Classification of diffraction patterns in Single Particle Imaging (SPI) experiments performed at X-ray free-electron lasers using a Convolutional Neural Network (CNN)

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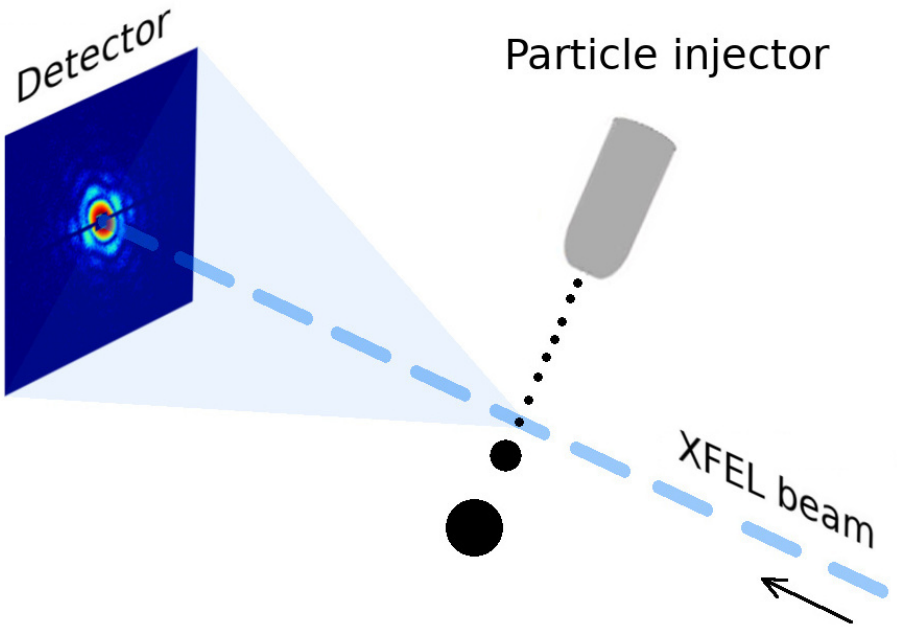
HELMHOLTZ RESEARCH FOR GRAND CHALLENGES

RSF Russian Science Foundation

DESY.

SPI experiment



LCLS 2018

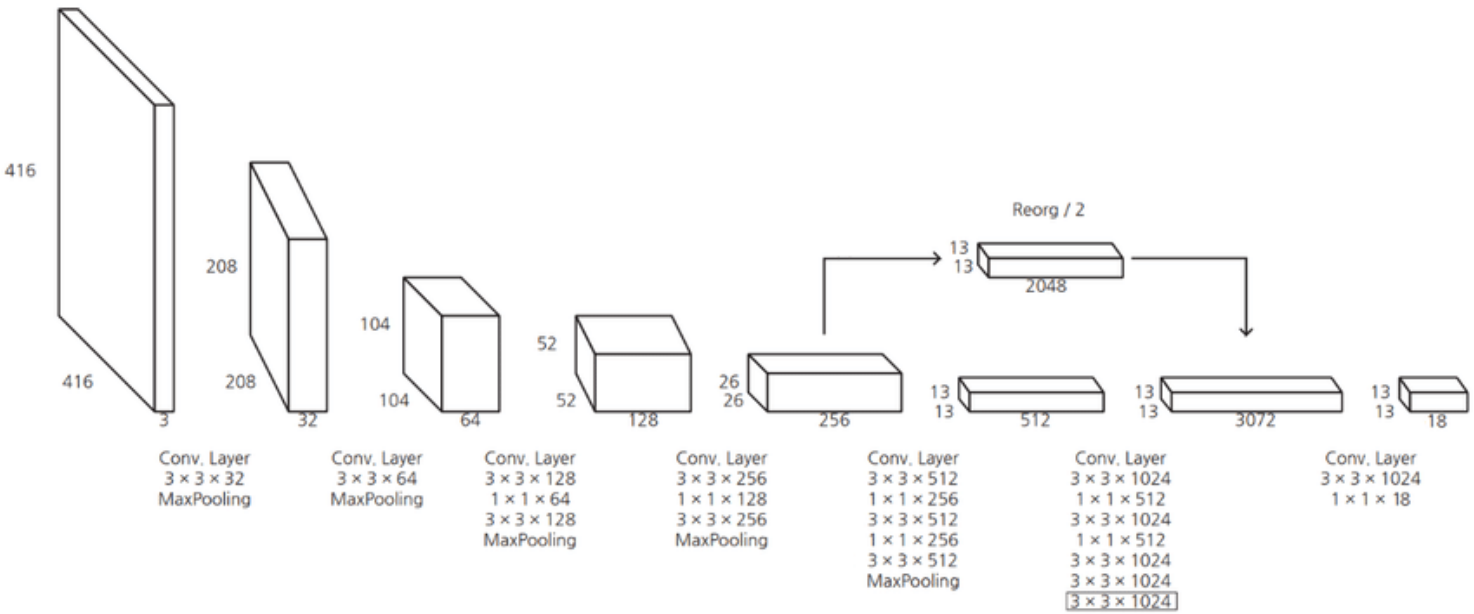
- AMO beamline at LCLS
- Sample – bacteriophage PR772, expected size 60-75 nm
- E = 1.7 keV (λ = 7.29 Å)
- Detector distance = 130 mm
- Detector – pnCCD, one plane (512×1024) was operational

Data processing pipeline:

Pre-processing → Classification → Orientation determination & background subtraction → Phase retrieval and structure reconstruction

Classification: hit finding, size filtering, single-hit classification

YOLOv2



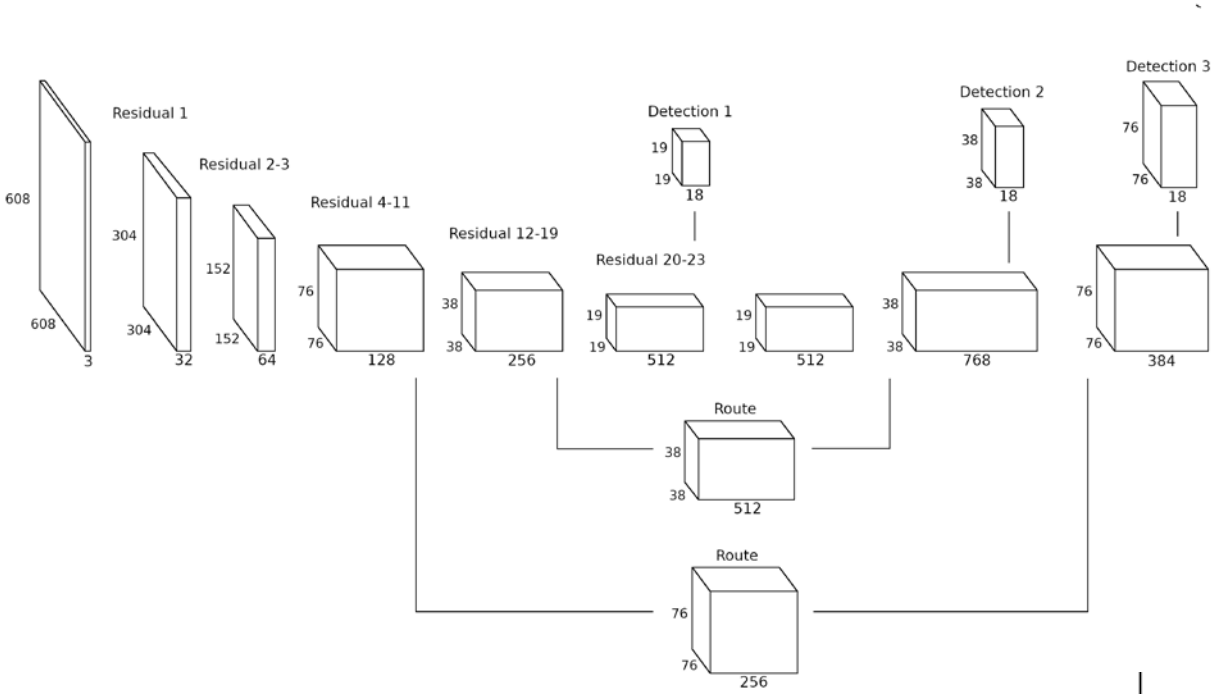
S. Seong et al., Determination of Vehicle Trajectory through Optimization of Vehicle Bounding Boxes using a Convolutional Neural Network. *Sensors* **2019**, *19*, 4263

Darknet-19 feature extractor trained on ImageNet
+ 1 convolutional layer: 20 convolutional layers

Loss function with classification and localization terms

Stochastic gradient descent (SGD) used for minimization
Batch size: 64

YOLOv3

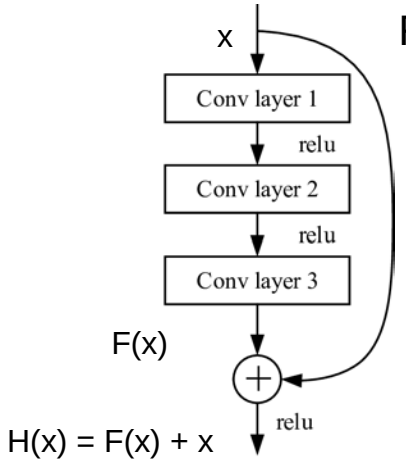


Darknet-53 feature extractor trained on ImageNet
53 convolutional layer in feature extraction

Residual architecture

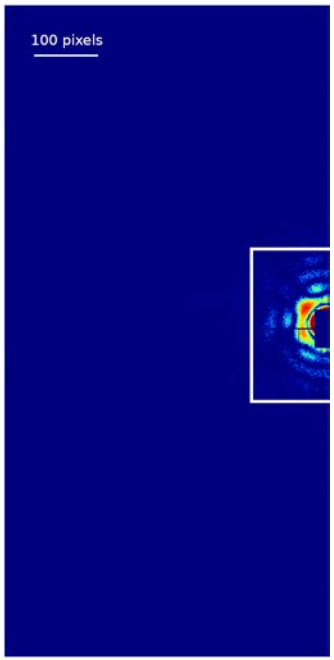
Loss function with classification and localization terms

Stochastic gradient descent (SGD) used for minimization
Batch size: 24



Residual block

Data preparation



HDF5 file

Pattern
512×1024

ROI
123×240

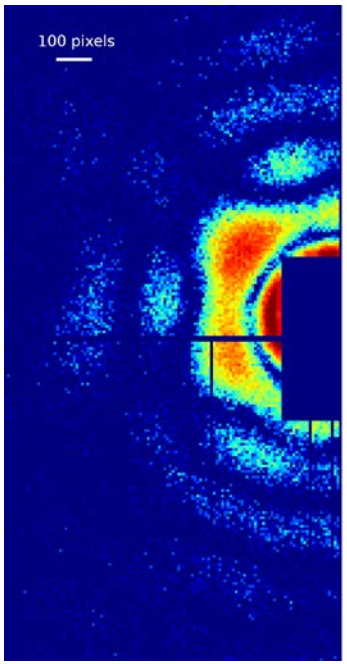


Image file

954×1855

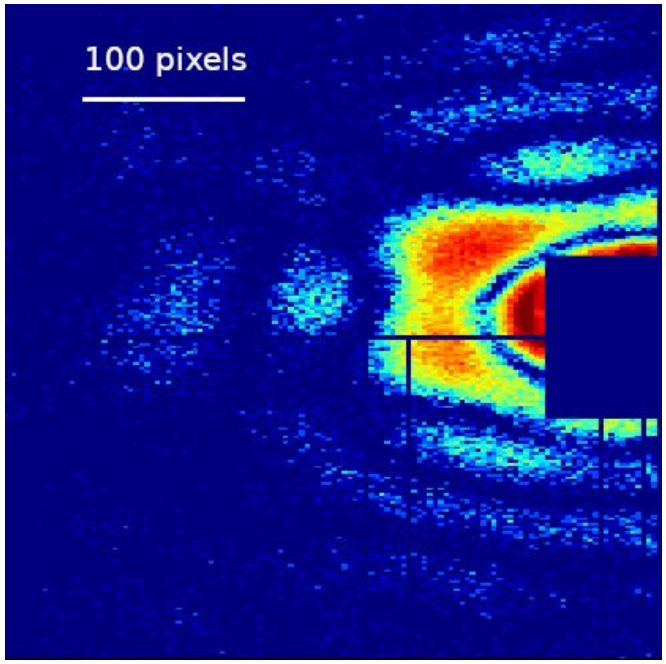


Image file

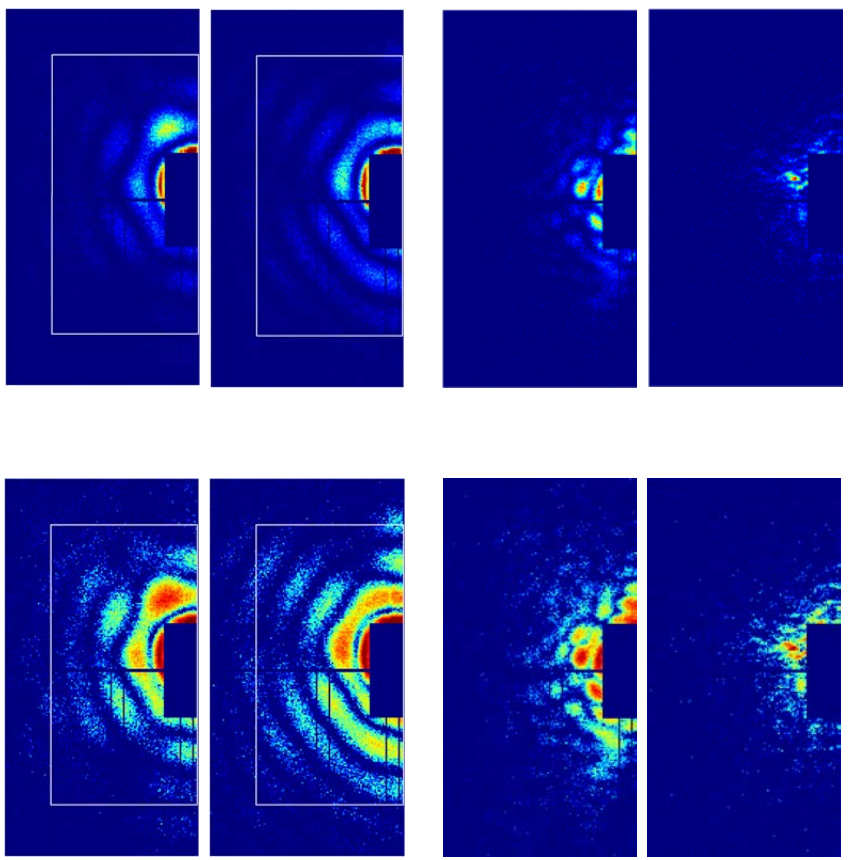
416×416
(YOLOv2)

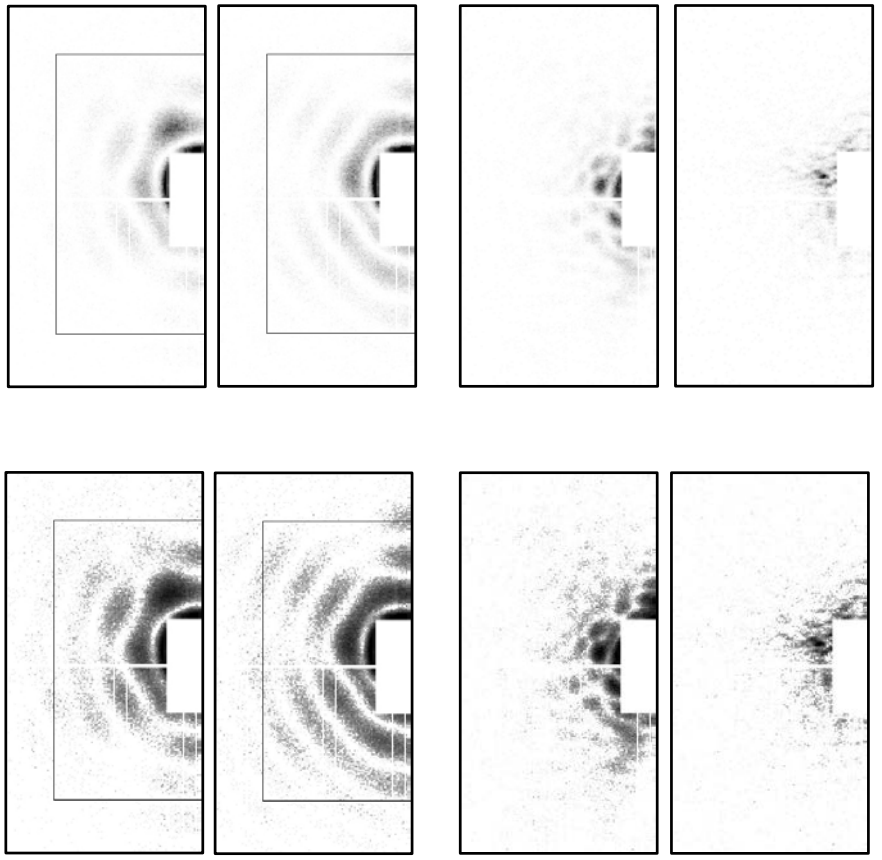
608×608
(YOLOv3)

Data representation

Color (3 RGB layers, “jet” color scheme)

Grayscale (3 identical layers)





Linear scale

Logarithmic scale

Positive

Negative

Positive

Negative

$I(q) \sim q^{-3} \div q^{-4}$

Training, validation and test sets

Training set

165 positive examples (single hits)

390 negative examples

Validation set

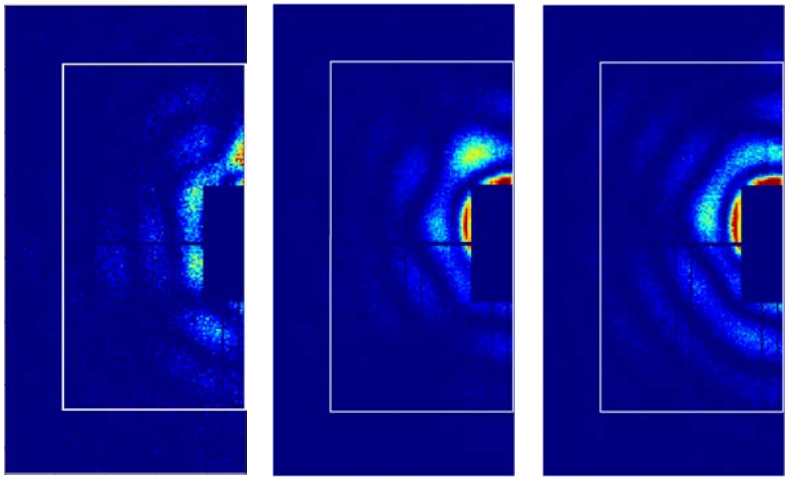
53 positive examples (single hits)

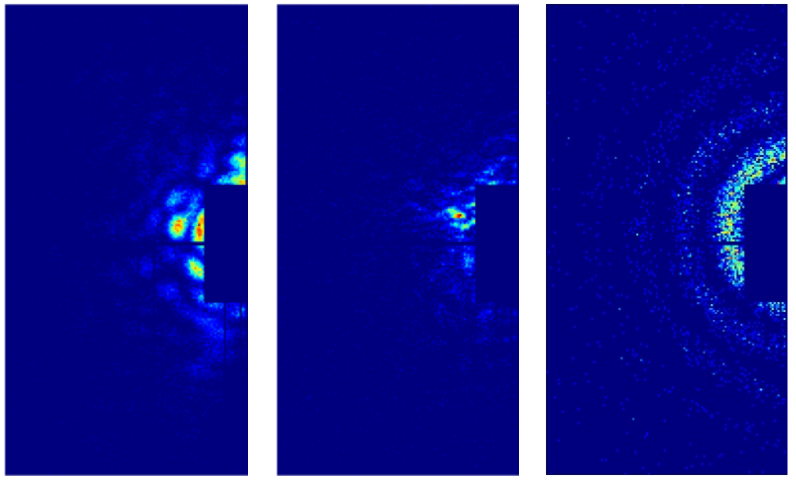
283 negative examples

Test set
(55-84 nm)

995 positive examples (single hits)

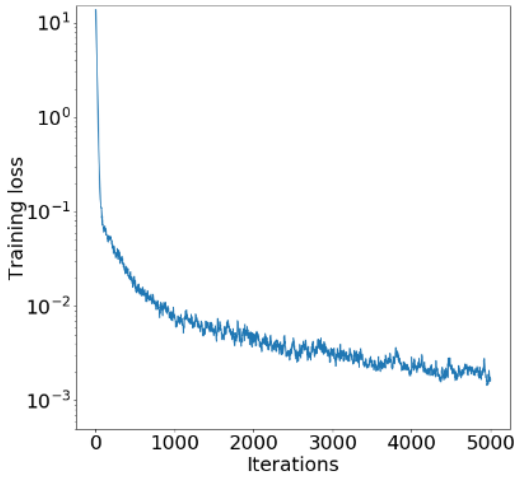
16 937 negative examples

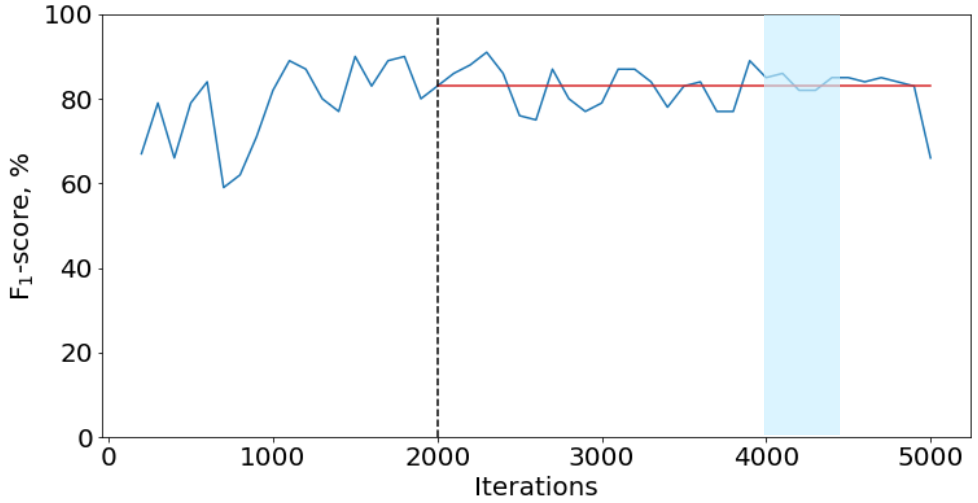




Training, validation and test

Observe training loss every iteration and save model every 100 iterations





Validation procedure to find an optimal training stage (not to optimize the hyper-parameters, *i.e.* size and number of filters, learning rate, batch size etc)

Calculate F_1-score on validation data set (every 100 iterations) to control overfitting

Intersection selection (4000, 4100, 4200, 4300 and 4400 iterations) for test

Results

Intersection selection

Model	Number of selected single hits	Intersection with manual selection	IoU for manual selection, %	Accuracy, %	Precision, %	Recall, %
YOLOv2, color, linear	1185	597	38	95	50	60
YOLOv2, color, log	1368	614	35	94	45	62
YOLOv2, grayscale, linear	1756	622	29	92	35	63
YOLOv2, grayscale, log	904	487	34	95	54	50
YOLOv3, color, linear	1041	505	33	94	49	51
YOLOv3, grayscale, linear	2316	465	16	87	20	47

Results

Comparison with a reference method

Model	Number of selected single hits	Intersection with manual selection	IoU for manual selection, %	Accuracy, %	Precision, %	Recall, %
YOLOv2, color, linear	1185	597	38	95	50	60
EM based	1085	574	34	94	53	48

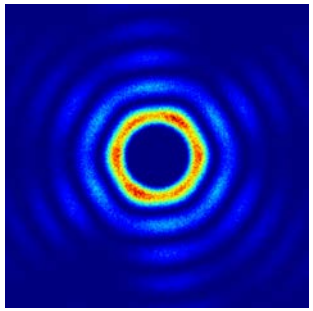
Ground truth: manual selection

A. Ignatenko et al. (2020) "Classification of diffraction patterns in single particle imaging experiments performed at X-ray free-electron lasers using a convolutional neural network", *Machine Learning: Science and Technology* (submitted). Preprint available http://arxiv.org/abs/2008.07288

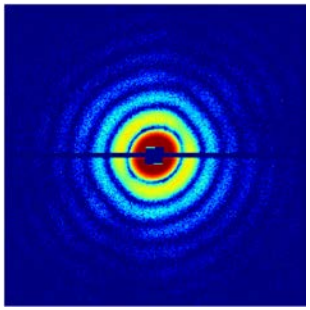
Outlook

- Build a custom CNN and train with diffraction patterns to the full depth
- Optimize hyper-parameters (use larger filters, reduce number of filters, increase batch size)
- Try state-of-the-art architectures
- Try methods of self-supervised and semi-supervised learning
- Attempt to generalize for many objects

Train with large amount of data: simulated+experimental data for many objects, extensive data augmentation



Simulated pattern (central part masked out)



Experimental pattern

Thank you for your attention!

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