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multi-contrast X-ray imaging-based study of aggregates in cement-based mortars

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Outlines

- Background and target of the project
- image analysis and results
  - image enhancement/artifact correction
  - image segmentation
  - feature analysis
- conclusion and outlook

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Background and target of the project

- **target**:

  segmentation and feature analysis of aggregate within a mortar sample (cement paste matrix with embedded aggregates)
- **origin of examined dataset**
  - time-lapsed inline phase-contrast X-ray tomography of drying in porous building materials at TOMCAT beamline, PSI
  - water pre-saturated mortar sample
  - acquisition at contact plane and at 90mm sample-detector distance
- **what do we have?**
  - 3D attenuation-contrast dataset (AC)
  - 3D edge-enhancement contrast dataset before phase retrieval (EC)
  - 3D phase-contrast dataset (PC)

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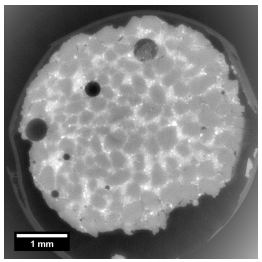
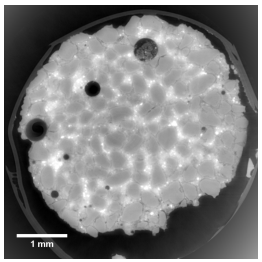
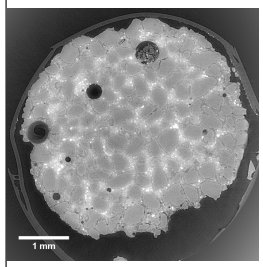
Attenuation-contrast images	Phase-contrast images	Edge-enhancement contrast images (before retrieval)
		
☺ Higher resolution ☺ Lower CNR and higher noise level	☺ Higher SNR and contrast for features ☺ Lower resolution	☺ Increased feature visibility from edge-enhancement

cross-section ("slice") from the X-ray phase-contrast, attenuation-contrast, edge-enhanced (before phase retrieval) tomographic datasets, respectively, taken at the same vertical position

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Background and target of the project

- **main difficulties**
  - large dataset (1140 x 1140 x 629 pixel^3 after cropping and binning, 32bit floating-point)
  - strong image artifacts
  - low contrast between aggregate and solid matrix (well-known issue for traditional attenuation-contrast mode)
- **methods:**
  - combination of high feature visibility from phase-contrast and high resolution from attenuation-contrast
  - comparison and testing of different image analysis methods
- **applied software/programming:**
  ImageJ, Matlab, Avizo

other information?

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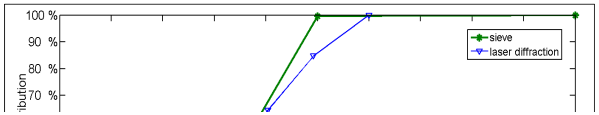
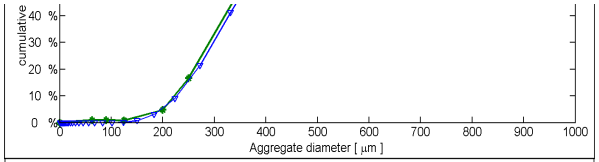
1. laser diffraction 2. sieving 3. product datasheet 4. mixing recipe

- volumetric fraction of aggregate in whole sample ≈ 50%
- Average aggregate size of 357µm
- majority of size 250-500µm, quite a few above 600µm



insufficient due to available techniques' limitation



cumulative aggregate size distribution from laser diffraction (blue) and sieving methods

Imaging analysis and results

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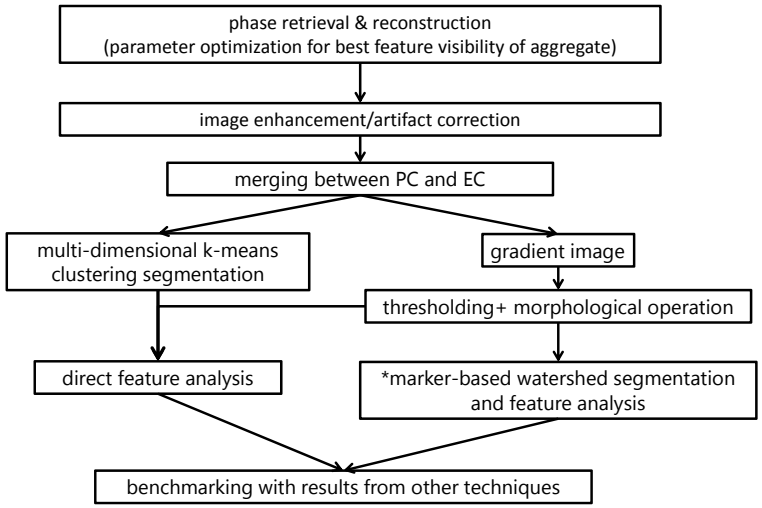

Imaging analysis and results

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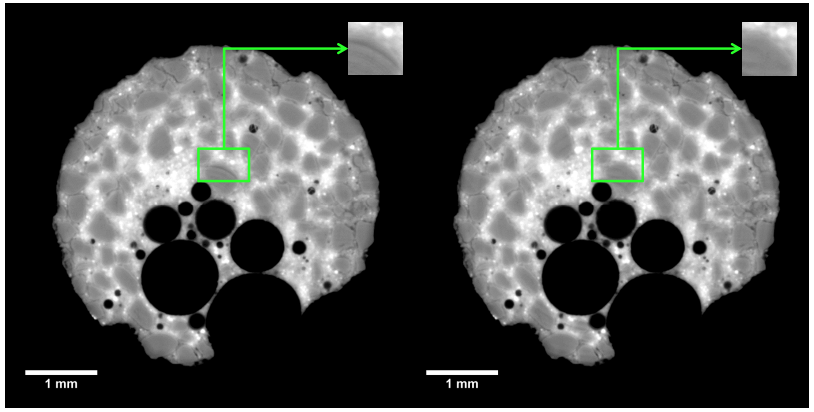
- **image enhancement/artifact correction**
  - main problem I : ring artifact for all three contrast-modes
    - → rings superimposed on structures
    - → influence on segmentation and qualitative analysis

Solution: combined wavelet- Fourier stripe filter *
- correction on sinogram (phase-contrast: before phase retrieval)
- in-house Java-based algorithm

Further improvement: tailored filtering slice-wisely*

*B. Münch, P. Trtik, F. Marone and M. Stampanoni, Stripe and ring artifact removal with combined wavelet-Fourier filtering, Optic. Express 17 (2009) 8567



cross-section ("slice") from the phase-contrast dataset before ring removal (left) and the respective one after removal (right). The top-right insets show a zoom-in of the ring artifact before and after removal

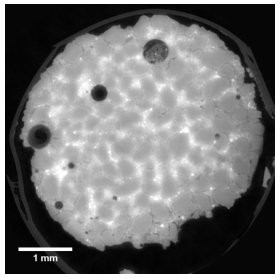
Imaging analysis and results

- **image enhancement/artifact correction**
  - main problem II : spatial background fluctuation within slice
    - → lower voxel value at sample boundary than center
    - → strongly influences segmentation and qualitative analysis

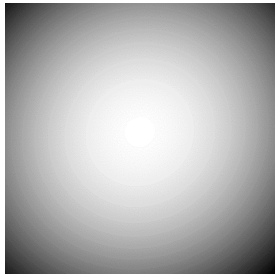
Solution: polynomial fitting-based background correction
- in-house Java-based algorithm

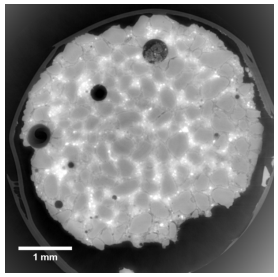
Possible reasons:
- temporal beam position shifting
- spatially nonlinear detector response

*B. Münch, P. Trtik, F. Marone and M. Stampanoni, Stripe and ring artifact removal with combined wavelet-Fourier filtering, Optic. Express 17 (2009) 8567

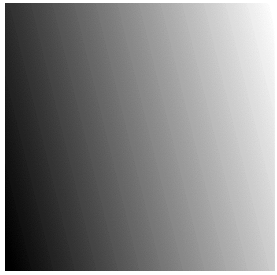


Left: cross-section from the phase-contrast dataset before background correction (top) and calculated background image (bottom)





Right: cross-section after background correction (top) and calculated background image (bottom)



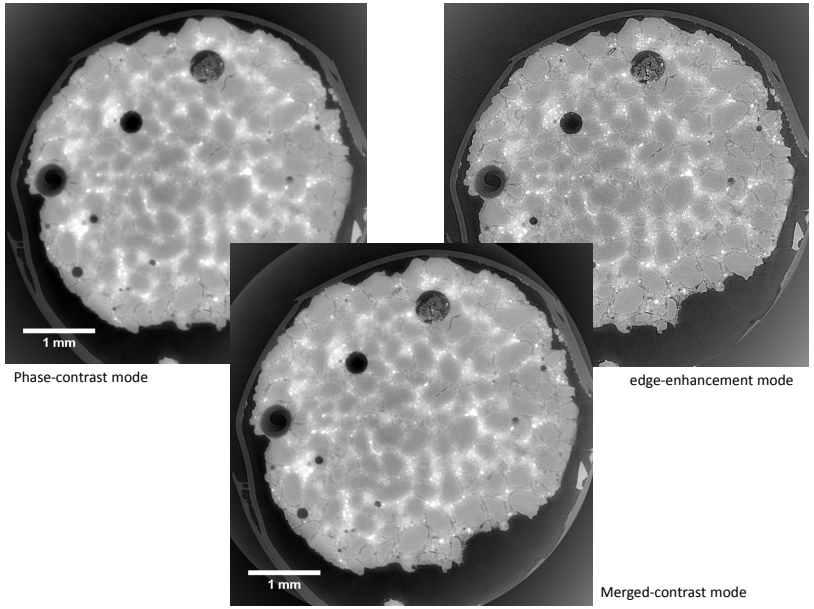
Imaging analysis and results

- **image enhancement/artifact correction**
  - main problem III : low contrast between aggregate and solid matrix
    - → difficulty for histogram-based unsupervised segmentation

Solution:
1) phase-retrieval parameter optimization
2) image merging between edge-enhanced (attenuation) contrast and phase-contrast mode in Fourier domain
   - *tuning weighing factor*
   - *using attenuation- or edge-enhanced contrast mode*
   - *merging in projection or reconstruction level*
   - *testing different filters, smoothing factor .....*

- criterion: comparison of resolution and CNR of aggregate to solid phases

*S. Irvine, R. Mokso, P. Modregger, Z. Wang, F. Marone, and M. Stampanoni, "Simple merging technique for improving resolution in qualitative single image phase contrast tomography," Optics express, vol. 22, no. 22, pp. 27257–27269, 2014



Phase-contrast mode

edge-enhancement mode

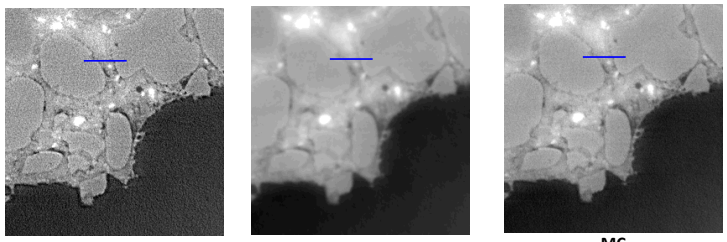
Merged-contrast mode

Qualitative comparison between the three modes

- Comparison of contrast-to-noise (CNR) between aggregate to surrounding solid phases from 3D datasets of the three contrast-modes

	• Edge-enhancement (EC)	• Phase-contrast (PC)	• Merged-contrast (MC)
• $CNR_{aggregate\text{-}to\text{-}CSH}$	• 0.12	• 0.17	• 0.15
• $CNR_{aggregate\text{-}to\text{-}[CSH+C_3S]}$	• 0.13	• 0.16	• 0.14

- Comparison of image resolution from the line profile of same feature on the corresponding 2D image of three contrast modes



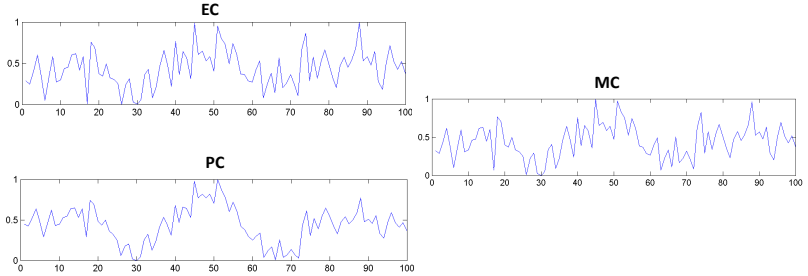
EC PC MC

Qualitative comparison between the three modes

- Comparison of contrast-to-noise (CNR) between aggregate to surrounding solid phases from 3D datasets of the three contrast-modes

	• Edge-enhancement (EC)	• Phase-contrast (PC)	• Merged-contrast (MC)
• $CNR_{aggregate\text{-}to\text{-}CSH}$*	• 0.12	• 0.17	• 0.15
• $CNR_{aggregate\text{-}to\text{-}[CSH+C_3S]}$*	• 0.13	• 0.16	• 0.14

- Comparison of image resolution from the line profile of same feature on the corresponding 2D image of three contrast modes



Imaging analysis and results

- **image segmentation**
  - two main current workable segmentation methods
    1. multi-dimensional (contrast-mode) K-means clustering segmentation
    2. manual thresholding on gradient images of merged-contrast mode + morphological refinement

✓ no prior feature characteristics→ unsupervised segmentation
✓ ability of self-tunable settings → fit data better
✓ take advantage of information from multi-contrast mode images

Imaging analysis and results

1. multi-dimensional K-means clustering segmentation

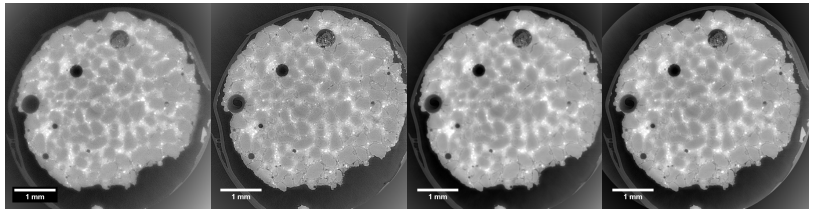
8-dimensional data combination

- ✓ 4 contrast-modes
  - attenuation-contrast, edge-enhanced contrast
  - phase-contrast, merged-contrast
- ✓ 2 types of images in each mode
  - original intensity image

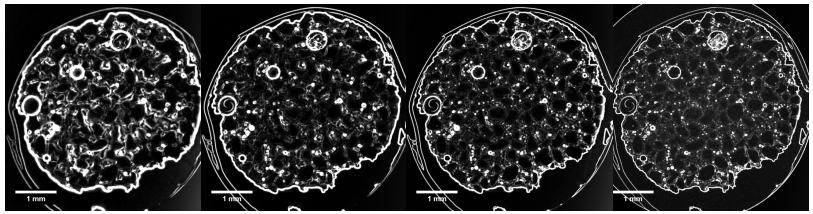
    aggregate: slightly lower voxel value than surrounding solid phases
  - variance image/ gradient image: edge-highlighted

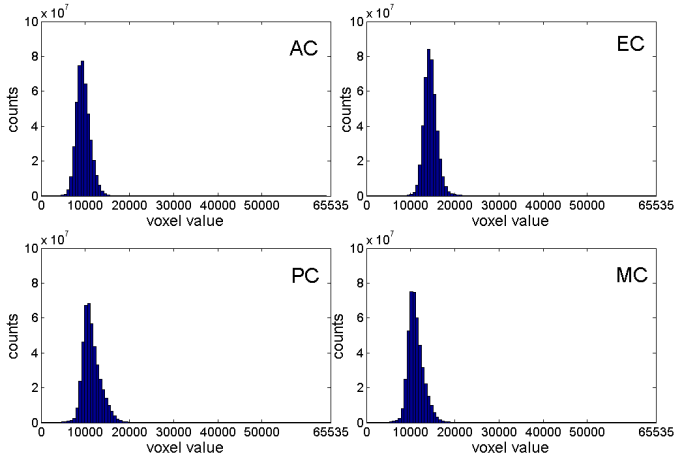
    aggregate: less structural pattern

    → voxel value decreases from aggregate boundary to aggregate center region

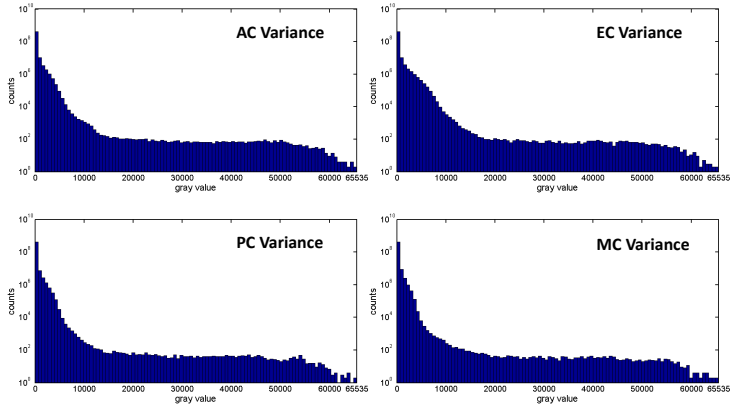


original 2D cross-section(image) from attenuation-/edge-enhancement-/phase-/merged- contrast dataset (top row, from left to right), and the respective variance images with window 3x3x3 voxel^3 (bottom row, from left to right)





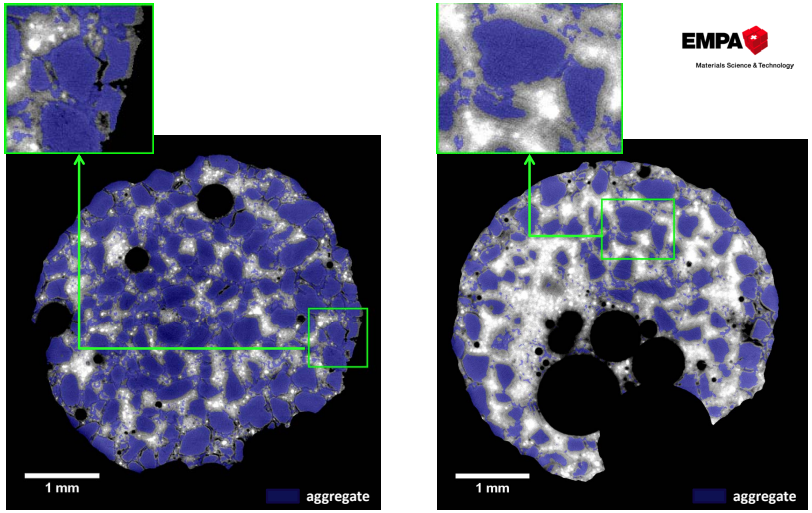
histogram of 4 original intensity 3D dataset, only considering the voxels in pre-segmented sample masks (most air voids excluded). voxel value has been linearly mapped to the range [0 65535] corresponding to minimum and maximum voxel value in the 3D pre-segmented sample ROI. top-left: attenuation- contrast; top-right: edge-enhancement contrast; bottom left: phase-contrast; bottom right: merged-contrast



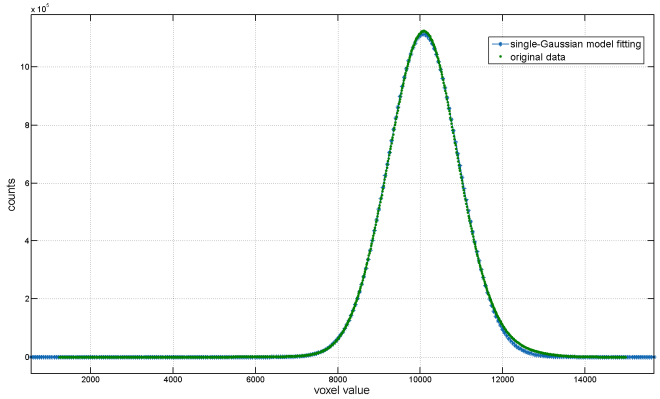
histogram of 4 Variance 3D dataset, only considering the voxels in pre-segmented sample masks (most air voids excluded). voxel value has been linearly mapped to the range [0 65535] corresponding to minimum and maximum voxel value in the 3D pre-segmented sample ROI, y axis is set to logarithmic scale. top-left: attenuation- contrast; top-right: edge-enhancement contrast; bottom left: phase-contrast; bottom right: merged-contrast

results of multi-dimensional k-means clustering

- ✓ variance images + original images (scaling factor 50:1)
  - variance images: calculation window 3x 3 x3 voxel^3
  - original images: pre-median filter to remove noise
- ✓ 2-time higher weighing on phase-contrast mode
- ✓ aggregate: single cluster in total 9 clusters (exclude large air void)
- ✓ selection criterions:
  - i. direct visualization
  - ii. ≈ 50% volumetric fraction of aggregate at mixing
  - iii. single phase ≈ single Gaussian-shaped peak in histogram of phase-contrast dataset



segmented aggregate ROI color-coded in blue on corresponding 2D merged-contrast cross-sections at the top (left) and bottom (right) of analyzed sample ROI volume. Background has been replaced with 0. The insets on top of each image show the zoom-in of segmented results.



voxel value histogram (green solid dot) from phase-contrast dataset considering only the voxels belonging to the segmented aggregate 3D binary image, 1-Gaussian best fit using in-built Matlab curve fitting toolbox (blue star).
Goodness of fit: R-square/adjusted R-square=0.9997

Imaging analysis and results

conclusion on the clustering results

- ☺ works fine for big aggregate
- ☺ results statistically under limitation (volumetric fraction≈ 40.43%)
- ☹ missing or fragmented small sized aggregates
- ☹ segmented particles still connected at the boundary

Further improvement:

- more qualitative optimization of different parameters for clustering
- testing on varying width of variance window, pre-filtering , etc.
- replace variance images with other types of images

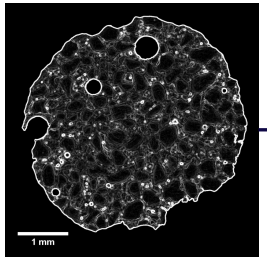
Imaging analysis and results

- **image segmentation**

2. manual thresholding on gradient images of merged-contrast mode + morphological refinement

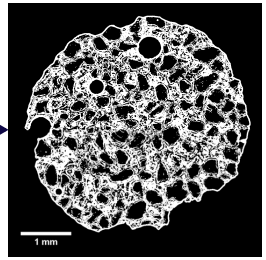
❖ merged-contrast mode: preserved contrast and image resolution

❖ pre-median filter, highest local gradient resolution



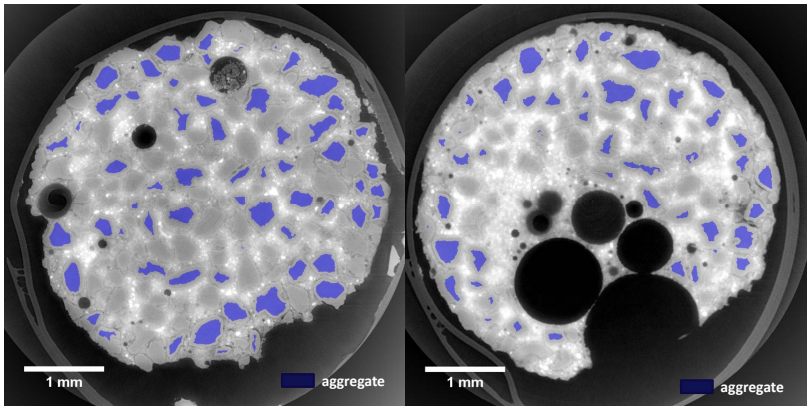
gradient image of 1st cross-section in 3D merged-contrast dataset, (Gaussian span 1*1*1 voxel³)

thresholded →



binary mask after manual-thresholding on gradient image

results of segmentation on gradient merged-contrast dataset using manual-threshold+ morphological operation



segmented aggregate ROI color-coded in blue on corresponding 2D merged-contrast cross-sections at the top (left) and bottom (right) of analyzed sample ROI volume. Background has been replaced with 0.

Imaging analysis and results

conclusion on the threshold result

☹ segmented volume of aggregate far smaller (VR≈10.11%)

☹ big influence from ring artifact and noise level

☺ further use in my project: signal threshold on differential phase-contrast dataset from water change in sample during drying

further improvement:

- systematical testing of different threshold value, pre-/post-filter on gradient images
- testing on edge-enhancement contrast dataset
- marker-based watershed segmentation

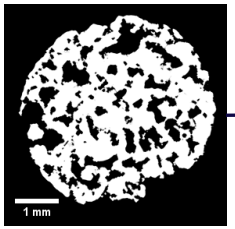
Imaging analysis and results

- **further steps on segmented results**

➢ finer morphological operation on binary mask

➢ disconnect particles
  - in-house Java-based algorithm*
  - need of high computation time: downsize dataset (8x8x8 binning/cropping)

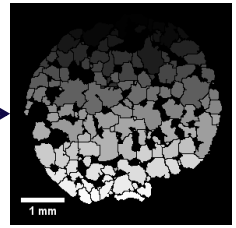
➢ component labeling



binary mask of 1st cross-section in 3D segmented aggregate volume by clustering methods, 8x8x8 binning of original dataset

disconnect and label →

volumetric fraction reduced from 35.09% to 32.00%



disconnected and labeled mask of 1st cross-section in 3D segmented aggregate volume by clustering methods (16 bit unsigned)

* Münch B., Gasser P., Holzer L., Flatt R., "FIB Nanotomography of Particulate Systems - Part II: Particle Recognition and Effect of Boundary Truncation.", Journal American Ceramics Society 89(8), pp.2586-2595, 2006

feature analysis

- **what do we want to know?**
  - particle size information (distribution, average value, etc)
  - shape information (anisotropy distribution, etc)
- **how to achieve these goals?**
  - PCA analysis on labeled segmentation results (Avizo)
  - 3-parameter elliptical model (3D) for each particle
  - defined size metrics:
    - i. extent along the 2nd longest principal axis (Vs. mechanical sieving)

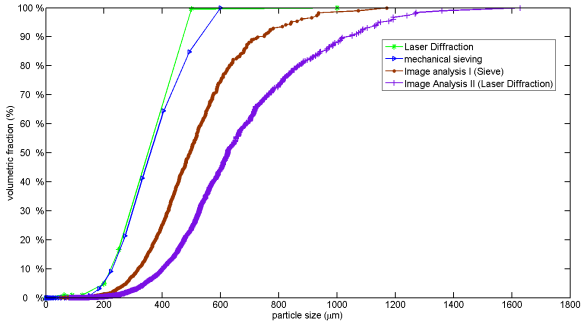
      below mentioned as 'image analysis I'
    - ii. extent along the 1st longest principal axis (Vs. Laser Diffraction)

      below mentioned as 'image analysis II'
    - iii. anisotropy= $1 - \frac{shortest\ eigenvalue}{longest\ eigenvalue}$

feature analysis

results I- size analysis

averaged particle size=333.655µm (calculated as the extent of 2nd longest principle axis)
averaged particle size=431.281µm (calculated as the extent of 1st longest principle axis)

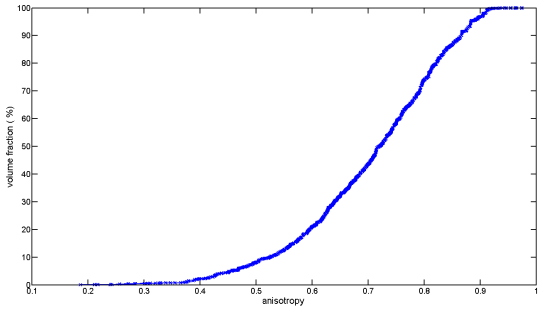


comparison of cumulative particle size distribution, described by the cumulative volumetric fraction as a function of particle size, among results from laser diffraction (green star), mechanical sieving (blue triangle) and results calculated mage analysis: I. extent of the 2nd longest principal axis, used to correlate the sieving results; II. extent of the 1st longest principal axis, used to correlate the laser diffraction results.

feature analysis

results II- shape analysis

averaged anisotropy= 0.692395



cumulative anisotropy distribution from image analysis results, expressed as the volumetric fraction as the function of corresponding anisotropy.

feature analysis

Conclusion on results of feature analysis

- image analysis results show shift of particle size spectrum to the higher value range , compared to those from mechanical sieving and laser diffraction
- larger deviation of results between image analysis (II) and laser diffraction, than between image analysis (I) and mechanical sieving.
- using size metric from image analysis (I) gives closer average particle size to the data from producer, and similar majority size range between 250-500 µm
- anisotropy from image analysis results shows highly elongated shape of aggregates.

feature analysis

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Possible reasons for the mismatch

I. mismatch between laser diffraction Vs. image analysis I
   i. limitation of laser diffraction machine to detect particles above 600µm
   ii. limitation of Fraunhofer theory: assuming all particles are spherical
   iii. missing of small aggregates/ out-of-border aggregates after segmentation → excessive segmented large aggregates
   iv. influence on the size of selected metric from the binning during particle disconnection (error might be larger when using extent along 1st longest principal axis than that long 2nd longest principal axis)

II. mismatch between mechanical sieving Vs. image analysis II
   i. lack of large quantity mechanical sieving measurements
   ii. missing of small aggregates/ out-of-border aggregates after segmentation → excessive segmented large aggregates
   iii. influence on the size of selected metric from the binning during particle

Conclusion and Outlook

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- **Conclusion**

current results still not optimal, but:

- ✓ potential of using image-based unsupervised analysis methods on aggregate study in mortars, concrete and other porous building material
- ✓ benefit of multi-dimensional data from in-line phase-contrast imaging technique
- ✓ familiarity with different image analysis methods
- ✓ further usage as noise calibration for signal change in time-differential phase-contrast dataset due to water change in sample during drying process

Conclusion and Outlook

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- **Outlook**
  - finer ring artifact removal slice-wisely
  - systematic testing and evaluation of clustering segmentation
  - optimization of thresholding methods
  - combination of other segmentation methods

    ex, clustering/threshold → marker-based watershed segmentation
  - reduction of computation time for full volume feature analysis
  - better correlation of feature analysis to real particle features

    ex. using known samples to characterize the precision of using the selected size metric
  - sensitivity testing on PCA analysis results to image binning

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