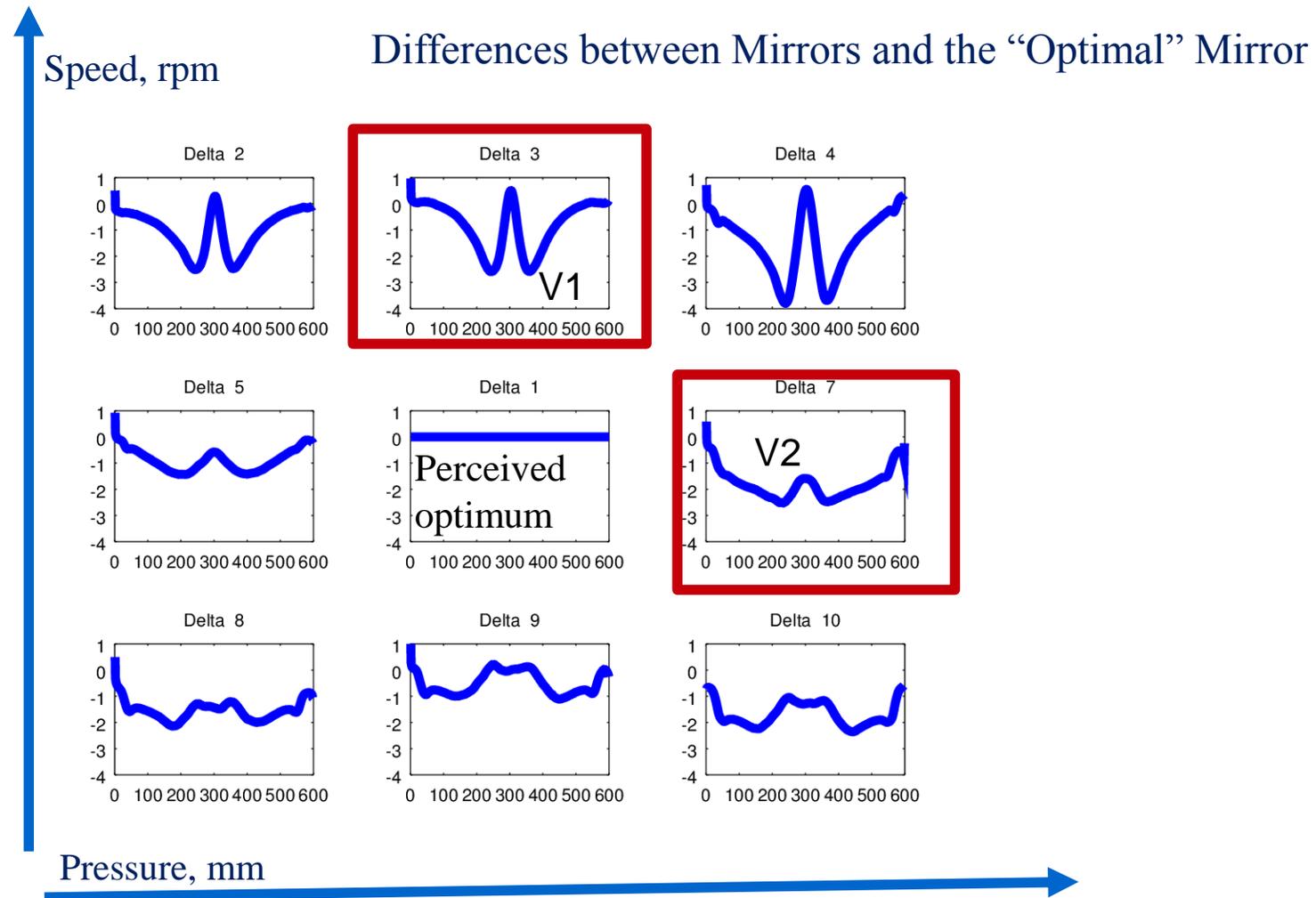
Pixels 1- 600

These are sections of the mirror samples (we checked that they are uniform about the angle)

# Two methods of mirror quality comparison

- Shape analysis (large effects)
- Stochastic analysis (finer effects)

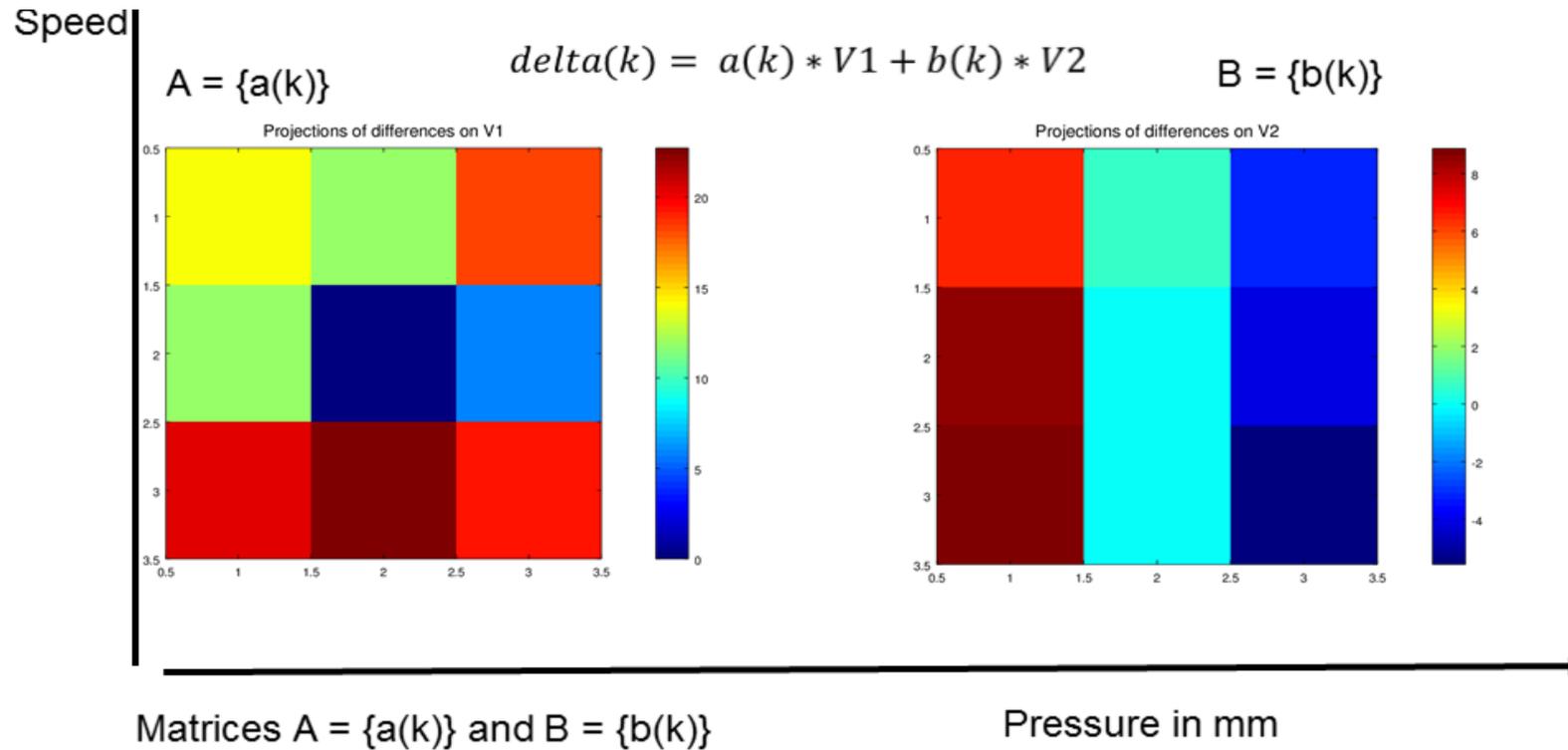
# Method 1: Sape analysis. “Basic” vectors (aka Characteristic vectors)



Express all other differences deltas as “vectors” in the space of functions as a linear combination of “vectors” V1 and V2:



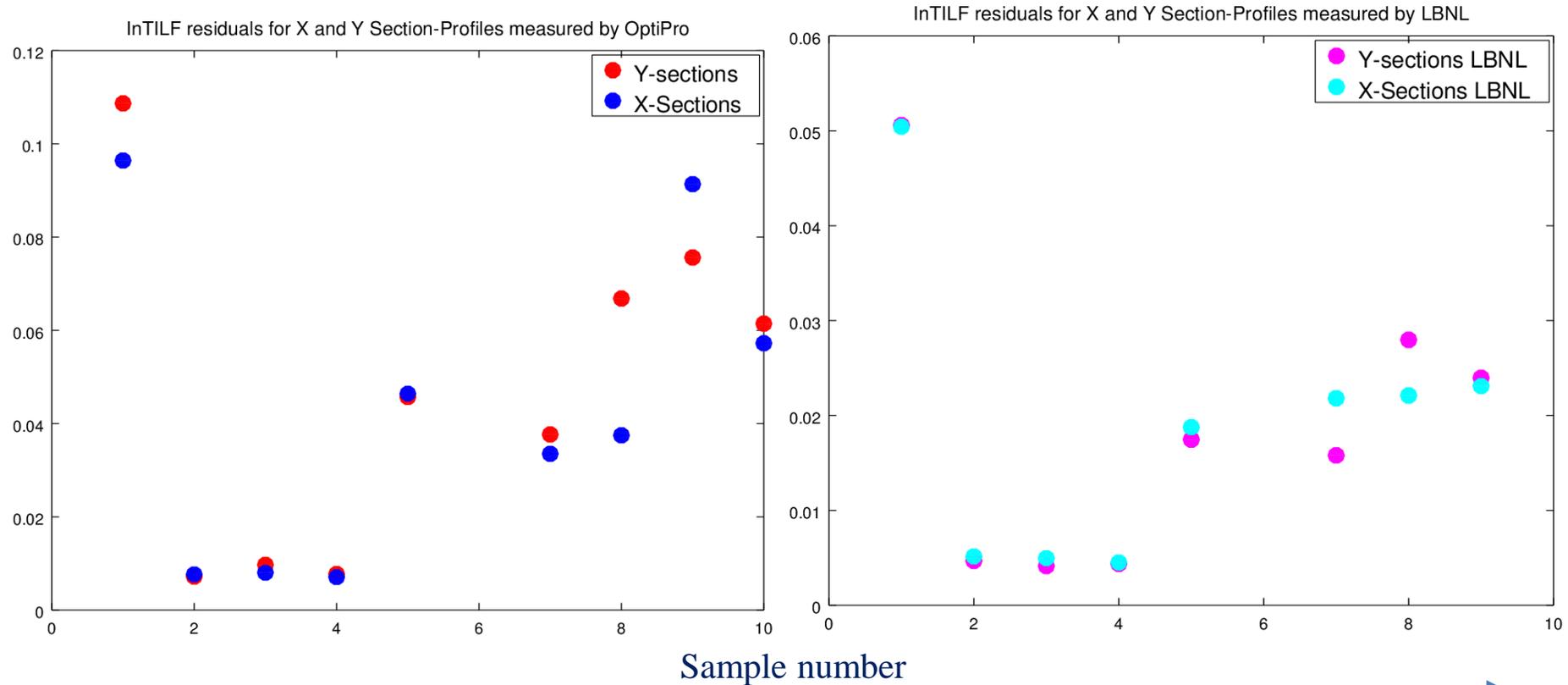
# Method 1: Vector decomposition with basic vectors



Method 1 shows good potential in optimizing for polishing parameter ‘pressure’. The dependence of a sample shape on pressure appears “linear” in its magnitude. Not so for the rotation speed.

# Method 2: InTILF-Quality indicator computed for OptiPro and LBNL data

Quality Indicator, based on InTILF was computed for samples using good quality **central segments**

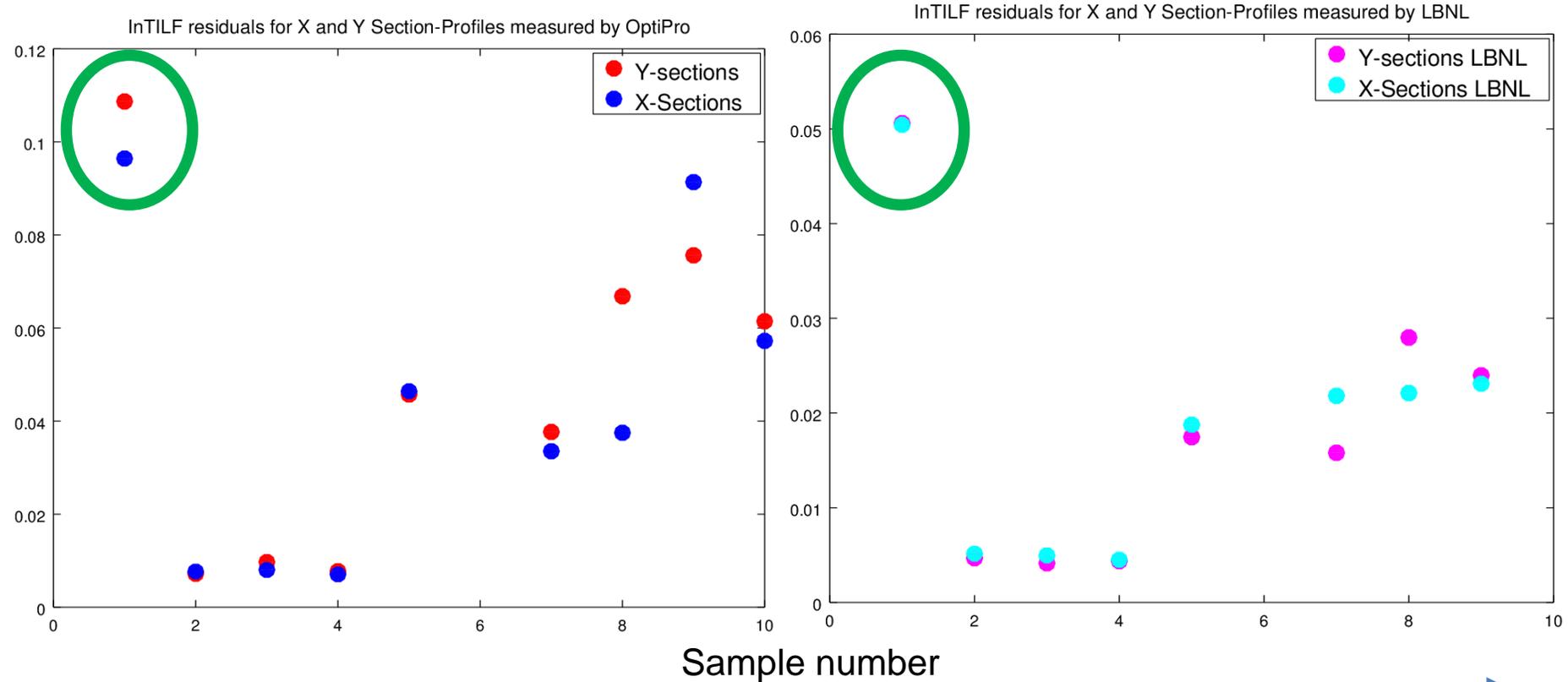


The data is numerically different (for sample measurement errors related issues), but qualitatively points to the same optimal sample 1



# Method 2: InTILF-Quality indicator computed for OptiPro and LBNL data

Quality Indicator, based on InTILF was computed for samples using good quality **central segments**



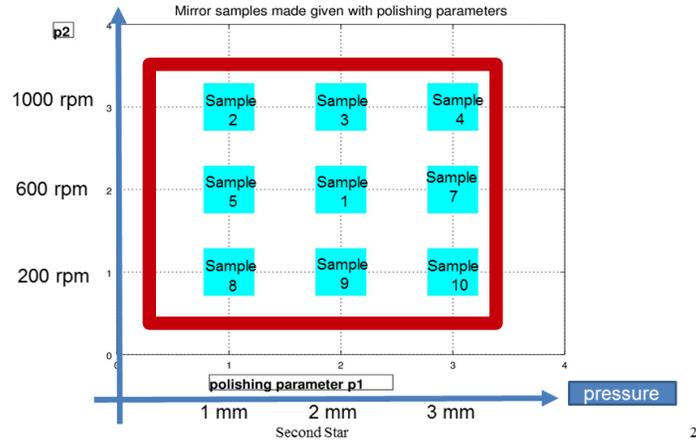
The data is numerically different (for sample size related normalization issues), but qualitatively points to the same optimal sample 1



# Design of data collection 2

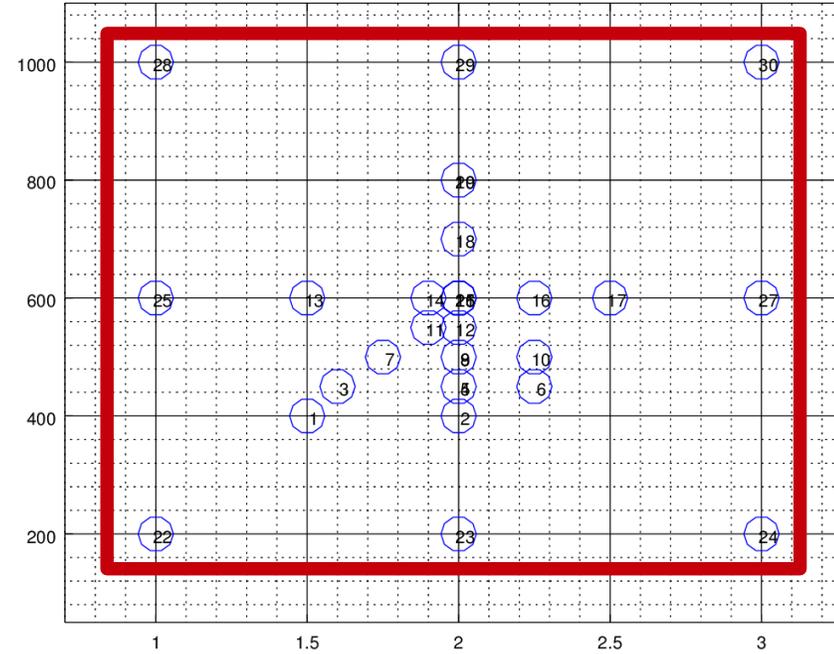
Recall experiment 1: Samples Polished with different polishing parameters

Two parameters: **speed** (in rpm) and **pressure** (in mm) were varied around perceived optimal values of 600 rpm and 2 mm.



10 samples

Test 2 samples polishing parameters and sample numbers



30 samples

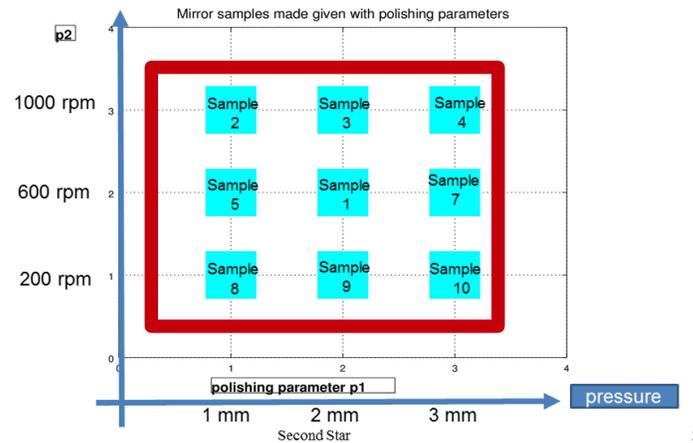


# Design of data collection 2

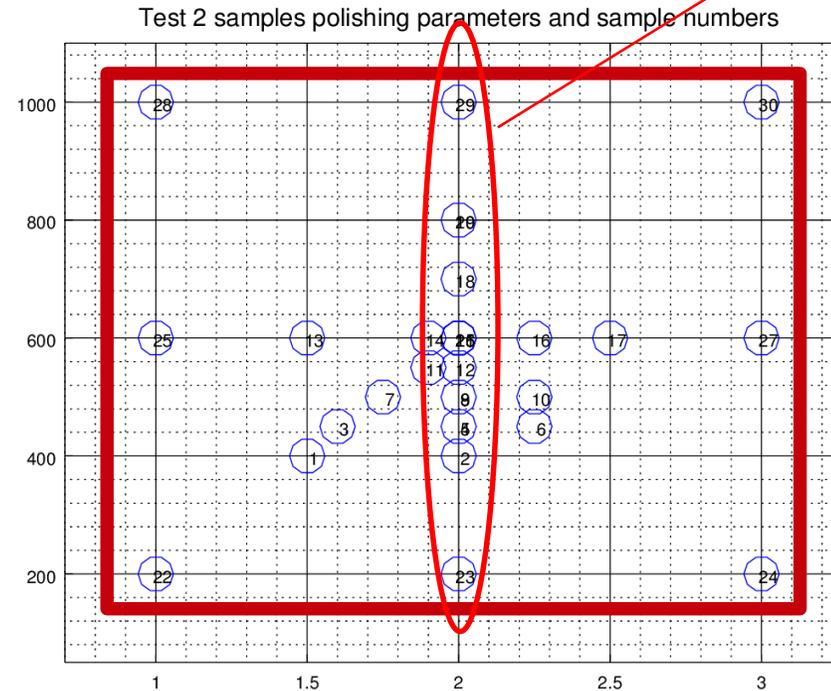
To study non-linear dependence on speed

Recall experiment 1: Samples Polished with different polishing parameters

Two parameters: **speed** (in rpm) and **pressure** (in mm) were varied around perceived optimal values of 600 rpm and 2 mm.



10 samples



30 samples

# Conclusions:

BeatMark software package – **the prototype implementation of InTILF**

- characterizes mirror surfaces with a **small number of parameters**
- needs only **modest amount of metrology data** to characterize **the entire surface**
- generates **simulated ‘metrology’ profiles** statistically equivalent to the original profile (1D or 2D )

We are working on using the BeatMark (and InTILF) to:

- provide the surface quality assessment through a **quality metric**
- look to work on validation of q-metrics with XFEL
- lead to **significant improvements in polishing**

Possible development of InTILF method may lead to comprehensive analysis of metrology data taken by instruments with different Modulation Transfer Function.



# Acknowledgments

This work was supported by NASA Small Business Innovation Research SBIR grant to Second Star Algonumerix, project No. 15-1 S2.04-9193. The Advanced Light Source is supported by the Director, Office of Science, Office of Basic Energy Sciences, Material Science Division, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231 at Lawrence Berkeley National Laboratory.



Thank you for your attention!



Second Star Algonumerix: <http://www.secondstaralgonumerix.com>

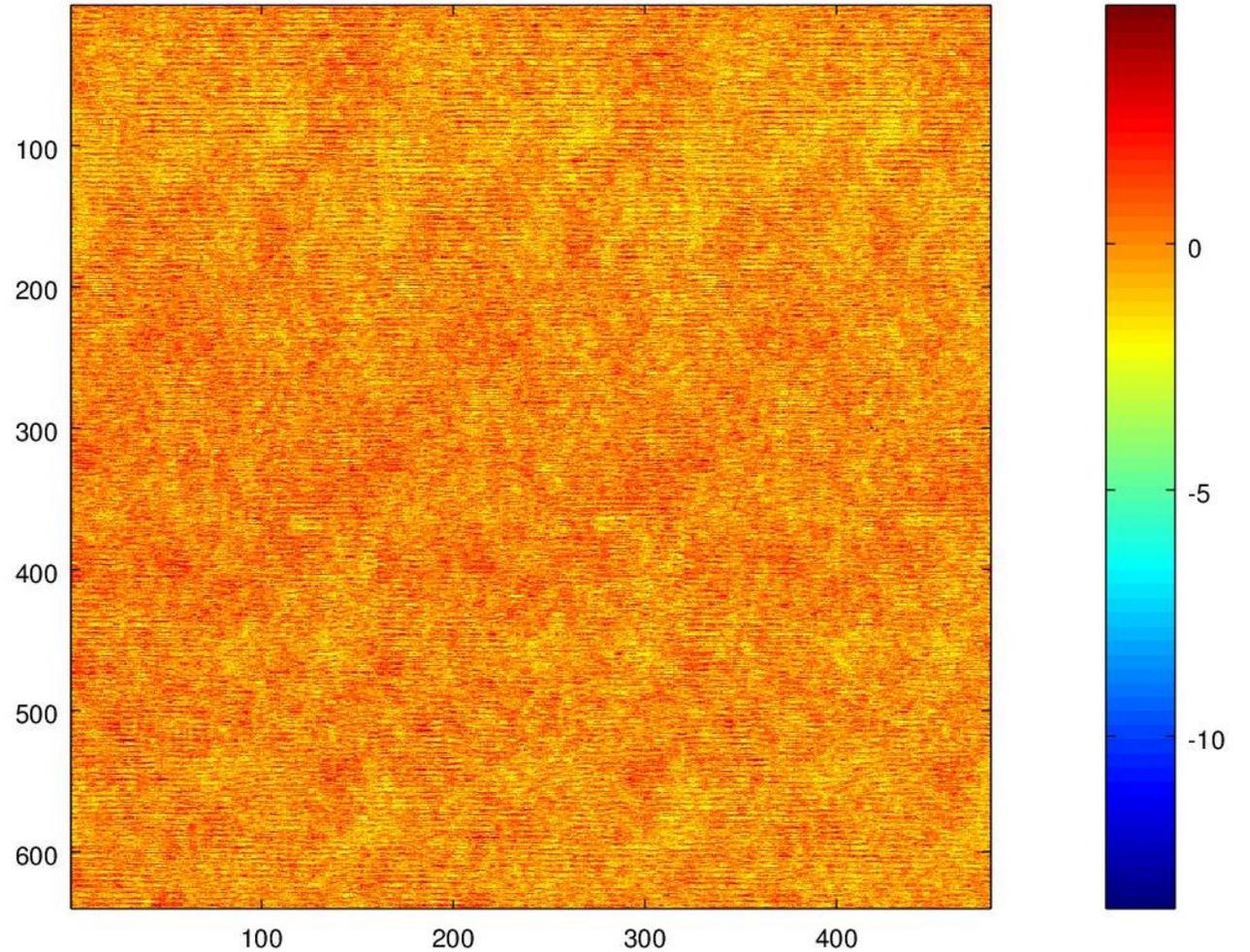
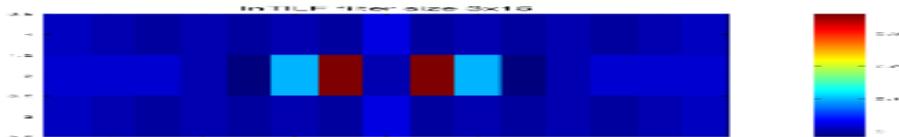
# Appendix



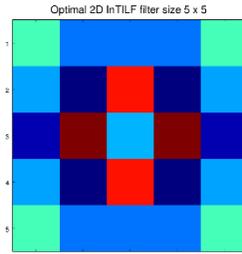
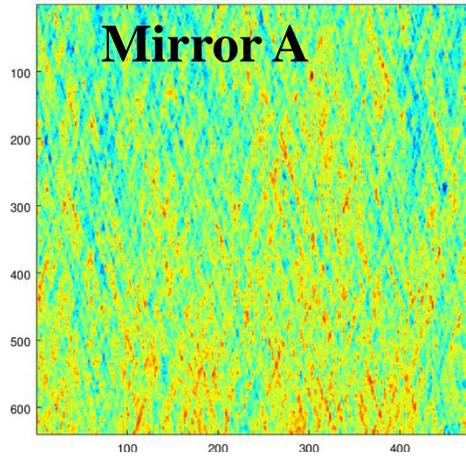
# InTILF analysis of mirror B

Height distribution of the mirror B  
measured with the ALS XROL interferometric microscope  
ZYGO NewView™-7300 equipped with 2.5× objective  
with ×2.0 zoom  
surface area 1.06 mm × 1.41 mm  
effective pixel size of 2.2 μm (640 pixels × 480 pixels)  
Measured surface topography has a structure of horizontal  
'strips' with rms variation of the surface height of 1.74 Å.

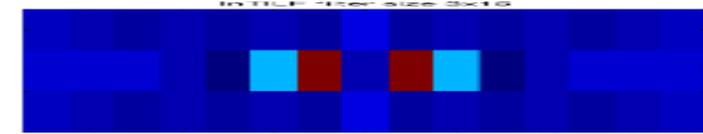
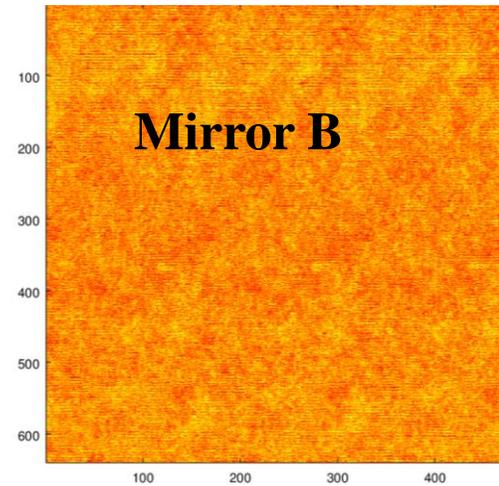
## InTILF matrix 3 × 15



# BeatMark-2D assessment of two mirrors



**BeatMark assessment of Mirror A:**  
**InTILF 5x5 matrix**  
**Residual < 1 %**



**BeatMark assessment of Mirror B:**  
**InTILF = 3 x15 matrix**  
**Residual = 23%**

**How many parameters do fully describe a mirror?**

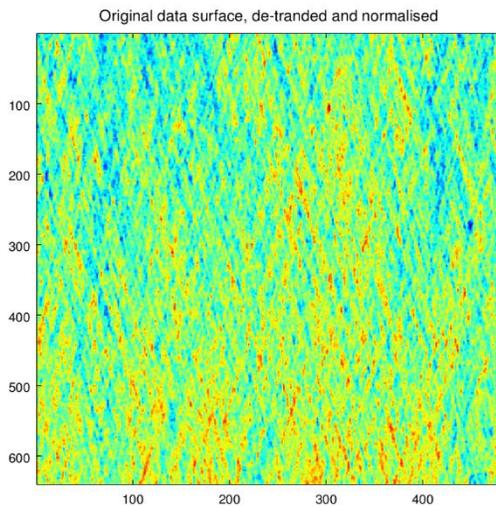
**A: 25**

**B: 45**

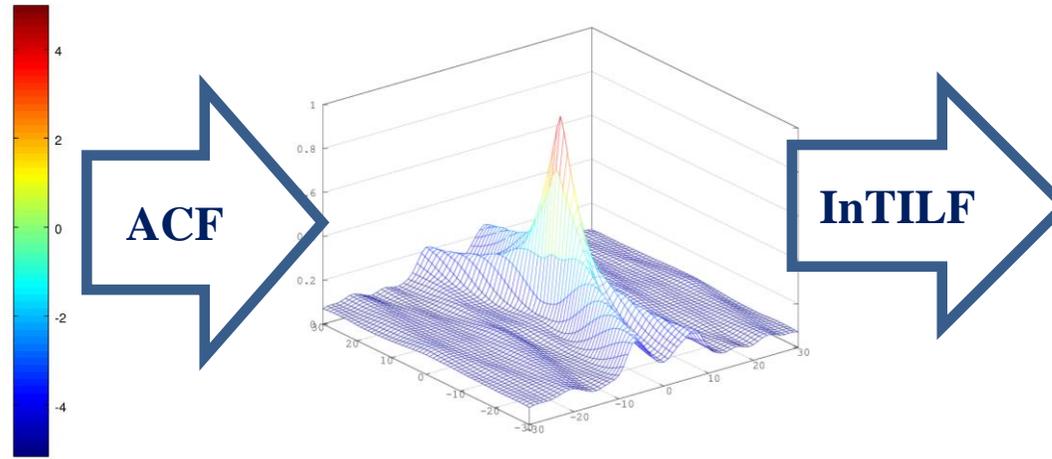


# Construction of 2D InTILF model, mirror A

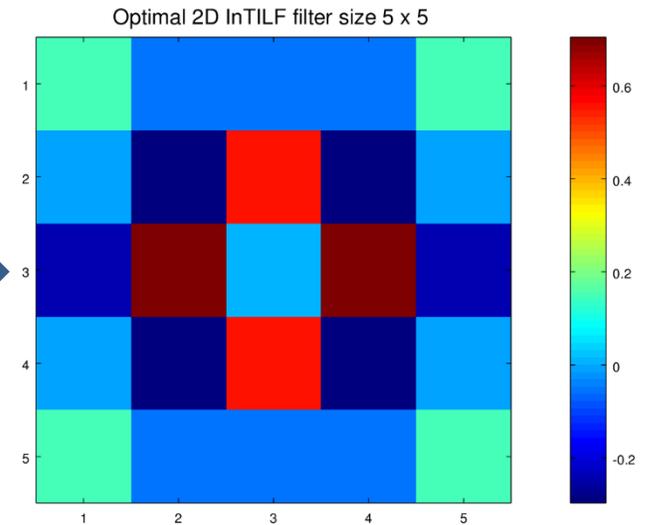
## 1. Start with 2D data



## 2. Compute Auto Covariance Function

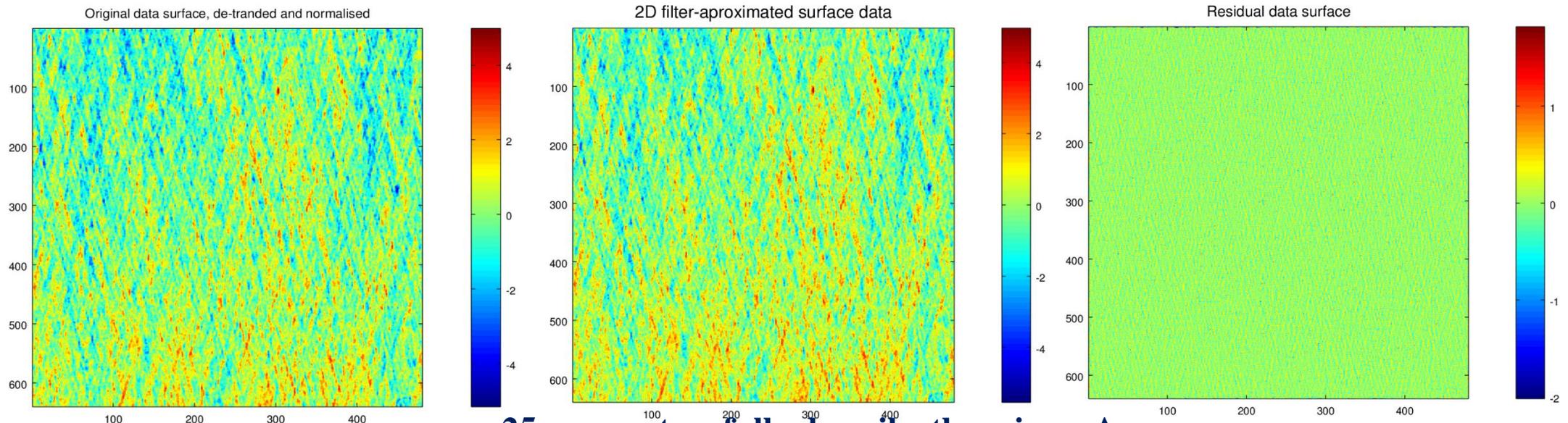


## 3. Compute InTILF (2D matrix)



# 2D InTILF analysis of Mirror A

**Mirror A data:** height distribution measured with an interferometric microscope ZYGO NewView™-7300 equipped with 2.5× objective with ×2.0 zoom. The Microscope is available at the ALS XROL.<sup>18,19</sup> The left-hand plot in Fig. 1 shows the rectangular surface area of 1.06 mm × 1.41 mm measured with the effective pixel size of 2.2 μm (the data set consists of 640 × 480 pixels<sup>2</sup>). The measured surface topography has a characteristic ‘diamond’ like pattern with rms variation of the surface height of 6.75Å.



**25 parameters fully describe the mirror A**

**2D InTILF model accuracy: residual rms ~1%**



# Stationary Random Process (SRP) and its Auto-covariance function (ACF) in 2D

Natural extension to 2D:

**SPR:**  $x(t_1, t_2): \mathbb{Z}^2 \rightarrow \mathbb{R}^2$  &  $E(X(t_1 + h_1, t_2 + h_2) * X(t_1, t_2)) = E(x(h_1, h_2)X(\mathbf{0}))$ ,  $\forall h = (h_1, h_2) \Rightarrow$  introduce ACF  $Q_x(h) = Q_x(h_1, h_2) = E\{x(t_1 + h_1, t_2 + h_2)x(t_1, t_2)\}$ .

In 2D b) means that for any natural number  $m$ , any  $m$  integers  $h_1, \dots, h_m$  and any real numbers  $z_1, \dots, z_m$

$$\sum_{i,j=1}^m q(h_i - h_j) z_i z_j \geq 0$$

ACF  $Q(\cdot, \cdot)$  of a stationary random process on a lattice  $\mathbb{Z}^2$  can be represented as:

$$q(h_1, h_2) = \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} e^{ih_1 x_1 + ih_2 x_2} \mu(dx_1, dx_2), (h_1, h_2) \in \mathbb{Z}^2$$

# Polishing optimization idea

- Ideal mirror surface deviates from its form very slightly and in an absolutely random manner – white noise random
- White noise is an absolutely random process completely devoid of pattern
- A polishing tool might leave a pattern (correlations) on a mirror. If it is detected and characterized, the mirror can be improved by optimizing polishing parameters.
- Our task is to detect and characterize the pattern

**We are in search of the stochastic pattern**