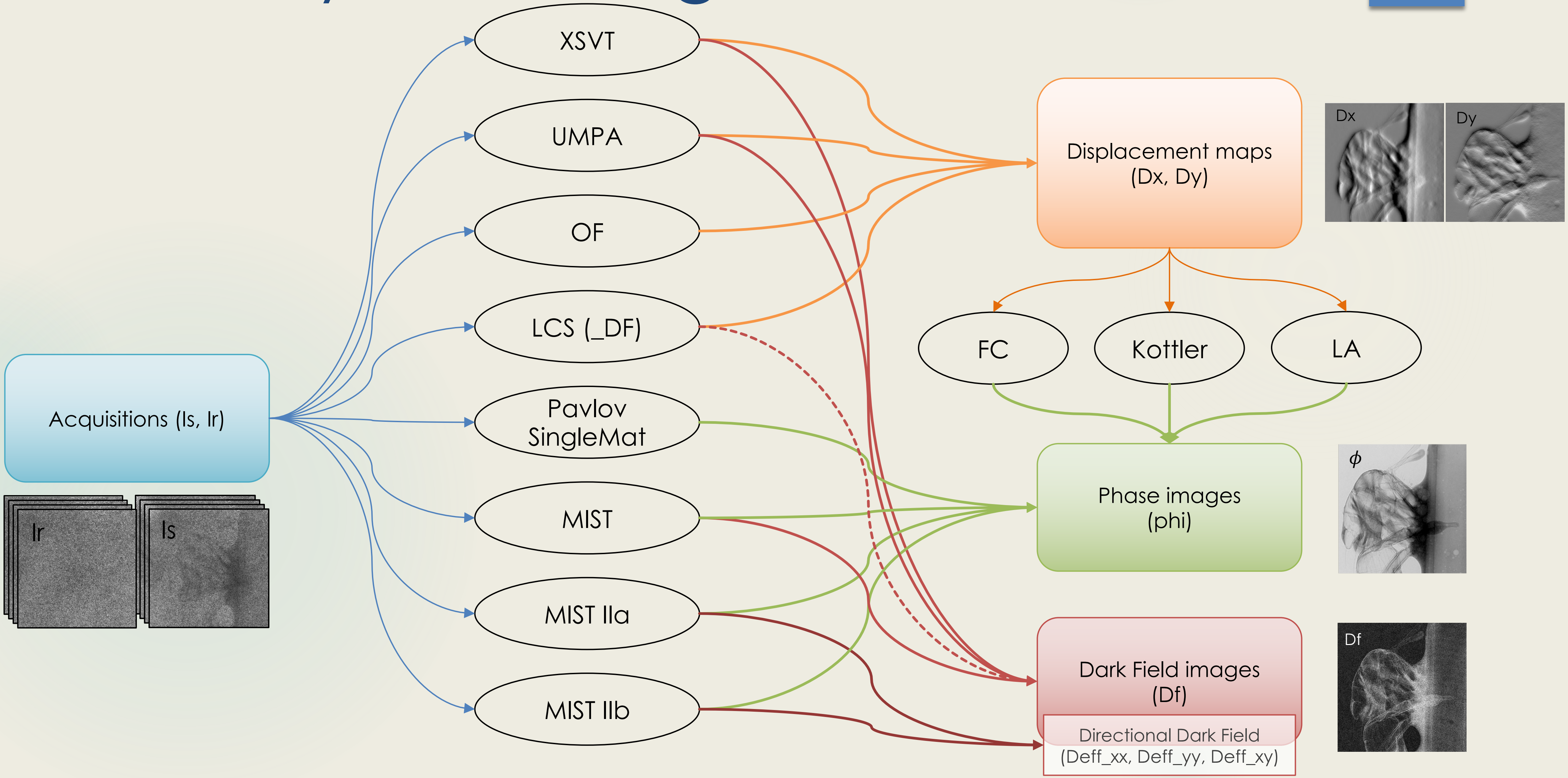
Phase retrieval algorithms

DATA SHEET AND USER GUIDE

Summary of the algorithms



Algorithms hypothesis and limitations

	Hypothesis	Limitations	Min number of acquisitions
UMPA	None	Resolution of the system	Several
XSVT	None	Resolution of the system	Several
OF	Phase object = NO attenuation	Attenuation	1
LCS (LCS_DF)	Low coherence but works also for quasi coherent systems	Noise, source blurring and PSF	3 (4)
Pavlov Single Material	Sample single material, sample weak absorption, membrane intensity gradients assumed small	A lot oh hypothesis…	1
MIST I	Phase object	Detector resolution/absorption	2
MIST IIa	Phase object	Detector resolution?	4
MIST IIb	Single material	Detector resolution?	4

Papers:

	Reference	Year
UMPA	Zdora, M. C., Thibault, P., Zhou, T., Koch, F. J., Romell, J., Sala, S., ... & Zanette, I. (2017). X-ray phase-contrast imaging and metrology through unified modulated pattern analysis. Physical review letters, 118(20), 203903.	2017
XSVT	Berujon, S., & Ziegler, E. (2015). Near-field speckle-scanning-based x-ray imaging. Physical Review A, 92(1), 013837.	2015
OF	Paganin, D. M., Labriet, H., Brun, E., & Berujon, S. (2018). Single-image geometric-flow x-ray speckle tracking. Physical Review A, 98(5), 053813.	2018
LCS (LCS_DF not published yet)	Quénot, L., Rougé-Labriet, H., Bohic, S., Berujon, S., & Brun, E. (2021). Implicit tracking approach for X-ray phase-contrast imaging with a random mask and a conventional system. Optica, 8(11), 1412-1415.	2021
Pavlov Single Material	Pavlov, K. M., Li, H. T., Paganin, D. M., Berujon, S., Rougé-Labriet, H., & Brun, E. (2020). Single-shot x-ray speckle-based imaging of a single-material object. Physical Review Applied, 13(5), 054023.	2020
MIST I	Pavlov, K. M., Paganin, D. M., Li, H. T., Berujon, S., Rougé-Labriet, H., & Brun, E. (2020). X-ray multi-modal intrinsic-speckle-tracking. Journal of Optics, 22(12), 125604.	2020
MIST Iia, MIST IIb	Pavlov, K. M., Paganin, D. M., Morgan, K. S., Li, H. T., Berujon, S., Quénot, L., & Brun, E. (2021). Directional dark-field implicit x-ray speckle tracking using an anisotropic-diffusion Fokker-Planck equation. Physical Review A, 104(5), 053505.	2021

User guide

- 3 files to modify:
  - ExperimentParameters.xml
  - AlgorithmParameter.xml
  - allPhaseRetrievalMethods.py

The first two contain all the parameters of the experiment and the ones to use for the phase retrieval.

The .py allows to chose which phase retrieval algorithms to use and to run the calculations.

User guide

ExperimentParameters.xml

Start by creating a new **experiment** and enter all the correct values

```xml
<experiment>
    <experiment_name>MoucheSimapAout2017</experiment_name>
    <exp_folder>/Data/SIMAP/MoucheSimapAout2017/</exp_folder>
    <output_folder>/PhaseRetrieval/Results/MoucheSimapAout2017/</output_folder>
    <energy unit="keV">27</energy>
    <pixel unit="m">48e-6</pixel>
    <dist_object_detector unit="m">0.6385</dist_object_detector>
    <dist_source_object unit="m">0.0316</dist_source_object>
    <delta>3.49E-07</delta>
    <beta>3.57E-10</beta>
    <source_size unit="um">2</source_size>
    <detector_PSF unit="pix">1.2</detector_PSF>
    <crop_on>False</crop_on>
    <cropDebX unit="pix">0</cropDebX>
    <cropDebY unit="pix">0</cropDebY>
    <cropEndX unit="pix">-1</cropEndX>
    <cropEndY unit="pix">-1</cropEndY>

</experiment>
```

/!\The experiment name must be consistent in all 3 files

Folder containing the data ref and sample images.
/!\ the folders must be called 'ref' and 'sample'

Folder that will contain the computed images (must already exist)

Mean energy of the experiment

Detector pixel size

Refraction and absorption indices (can be found there: http://ts-imaging.science.unimelb.edu.au/Services/Simple/)

FHWM (not actually useful for now…)

Value used for de-blurring of the acquisitions. Corresponds to the standard deviation of the blurring gaussian

To choose a region of interest

/!\ all units given in the .xml files are only here to help the user fill the file, they must not be changed! They are not read in the program.

User guide

AlgorithmParameters.xml

Start by creating a new **experiment** and enter all the correct values

```xml
<experiment>
    <experiment_name>MoucheSimapAout2017</experiment_name>
    <nb_of_point>20</nb_of_point>
    <pad_size>0</pad_size>
    <pad_type>reflect</pad_type>
    <do_deconvolution>False</do_deconvolution>
    <deconvolution_type>unsupervised_wiener</deconvolution_type>
    <absorption_correction_sigma>15</absorption_correction_sigma>
    <max_shift>1</max_shift>
    <sigma_regularization>1</sigma_regularization>
    <LCS_median_filter>3</LCS_median_filter>
    <umpaNw>5</umpaNw>
    <MIST_median_filter>3</MIST_median_filter>
</experiment>
```

/!\The experiment name must be consistent in all 3 files

Number of measurement {Is, Ir} to use

Padding acquisitions to reduce edge effects in some methods (may be usefull for OF, Pvlov et MISTx)

De-blurring of the acquisitions (uses the PSF value) greatly improves results in some cases

In some cases we assume no absorption, it can be corrected using the ratio Is/Ir with a small blurring of this size. This correction is not great in most cases because it induces a edge enhancement that will be confused with phase. To exclude this correction use “0”.

Limit of displacement in pixel that should be measured (usefull for filtering outliers)

Filtering very low frequencies for methods using Fourier transforms (OF, Pavlov, MISTx)

Filtering of shot noise in displacement maps retrieved with LCS

Size of the cross correlation windows for UMPA: window=(2*umpaNw+1)x(2*umpaNw+1)

Median filter used on the retrieved directional dark field images

/!\ all units given in the .xml files are only here to help the user fill the file, they must not be changed! They are not read in the program.

User guide

ExperimentParameters.xml – TOMOGRAPHY CASE

Start by creating a new **experiment** and enter all the correct values

Experiment folder without the number of the speckle point (here the entire path of the first point folder is "/data/visitor/md1217/id17/HA750_33keV_6um_SP_025_SD_Fe90_3layers__004__001/"

```xml
<experiment>
    <experiment_name>Tomo_md1217</experiment_name>
    <exp_folder>/data/visitor/md1217/id17/HA750_33keV_6um_SP_025_SD_Fe90_3layers__004__</exp_folder>
    <output_folder>/data/visitor/md1217/id17/HA750_33keV_6um_SP_025_SD_Fe90_3layers__004__Retrieval/
</output_folder>
    <tomo>True</tomo>
    <number_of_projections>2602</number_of_projections>
    <energy unit="keV">33</energy>
  …
  …
</experiment>
```

Must be True to be treated as a tomo

Total number of projections acquired

/!\ The references must have been averaged under the name refHST0000 and refHSTXXXX with XXXX=**number_of_projections**

User guide

AlgorithmParameters.xml

Start by creating a new **experiment** and enter all the correct values

```
<experiment>
    <experiment_name>MoucheSimapAout2017</experiment_name>
    <nb_of_point>20</nb_of_point>
    <pad_size>0</pad_size>
    <pad_type>reflect</pad_type>
      …
      …
    <proj_to_treat_start>3</proj_to_treat_start>
    <proj_to_treat_end>5</proj_to_treat_end>
</experiment>
```

All the same parameters as for a projection experiment

To choose to treat only a range of projections (for testing for example)
Those parameters are optional: if not in the .xml the algorithm treats all the projections

Python end of range 5 actually means that it will stop after treating projection 4.

User guide

allPhaseRetrievalMethods.py

Set the value of “studied_case”

studied_case = 'MoucheSimapAout2017’ same experiment name as in the other files

Choose the phase retrieval methods you want to use by setting them to “True” (“False” otherwise)

Run the script!

Calculations – XSVT

- **XSVT()**

  → Crossed correlation

$$D_{\perp}(x_0, y_0) = \underset{\delta_x,\delta_y}{\operatorname{argmax}} \iint \widehat{I_s}\,(P_x, P_y, x, y)\widehat{I_R}\,\left(P_x, P_y, x - \delta_x, y - \delta_y\right)dxdy$$

  Returned images:

  - Phase gradients (+integrated phase images)
  - Dark-field image

+ No hypothesis on the experiment or the sample

- Limited sensitivity (~ 0.1 pixel)
- Heavy computation (time consuming)

Calculations - UMPA

- **UMPA()**

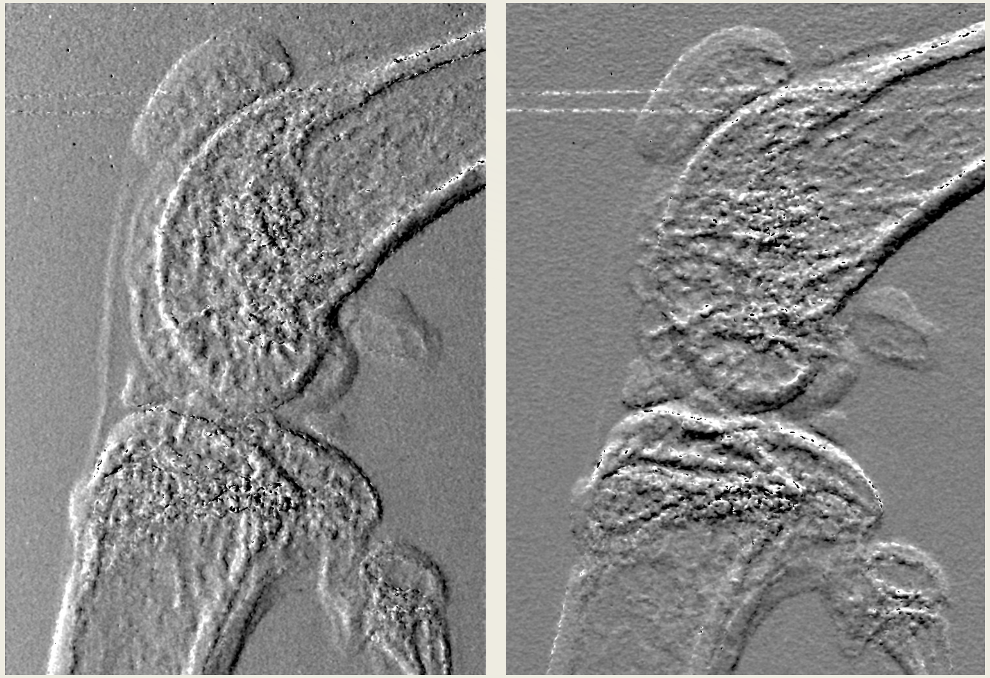
  Calculates the displacement images of a pure phase object from sample and reference images.

  → Minimization of the mean squared error:

$$D_{\perp}(x_0, y_0) = \underset{\delta_x,\delta_y}{\operatorname{argmin}} \iint w(x - x_0, y - y_0)\left[T I_r(x - \delta_x, y - \delta_y) - I_s(x, y)\right]^2 dxdy$$

Returned images:

- Phase gradients (+integrated phase images)
- Dark-field image
- Thickness image (not very accurate)



+ No hypothesis on the experiment or the sample

- Limited sensitivity (~ 0.1 pixel)
- Heavy computation (time consuming)

Calculations - OF

- **OF()**

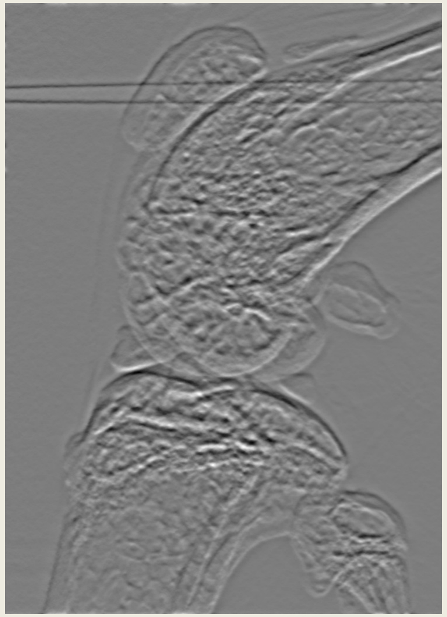
  Calculates the displacement images of a pure phase object from sample and reference images.

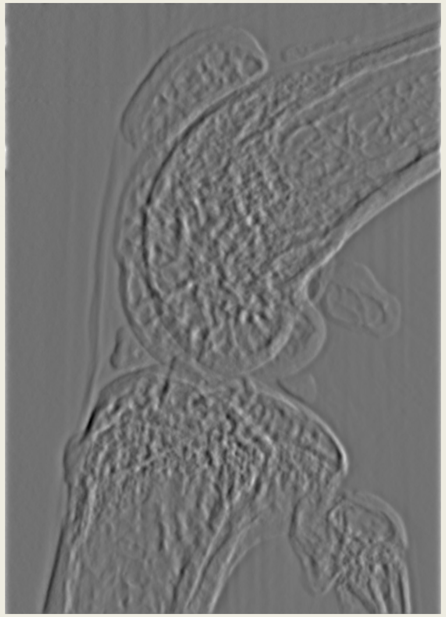
  Transport of intensity equation: $I_s(x,y) - I_r(x,y) = \nabla_\perp \cdot [I_r(x,y) D_\perp(x,y)]$

  Numerical resolution method: $D_\perp(x,y) = \frac{i}{I_r(x,y)} \mathcal{F}^{-1}\left\{(k_x, k_y)\left[\frac{\mathcal{F}[I_s(x,y) - I_r(x,y)]}{k_x^2 + k_y^2}\right]\right\}$

Returned images:

- Phase gradients (+integrated phase images)





+ Very fast computation

- Assumes non attenuating sample

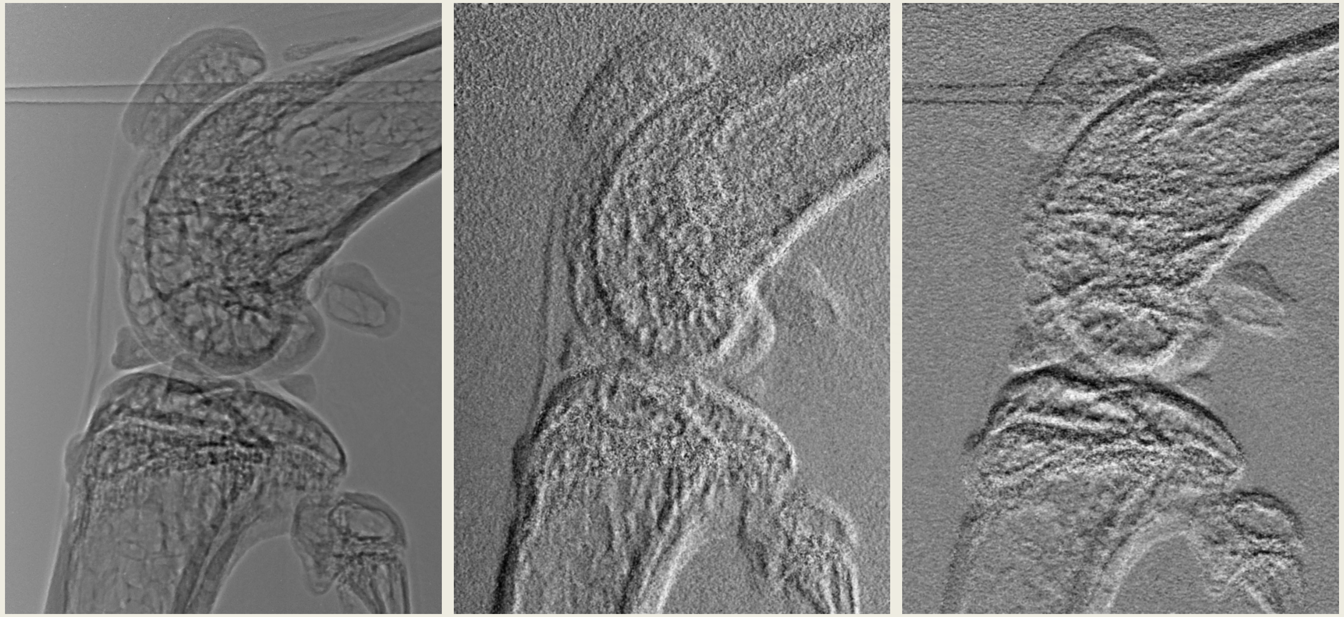
Calculation - LCS

- **LCS()**

Calculates the displacement images from sample and reference images using the LCS system

- System to solve (Variables are in red)

$$\begin{cases} I_r^{(1)}(x,y) = \frac{1}{I_{abs}(x,y)} I_s^{(1)}(x,y) + D_x(x,y)\frac{\partial I_r^{(1)}(x,y)}{\partial x} + D_y(x,y)\frac{\partial I_r^{(1)}(x,y)}{\partial y} \\ I_r^{(2)}(x,y) = \frac{1}{I_{abs}(x,y)} I_s^{(2)}(x,y) + D_x(x,y)\frac{\partial I_r^{(2)}(x,y)}{\partial x} + D_y(x,y)\frac{\partial I_r^{(2)}(x,y)}{\partial y} \\ I_r^{(3)}(x,y) = \frac{1}{I_{abs}(x,y)} I_s^{(3)}(x,y) + D_x(x,y)\frac{\partial I_r^{(3)}(x,y)}{\partial x} + D_y(x,y)\frac{\partial I_r^{(3)}(x,y)}{\partial y} \end{cases}$$



Returned images:

- Phase gradients (+integrated phase images)
- Attenuation image

+ Fast computation

- Can be sensitive to noise

Calculation – LCS_DF

- **LCS_Df()**

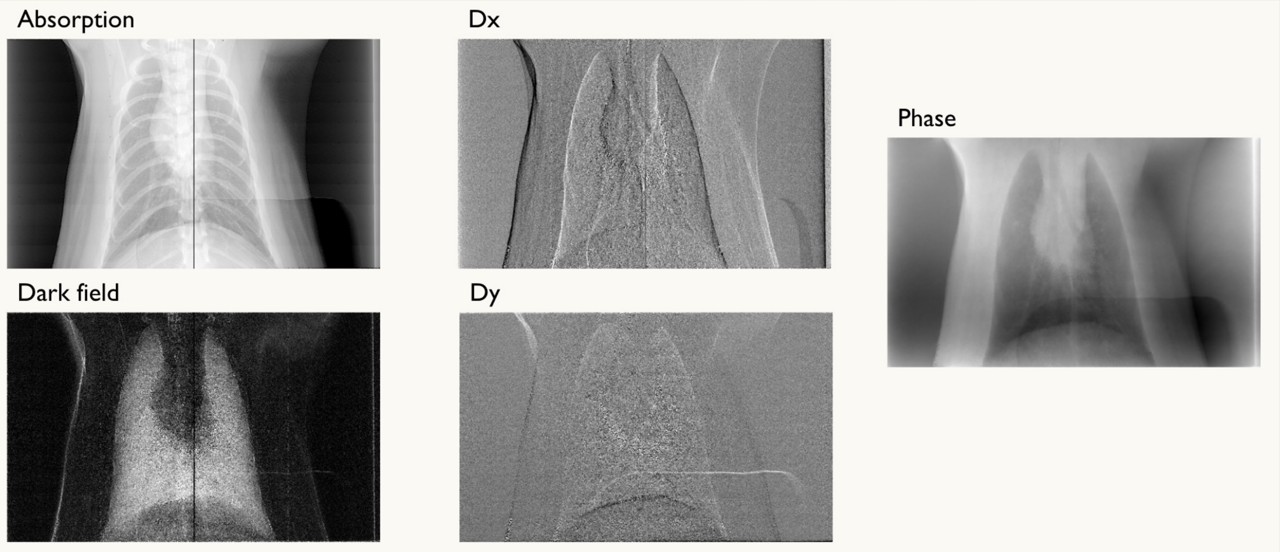
Calculates the displacement images and dark-field image from sample and reference images using the LCS system

- System to solve (Variables are in red)

$$I_r(x,y) = \frac{1}{I_{obj}(x,y)} I_s(x,y) + D_x(x,y)\frac{\partial I_r(x,y)}{\partial x} + D_y(x,y)\frac{\partial I_r(x,y)}{\partial y} - \Delta D_{eff}(x,y)\nabla_{\perp}^2 I_r(x,y)$$

Returned images:

- Phase gradients (+integrated phase images)
- Attenuation image
- Dark-field image



+ Fast computation

- Can be sensitive to noise

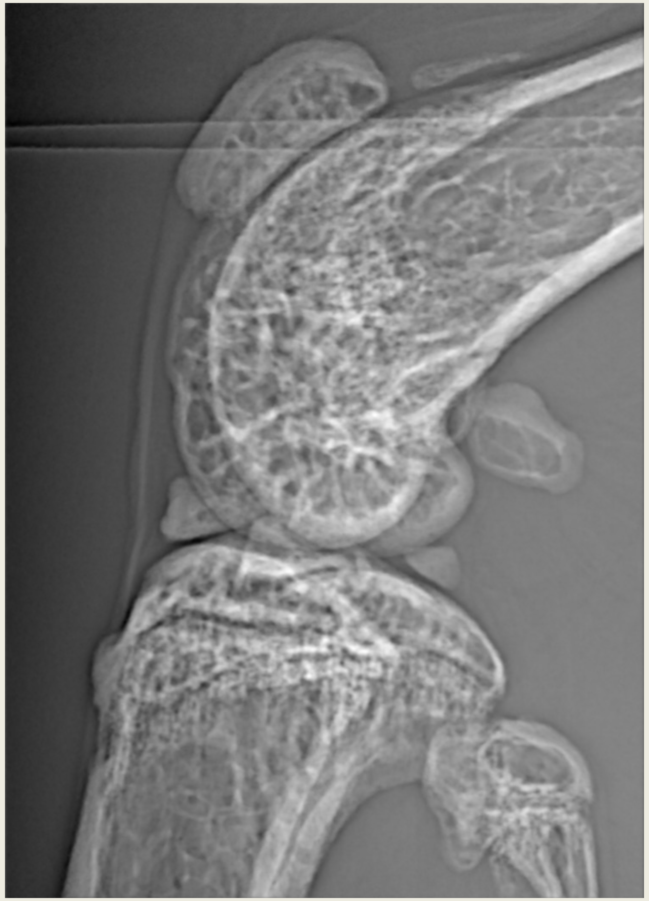
Calculation – Pavlov Single Material

- **tie_Pavlovetal2020()**

→ Calculates the thickness (equivalent to phase in this case) of a single material object form sample and reference images (starting from the TIE).

  - $t(x, y) = \frac{1}{\mu} \mathcal{F}^{-1} \left\{ LFF \left[\frac{\mathcal{F}\{1 - I_s(x,y)/I_r(x,y)\}}{1 + \pi\gamma L\lambda\left(k_x^2 + k_y^2\right)} \right] \right\}$
  - $\phi(x, y) = -k\delta t(x, y)$ (Proportionality between phase and thickness of a single material object)

Returned image: thickness



\+ Fast computation

\- Requires quasi-coherent source
\- Assumes single-material
\- Assumes non attenuating sample?

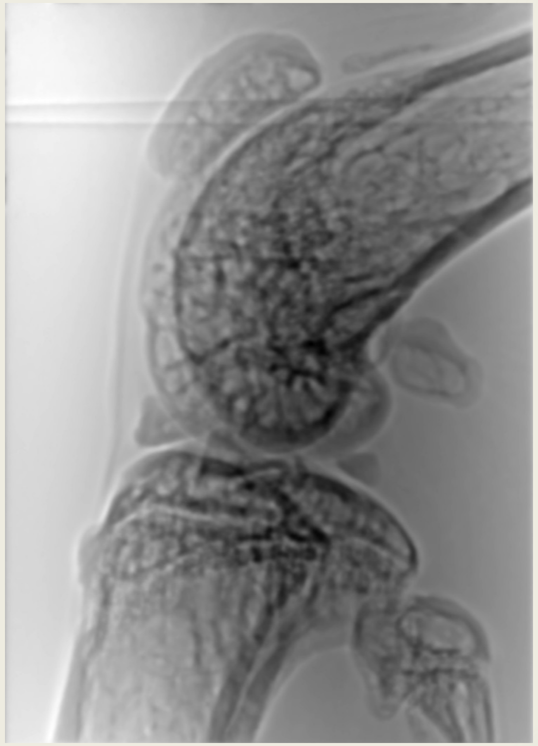
Calculations – MISTI

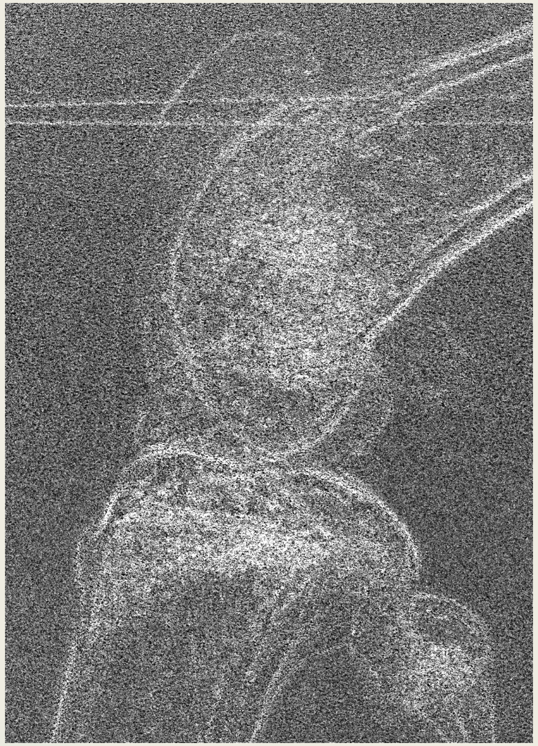
- **MISTI():** calculates the dark field and the phase of a single-material object from sample and reference images.
  - $Deff$ [numpy arrays]: the Dark-Field
  - phi [numpy array]: the phase of the object

Returned images:
- Phase image
- Dark-field image

+ Fast computation

- Assumes quasi-coherent source





Calculations – MISTII_1/2

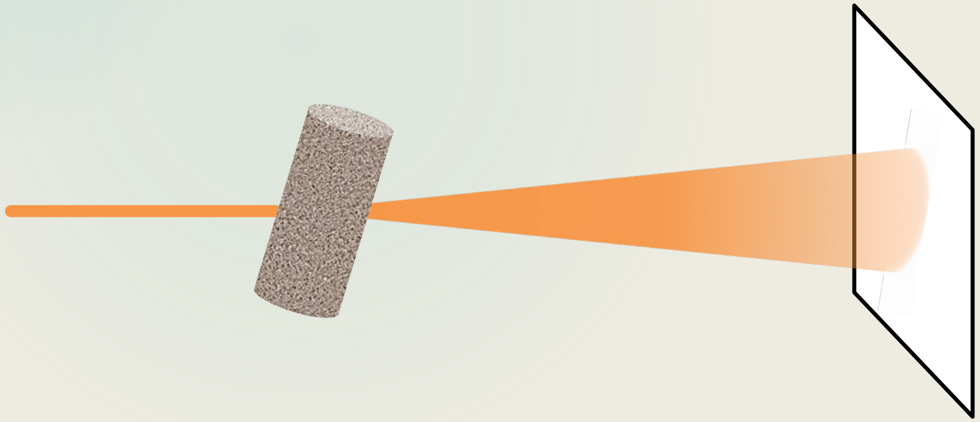
- MISTII_1/2() : Calculates the directionnal dark field of a phase sample (1) or a single material object (2) from sample and reference images Solves the system:

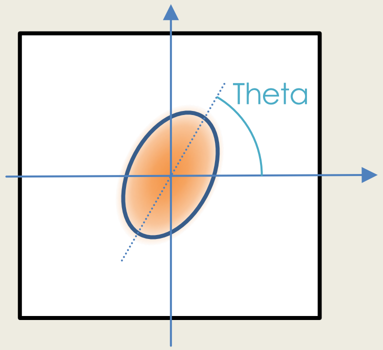
$$\frac{I_s^{(i)}(x,y)}{I_r^{(i)}(x,y)} = \left(1 - \frac{\gamma\Delta}{2k}\nabla_\perp^2\right) I_{ob}(x,y) + \Delta D_{eff}^{(xx)} \frac{\partial^2}{\partial x^2} I_{ob}(x,y) + \Delta D_{eff}^{(yy)} \frac{\partial^2}{\partial y^2} I_{ob}(x,y) + \Delta D_{eff}^{(xy)} \frac{\partial^2}{\partial x \partial y} I_{ob}(x,y) + \Delta D_{eff}^{(xx)} I_{ob}(x,y) \frac{\frac{\partial^2}{\partial x^2} I_r^{(i)}(x,y)}{I_r^{(i)}(x,y)} + \Delta D_{eff}^{(yy)} I_{ob}(x,y) \frac{\frac{\partial^2}{\partial y^2} I_r^{(i)}(x,y)}{I_r^{(i)}(x,y)} + \Delta D_{eff}^{(xy)} I_{ob}(x,y) \frac{\frac{\partial^2}{\partial x \partial y} I_r^{(i)}(x,y)}{I_r^{(i)}(x,y)}$$

Returned images:

- Thickness/phase image
- Dark-field tensors images
- A bunch of other transformed values related to the ellipse

- $\nabla_\perp^2$: orthogonal Laplacien (along x and y)
- Δ distance object detector
- $k = 2\pi E \frac{e}{hc}$ wavenumber

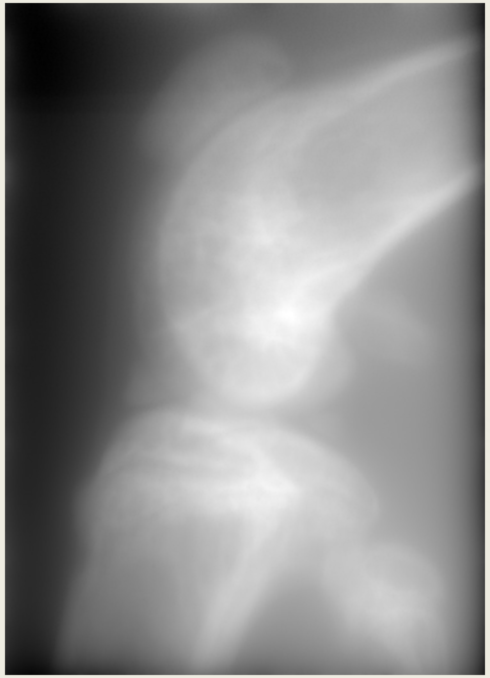




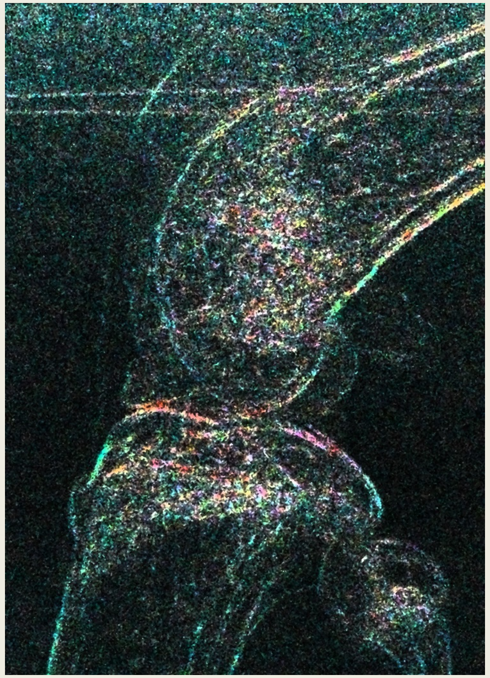
Calculations – MISTII2

Dark field tensors

Thickness



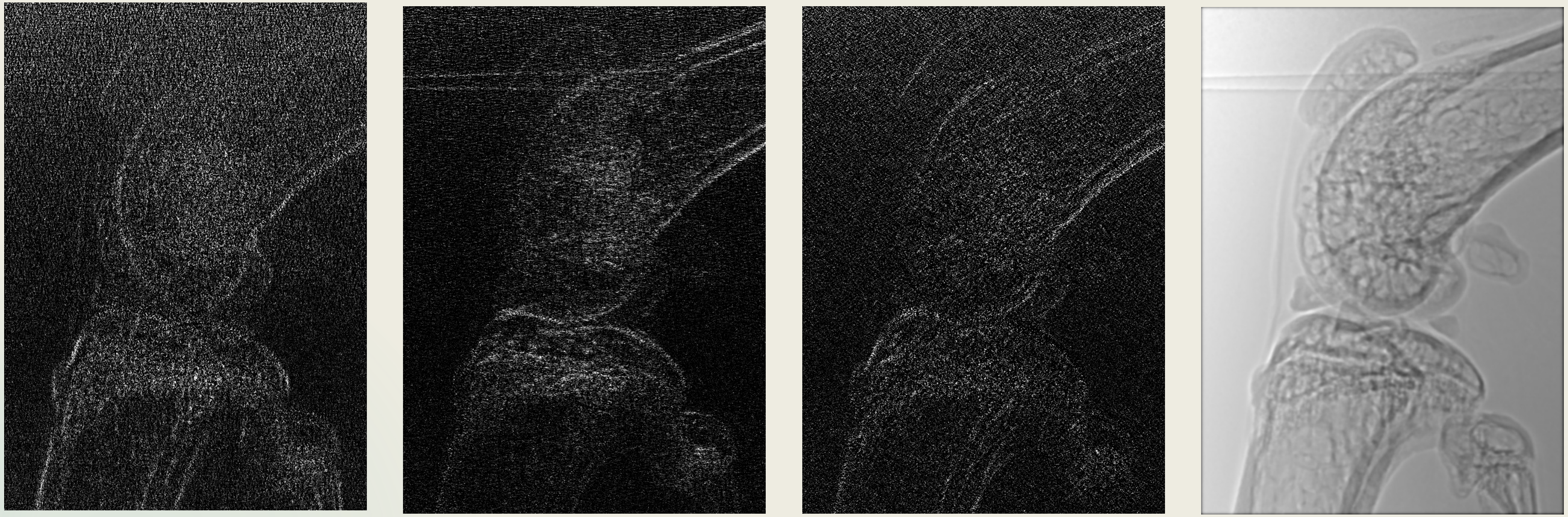
Ellipse area & theta



+ Directional dark field information

- Assumes quasi-coherent source
- Assumes single-material

Calculations – MISTII1



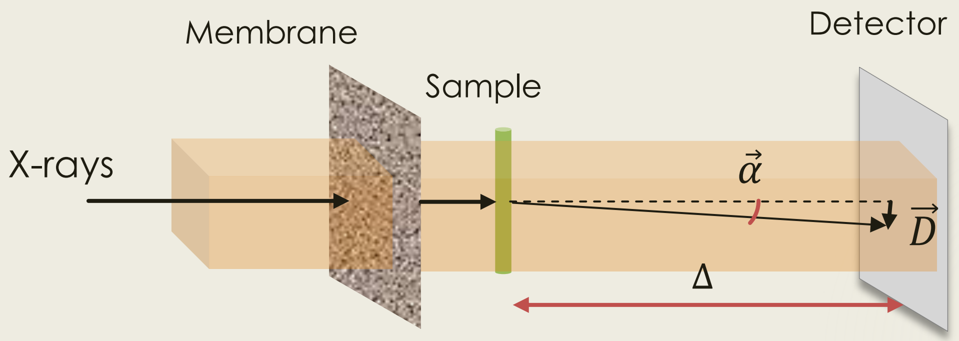
+ Directional dark field information

- Assumes quasi-coherent source
- Assumes non absorbing sample

Image integration

$$\frac{d\phi}{dx} = \frac{2\pi\alpha_x}{\lambda} = \frac{2\pi D_x}{\lambda\Delta}$$

$$\frac{d\phi}{dy} = \frac{2\pi\alpha_y}{\lambda} = \frac{2\pi D_y}{\lambda\Delta}$$



Algorithm	Reference	Year
FC	R. T. Frankot and R. Chellappa, "A Method for Enforcing Integrability in Shape from Shading Algorithms," 1988.	1988
LA	M. R. Arnison, K. G. Larkin, C. J. R. Sheppard, N. I. Smith, and C. J. Cogswell, "Linear phase imaging using differential interference contrast microscopy," *J. Microsc.*, vol. 214, no. 1, pp. 7–12, Apr. 2004.	2004
Kottler	C. Kottler, C. David, F. Pfeiffer, and O. Bunk, "A two-directional approach for grating based differential phase contrast imaging using hard x-rays," 2007.	2007

Image integration - FC

- frankoChellappa.py
  - frankotchellappa()

$$\phi(x,y) = \mathcal{F}^{-1}\left\{\frac{1}{k_x^2 + k_y^2}\left(-ik_x\mathcal{F}\left\{\frac{\partial\phi}{\partial x}(x,y)\right\} - ik_y\mathcal{F}\left\{\frac{\partial\phi}{\partial y}(x,y)\right\}\right)\right\}$$

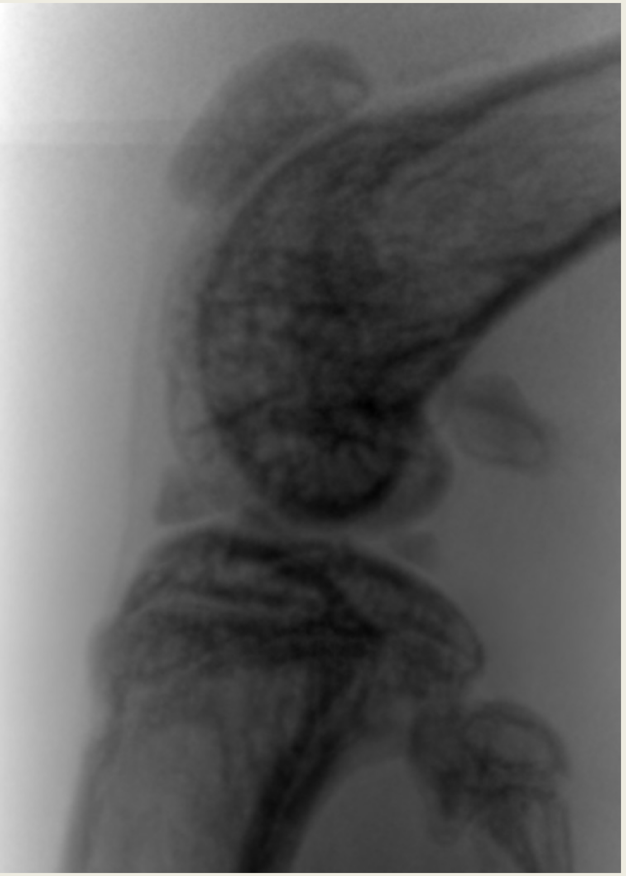


Image integration - LA

- phaseIntegration.py
  - LarkinAnissonSheppard()

$$\phi(x,y) = \mathcal{F}^{-1}\left\{\frac{1}{ik_x - k_y}\mathcal{F}\left\{\frac{\partial\phi}{\partial x}(x,y) + i\frac{\partial\phi}{\partial y}(x,y)\right\}\right\}$$

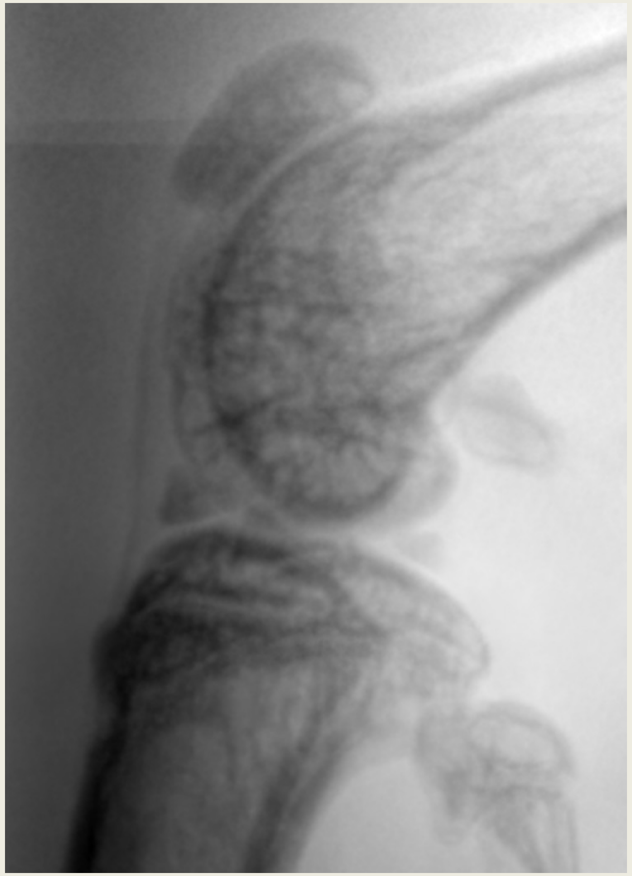
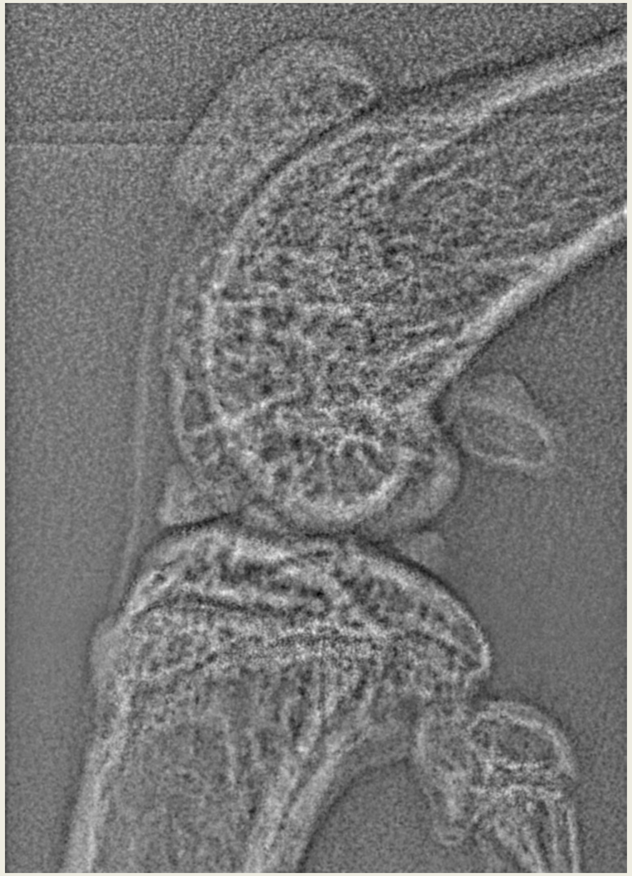


Image integration - kottler

- phaseIntegration.py
  - kottler()

$$\phi(x,y) = \mathcal{F}^{-1}\left\{\mathcal{F}\left\{\frac{\partial\phi}{\partial x}(x,y) + i\,\frac{\partial\phi}{\partial y}(x,y)\right\} * e^{i\tan^{-1}(k_x/k_y)}\right\}$$



Code architecture

- allPhaseRetrievalMethods.py
  - Main():
    - Receives all interesting parameters
    - Calls readStudiedCase()
    - Calls one by one each processers of phase retrieval algorithms « process… ()»

  - readStudiedCase(): contains and reads the data specific to an experiment,
    - opens the acquisitions and normalizes
    - Arguments:
      - sCase [string]: the experiment name
      - nbImages [int]: the number of pairs of acquisitions to take into account
      - machinePrefix [string]: the name of the machine you are working on
    - Outputs:
      - Is [numpy array]: contains the nbImages sample images
      - Ir [numpy array]: contains the nbImages reference images

Code architecture

- allPhaseRetrievalMethods.py
  - ProcessXXX(): calls the XXX() phase retrieval function and saves all the calculated images

- OpticalFlow2020.py, UMPA.py, LCS.py
  - processProjectionXXX():
    - calls XXX()phase derivative calculators
    - Converts displacements to phase derivative
    - Calls, frankotchellappa(), kottler() and LarkinAnissonSheppard() integration functions to calculate the phase 3 different ways.
    - Returns displacement maps and phases images