LNLS

sirius

Brazilian Synchrotron
Light Laboratory

Scientific Computing @ Sirius / LNLS

Yuri Rossi Tonin, M. Sc.
Scientific Computing Specialist
on behalf of the Scientific Computing group

LNLS Brazilian Synchrotron Light Laboratory sirius
CNPEM Brazilian Center for Research in Energy and Materials
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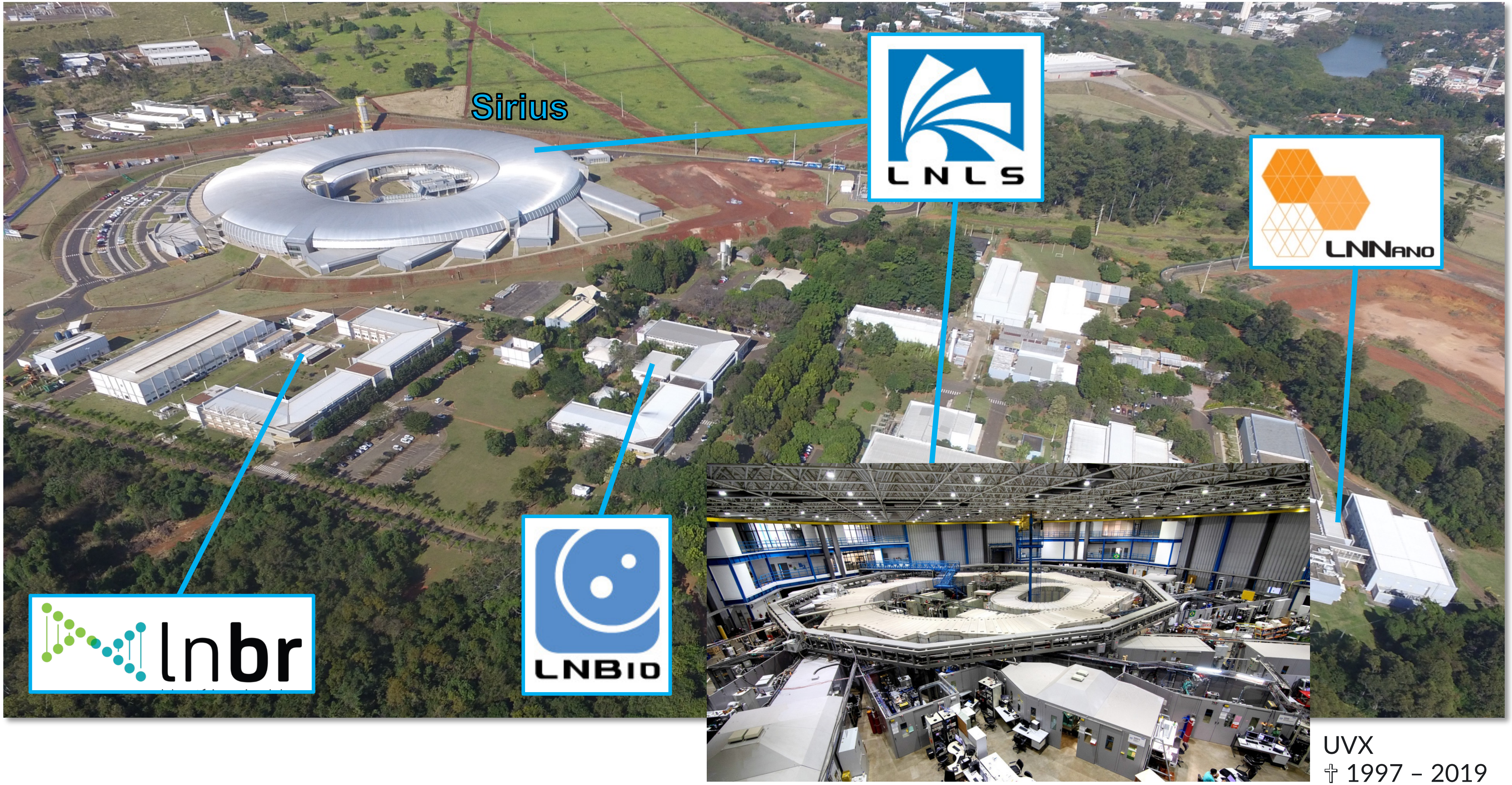
BRAZILIAN GOVERNMENT BRASIL UNITING AND REBUILDING

Outline

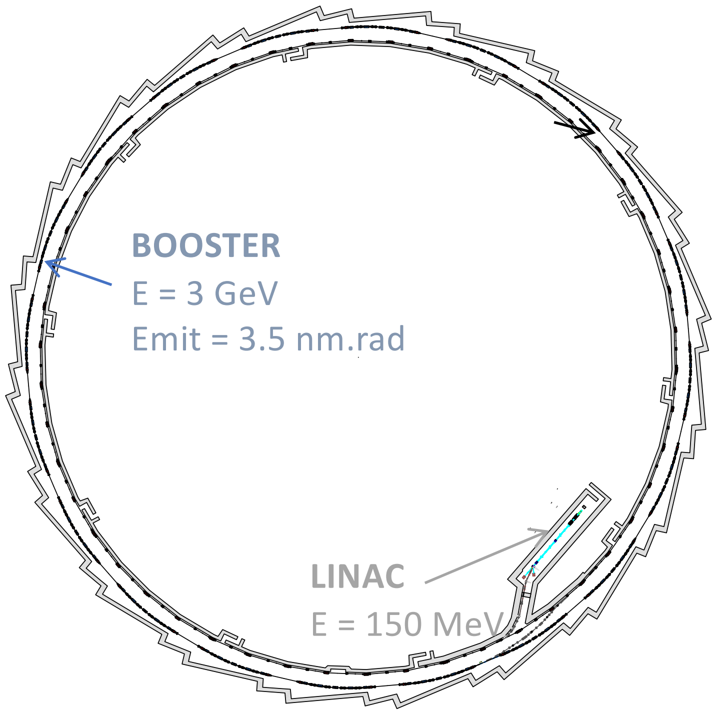
- SIRIUS, the new lightsource
- The scientific computing team
- Computing Infrastructure
- Detectors
- Processing pipeline
- Beamline results

CNPEM



UVX
† 1997 – 2019

Sirius Overview



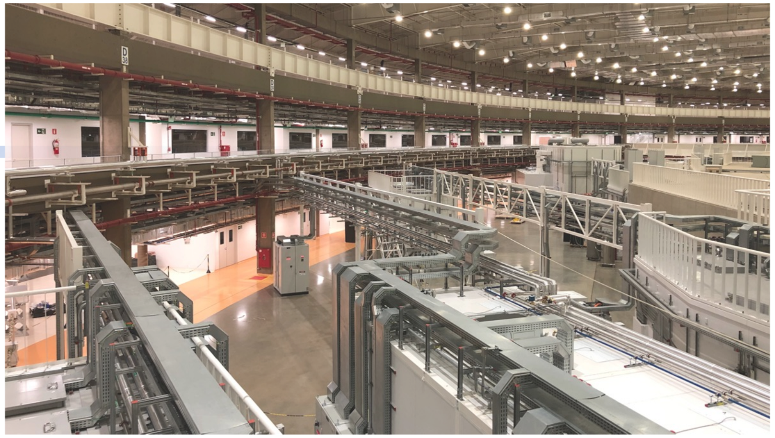
Storage Ring design parameters	
Beam energy	**3.0 GeV**
Circumference	518 m
Lattice	20 x 5BA
Current, top up	350 mA (100 mA)
Bunch length	8 ps
Energy spread	0.09 %
RF frequency	500 MHz
Hor. emittance (bare⇢ ids)	**250 ⇢ 150 pm.rad**
Vert. emittance	**2.5 ⇢ 1.5 pm.rad**
Straight section low β_x/β_y	**1.5 m / 1.4 m**

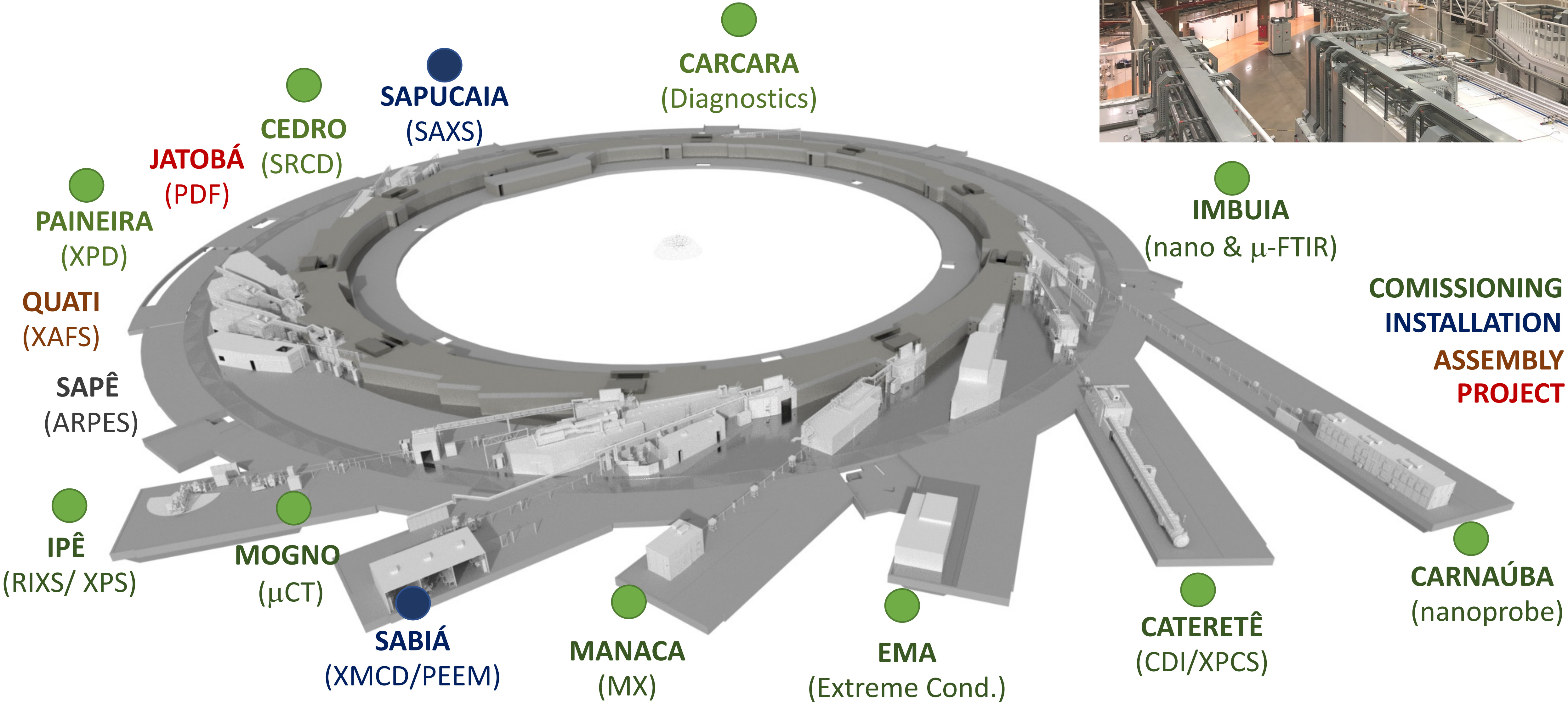
First beam: Dec 2019

First external users: Sep 2020

* Courtesy of Harry Westfahl Jr.

Phase 1A & 1B Beamlines





* Courtesy of Harry Westfahl Jr.

https://www.lnls.cnpem.br/beamlines/

“How many beamline does Sirius synchrotron has?”

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O Sirius tem 13 linhas de luz em operação atualmente, cada uma projetada para atender a uma área específica de pesquisa. Os nomes das linhas de luz são os seguintes:

1. Manacá
2. Ipê
3. Abacate
4. Jequitibá
5. Cajuí
6. Uva
7. Graviola
8. Açaí
9. Pitanga
10. Sirius MX
11. Macaúba
12. Cateretê
13. Caracará

2019-21 : X-Ray Optics Lab

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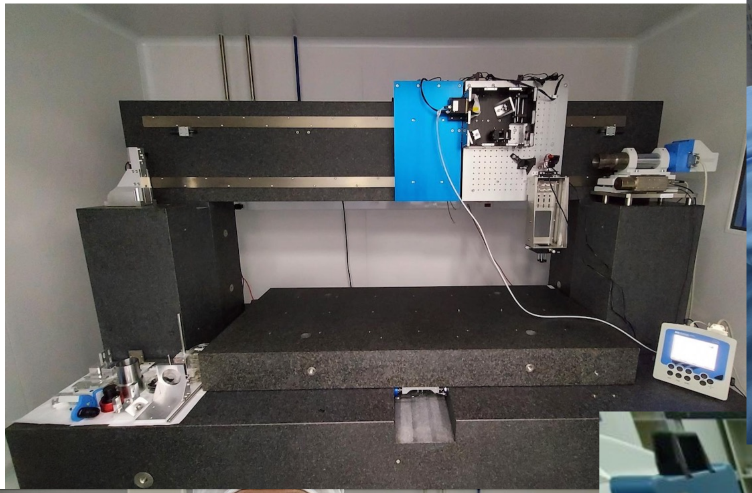
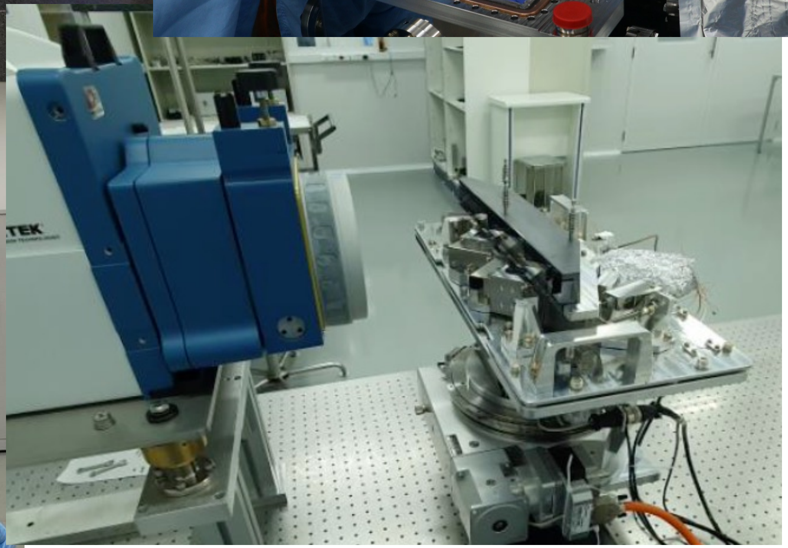
Long-trace profiler

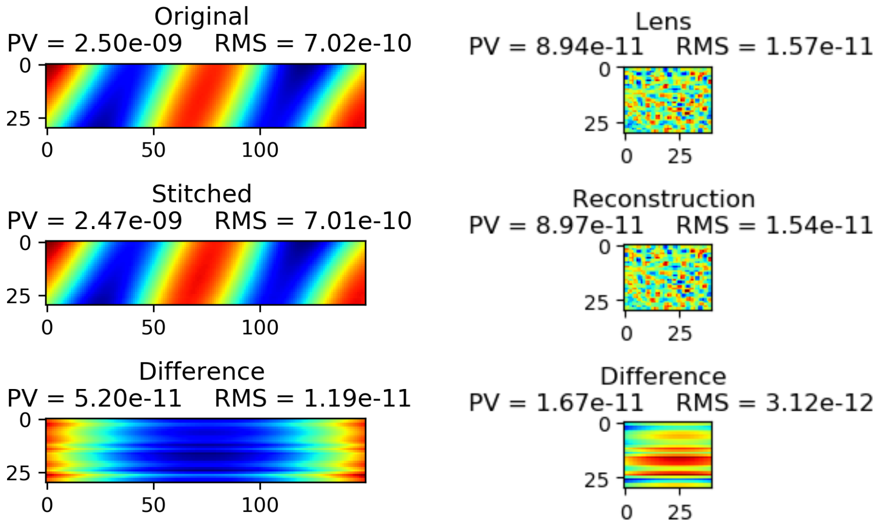


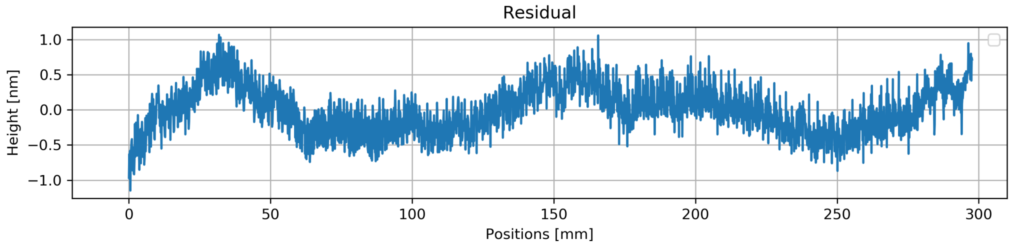


Fizeau interferometer

- Self-calibrating stitching interferometry

$$\left\| \begin{bmatrix} \mathbf{G} & \mathbf{D} \end{bmatrix} \begin{bmatrix} \mathbf{t}^\top \\ \mathbf{r}^\top \end{bmatrix} - \mathbf{d}^\top \right\| \rightarrow min,$$





21-Present: Scientific Computing

The team:

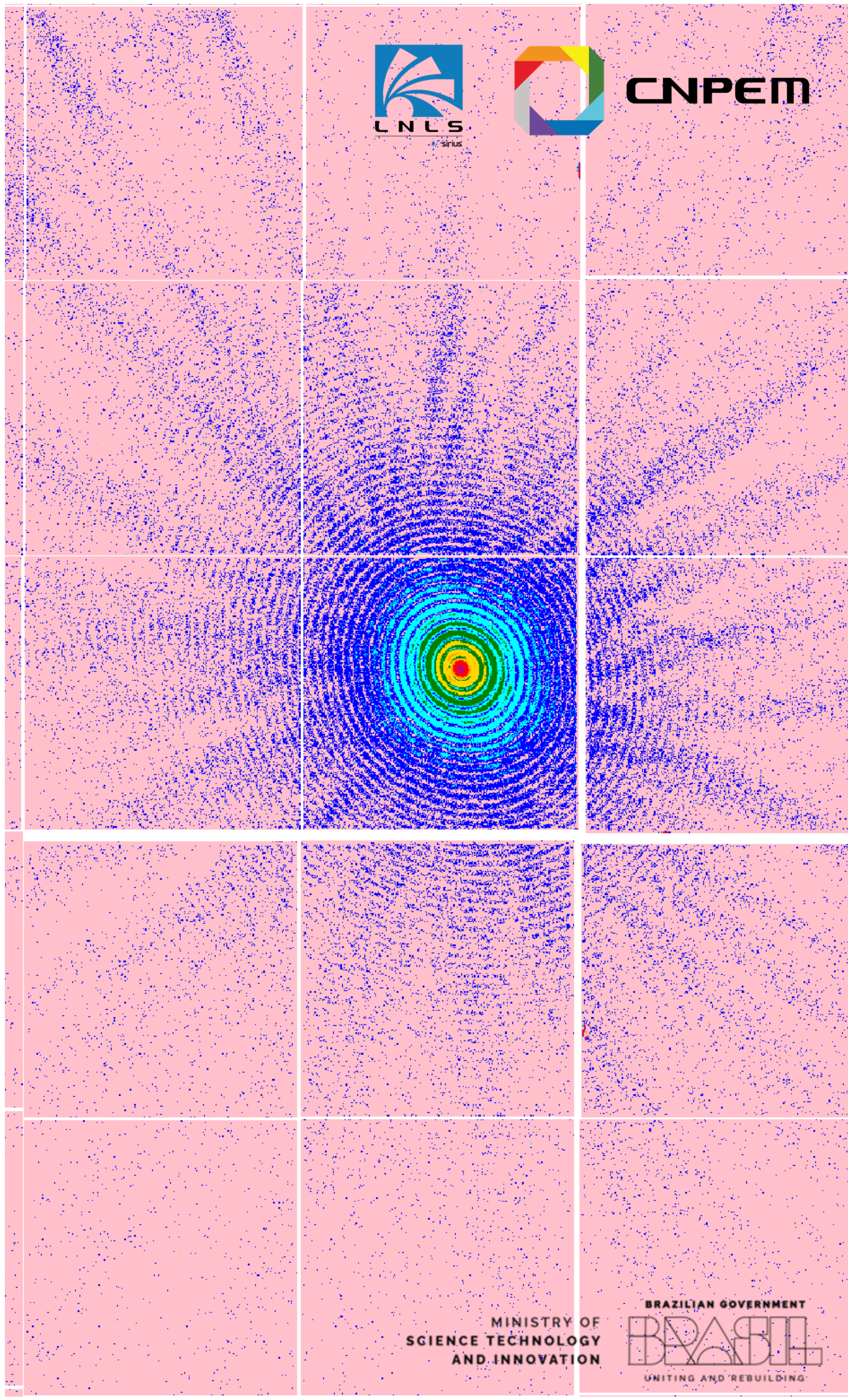
(A) Ricardo Grangeiro / (B) João F. Gondim / (C) Daniel Tavares / (D) Eduardo Miqueles

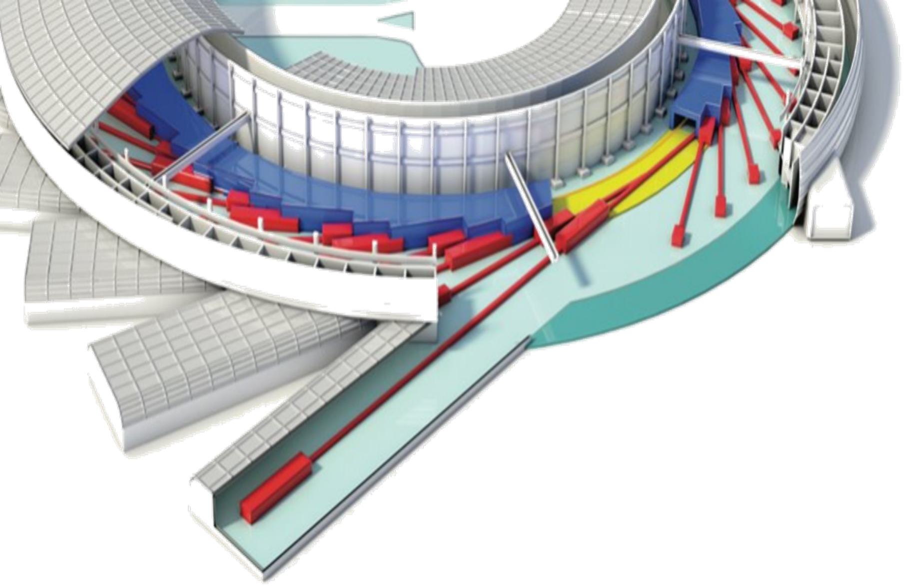
(E) Yuri R. Tonin / (F) Paola C. Ferraz / (G) Julia Carvalho / (H) Gabriel Borin

(I) Larissa Moreno / (J) Alice Kageyama / (K) Larissa Rosa / (L) Camila Lages / (M) Otávio Paiano

- *MOGNO / Petrobras: (A), (B), (H), (M)*

BR
PETROBRAS





Main activities

- *Detector corrections*
- *Plane-wave CDI*
- *Ptychography*
- *Tomography*
- *Diffraction*
- *ARPES*
- *Jupyter interfaces for analysis*
- *Overall mathematical modelling*
- *Beamline and user support*

- ➢ Make it work (Python)
- ➢ Make it fast (C/CUDA)
- ➢ Well written, well documented
  - ➢ Fast to debug
  - ➢ Fast to maintain
- ➢ Automatize as much as possible
  - ➢ “Single button processing”

TEPUI: Throughput Enhanced Processing Unit

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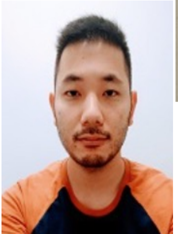
Storage
- Storage Unit
- Controllers
- Protocol Gateways

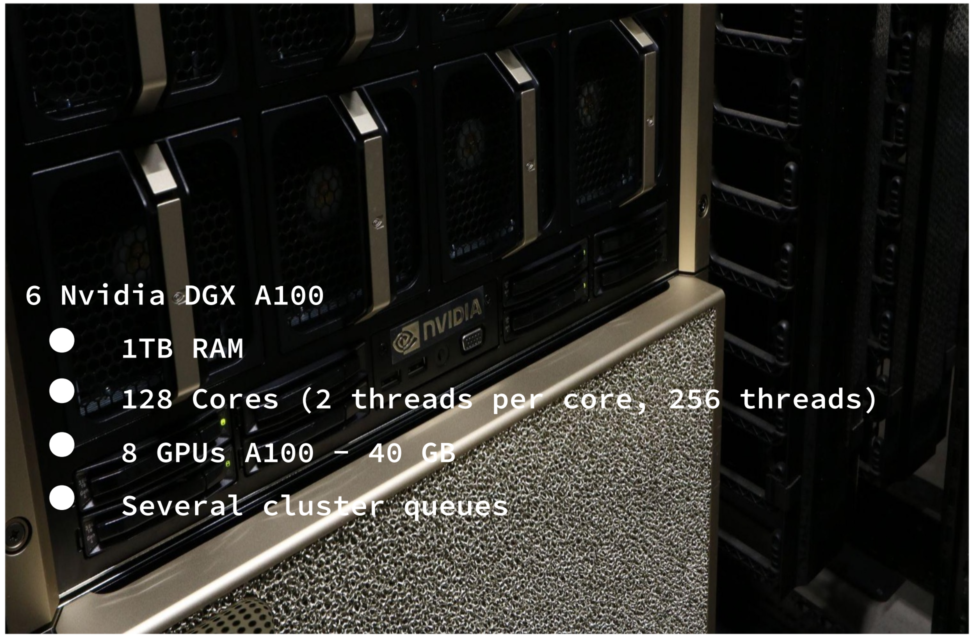
Network
- Core Switch
- Management Switch

Servers
- Standalone Servers
- GPU Cluster
- CPU Cluster



* Courtesy of F. Furusato

Infrastructure

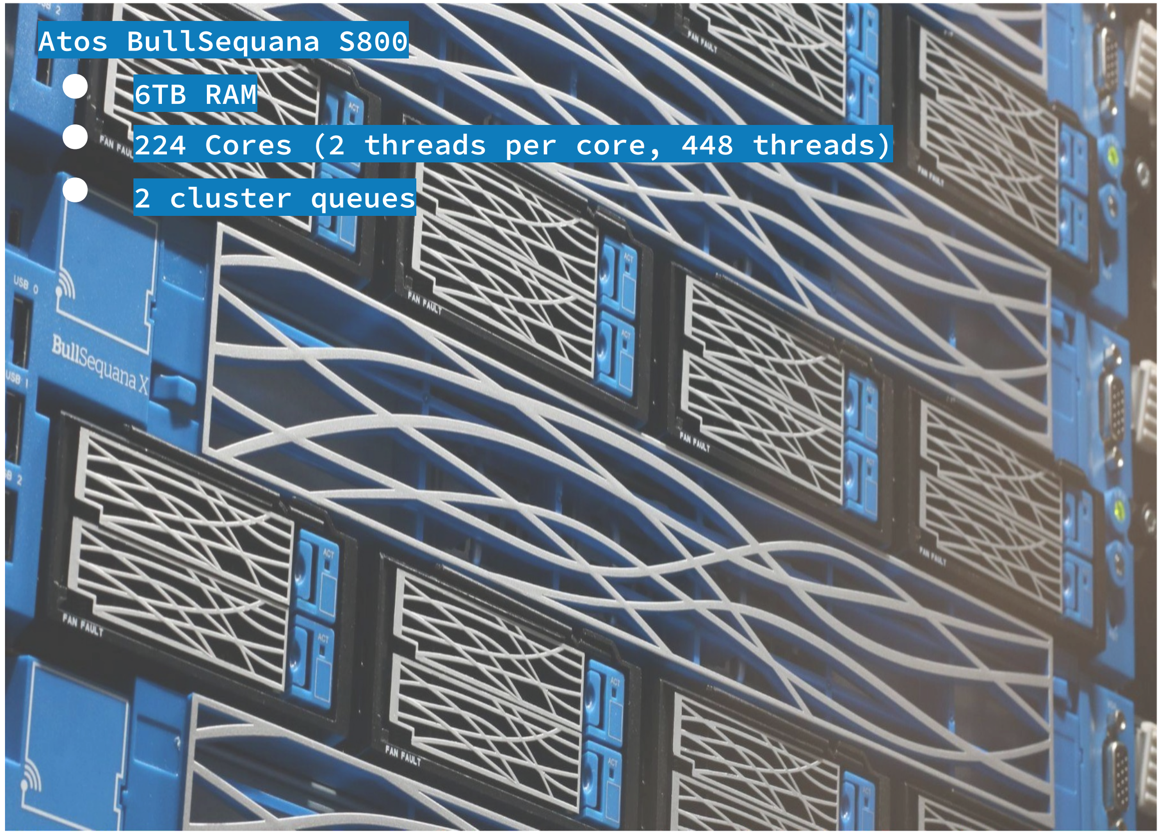


6 Nvidia DGX A100

- 1TB RAM
- 128 Cores (2 threads per core, 256 threads)
- 8 GPUs A100 – 40 GB
- Several cluster queues

GPU Node

CPU Node



Atos BullSequana S800

- 6TB RAM
- 224 Cores (2 threads per core, 448 threads)
- 2 cluster queues

HPE Cray ClusterStor E1000

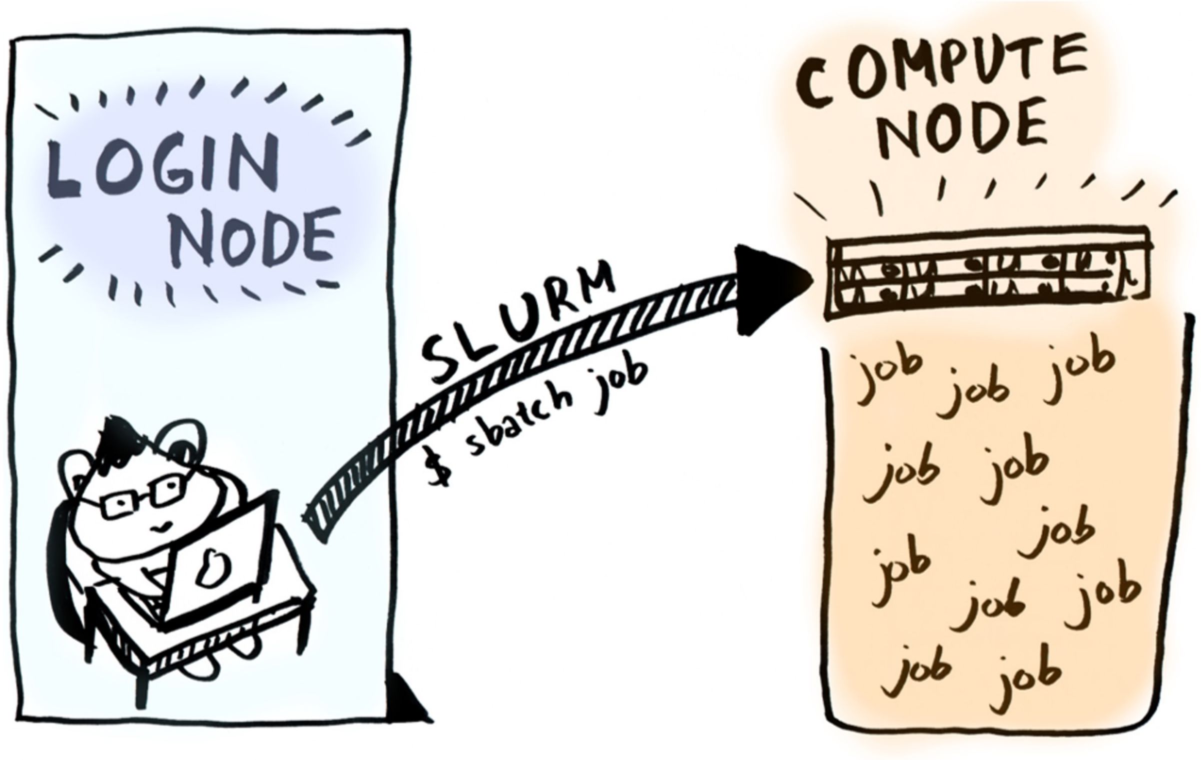
- 4PB
- Lustre Filesystem
- HTTP, FTP, NFS, CIFS gateways

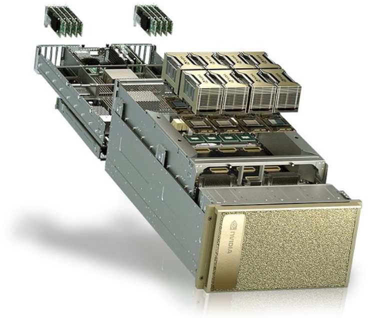
Storage

* Courtesy of F. Furusato

Cluster

- Slurm Worload Manager for job scheduling





- Beamline dedicated queues for processing and visualization:

PARTITION	NODELIST	CPUS(A/I/O/T)	FREE_MEM	GRES	GRES_USED	STATE	TIMELIMIT	GroupResources
cpu	enedina	100/348/0/448	6148752	(null)	gpu:0	mixed	5-00:00:00	
imb	enedina	100/348/0/448	6148752	(null)	gpu:0	mixed	3-00:00:00	cpu=32,mem=256G
mgn	mabel	0/256/0/256	887822	gpu:8	gpu:0	idle	3-00:00:00	cpu=160,gpu=5,mem=640G
cnb	mabel	0/256/0/256	887822	gpu:8	gpu:0	idle	3-00:00:00	cpu=96,gpu=3,mem=384G
cat	rosalind	0/256/0/256	730776	gpu:8	gpu:0	idle	3-00:00:00	cpu=160,gpu=5,mem=640G
ema	rosalind	0/256/0/256	730776	gpu:8	gpu:0	idle	3-00:00:00	cpu=32,gpu=1,mem=128G
ipe	rosalind	0/256/0/256	730776	gpu:8	gpu:0	idle	3-00:00:00	cpu=32,gpu=1,mem=128G
pnr	rosalind	0/256/0/256	730776	gpu:8	gpu:0	idle	3-00:00:00	cpu=32,gpu=1,mem=128G
dev-gcc	nise	96/160/0/256	828980	gpu:8	gpu:4	mixed	3-00:00:00	
tepui	harriet	0/256/0/256	993745	gpu:8	gpu:0	idle	3-00:00:00	
petro	aida	32/224/0/256	954461	gpu:8	gpu:2	mixed	3-00:00:00	

PIMEGA detectors

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- Part of Medipix3 collaboration
- Developed in partnership between Detectors group and PiTEC
- https://www.pitec.co/



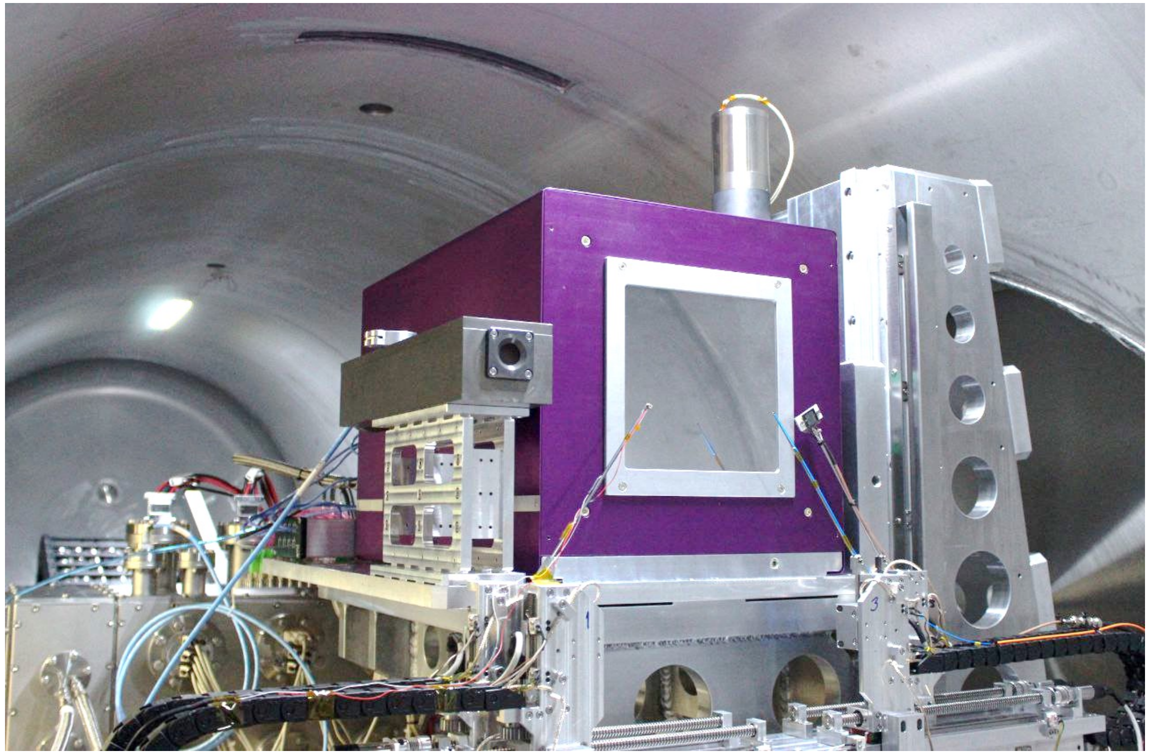


	MOBIPIX 15D	PIMEGA 45D	PIMEGA 135D	PIMEGA 450D	PIMEGA 450DS	PIMEGA 540D
Sensors (µm material)	300 Si / 1000 CdTe	300 Si	300 Si / 675 Si /1000 CdTe	675 Si	675 Si	300 Si / 675 Si
Pixels (number / arrangement)	262 kpx / 512 x 512	786 kpx / 512 x 1536	2,4 Mpx / 1536 x 1536	7,9 Mpx / 256 x 30720	7,9 Mpx / 512 x 15360	9,4 Mpx / 3072 x 3072
Pixel size (µm²)	55 x 55	55 x 55	55 x 55	55 x 55	55 x 55	55 x 55
Detection area (mm²)	28 x 28	28 x 85	85 x 85	14 x 1692	28 x 850	170 x 170
Active area (%)	99.7	99.6	99	90	90	99
Dynamic range (counts/px/s)	3×10^5	3×10^5	3×10^5	3×10^5	3×10^5	3×10^5
Frame rate @ 12bits (fps)	2000	600	2000	1000	1000	2000
Throughput @ 12bits (Gb/s)	5.9	5.3	52.7	87.9	87.9	211
Readout mode	Continuous or burst	Continuous or burst	Continuous or burst	Continuous or burst	Continuous or burst	Continuous or burst
Vacuum (10^{-3} mbar)	No	No	Yes	No	No	Yes

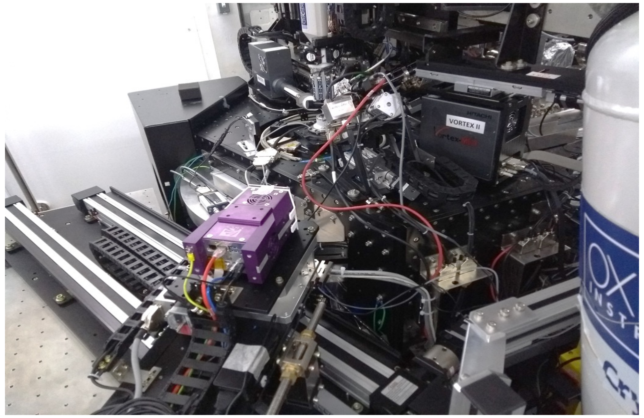
* Courtesy of Jean Polli

PIMEGA detectors

Pimega 135D @ Carnaúba

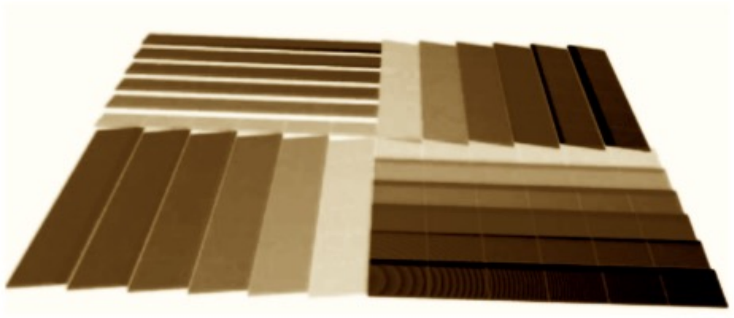


Pimega 540D @ Cateretê



Mobipix @ Carnaúba

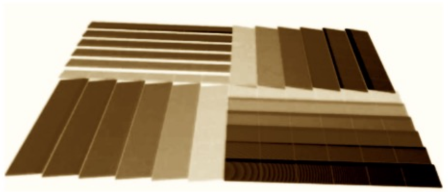
Geometry:



https://www.pitec.co/

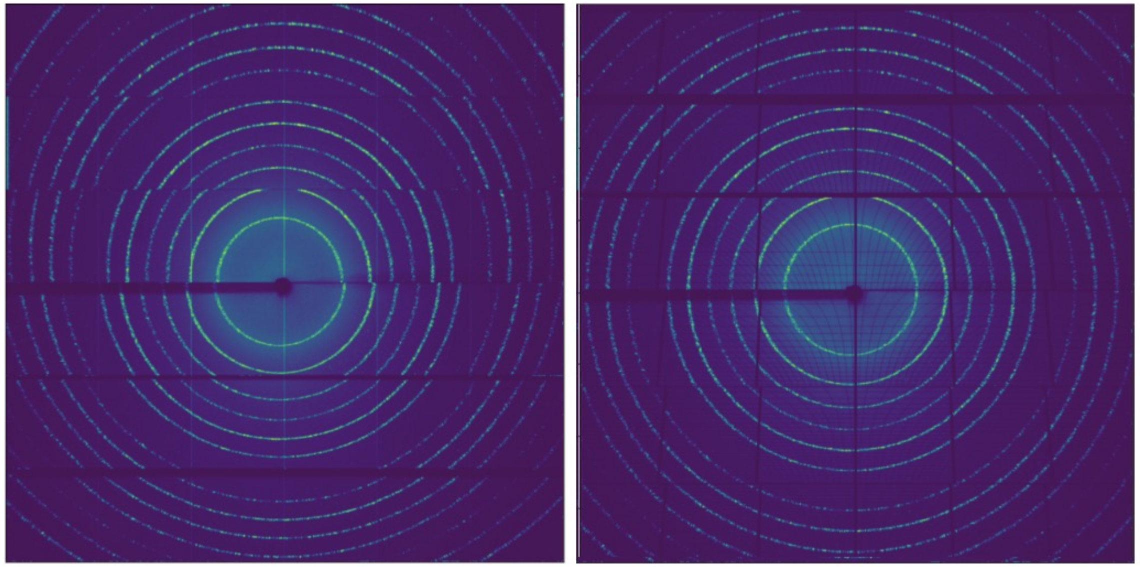
Restoration

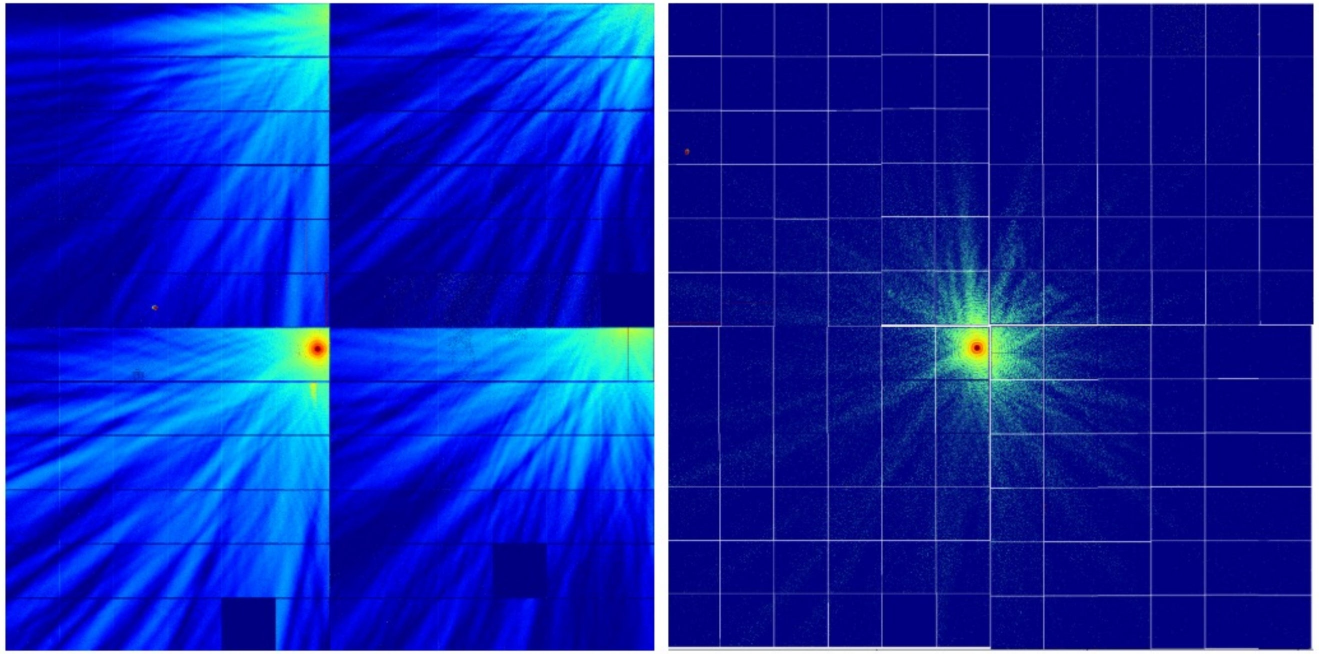
- Tilted chips to minimize gaps
- Geometric corrections necessary to adjust measured images from “tilted” to “virtual plane” chips



Four modules, 540D

Single module, 135D





- Restoration time < 1 second per DP (CPU, Python)
- 500 frames: <1 second with GPUs

Restoration of diffraction patterns through different imaging planes, E. X. Miqueles, under review

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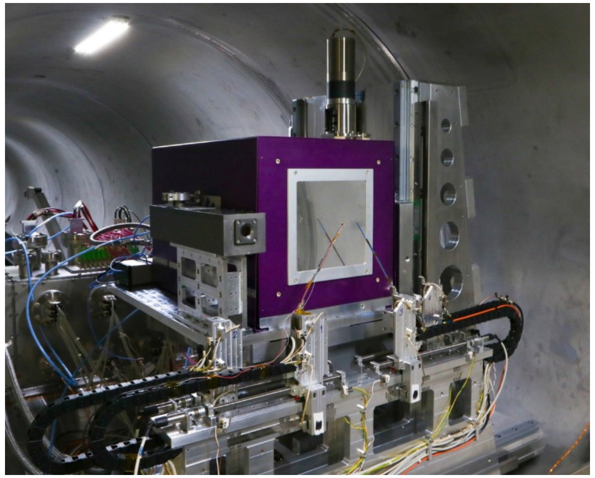
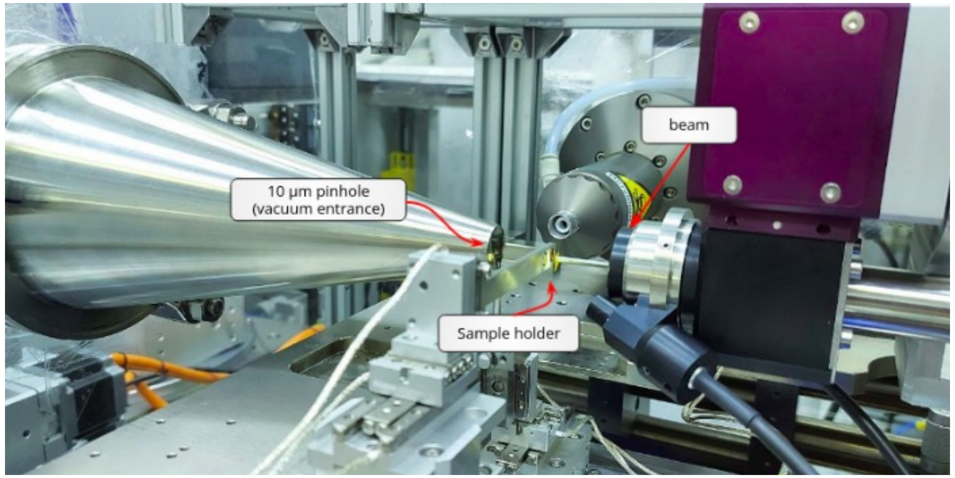
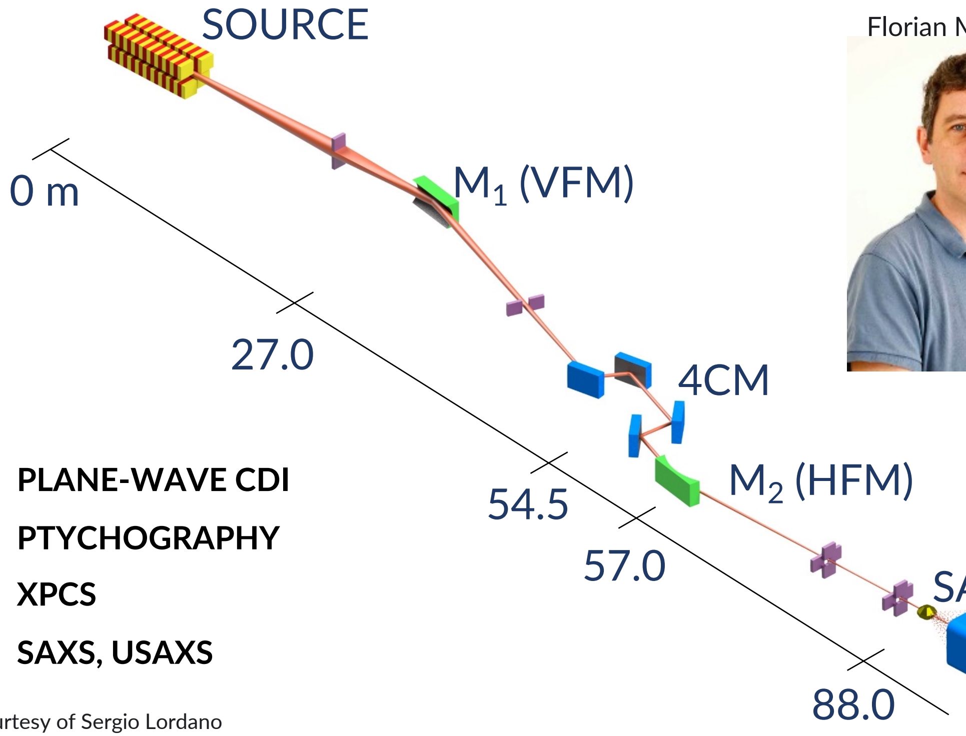
Coherent and Time-resolved X-ray Scattering

CATERETÊ beamline

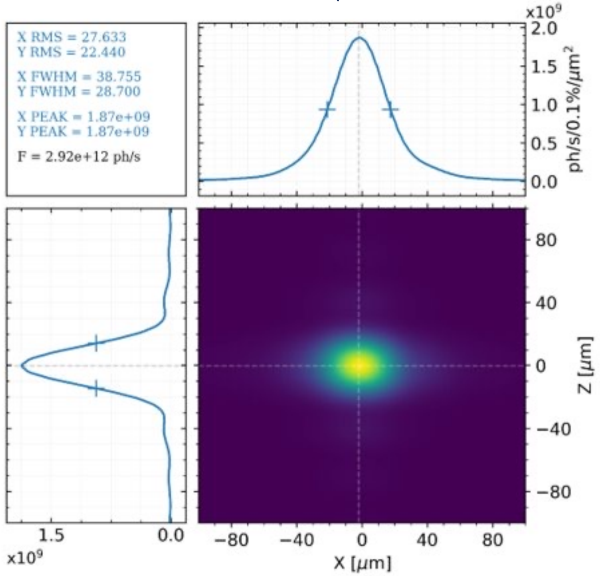




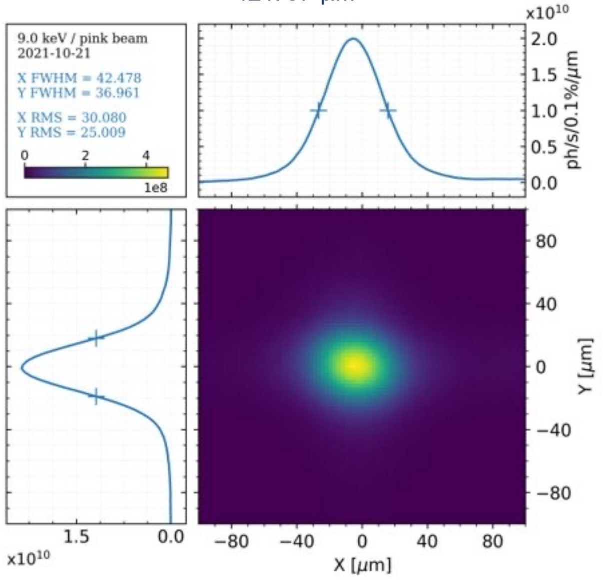


Florian Meneau

SIMULATED
39 x 29 µm²



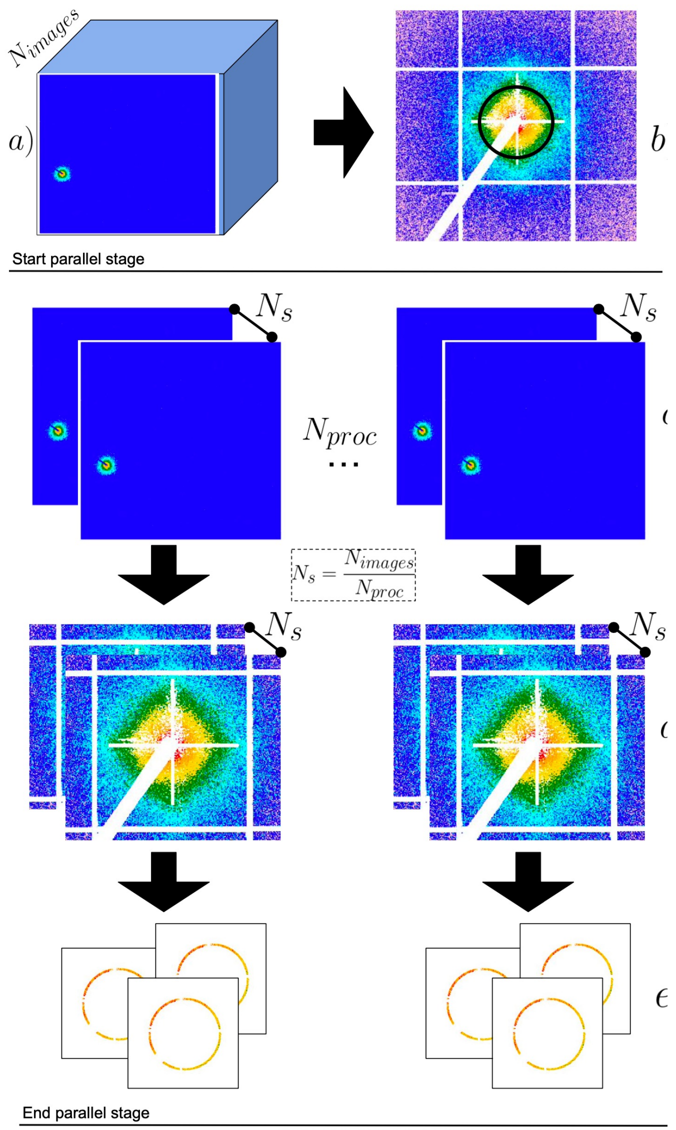
MEASURED
42 x 37 µm²



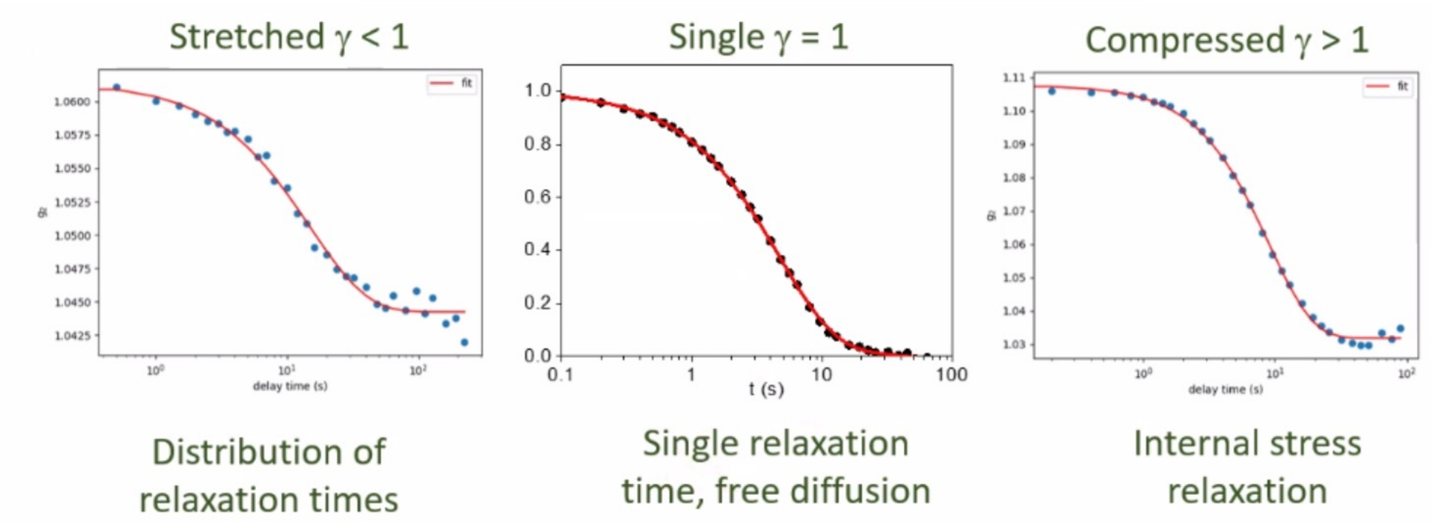
- **PLANE-WAVE CDI**
- **PTYCHOGRAPHY**
- **XPCS**
- **SAXS, USAXS**

* Courtesy of Sergio Lordano

Cateretê - XPCS



$$g^2(q,t) = \frac{\langle I(q,0)I(q,t)\rangle}{\langle I(q)\rangle^2} = 1 + \beta exp(-2(\tau/\tau_r)^\gamma)$$



- XPCS pipeline:
  1. Restoration
  2. Data reduction
  3. Correlation function
- Parallelism in CPU → huge decrease computational time
  - 32 minutes to 18 seconds for 1000 images
- Margin for future improvements using CUDA

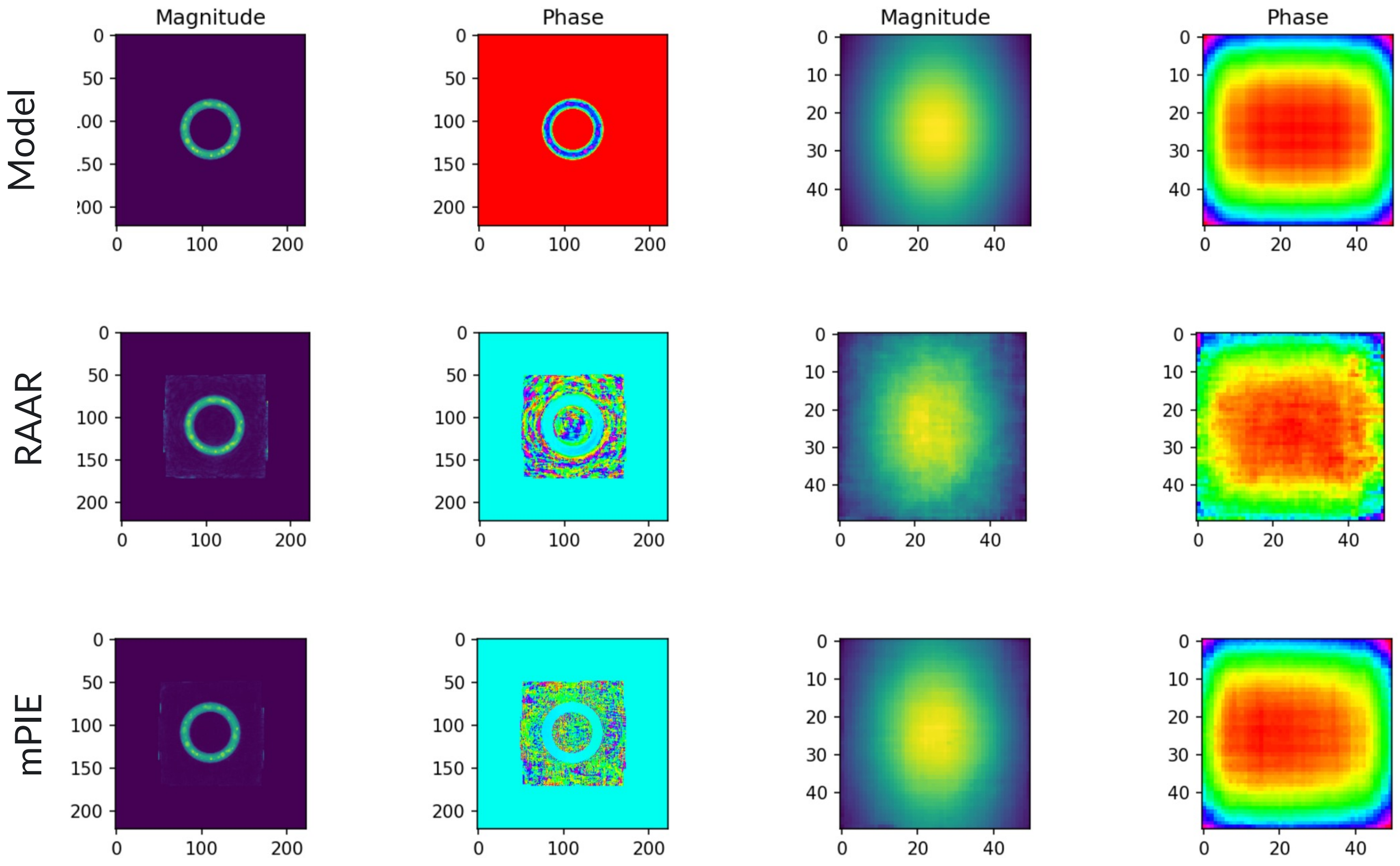
Aline Passos

* Courtesy of Aline Passos

see LINXS webinar from last week: “Evolution of dynamics during soft-chemistry synthesis of catalysts”

Ptychography engines

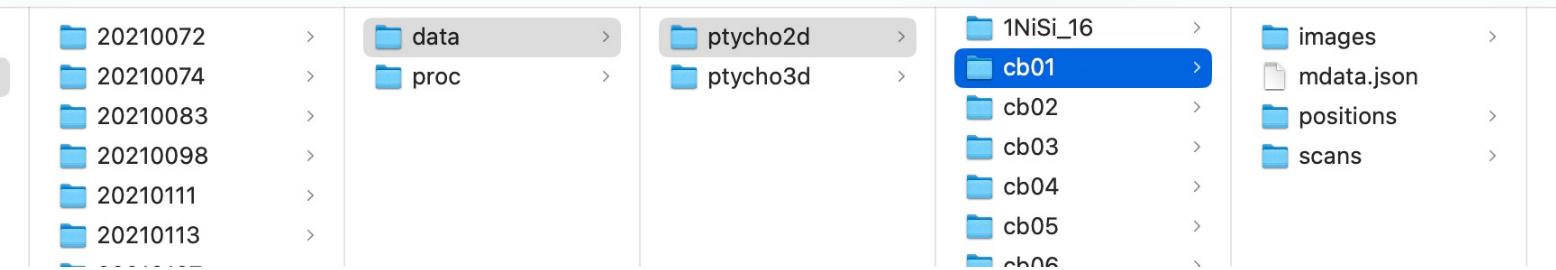
- High-level pre and post processing (Python)
- Current algorithms (CUDA):
    - RAAR
    - Alternating Projections + momentum
- Upcoming (Python + CUDA):
    - mPIE
    - Probe Decomposition
    - Position Correction
    - Plane Wave CDI:
        - ER, HIO, RAAR
- Tools from the community for benchmarking
    - PyNX
    - PtyPy
    - …
- On the way to open science…

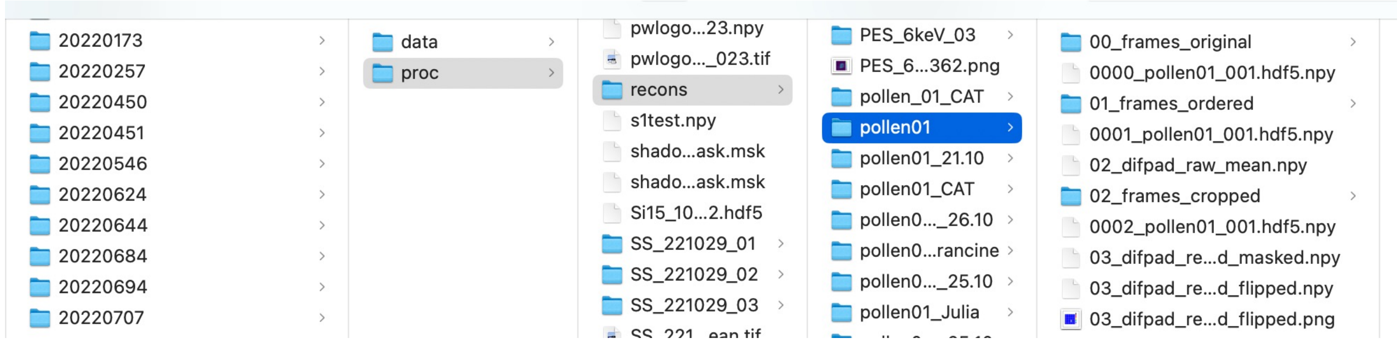


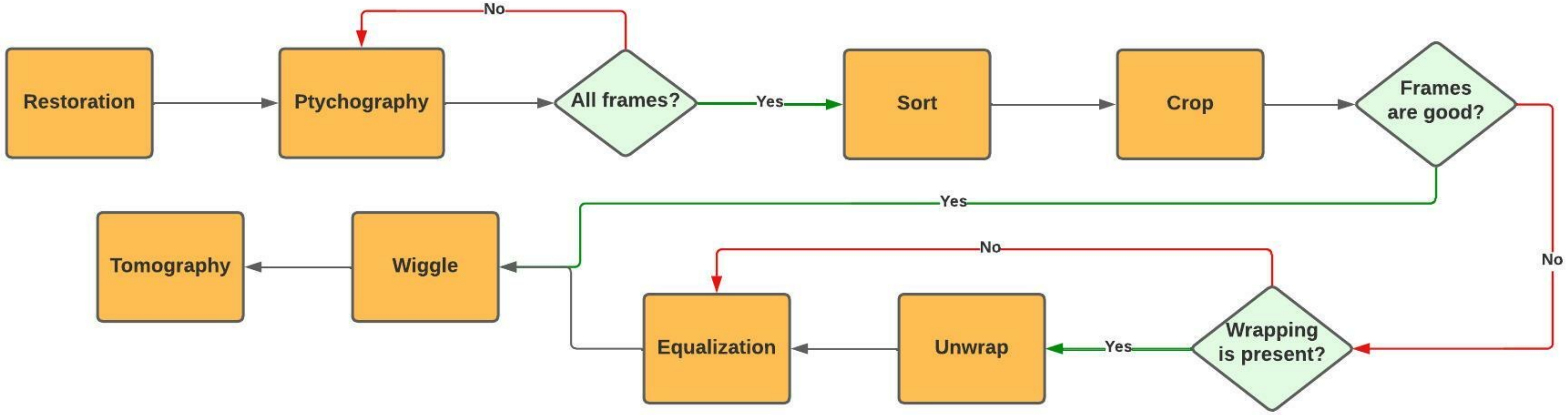
Baraldi, G. L. et. Al. (2020). Fast reconstruction tools for ptychography at Sirius, the fourth-generation Brazilian synchrotron. *Journal of Applied Crystallography*, *53*, 1550–1558.

Ptycho-tomo Pipeline

- Input and output data saved using predefined standard:
  - images
  - positions
  - scans
  - metadata
- Tomography: intermediate sinograms saved at each step
- Fast to adjust and optimize parameters







Improved UX for Ptycho-Tomography reconstructions using Jupyter Notebooks, Tonin et. al, submitted, Journal of Applied Crystallography, SAS2022

Jupyter Interface for Ptychography

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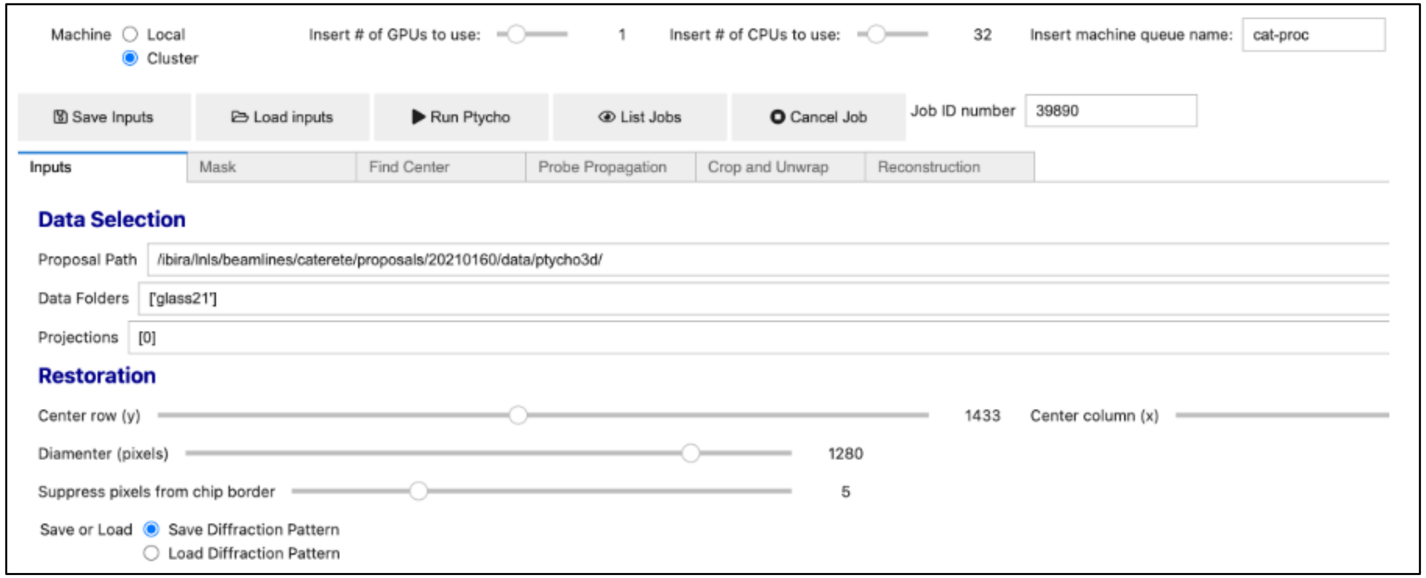
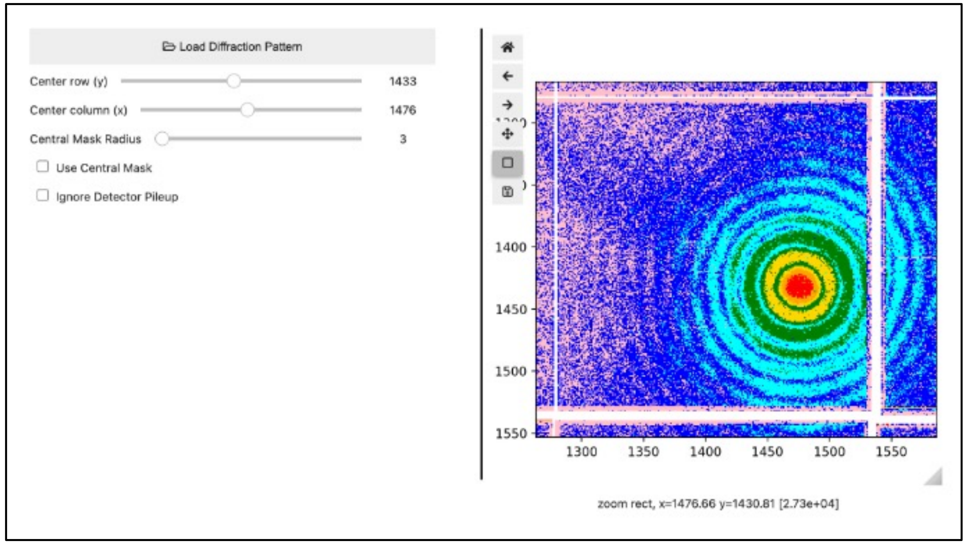
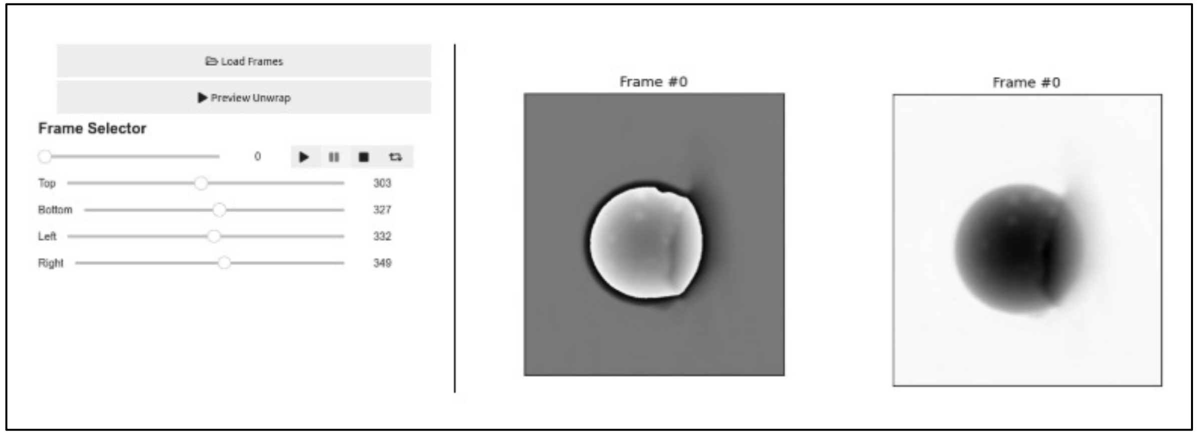
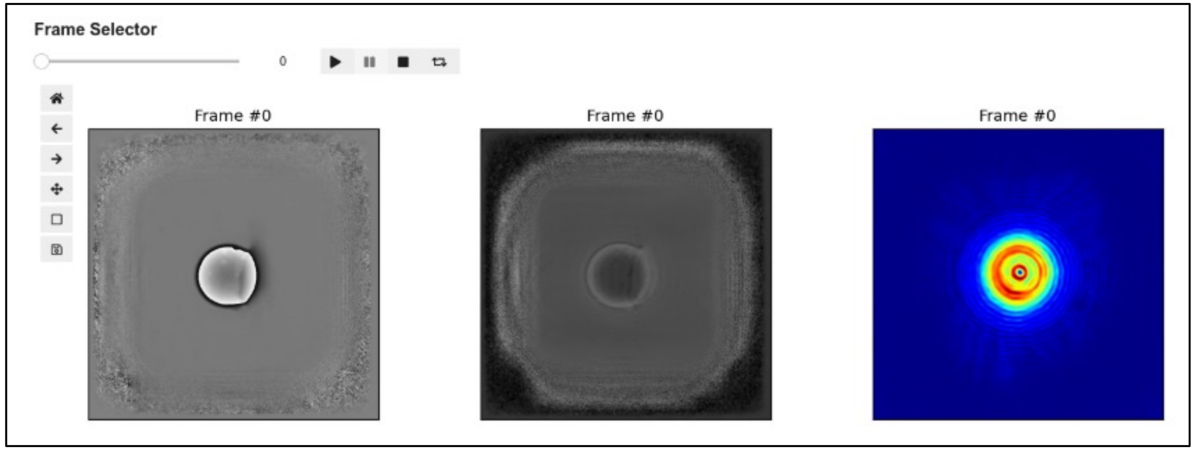
Local vs Cluster



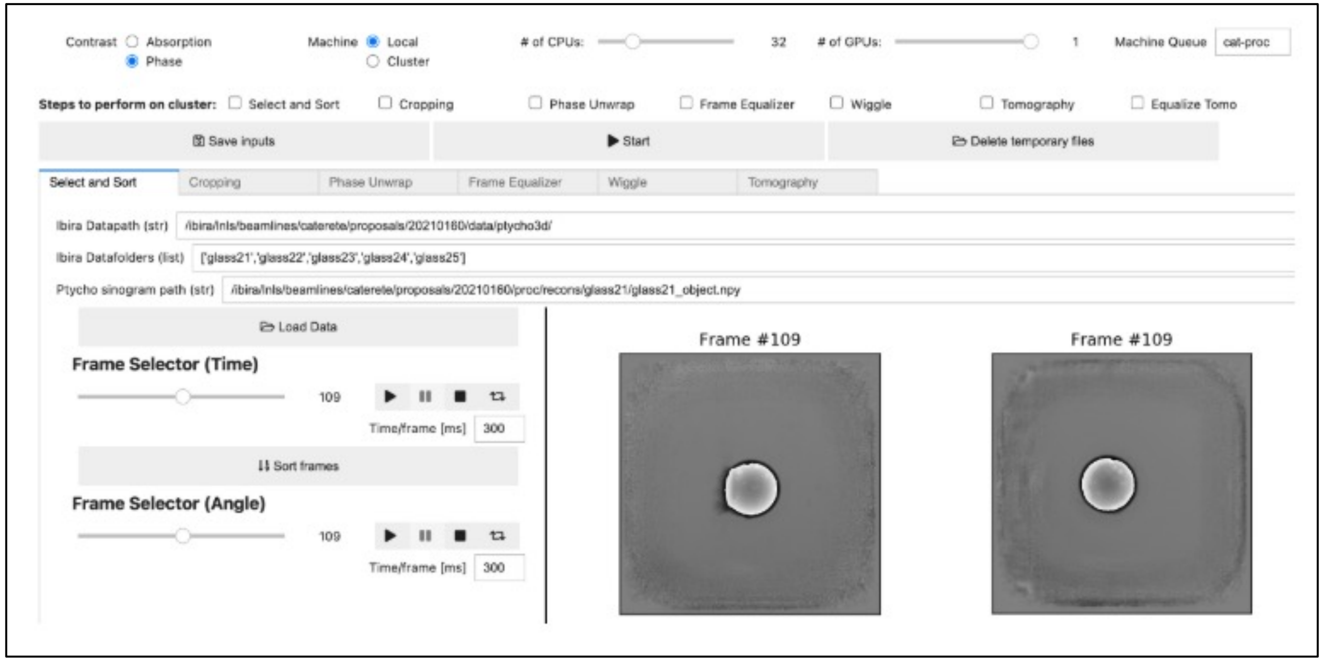


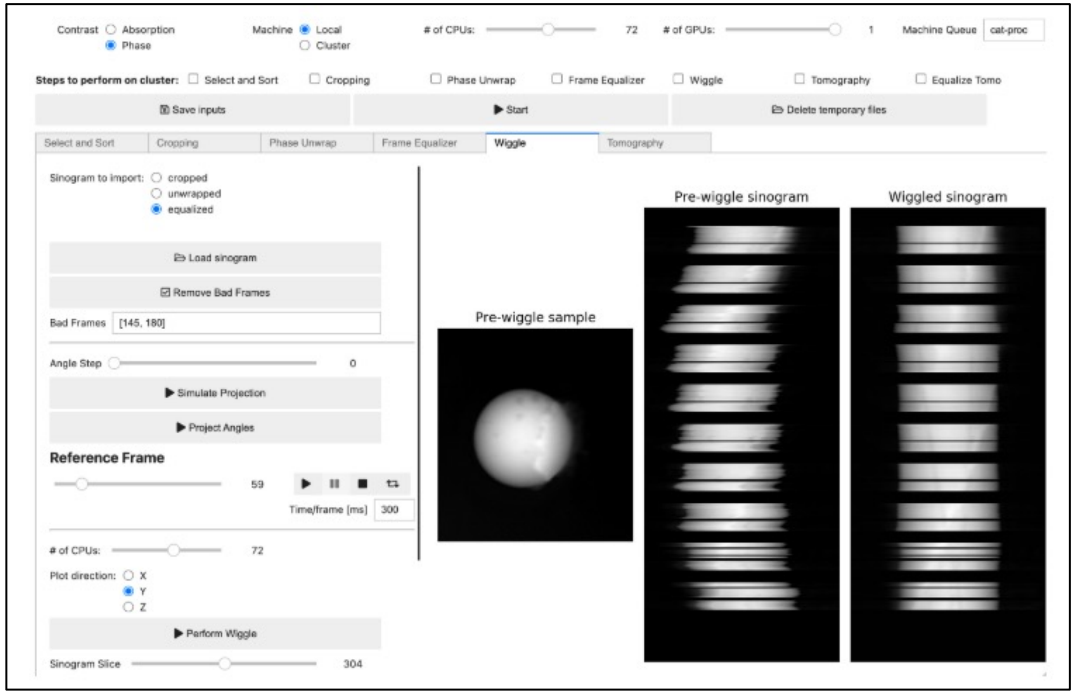


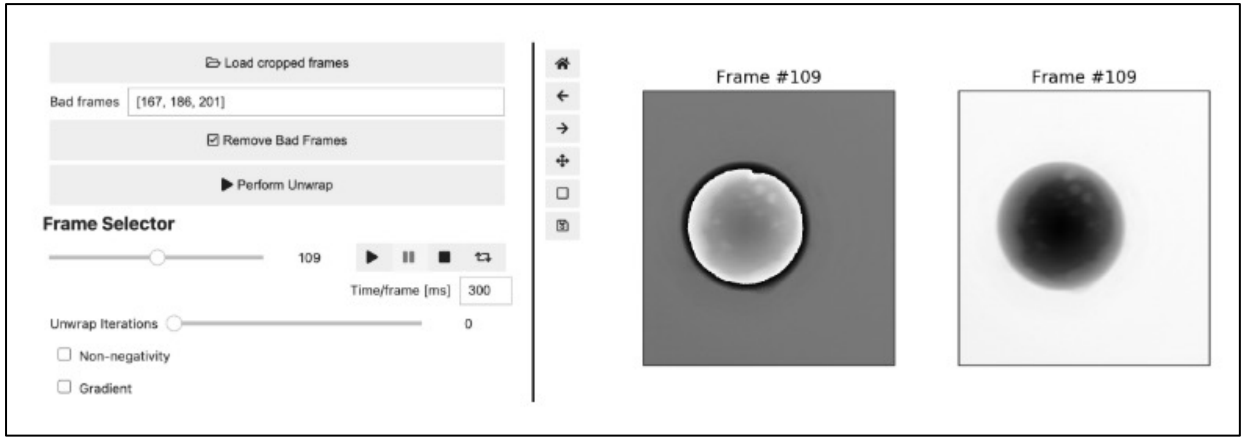


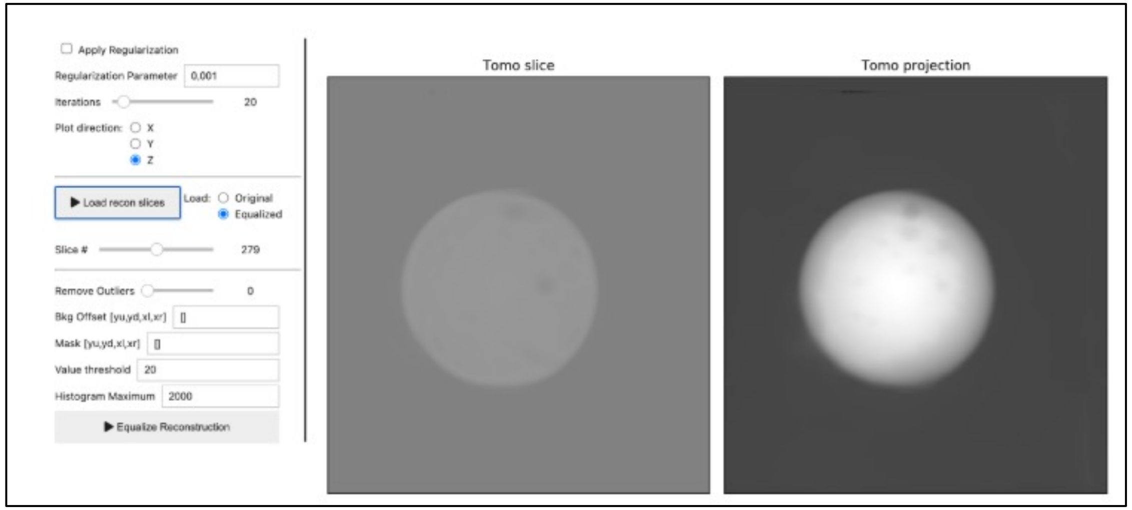
Y. R. Tonin et al, Improved UX for Ptycho-Tomography reconstructions using Jupyter Notebooks, submitted

Jupyter for Ptycho-tomography



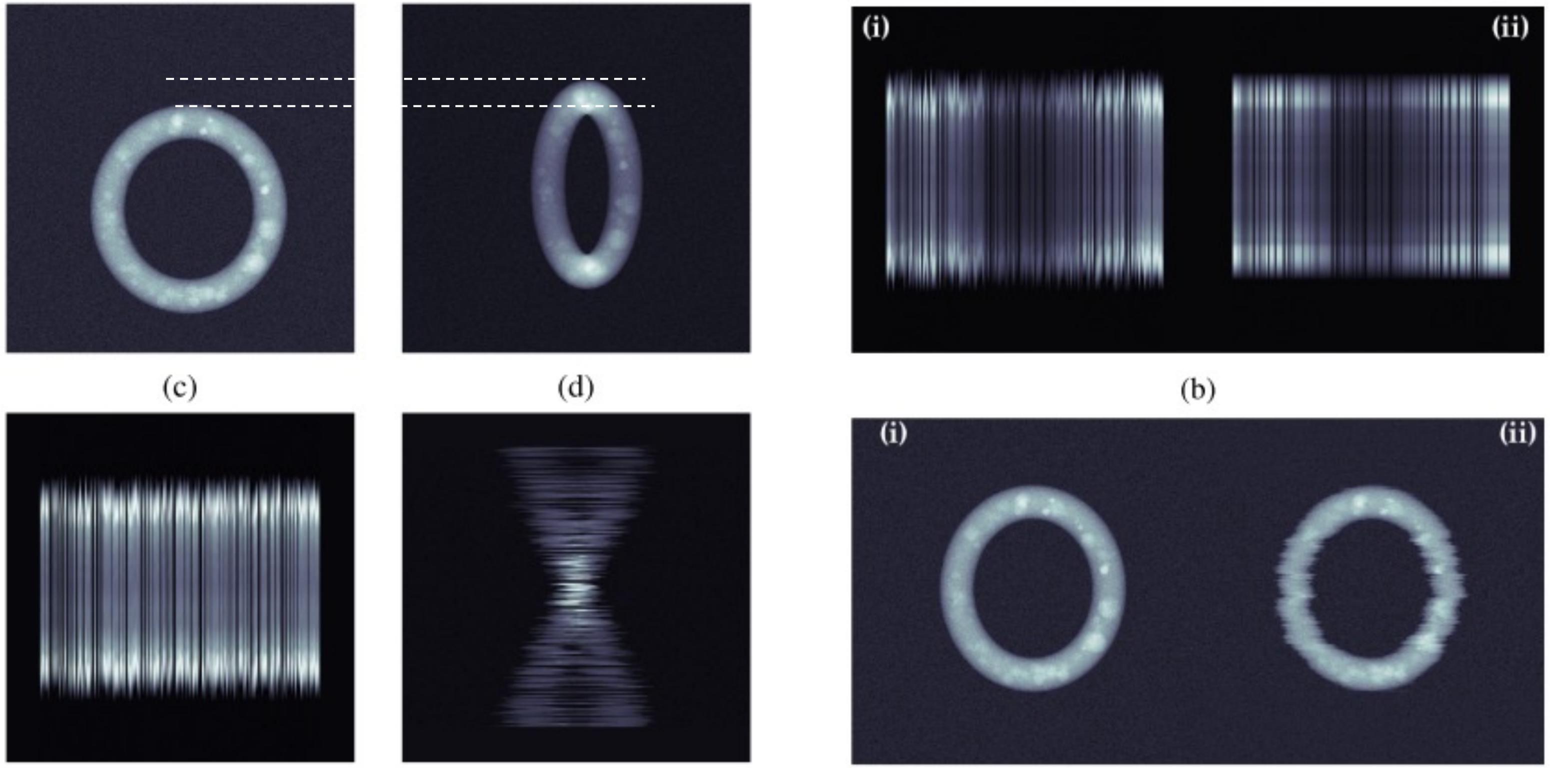




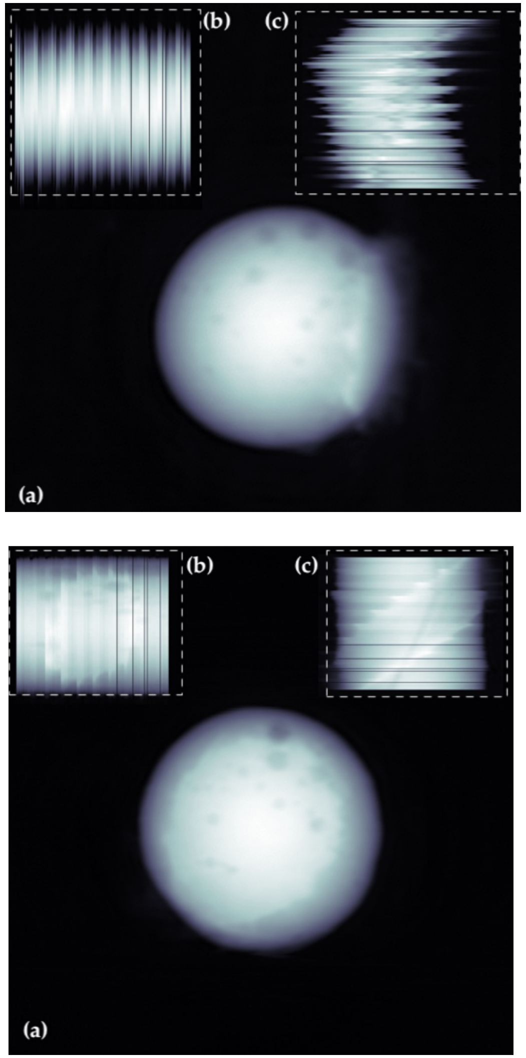


Y. R. Tonin et al, Improved UX for Ptycho-Tomography reconstructions using Jupyter Notebooks, submitted

Frame alignment: *"wiggle"*



Ptychography @ Cateretê



Ludwig-Helgason consistency conditions:

$$\frac{\int \mathrm{d}x\mathrm{d}y \; yF(\theta, y-h, x)}{\int \mathrm{d}x\mathrm{d}y \; F(\theta, y-h, x)} = \frac{\int \mathrm{d}x\mathrm{d}y \; yF(\theta_{\mathrm{REF}}, y, x)}{\int \mathrm{d}x\mathrm{d}y \; F(\theta_{\mathrm{REF}}, y, x)}$$

Automatic three-dimensional alignment for large volume tomographic samples, E. X. Miqueles, to be published

CATERETÊ - Ptychography

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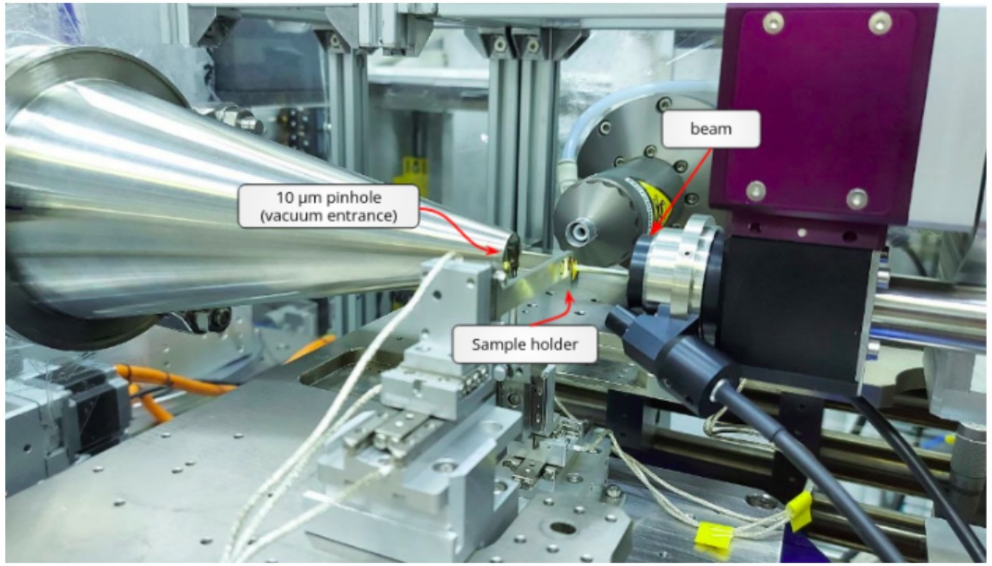
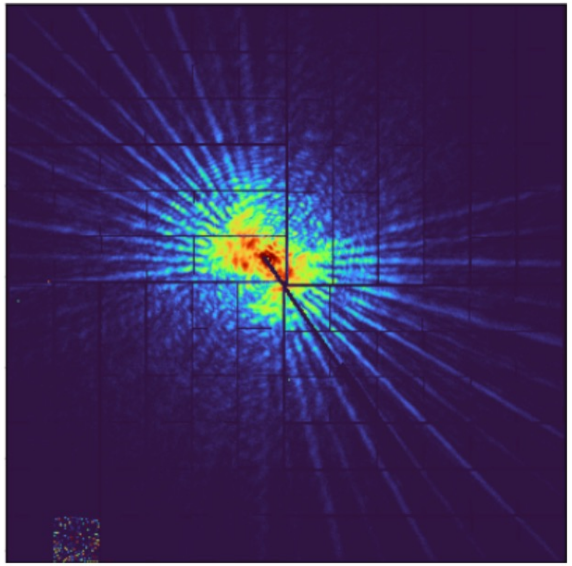
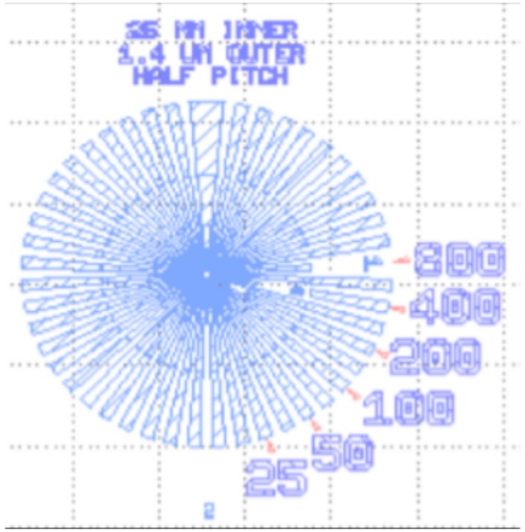
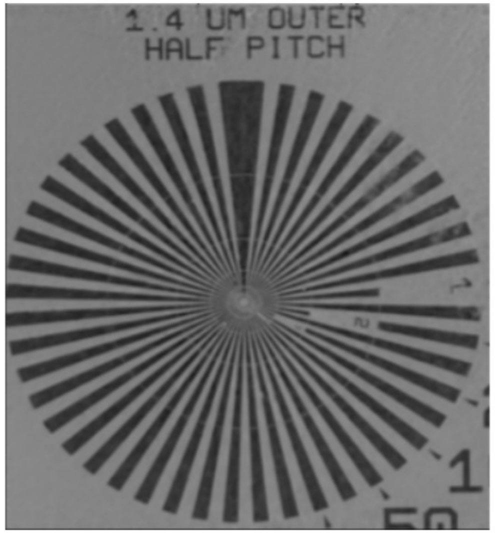
- Step-scan tele-ptychography, pink-beam

www.lnls.cnpem.br/sirius-updates

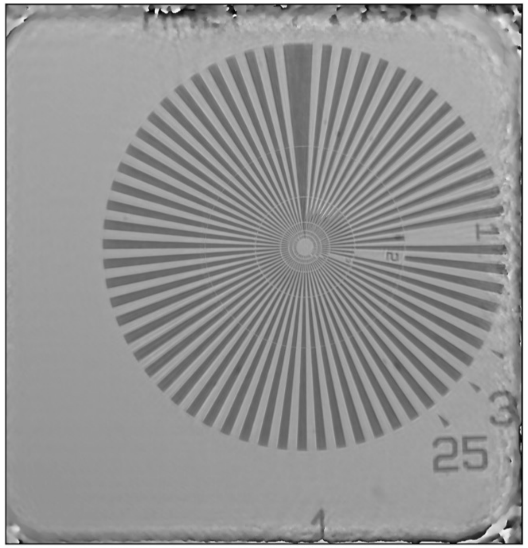




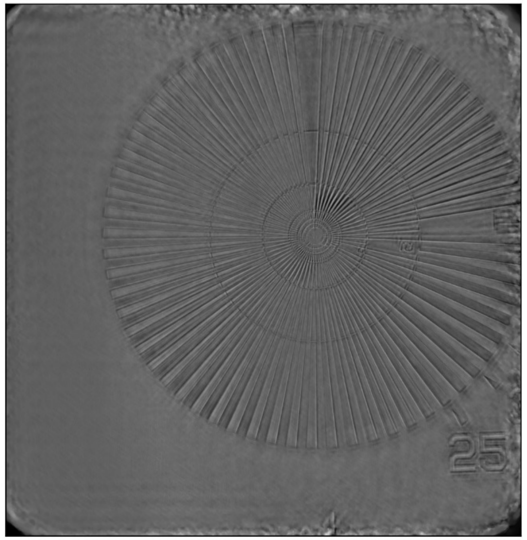




- Monochromatic beam



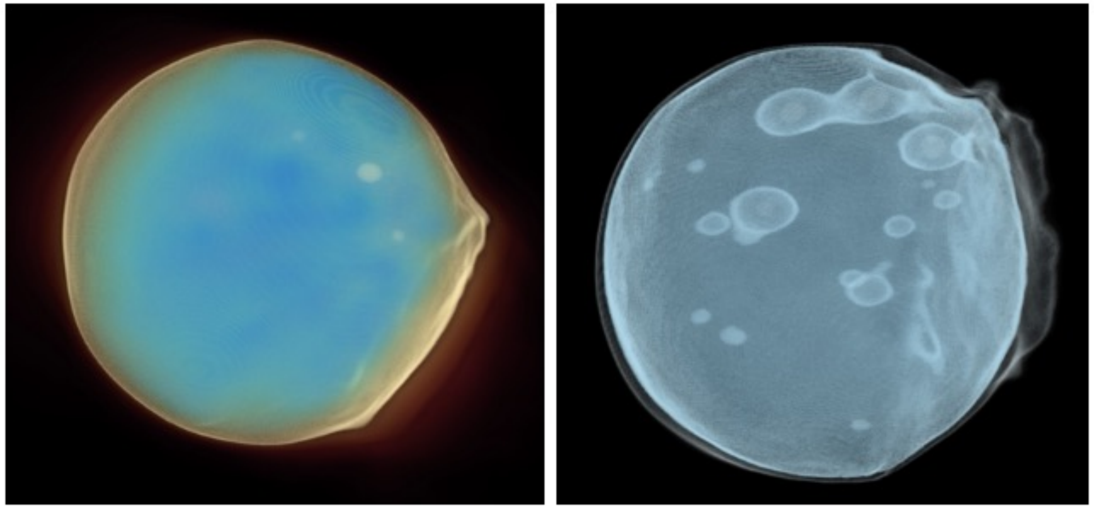
Phase



Absorp.

3D Visualization

- NVIDIA Index rendering
  - Many shader options
  - Fast rendering powered by NVIDIA
  - Customizable shaders for specific materials



Click “Watch Now” to login or join the NVIDIA Developer Program.

WATCH NOW

High-Throughput 3D Image Reconstruction, Visualization, and Segmentation of Large-Scale Data at the Sirius Synchrotron Light Source

Thiago Vallin Spina, Brazilian Synchrotron Light Laboratory / CNPEM

GTC 2020

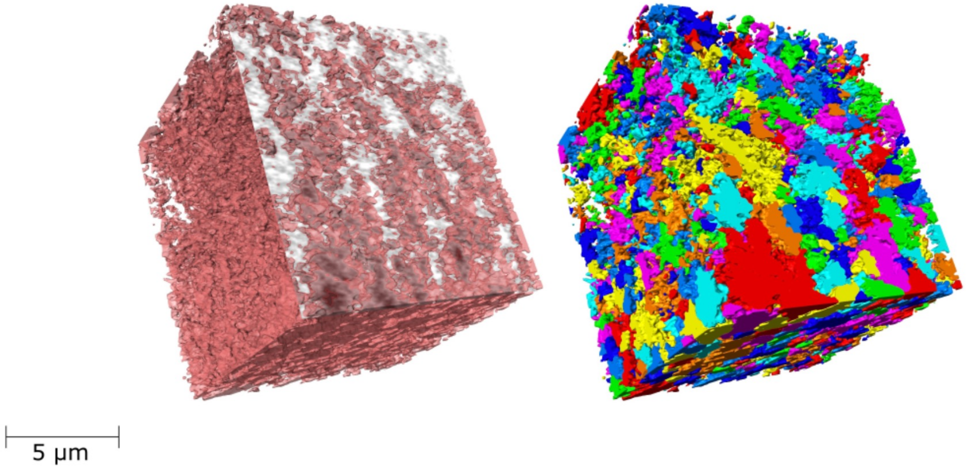
We'll present highly efficient tools for large-scale 3D image reconstruction, visualization, and segmentation being developed for the Sirius synchrotron light source. Sirius will be the second fourth-generation synchrotron in the world, and will acquire 3D/4D images with resolution up to <50 nm using hard X-rays. With NVIDIA, we're creating integrated pipelines to reconstruct 3D images from modalities such as coherent-diffraction imaging and transmission tomography, visualize the data in streaming mode, and segment the images to provide almost real-time feedback. We rely on multi-GPU/node CUDA programming and machine/deep learning-optimized inference to address the issues, given that each 3D image may be larger than 100 GB and may be acquired down to 1s, resulting in around 50 TB of data of a wide variety of samples (for example, biological and geological) expected to be produced every day.

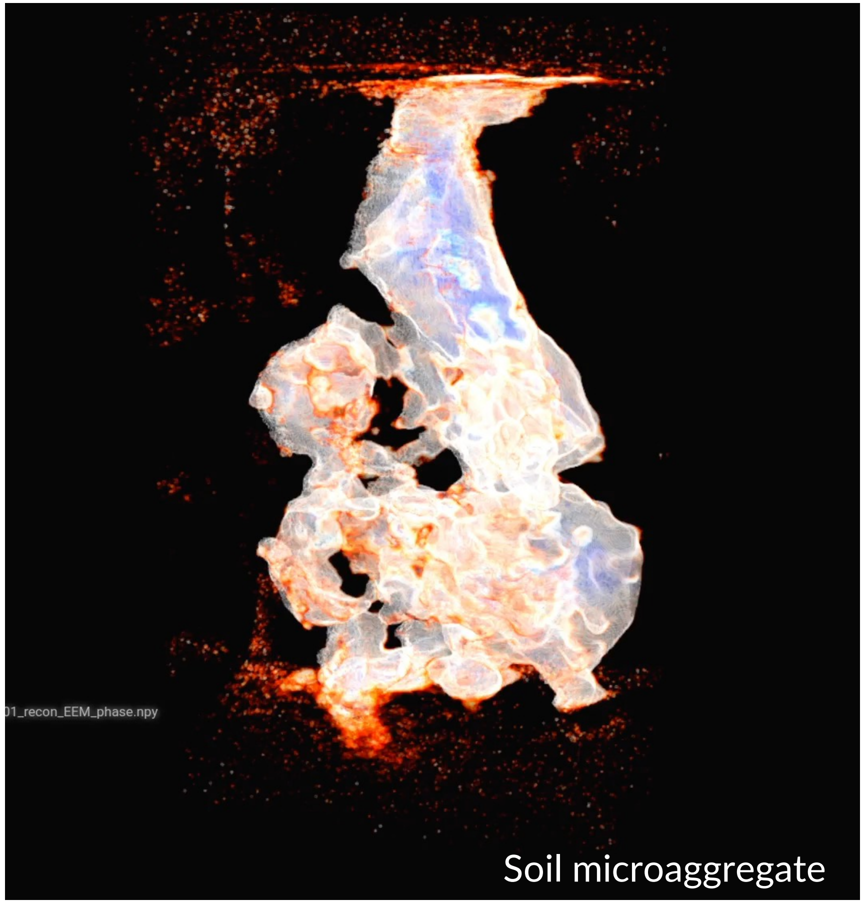
https://developer.nvidia.com/gtc/2020/video/s21278-vid

CATERETÊ – Ptycho-tomography

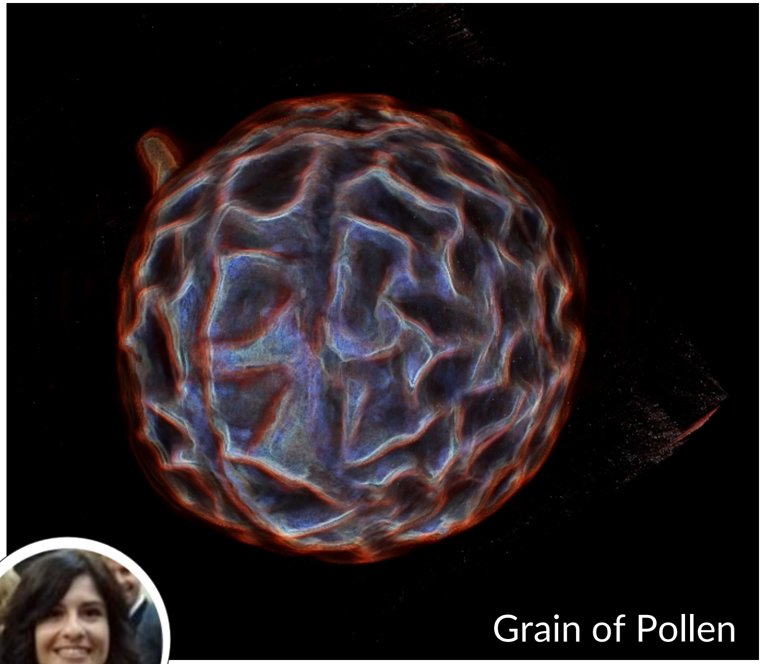
Dean

Talita

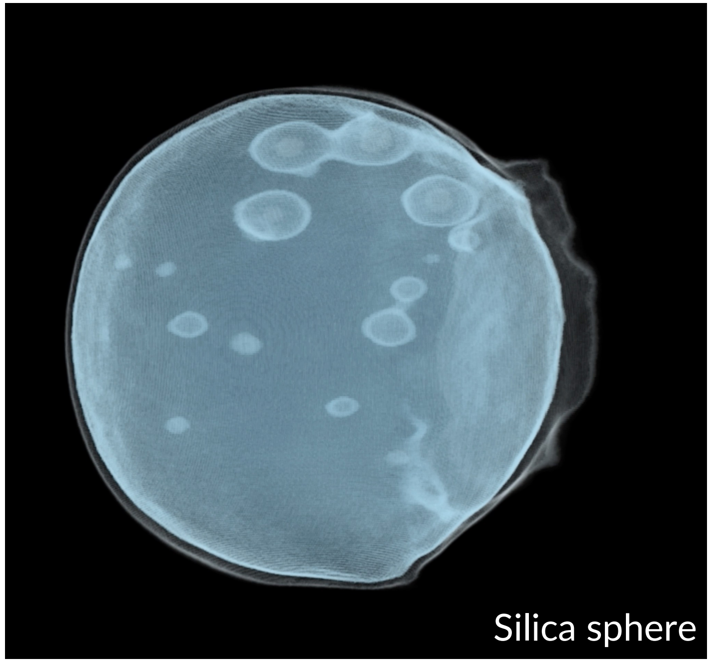




Soil microaggregate



Grain of Pollen



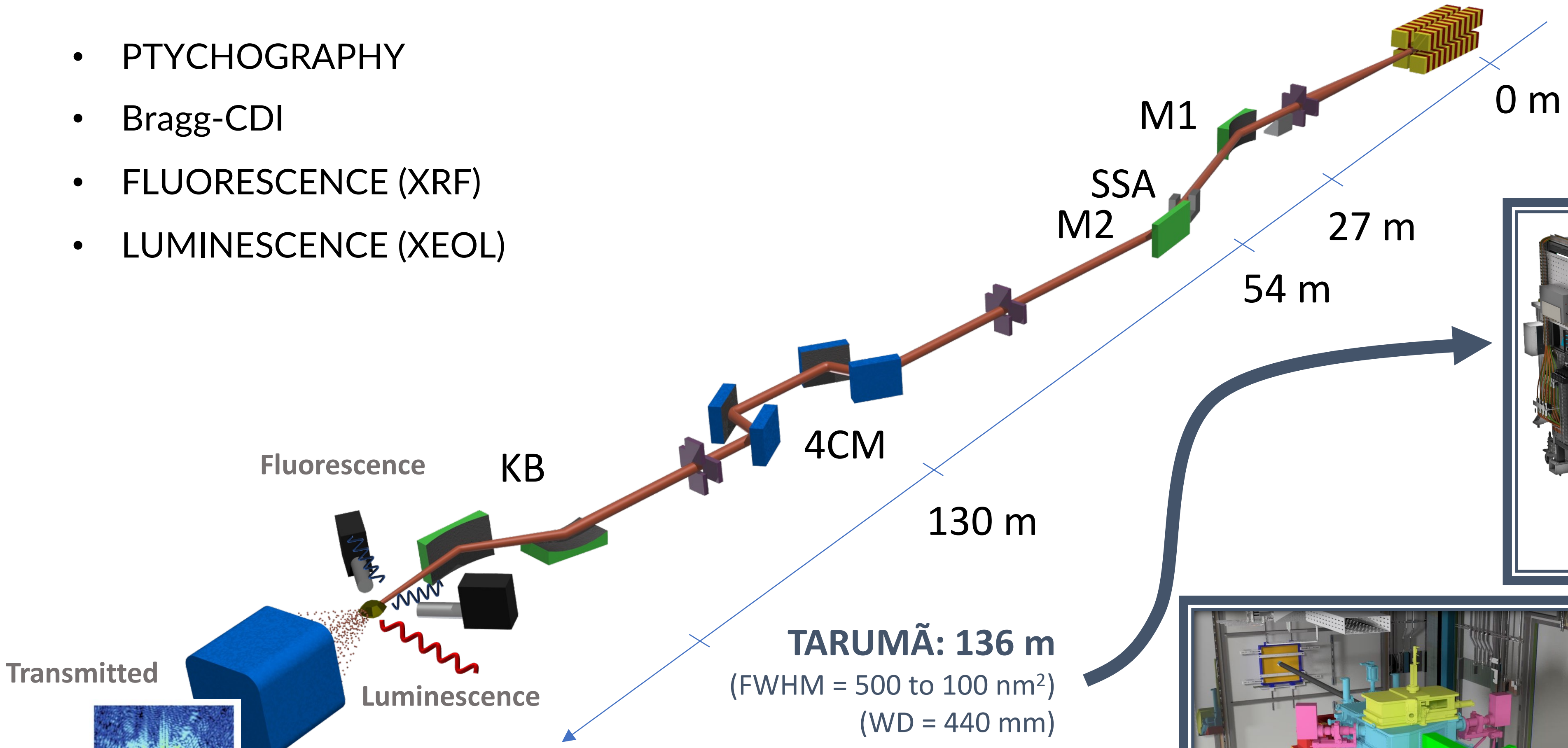
Silica sphere

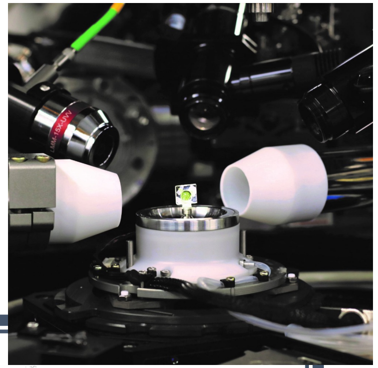
Carla

X-ray Nanoscopy

CARNAÚBA beamline

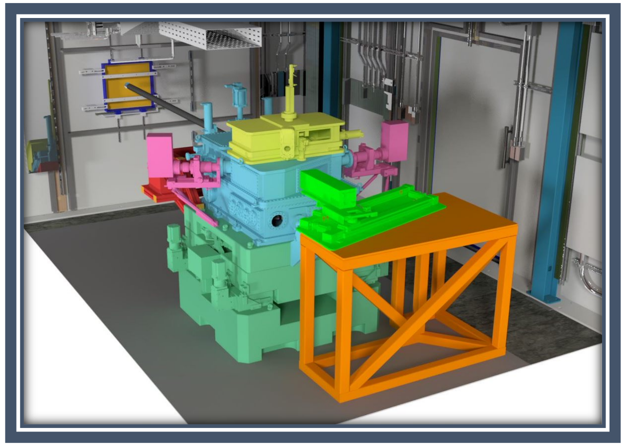
- PTYCHOGRAPHY
- Bragg-CDI
- FLUORESCENCE (XRF)
- LUMINESCENCE (XEOL)





TARUMÃ: 136 m
(FWHM = 500 to 100 nm²)
(WD = 440 mm)

SAPOTI: 142 m
(FWHM = 140 to 35 nm²)
(WD = 55 mm)



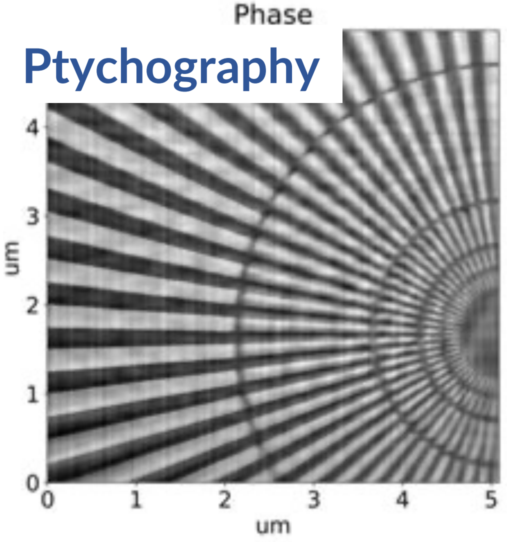
RMS PITCH STABILITY

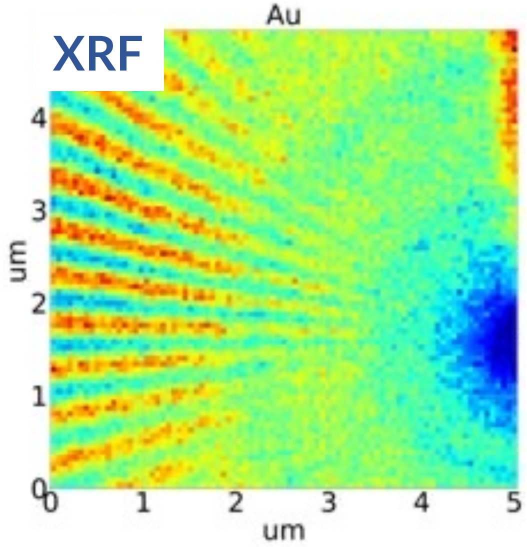
TARUMA: 10 nrad
SAPOTI: 4 nrad

R. Geraldes, *15th Intern. Conf. on X-ray Microscopy* (XRM 2022)

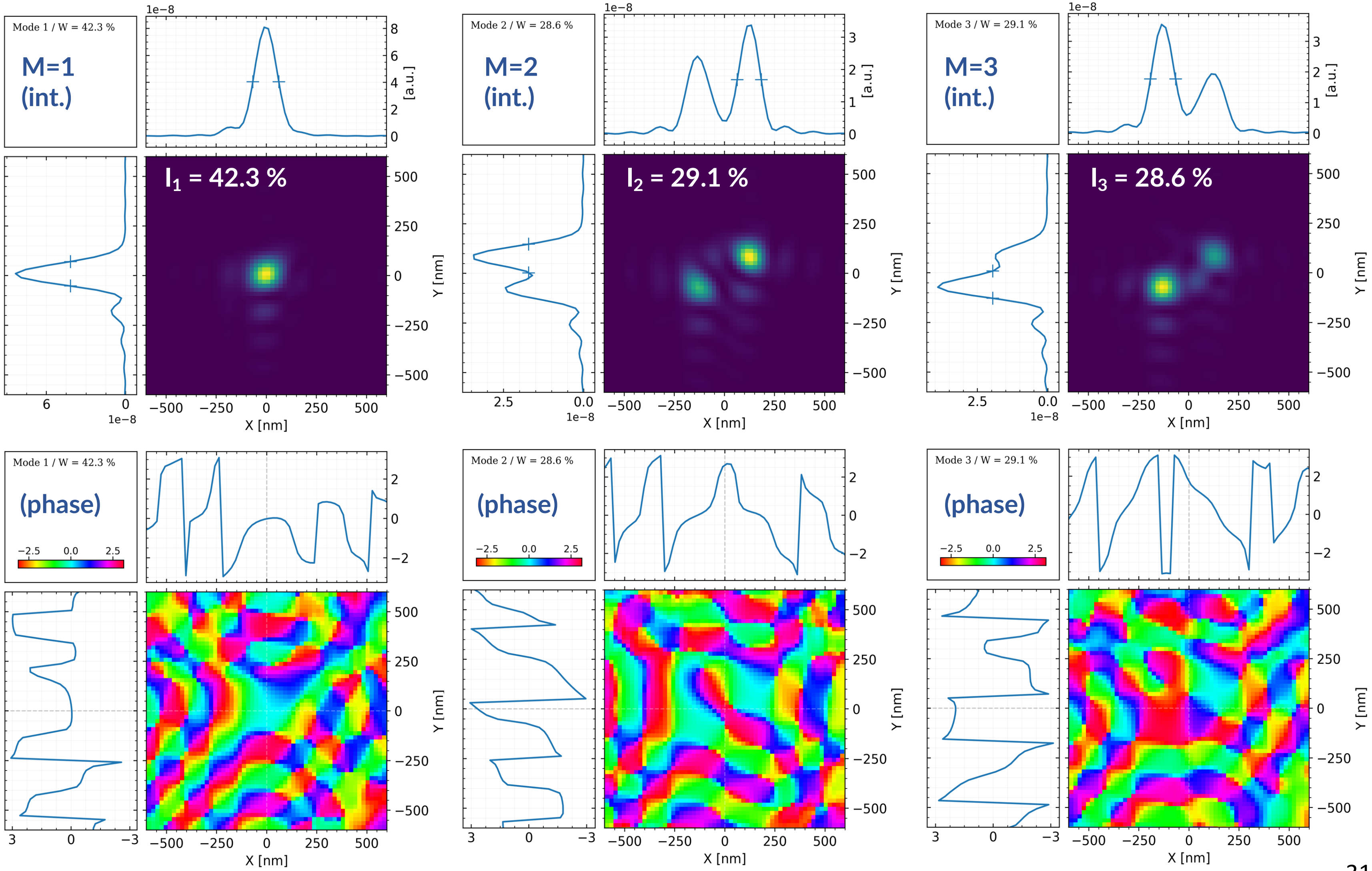
CARNAÚBA: Ptychography

MINISTRY OF SCIENCE TECHNOLOGY AND INNOVATION
BRAZILIAN GOVERNMENT
UNITING AND REBUILDING

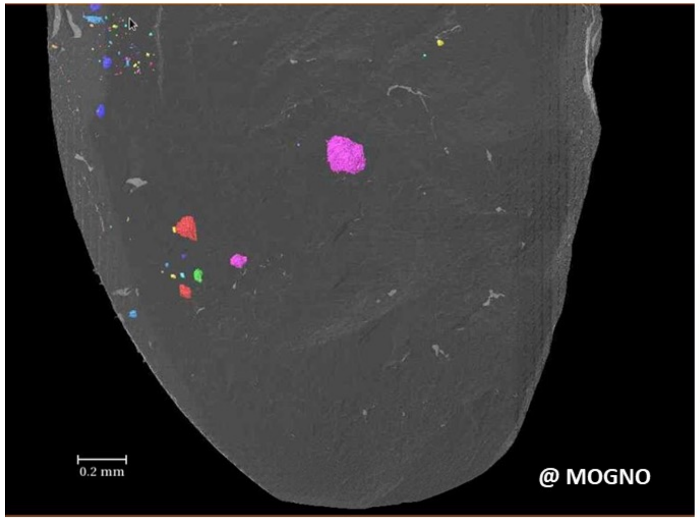


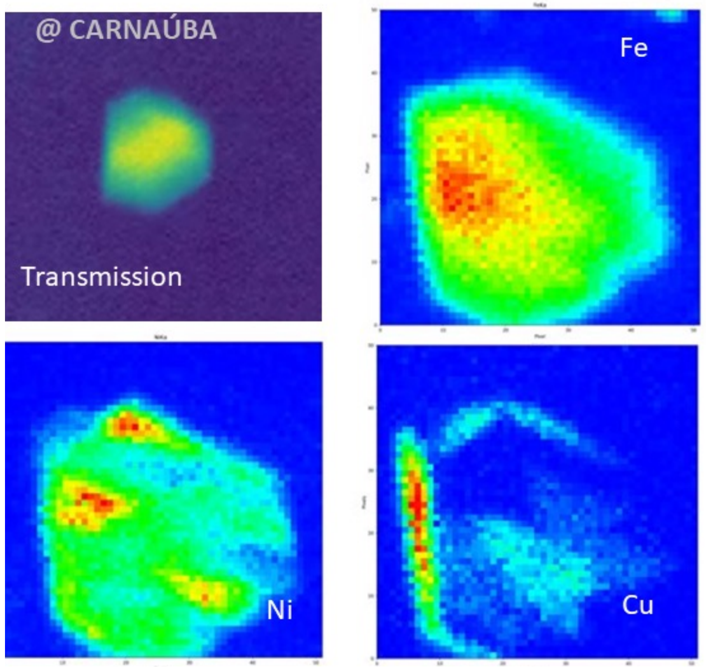
Incoherent modes



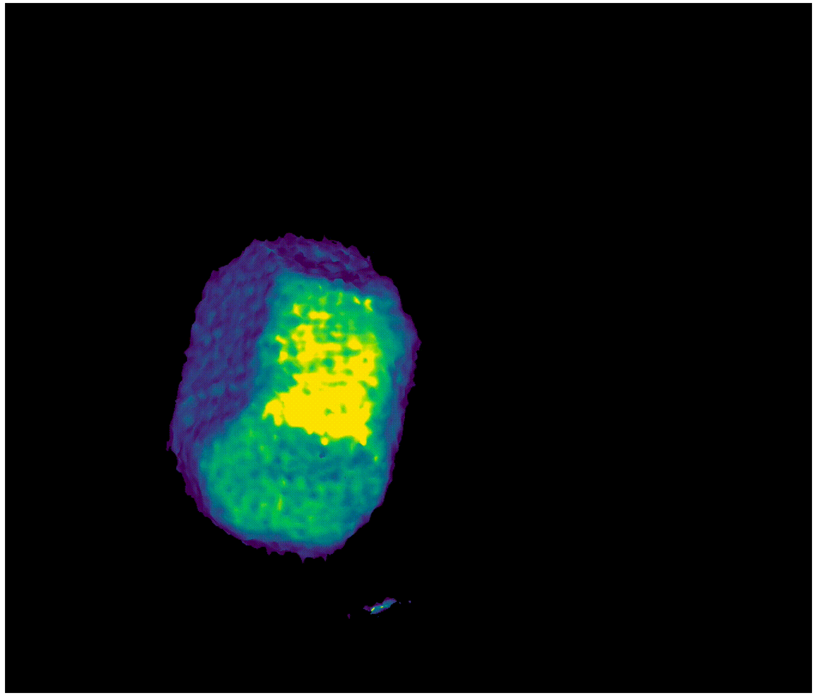
S. Lordano, X-Ray beam diagnostics using ptychography for optics alignment: https://doi.org/10.13140/RG.2.2.19430.09280

CARNAÚBA: Fluorescence

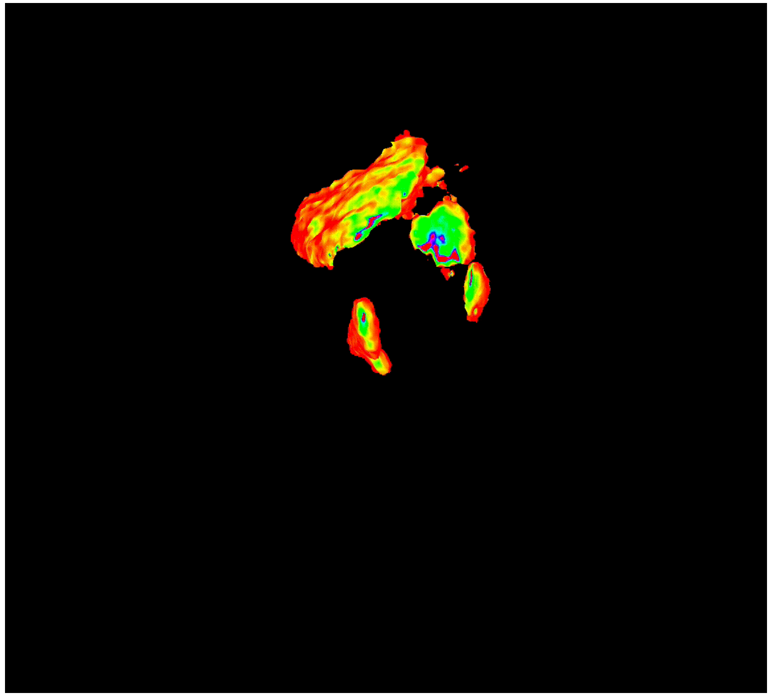




Tomography of a diamond sample with solid mineral inclusions



Transmission tomography



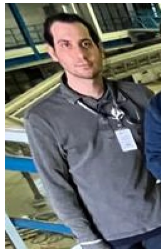
Fluorescence tomography
(Cu layer)

Fluorescence mapping of one solid mineral inclusion

https://www.lnls.cnpem.br/sirius-updates

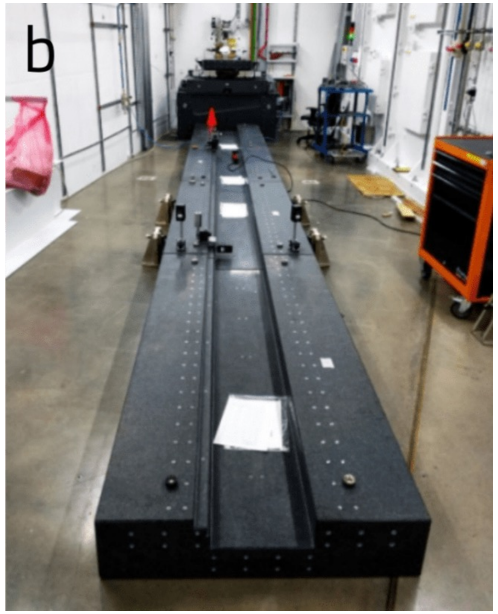
X-ray Micro and Nanotomography

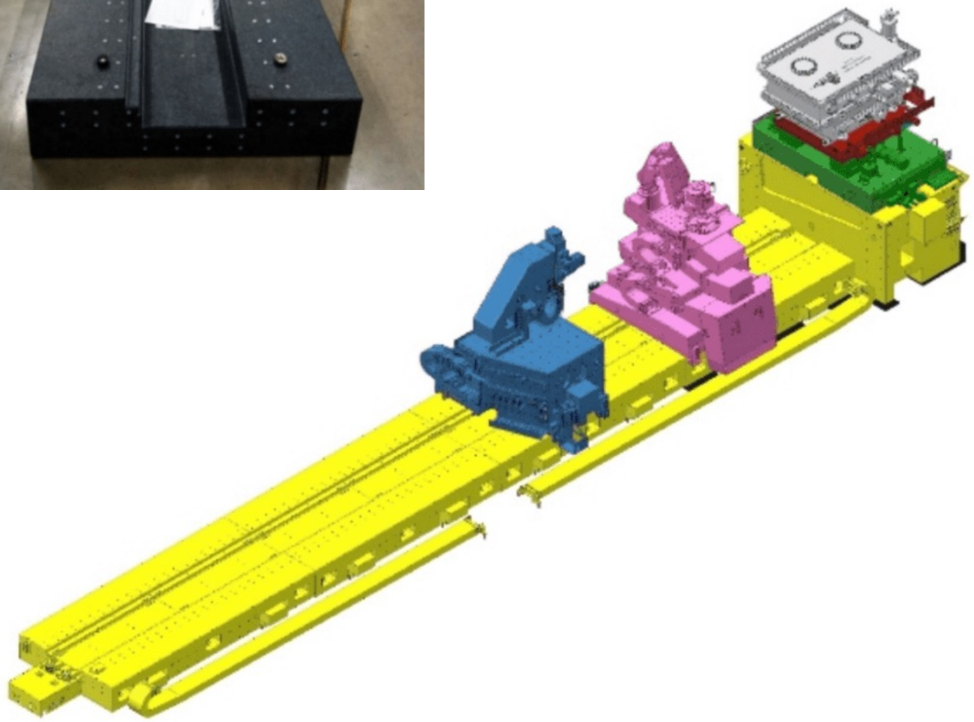


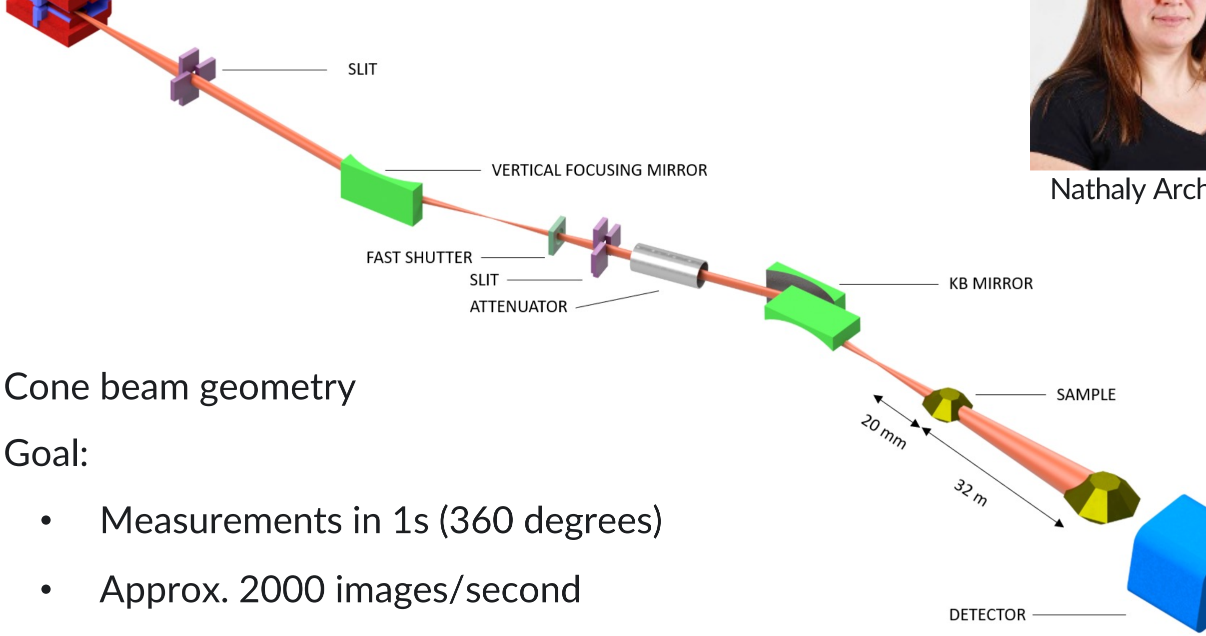



PETROBRAS

MOGNO beamline





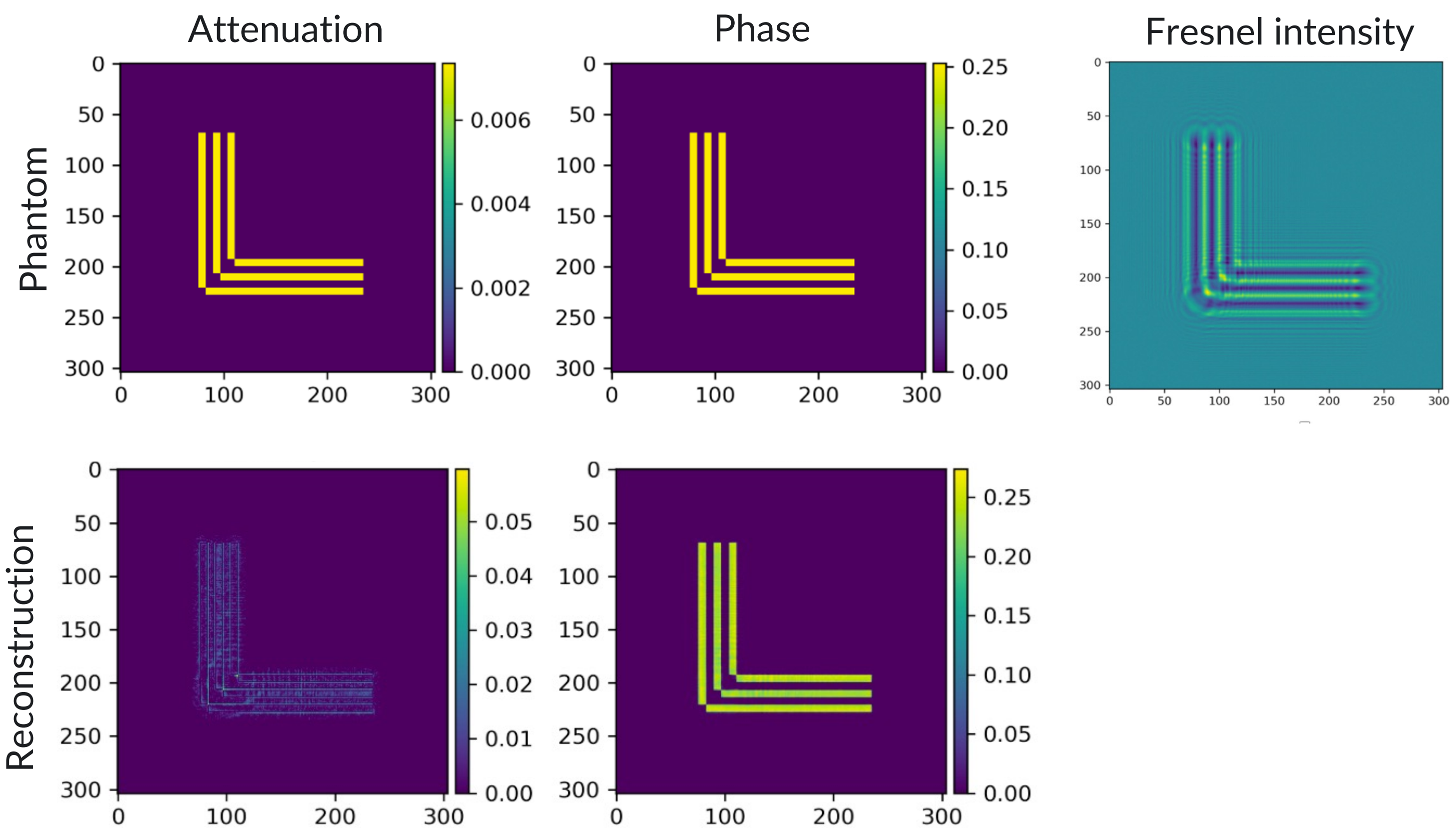


Nathaly Archilha

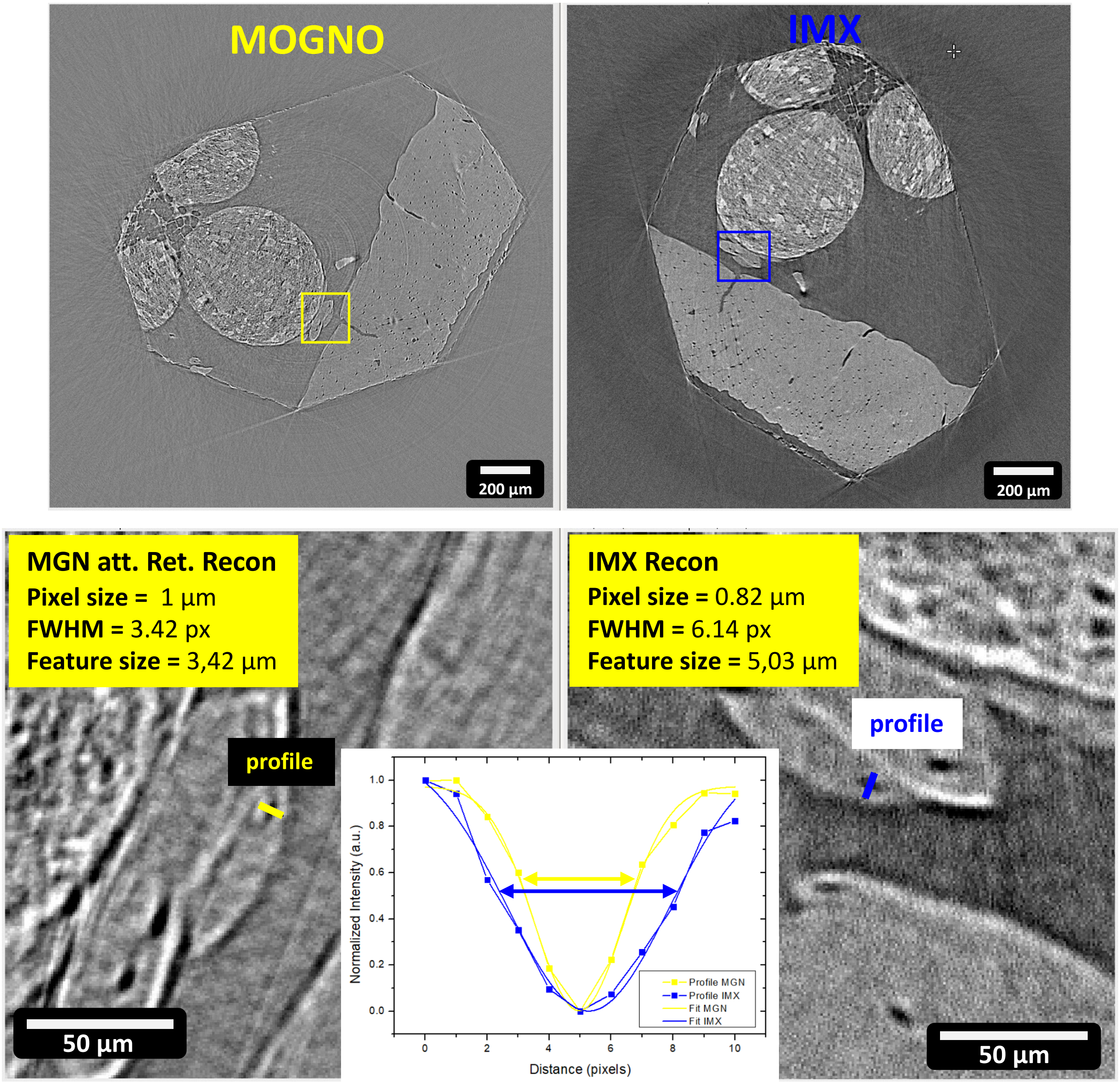
- Cone beam geometry
- Goal:
  - Measurements in 1s (360 degrees)
  - Approx. 2000 images/second
  - 150 nm target resolution @ nano-station
  - Reconstruction in quasi-real time (analytical)
- N x 2048^2 -> 35 GBs (PCO edge 4.2 CLHS)
- N x 1536^2 -> 20 GBs (PIMEGA 135D)
- 4D tomography (X, Y, Z, time):
  - in vivo samples
  - fluid injection in porous media

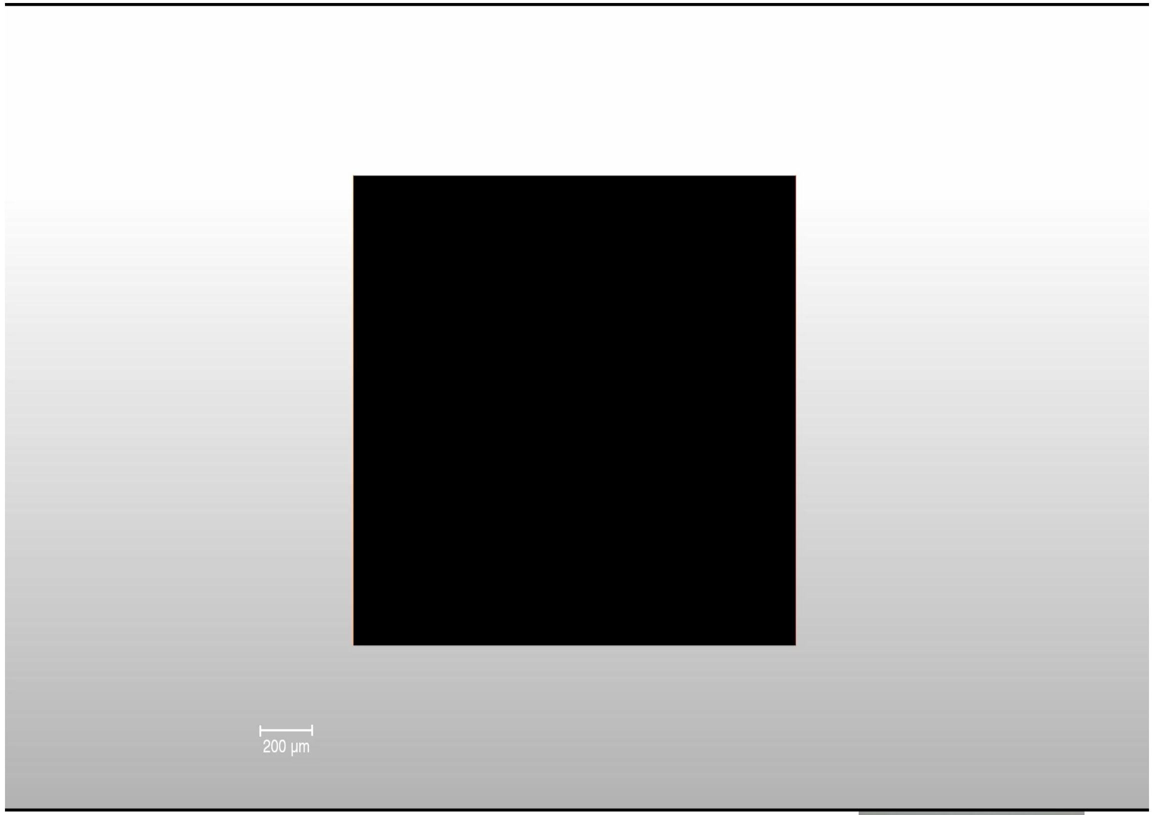
Phase Retrieval

- Iterative Regularized Gauss-Newton Method for Phase Retrieval
  - ”Regularized newton methods for x-ray phase contrast and general imaging problems,” Opt. Express, vol. 24, no. 6, pp. 6490–6506, 2016
- PCO (planar detector chips); future measurements using Pimega135D



Nano-hydroxyapatite-based microspheres implanted in rat tibia defect as a bone graft substitute

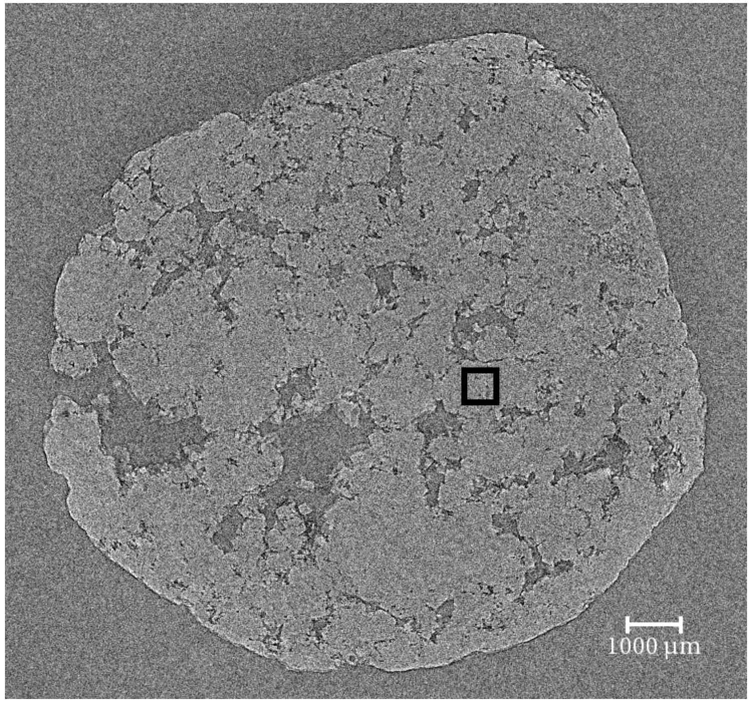


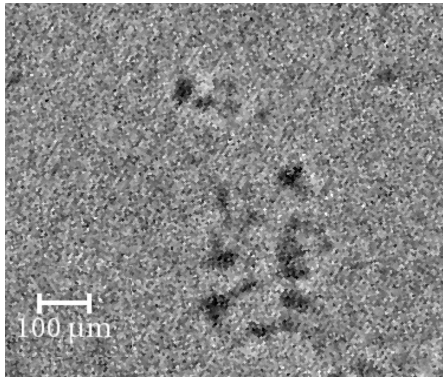


Vitor Zelaya

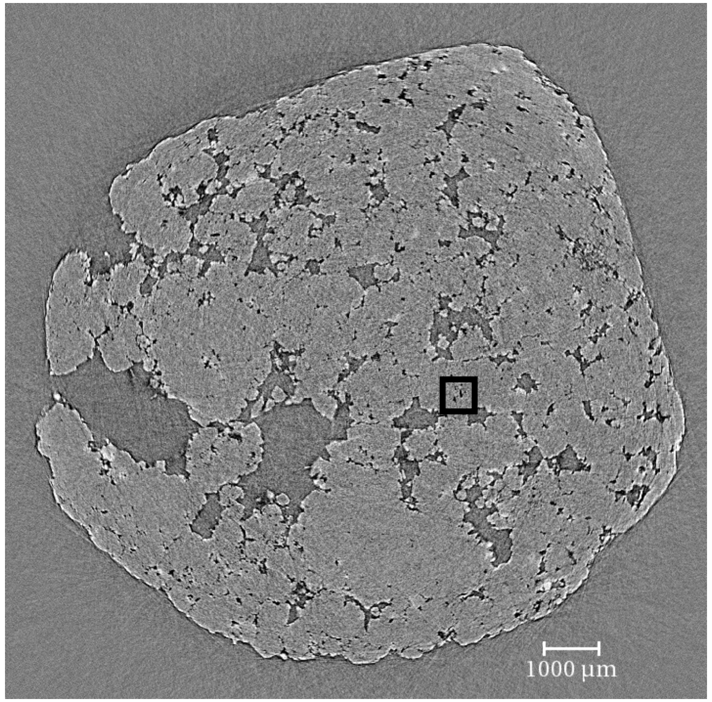
Pre-Salt limestone

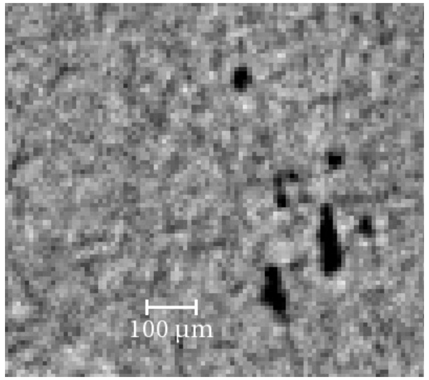
Feb/2021 – Mogno A

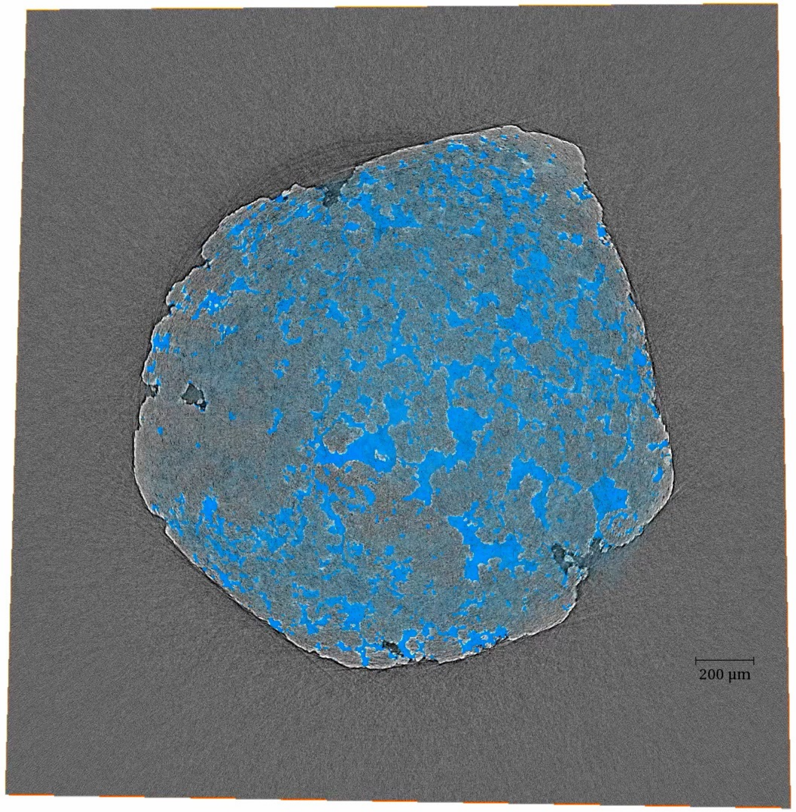




Oct/2022 - Mogno

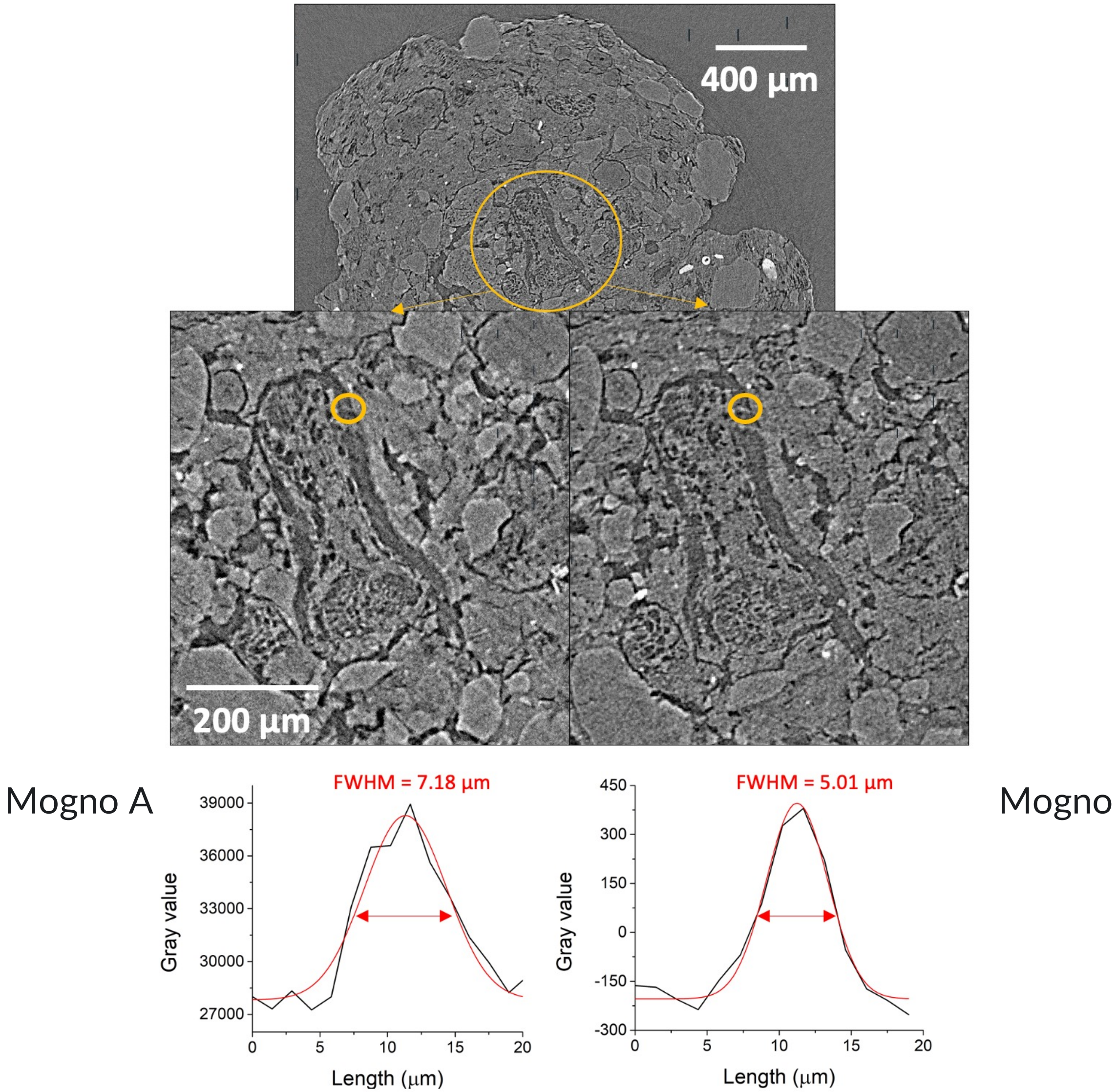


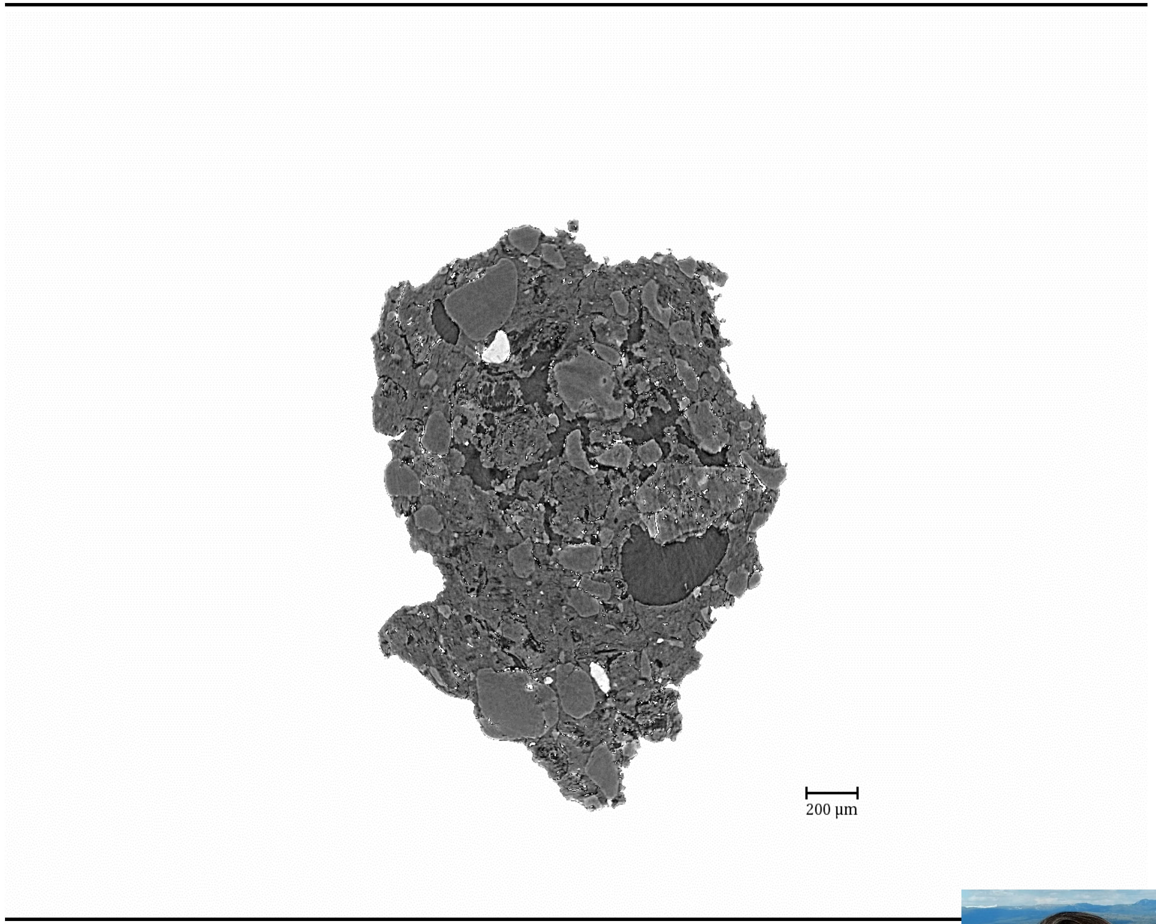




Daphne Pino

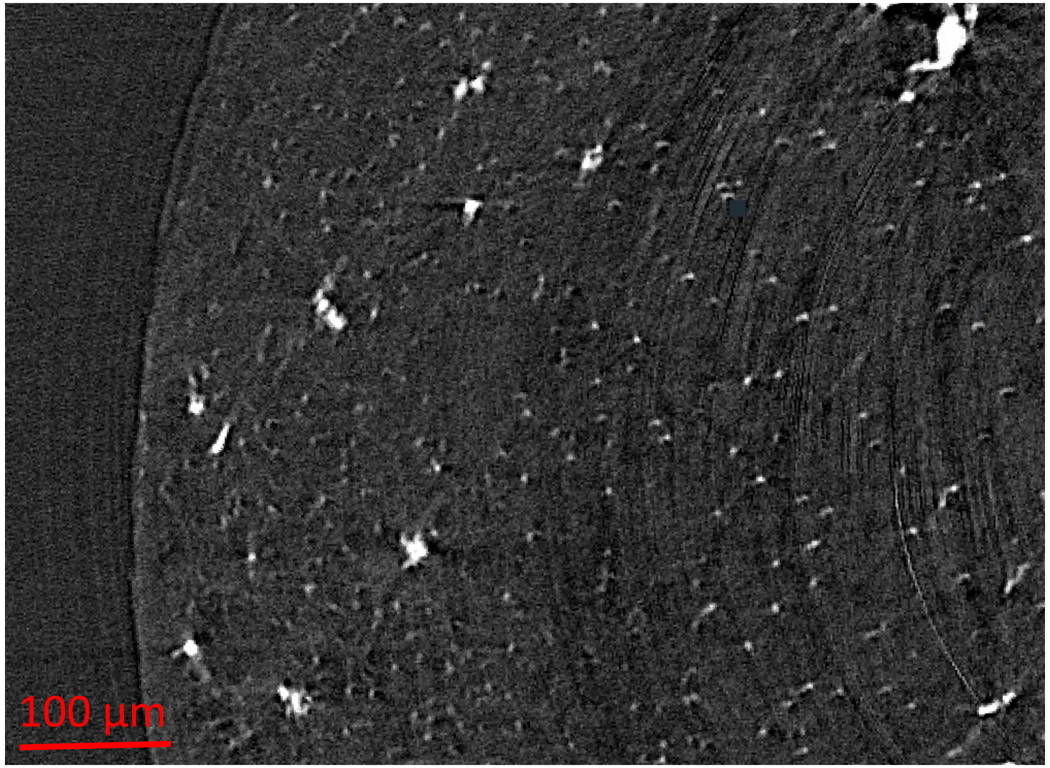
Soil Aggregate



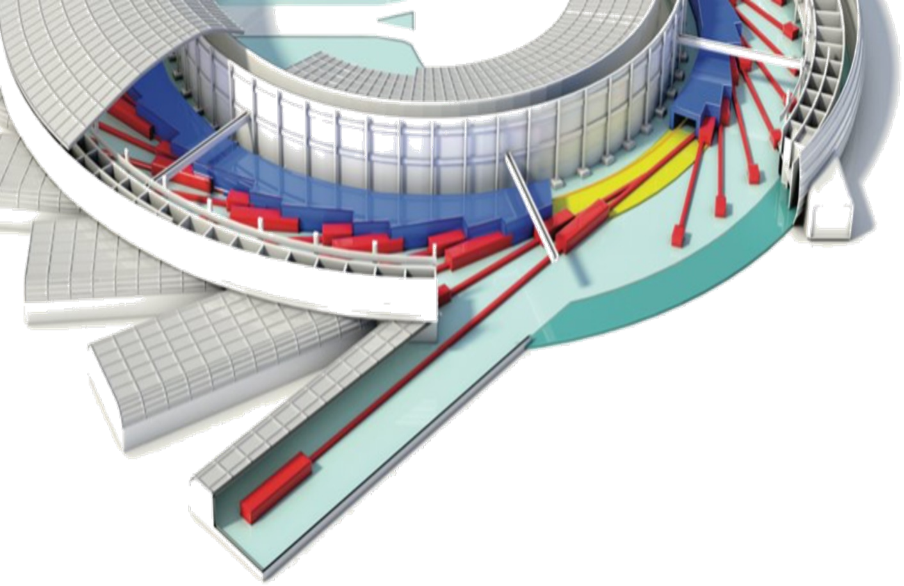


Talita Ferreira

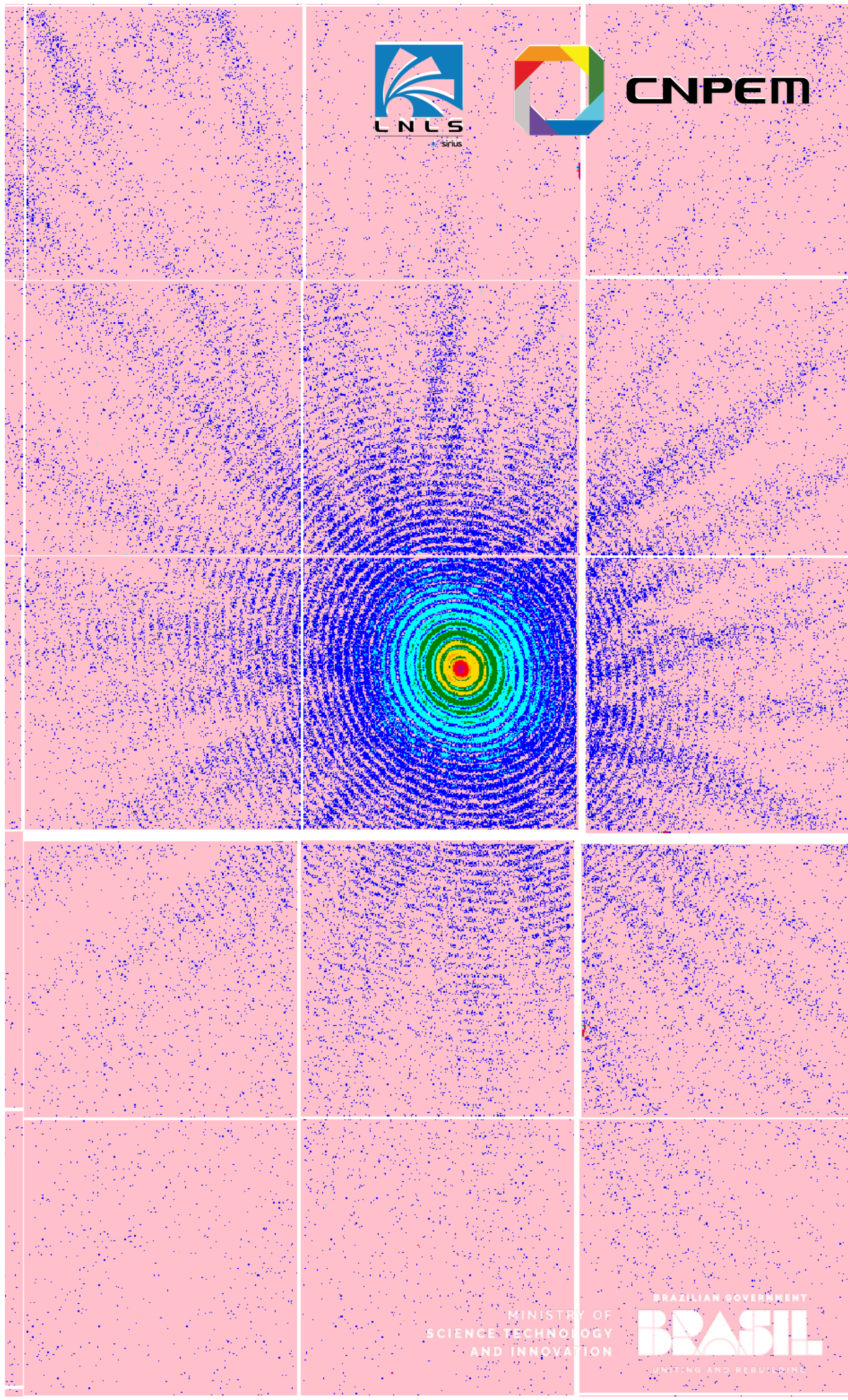
Golgi-cox stained Neurons



Murilo de Carvalho



Conclusion



- Scientific Computing at Sirius
  - has been steadily growing
  - target towards excellency in inverse problems
  - R&D + user support
  - Up to 2023, focus on imaging problems

    … but more fields to come in the future!
  - Preliminary results seem promising!
  - Margin for much improvement; numerous challenges ahead
- Looking forward to discuss and collaborate!

Thank you!

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lnls.cnpem.br

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Brazilian Center for Research in Energy and Materials

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