AI-based High-throughput X-ray Imaging

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Outline

- **Motivation**
  - Synchrotron-based X-ray Imaging
  - Methods for Life and Material Sciences
- **Components**
  - Deep Learning for Image segmentation
  - Simulation and Generative Modelling
  - Virtual Experiments
  - Neural Networks for Inverse problems
  - Evaluation of ML algorithms
- **Domain adaptation and Transfer Learning**
- **Unsupervised Learning**
- **Data and Experiment Lifecycle**
- **Outlook**

Motivation

Synchrotron-based X-Ray Imaging

Modern **synchrotron** light sources provide enormous photon flux densities.

Huge progress in detector technologies:

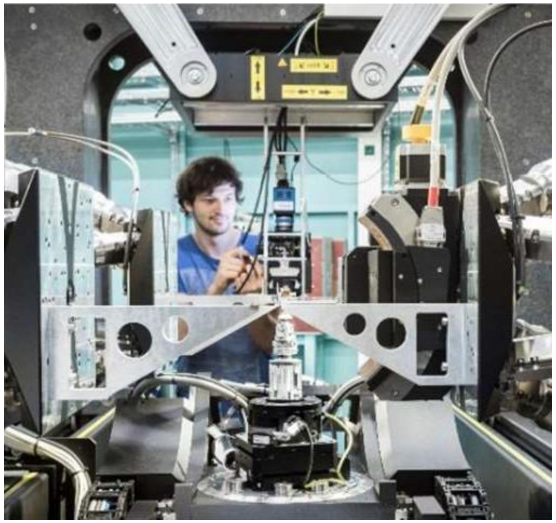
- High resolution
- Fast data acquisition
- Large storage capacity

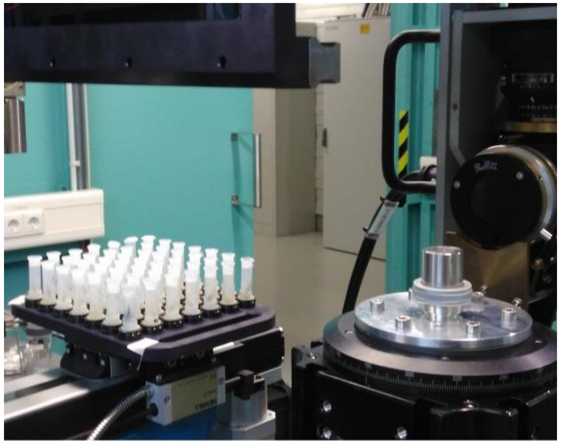
Methods:

- *In vivo* & *in situ* radiography and tomography
- **High-throughput** experiments with robotic sample changer

As a result:

- up to **10M** frames/s
- 20 tomograms/s
- 40 high resolutions (30 GB) samples/hour
- **hundreds** of samples per day!





robotic sample changer

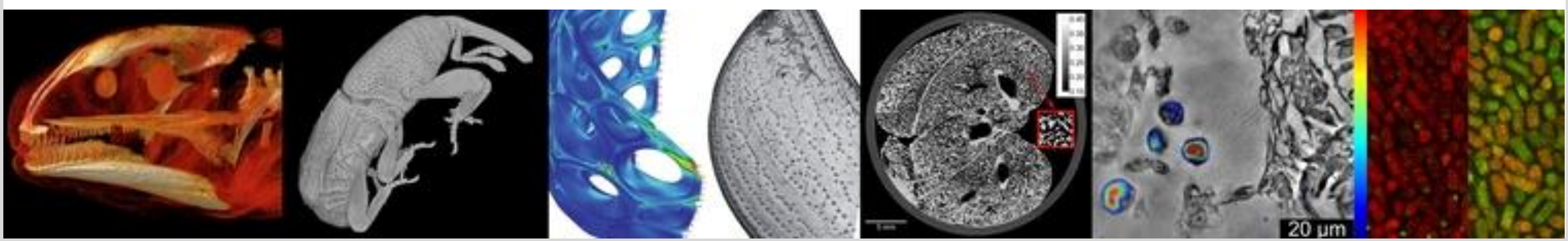
X-Ray Imaging for Life Sciences

Methods for hierarchical, correlated, *in vivo* imaging of organisms, tissues and cells:

- 3D phenotype atlases of model organisms
- Comparative 3D morphometrics of small animals
- 4D developmental studies of embryos
- 4D morphodynamics: mating, feeding, etc

Application fields:

- Developmental biology
- Genetics
- Medicine
- Zoology
- Palaeontology
- Environment
- Biotechnology
- Tissue Engineering
- Biomimetics



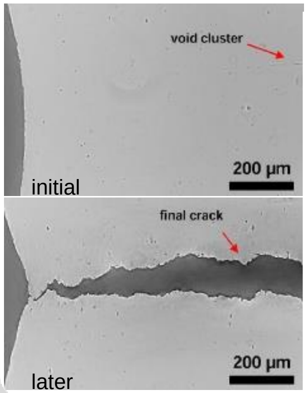
X-Ray Imaging for Material Sciences

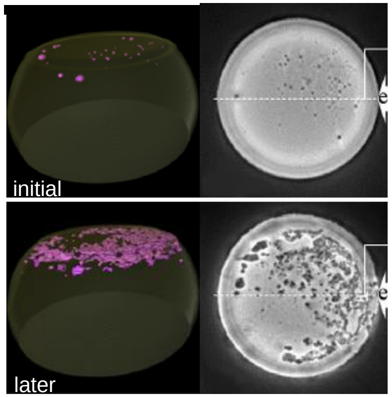
Methods for correlated, *in situ & operando* imaging of materials and processes

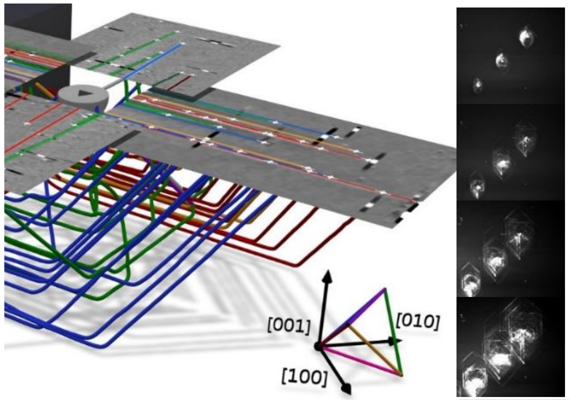
- Non-destructive 3D imaging
- Multi-contrast (absoption, phase-contrast, fluorescence)
- **Hierarchical** imaging (2D/3D screening and zooming into ROIs)

Application fields:

- Energy
- Nanotechnology
- Information Tech.
- Transport
- Fluid dynamics
- Aerospace

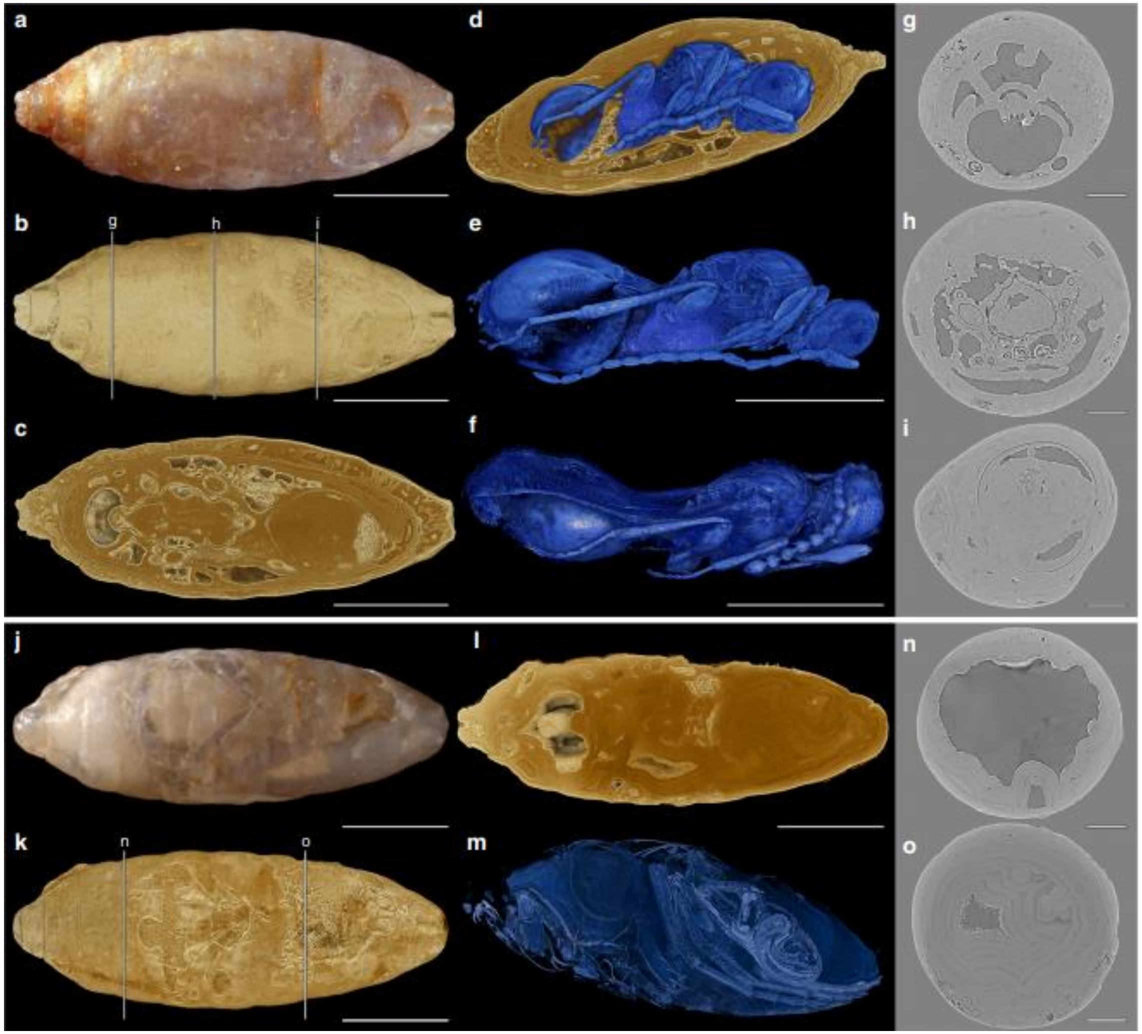






Deep Learning
for Image Segmentation

High Throughput Tomography of Fossils

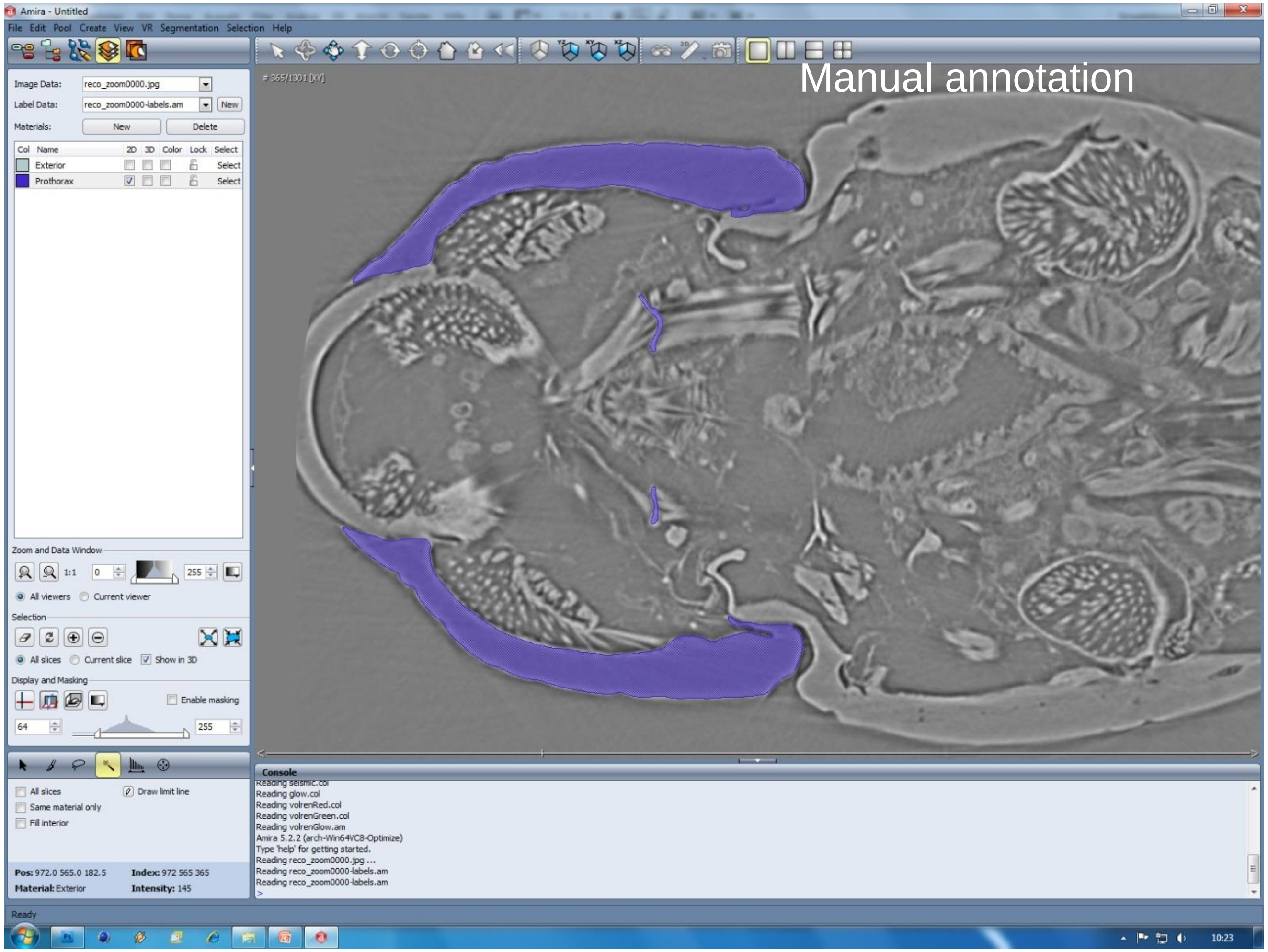


- **1510** fly pupae scanned in one week
- **55** parasitoid wasps found

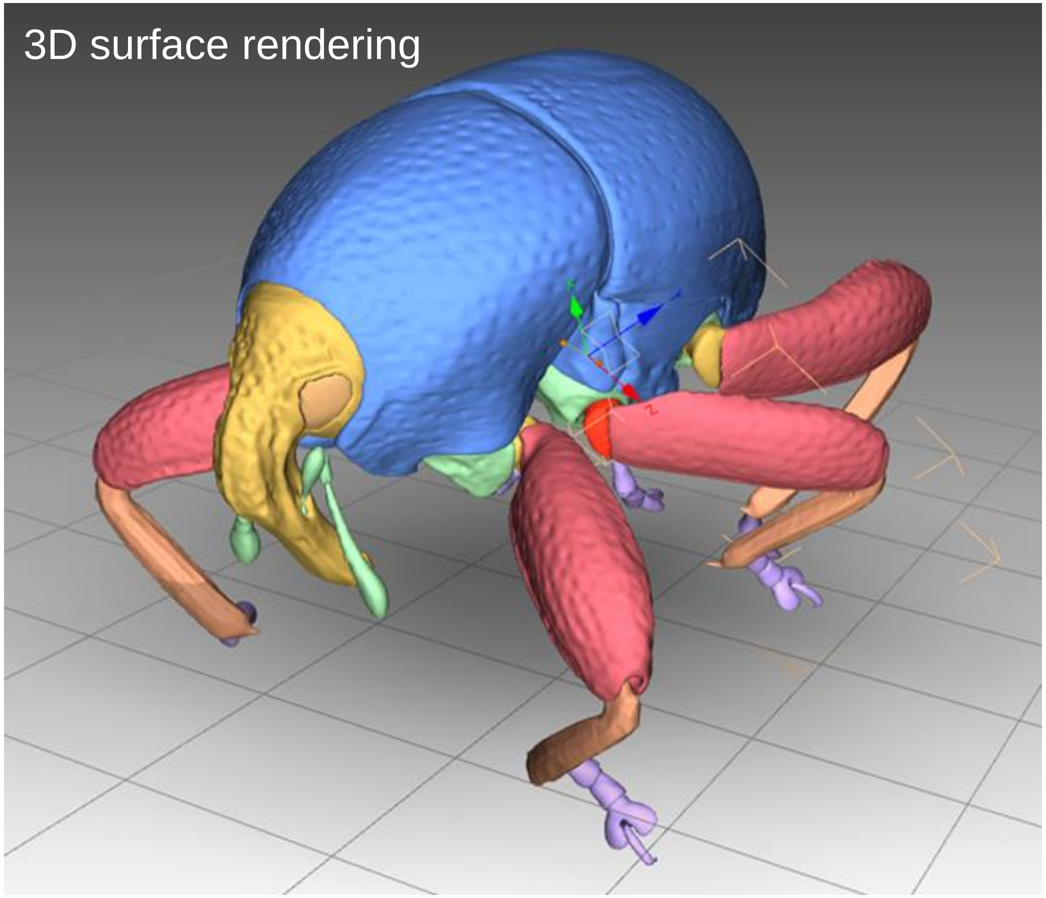
Van De Kamp et al. 2018: **Nature Communications**

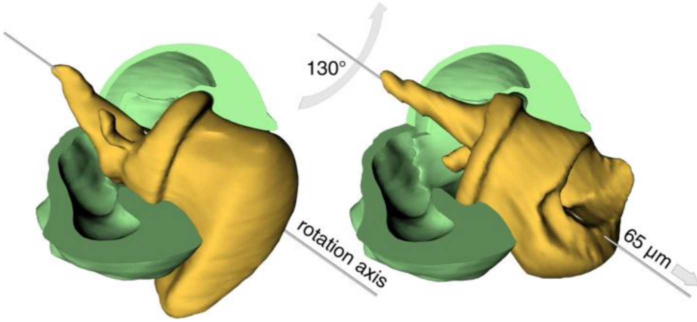
Segmentation: Manual approach

Aim: High quality **segmentation** of morphological structures in specimens.



Segmentation: Manual approach





Biological screw joint

Trigonopterus weevils

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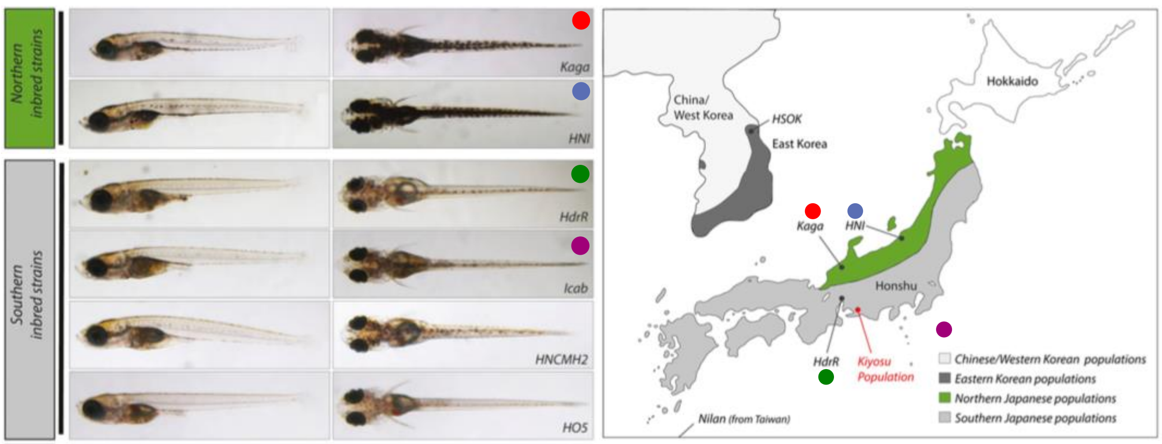
3D Morphometric Analysis

Model organisms provide insight into the working of other organisms.

- Aims:
  - Study of morphological data as basis for genotype-phenotype association
  - **Ultimate**: A smart way to decode the genome of a specimen



different phenotypes

Oryzias latipes (Medaka)

In collaboration with:

Centre for Organismal Studies Heidelberg

UNIVERSITÄT HEIDELBERG ZUKUNFT SEIT 1386

EZRC

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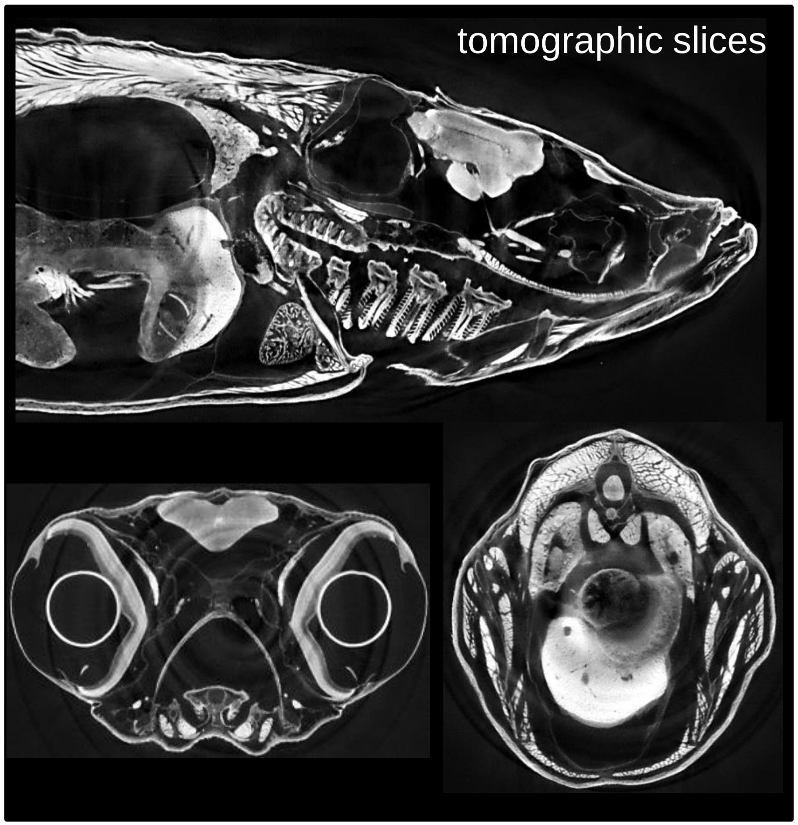
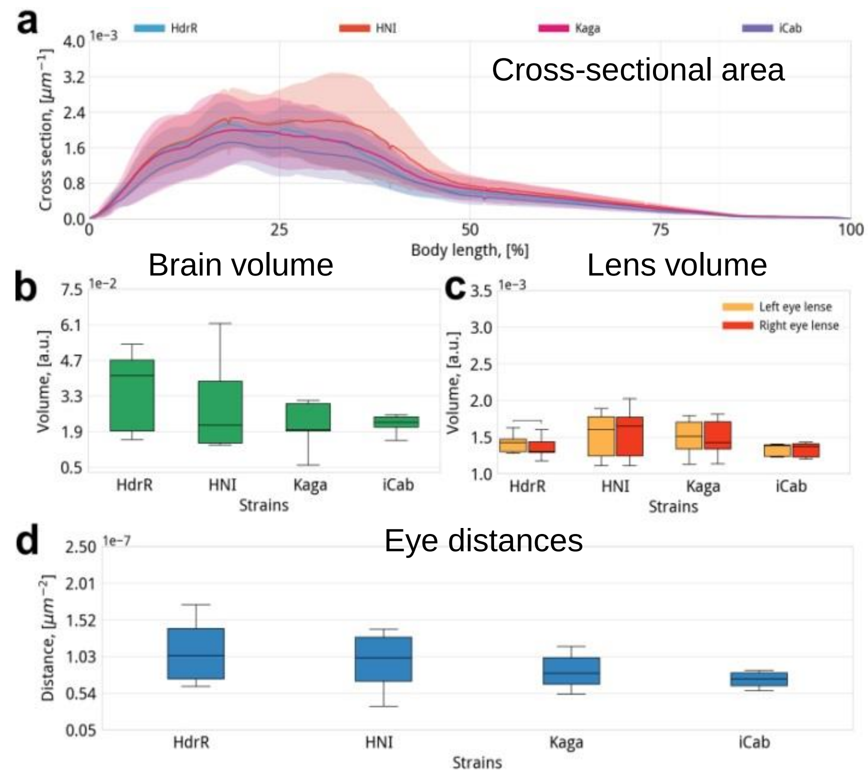
3D Comparative Studies

Model organism: Medaka fish, different inbred lines

Comparative study of inbred lines for the identification of line-specific characters





Statistical analysis

V. Weinhardt et al., SREP 2018

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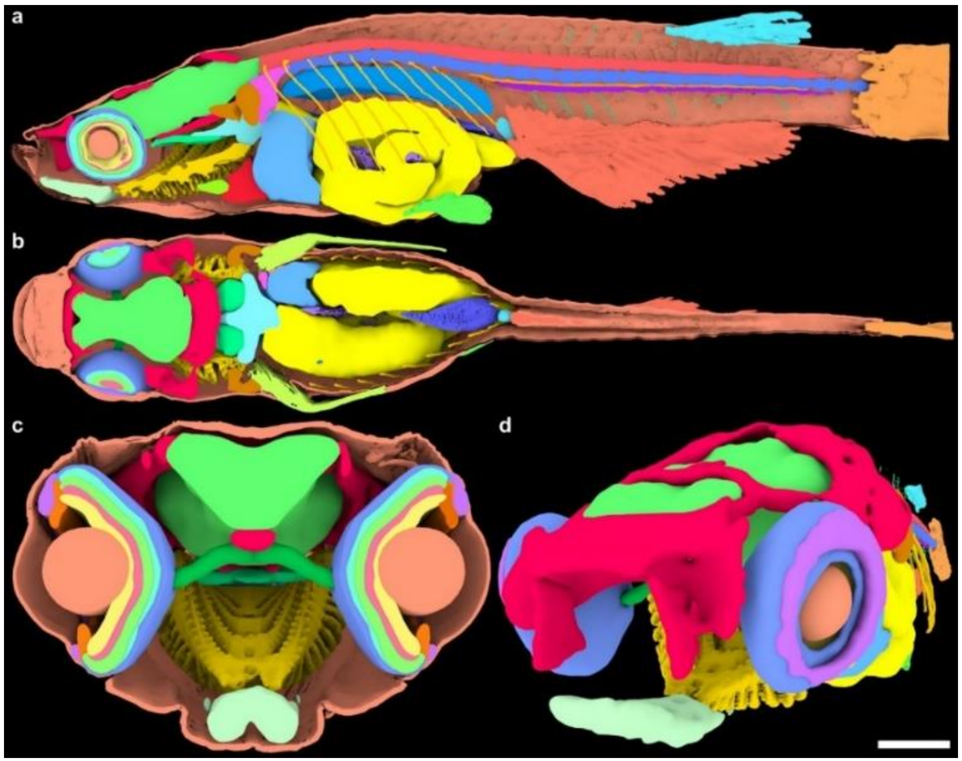
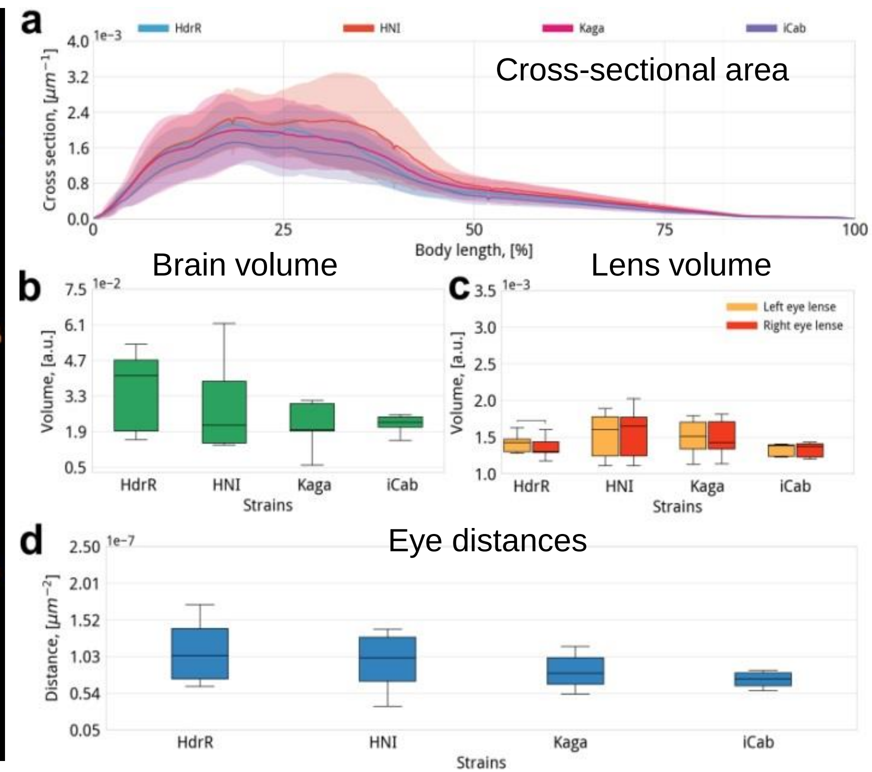


full body 3D digital atlas



Statistical analysis

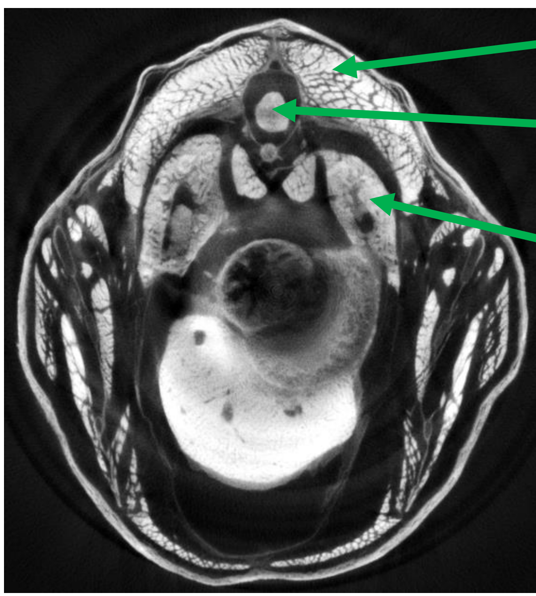
V. Weinhardt et al., SREP 2018

Challenges

Shape variation among specimens

Hearts

Contrast variations between organs



Muscles

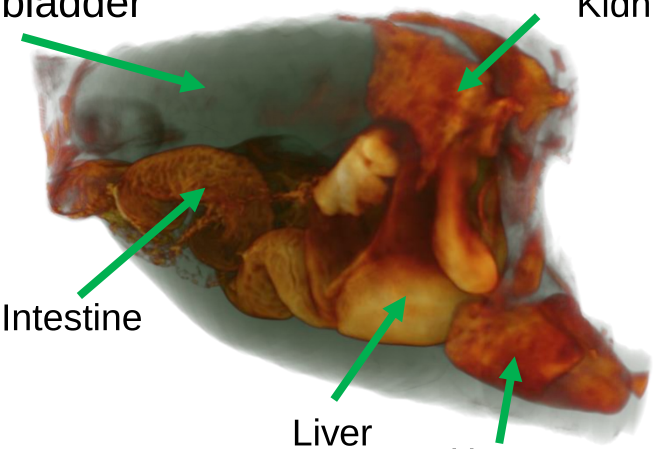
Spinal cord

Kidneys

Tightly **packed** organs.

Swim bladder

Kidneys

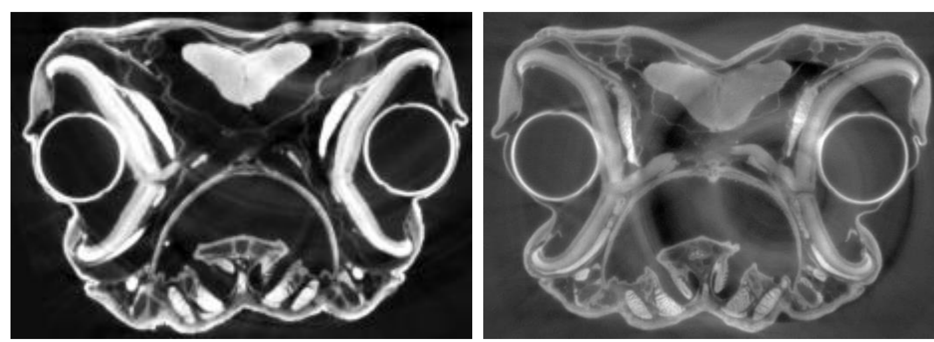


Intestine

Liver

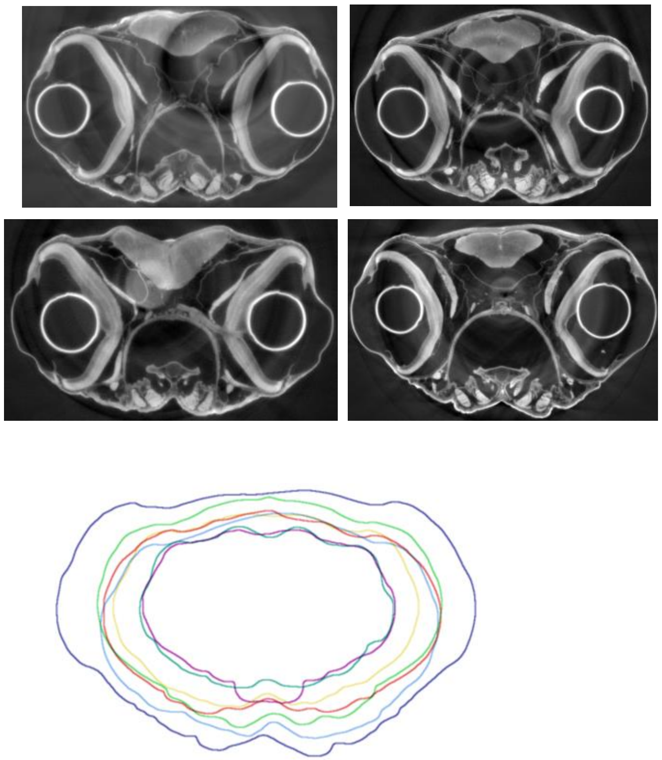
Heart

Contrast **variations** between **specimens**

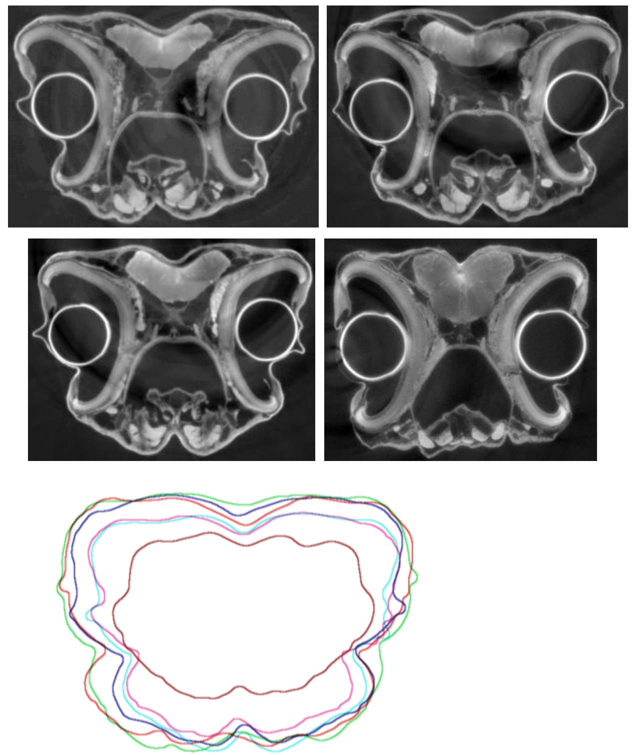


Challenges

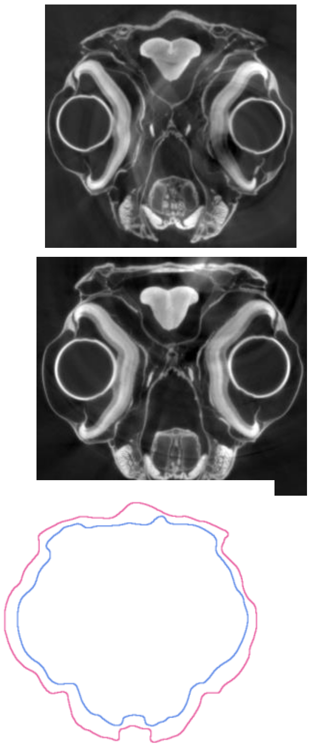
Large **morphological variability** which we want to measure with high precision.



fish line 1



fish line 2

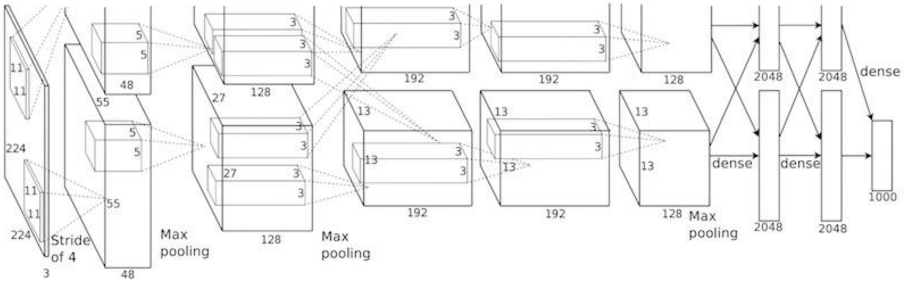


fish line 3

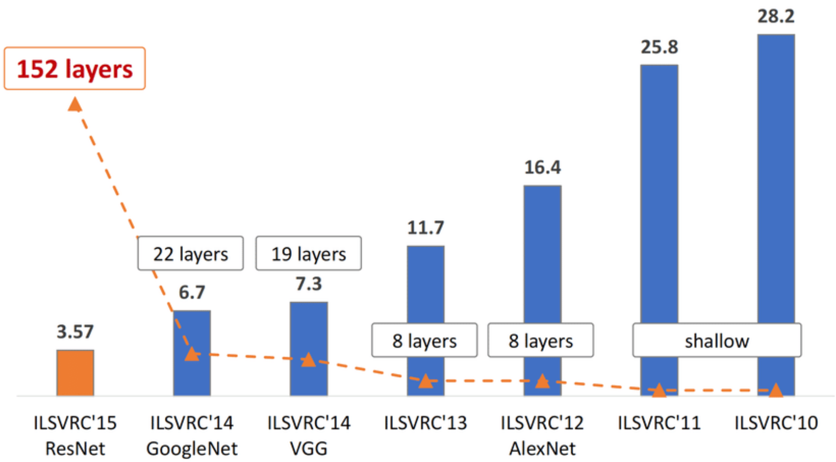
How to design **accurate**, **robust**, but also **general** segmentation procedure?

Computer Vision: Automated classification

AlexNet: Approach based on **deep neural networks**.

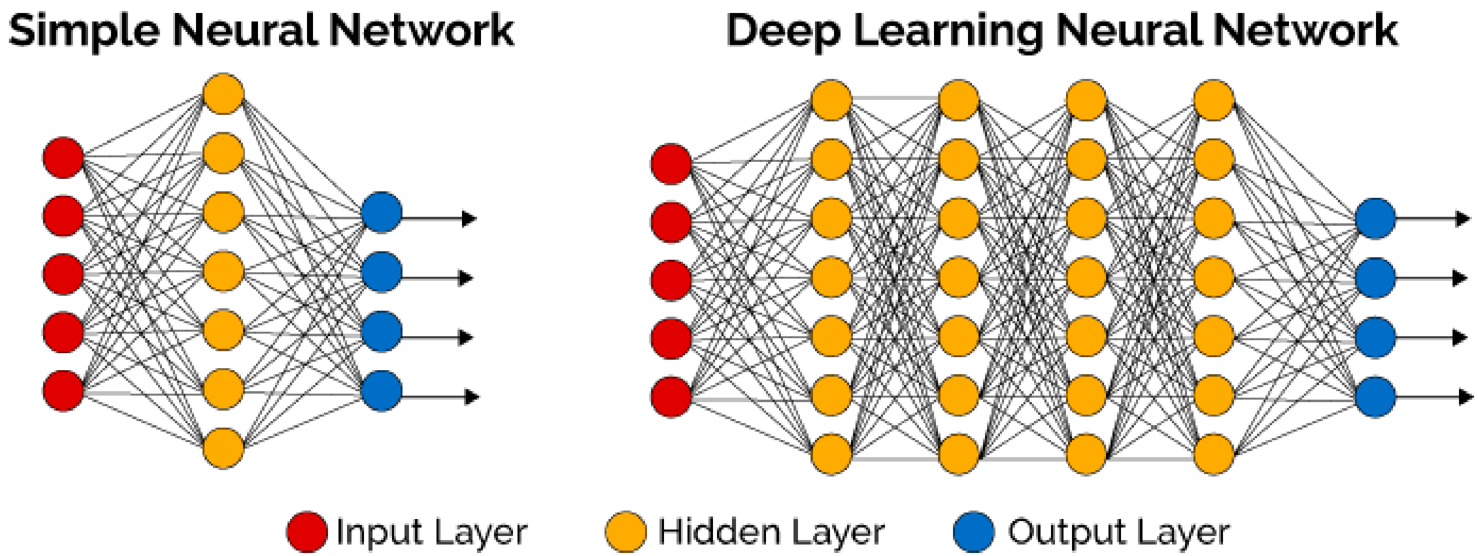


Krizhevsky et al., arXiv, 2012



Russakovsky et al., arXiv, 2014

Deep Learning



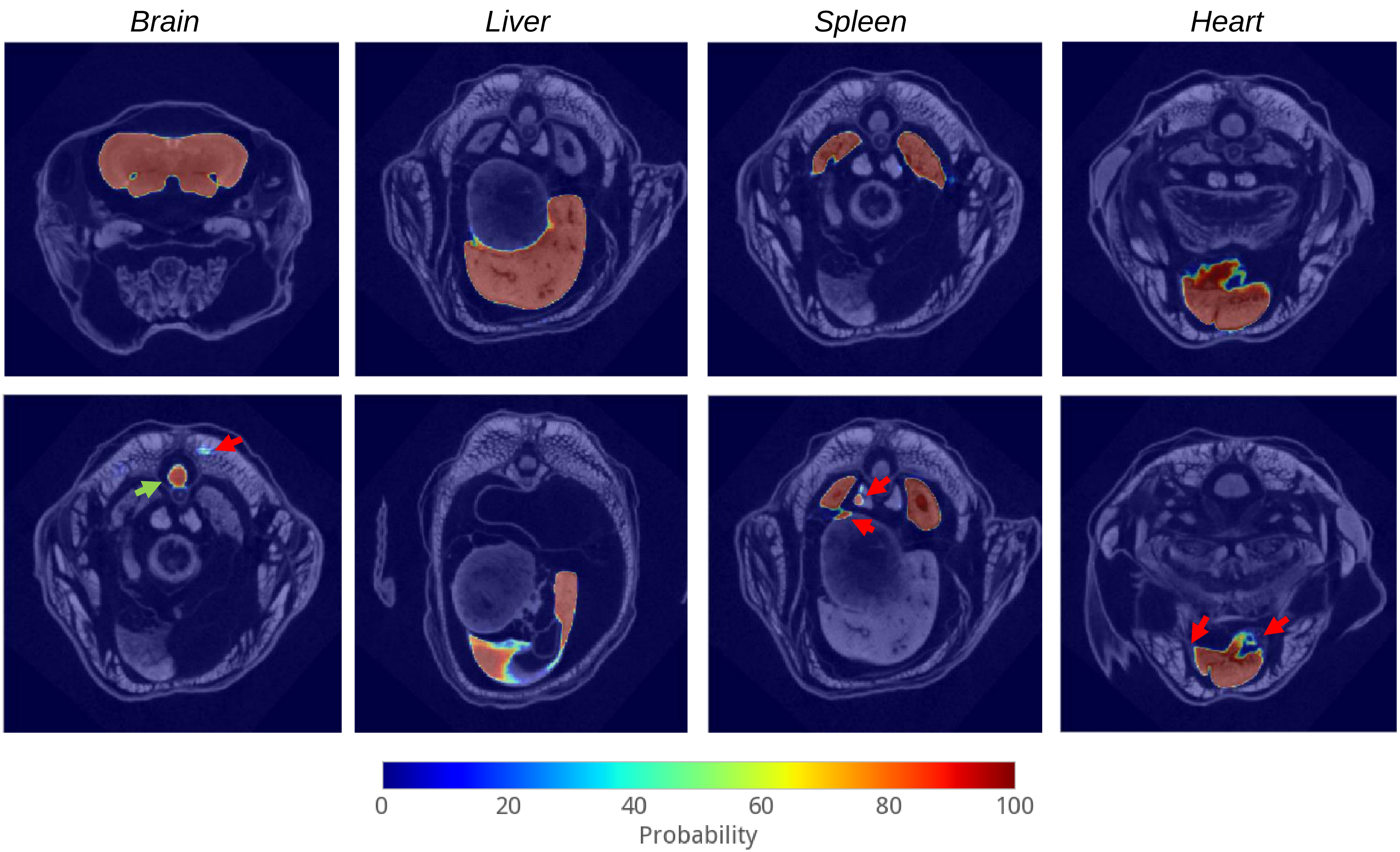
Learnable linear classifier

Deep, hierarchical, non-linear model

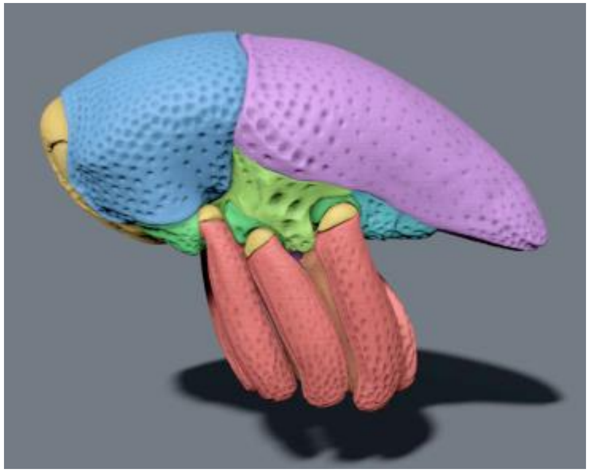
Idea:

- Train the model on a large amount of manually labeled data
- Optimize on each step to improve a certain metric (find best mapping)
- Apply on the new data

Deep Learning: Organ Segmentation



Processing Time and Costs



Full body segmentation, **1500** samples, **10** organs

	Manual	Neural Networks
Time: One dataset	77 h (215 slices + inter.)	(24 h + 2 min) * 10 ~ **240 h**
Time: All	77 * 1500 = **13 years**	(24 h * 10) + (2 min * 1500) ~ **30 days**
Computation cost	**a lot**	30 * 24 * **0.5** Euro / h = **360** Euro

Google Cloud Platform

Deep learning outperform classical methods on large datasets: both more precise and cost effective

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Challenges for Deep Learning

Deep learning methods provide very promising results.
But there are some open questions and challenges.

- Training ➡ **Ground truth** data
- Variation in data ➡ **Generalization** of NN Models
- Common data features ➡ Model Sharing and **Transfer Learning**
- Different conditions / experiments / methods ➡ **Domain adaptation**
- New applications / methods ➡ **Unsupervised Learning**

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Karlsruhe Institute of Technology

Simulation and Generative Modelling

syris: Virtual X-ray Imaging Lab

Karlsruhe Institute of Technology

- Aims
  - Design and **optimize experiments** and **imaging conditions**
  - Evaluate image processing **algorithms**, choose best parameters
  - **Train Machine Learning** methods on **synthetic** data
- Approach
  - Model complete experiment and data acquisition
  - Python API for easy usage
  - GPU accelerated computation

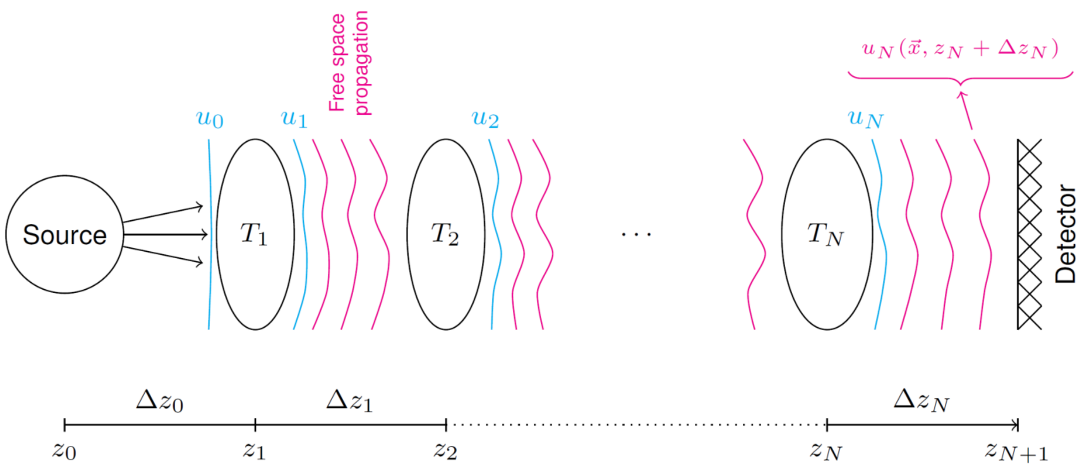


Image formation in ***syris***

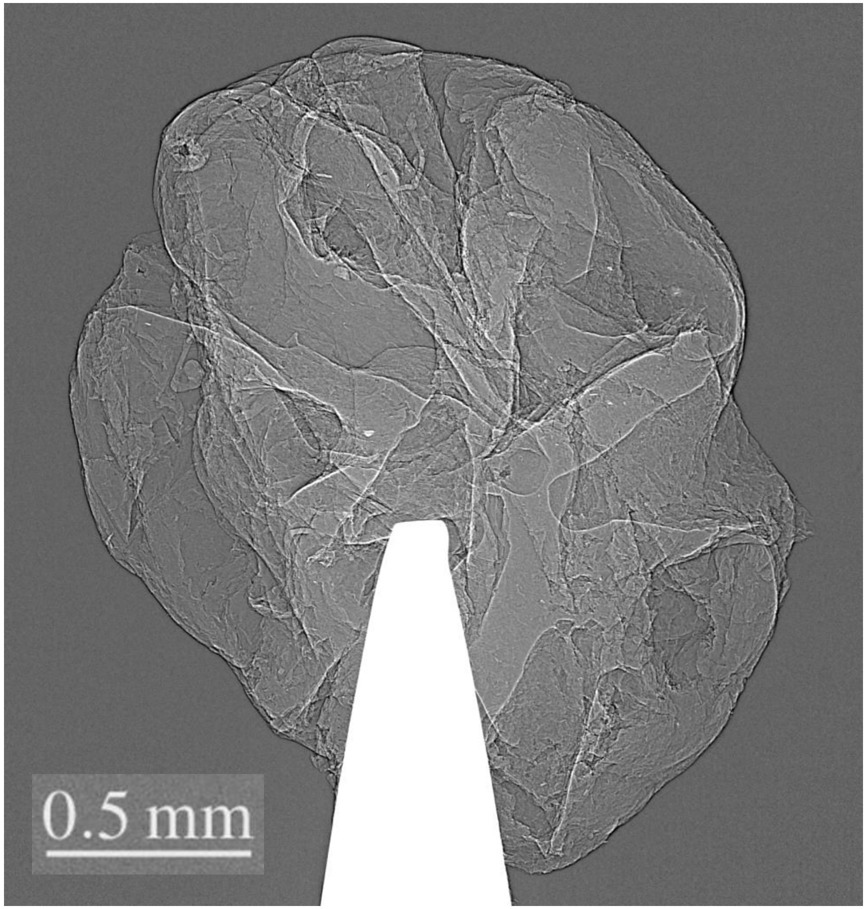
syris: Simulation Parameters

Category	Parameter	Value
Source	Storage ring energy	2.5 GeV
	Source type	Bending magnet
	Source size (FWHM)	–
	Magnetic field	1.5 T
	Electric current	106 mA
	Beam mode	White beam
	Energies	8 keV to 30 keV, 1 keV step
	Filters	0.7 mm aluminium
	Slit position	–
	Slit opening	–
Sample	Material	Wax on a steel needle
	Dimensions	1.5mm × 1.5 mm × 1.5 mm
	Source distance	–
	Detector distance	82 mm
Acquisition	Experiment	Tomography
	Number of projections	3000
	Data processing	Flat-field correction
	Reconstruction algorithm	Filtered back projection

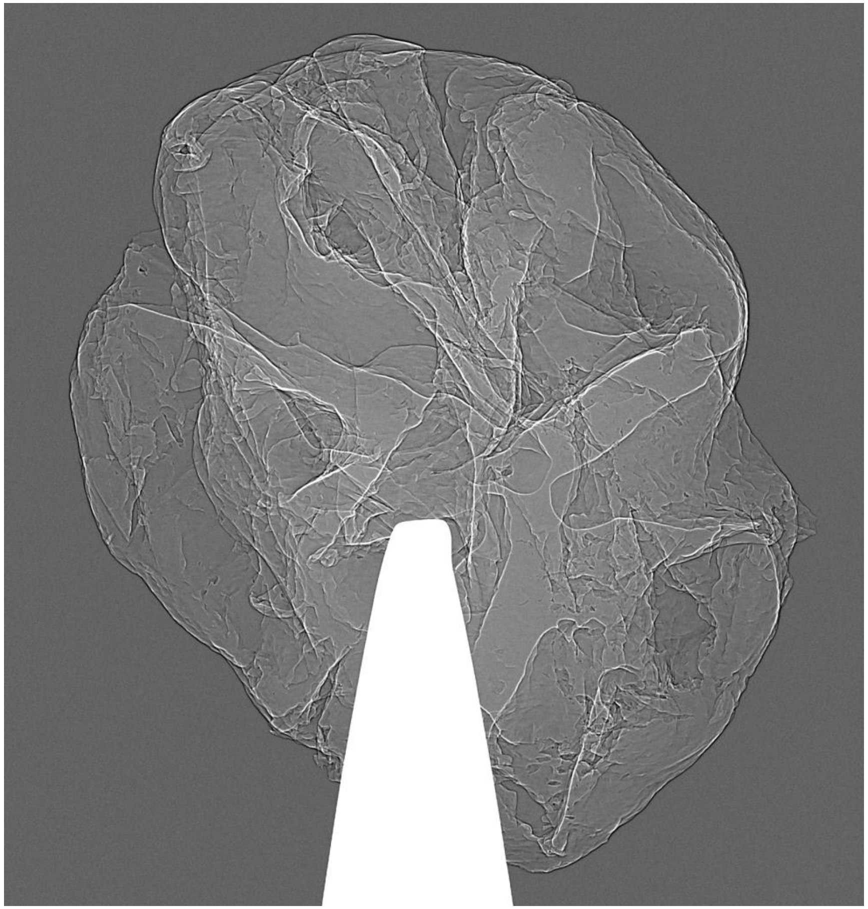
Detector system

Parameter	Value
Type	Indirect
Effective pixel size	1.22 µm
Objective lens	Mitutoyo Plan Apo
Magnification	10×
Numerical aperture	0.28
Scintillator	LSO:Tb (Lu_2SiO_5)
Density	7.4 g cm^{-1}
Thickness	12 µm
Light yield	36 photons keV^{-1}
Emission peak	545 nm
Camera	PCO.dimax
Sensor size	2016 × 2016
Sensor pixel size	11 µm
A/D factor	10 e^- per count
Quantum efficiency	49% at 525 nm
Dynamic range	1600:1
Frame rate	25 frames s^{-1}

syris: Simulation of a Complex Shape



Real data

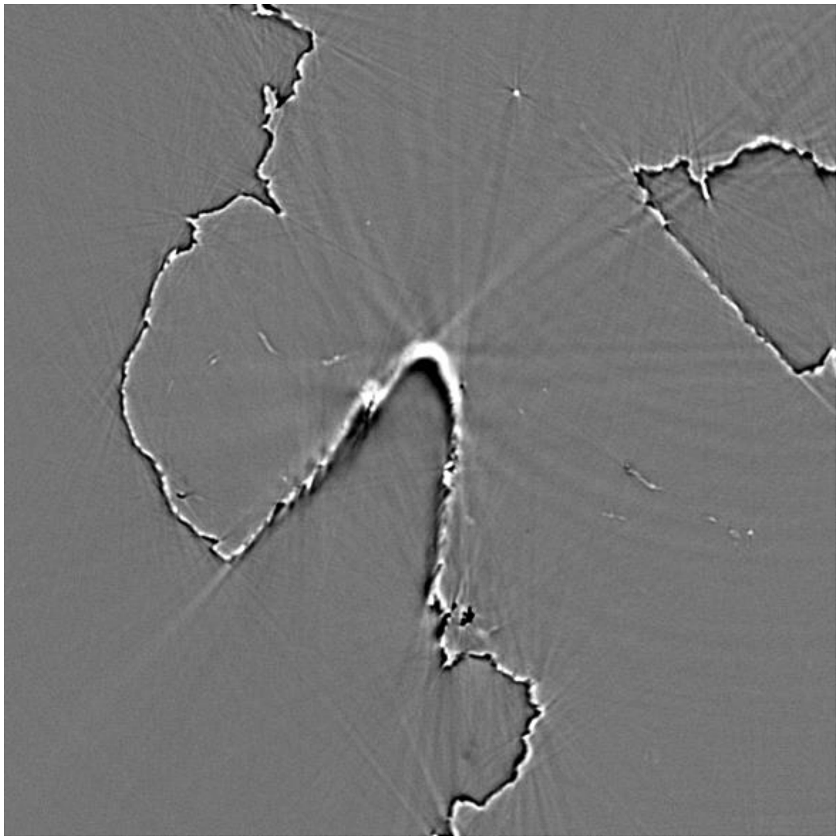


Simulation

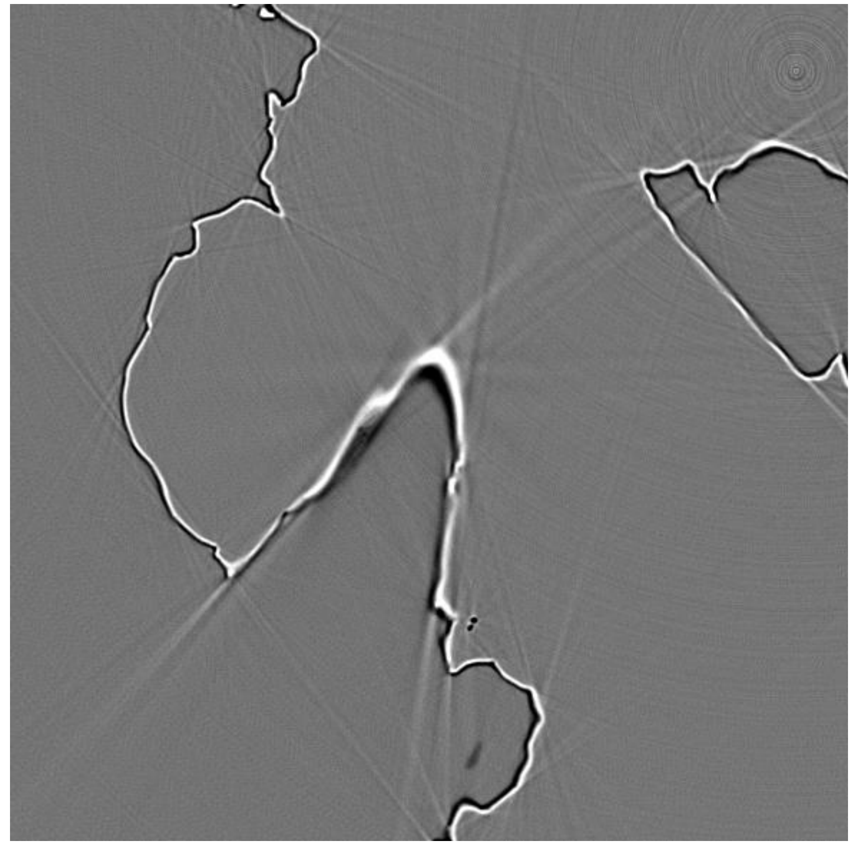
T. Farago et. al. ***syris***: *a flexible and efficient framework for X-ray imaging experiments simulation*, Journal of Synchrotron Radiation (2017)

syris: 3D Reconstruction

2D slice through the reconstructed volume



real data



simulated data

Use as **ground truth** data to train **Machine Learning** methods

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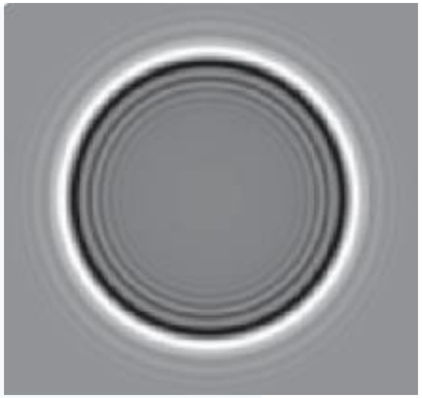
syris: Simulation example

A simple script to simulate a plastic ball in Python programming language.

```
syris.init()
energies = np.arange(10, 30) * q.keV
n = 1024
pixel_size = 0.4 * q.um
distance = 2 * q.m
material = make_henke('PMMA', energies)

sample = make_sphere(n, n / 4 * pixel_size, pixel_size, material=material)
image = propagate([sample], (n, n), energies, distance, pixel_size).get()
plt.imshow(image)
plt.show()
```



Open-source:

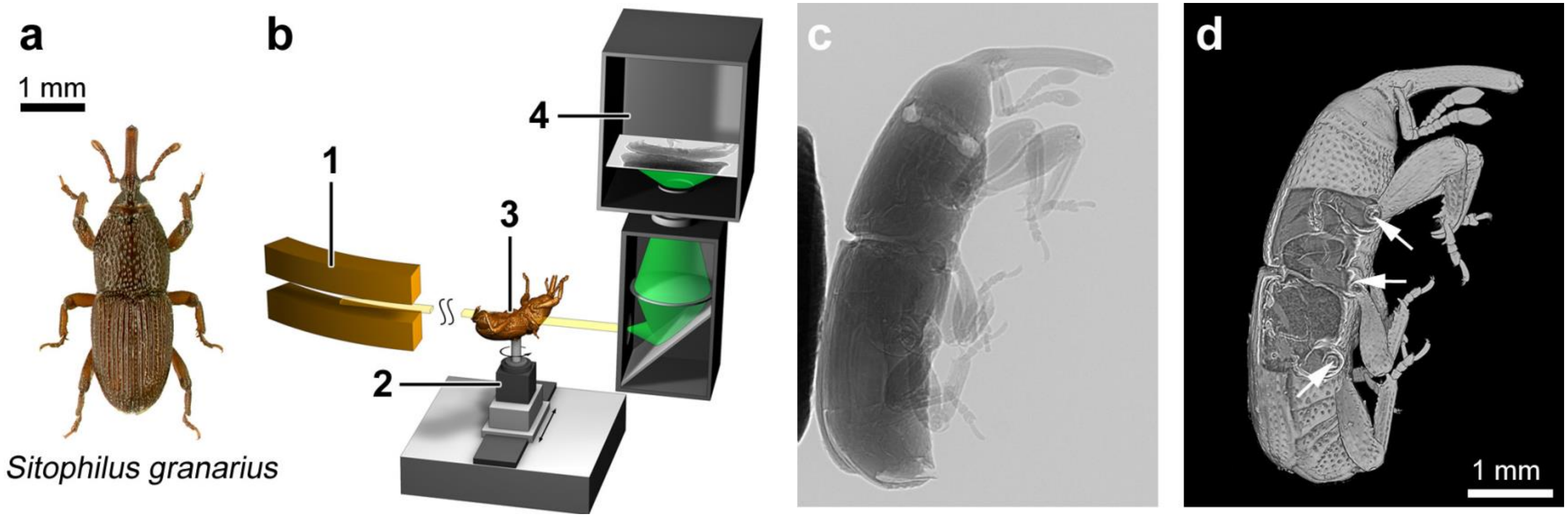
https://github.com/ufo-kit/syris

Virtual Experiments

Ultrafast *in vivo* 4D Cine-tomography

Application: Analyze the function of hip joints during defense mechanism in living insect.
Aim: Real-time study of structure **+** motion

Fast setup: **20** tomograms/s

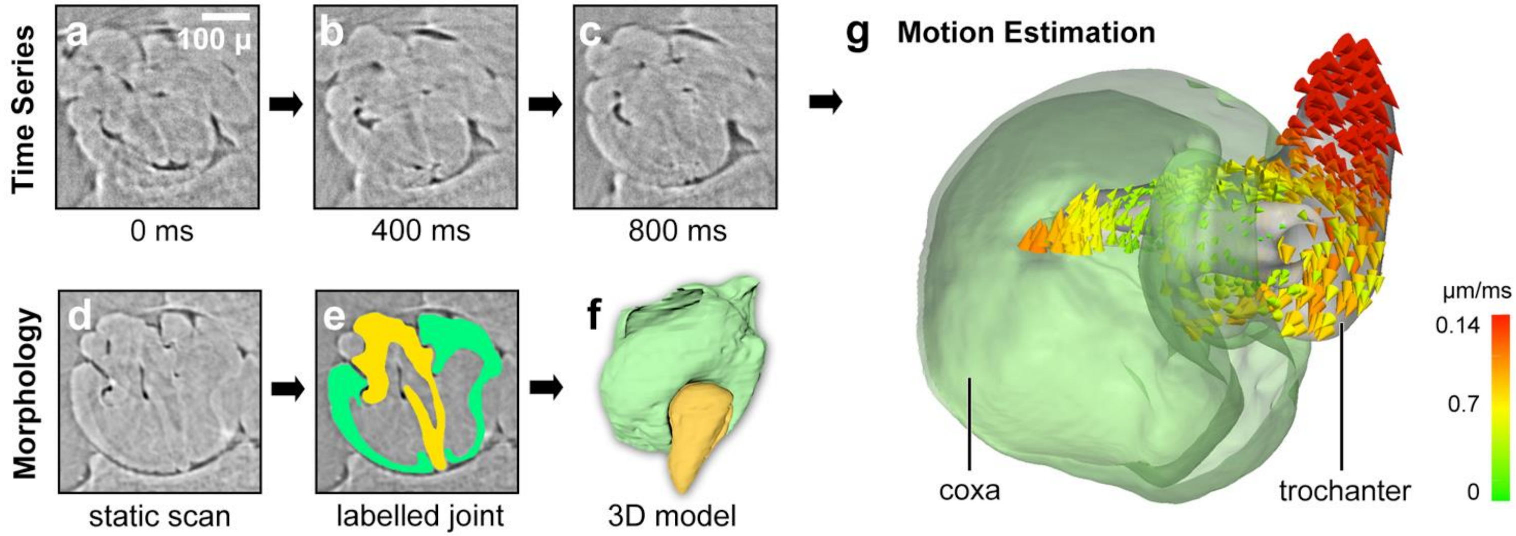


Experimental setup   Radiographic projection   Volume rendering

Source: beam energy E = 30 keV, photon flux = 10^{12}photons/s/mm^2

T. dos Santos Rolo et al. *In vivo X-ray 4D Cine-tomography for Tracking Morphological Dynamics*
Proceedings of the National Academy of Sciences 2014

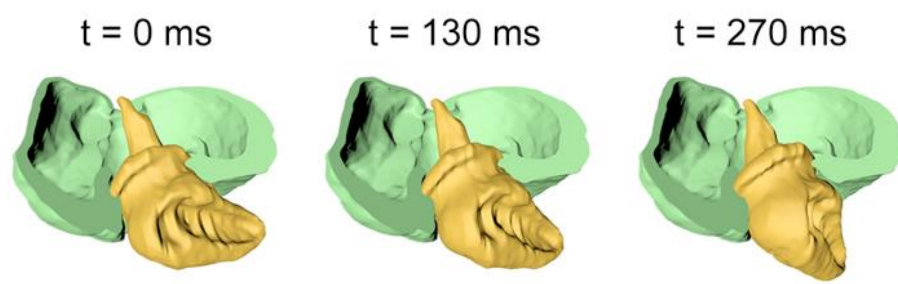
Motion Analysis and Kinematics



Challenge: How to design an experiment and find optimal conditions?

- We want:
  - **High**-resolution 3D data
  - **Ultra** fast acquisition
  - **Good** image quality
- But:
  - **Low** dose, longevity of a sample
  - **No** image artifacts

Reconstructing **Morphodynamics**



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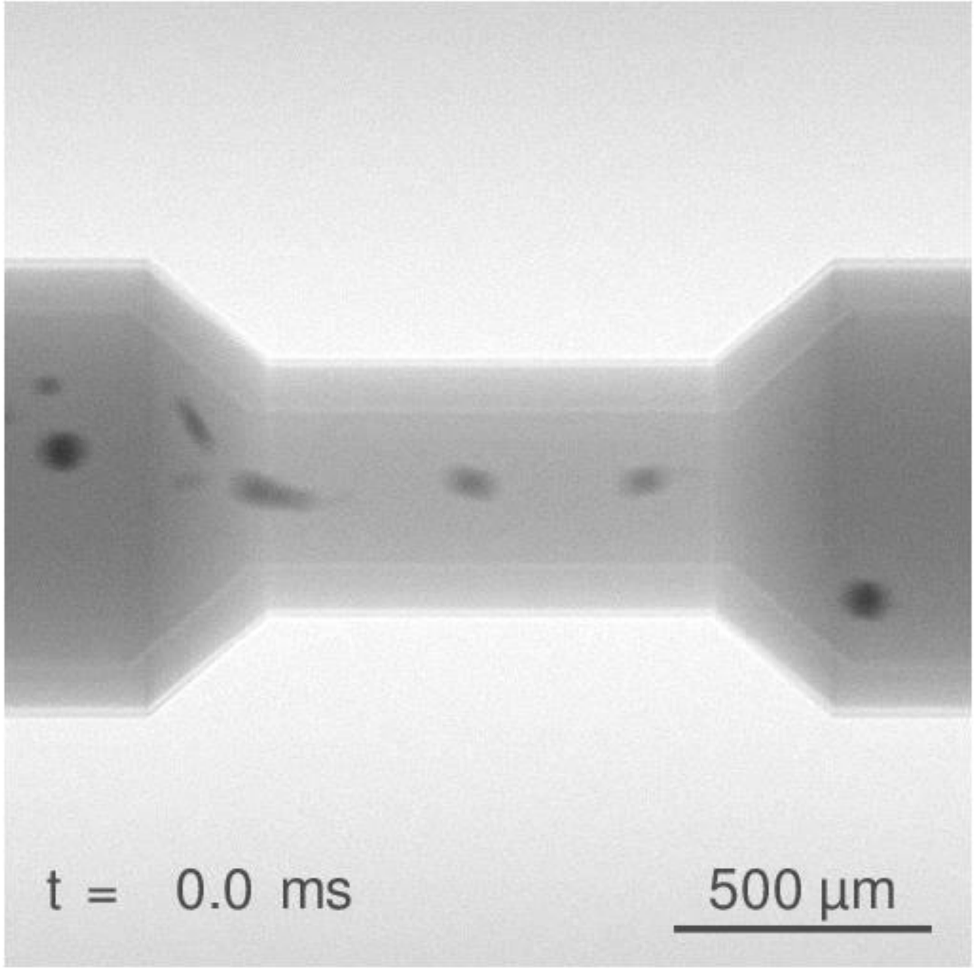
syris: Virtual *in-situ* Experiment

- *syris* accounts for:
  - Motion modeling
  - Noise
  - Beam variations
- Extendable for:
  - Elastic deformations
  - Artifacts modeling

Example:

Simulation of liquid droplets

- Camera: 5 000 frames/s
- Speed: 20 pixels/frame



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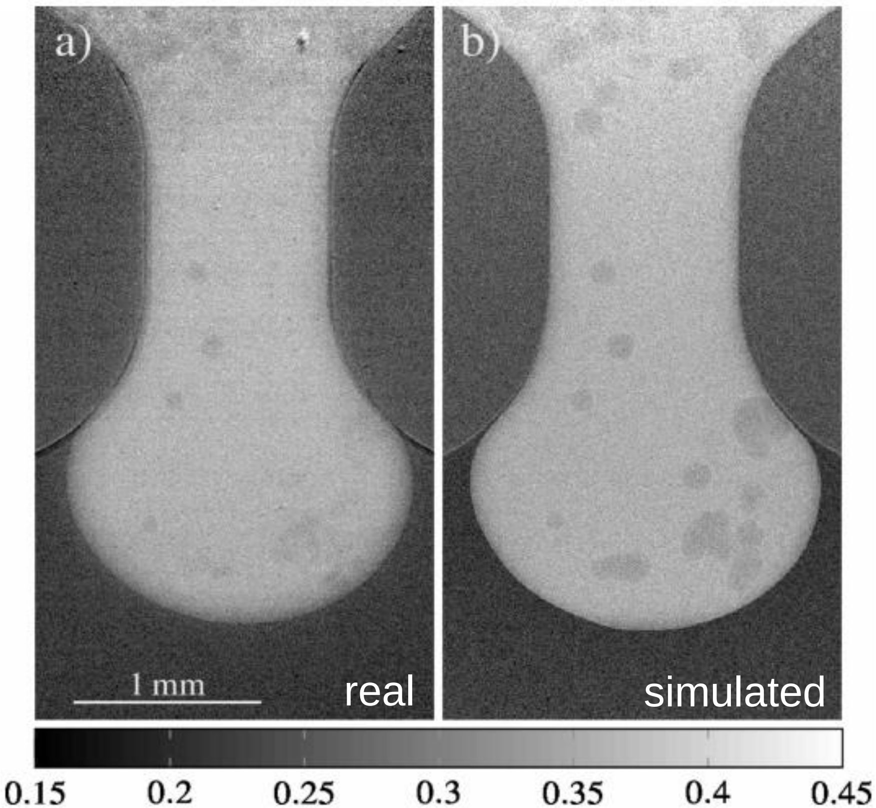
Evaluation of data processing methods



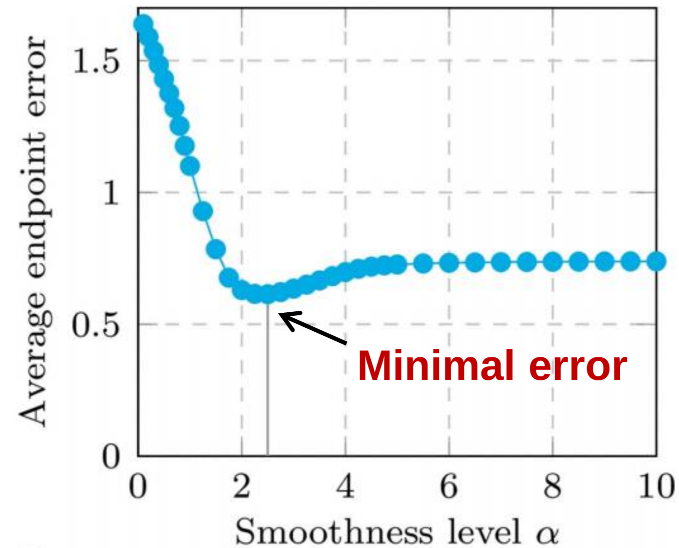


Figure 11
Motion estimation accuracy of algorithm M_4 as a function of the smoothness parameter α.

Computational model:

$$E_{\mathrm{HS}}(u, v) = \int_{\Omega_2} (I_x u + I_y v + I_t)^2 + \alpha(|\nabla_2 u|^2 + |\nabla_2 v|^2) \mathrm{d}x\mathrm{d}y$$

Optimization parameter

- **Optimize** parameters on **simulated** data
- **Apply** on real data
- **Verify** correctness and estimate **confidence**

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Neural networks
for Inverse problems

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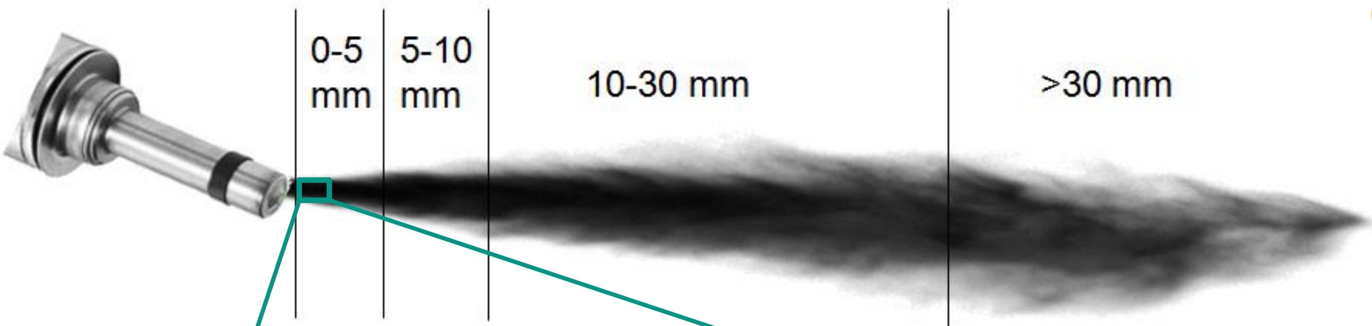
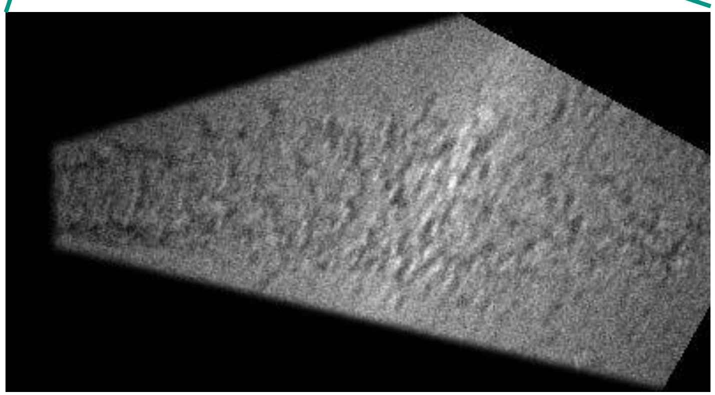
Fast Radiography of Fuel Sprays



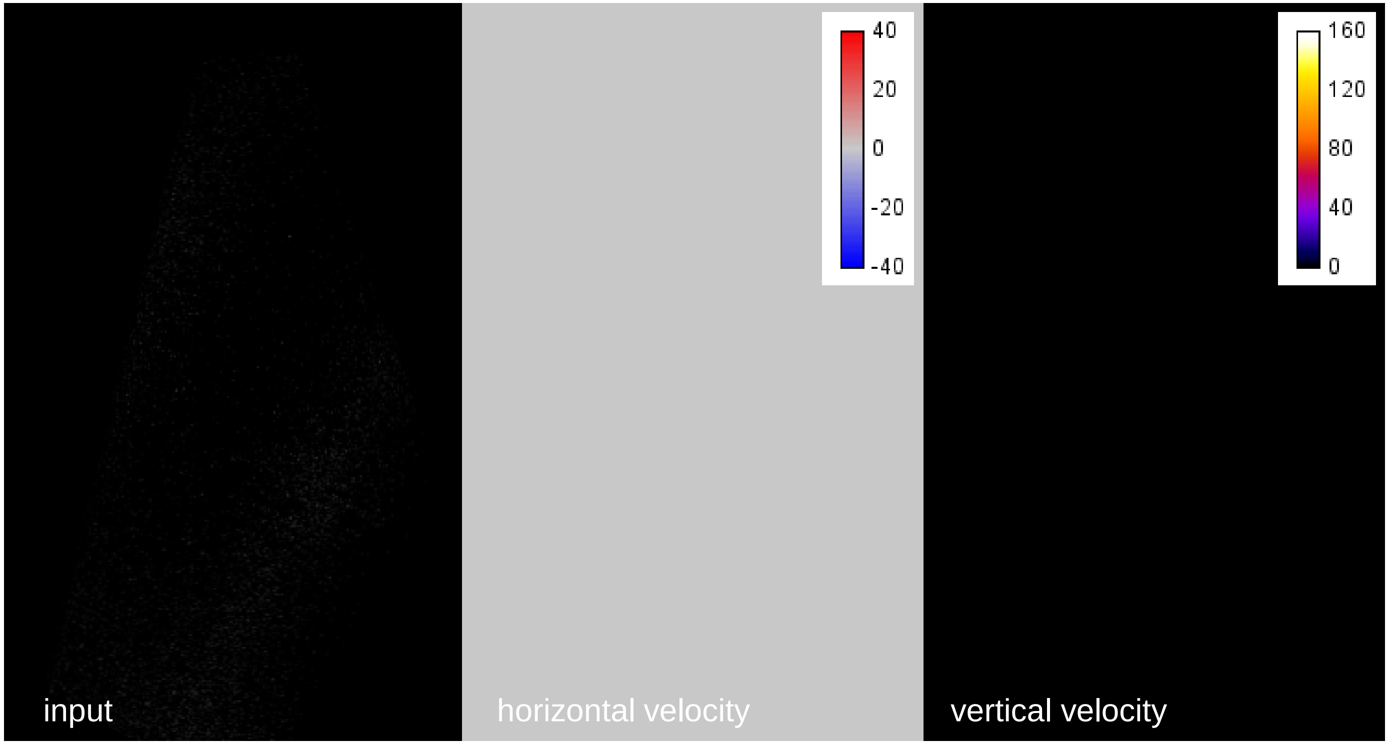
Shadowgraphy



X-ray radiography

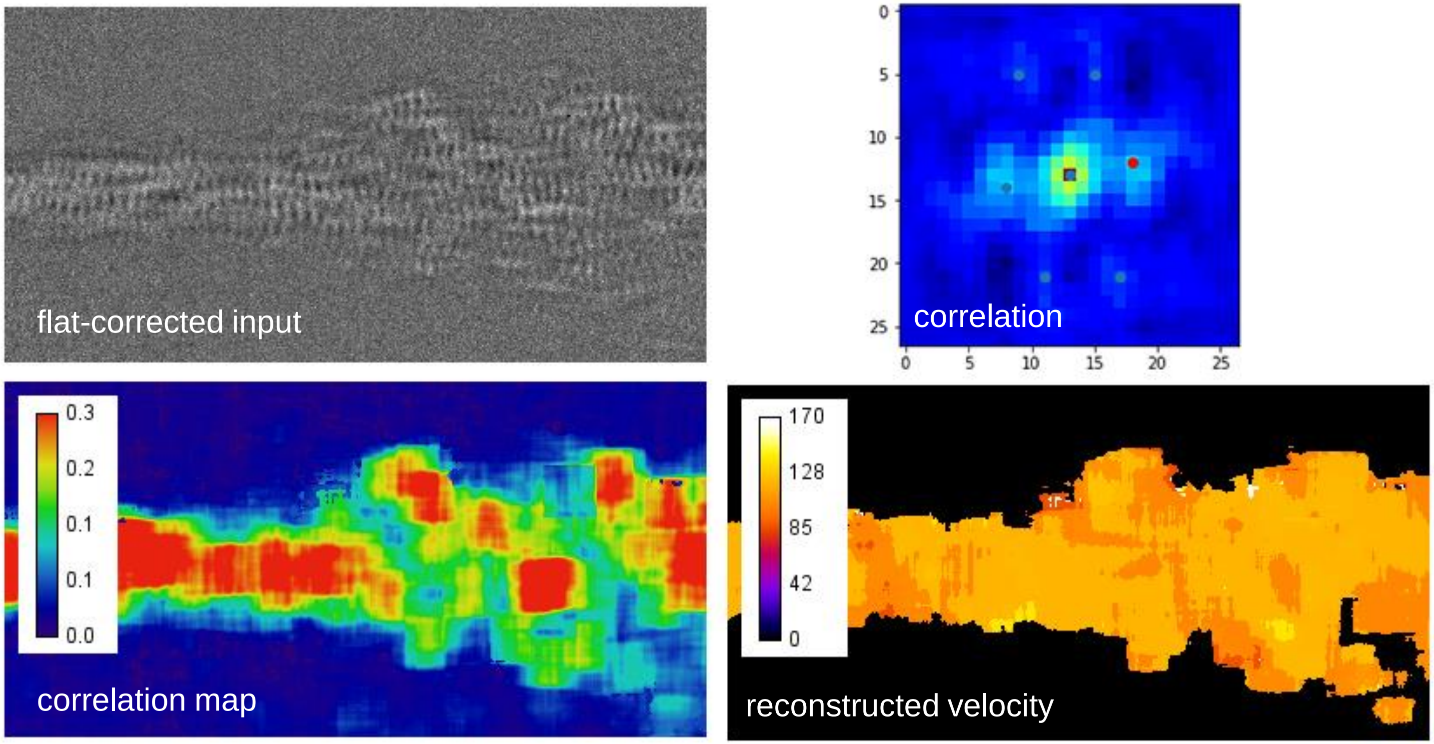
Project goal: reduce particle emission of injector-based motors by designing novel injector geometries. Highly accurate models are need

Fuel Sprays: Continuous Process



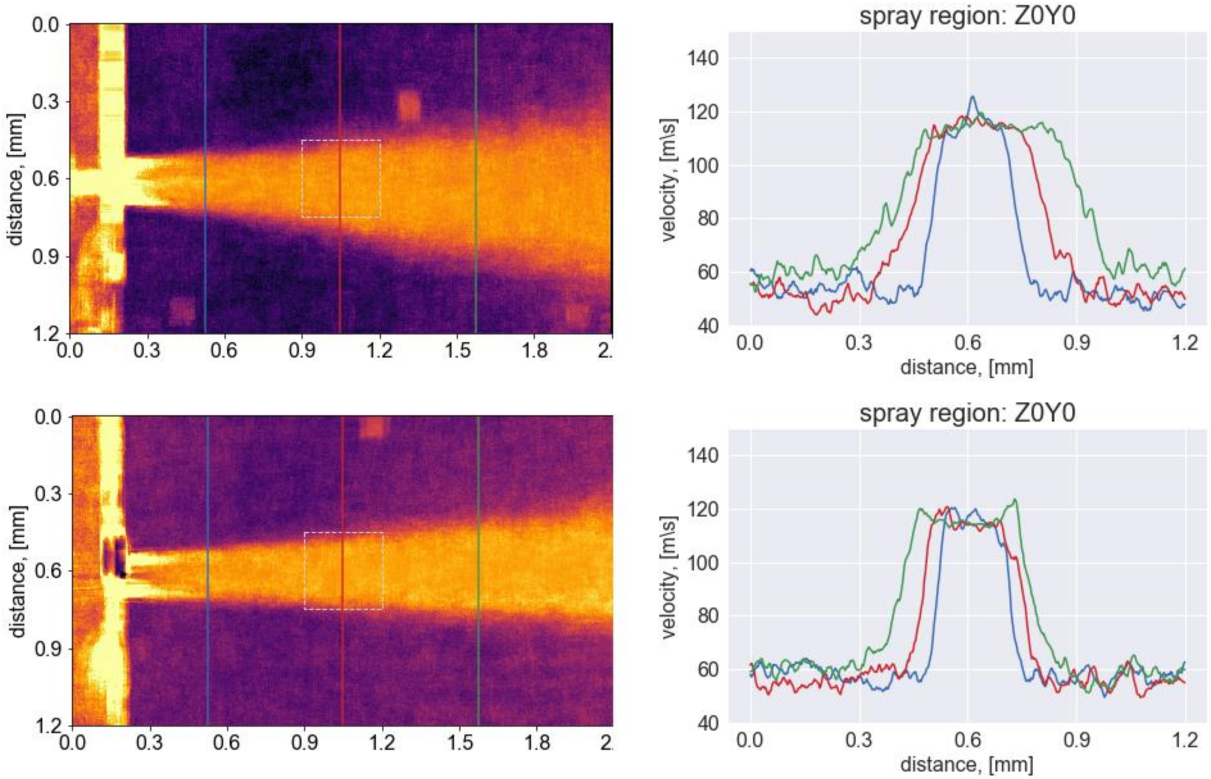
- **5 million** frames/s at ID19, ESRF
- Phase contrast
- One frame illuminated by a single photon bunch (30 -100 ps)
- **Continuous** process, **Short** sequence (128 image frames)

Fuel Sprays: Stochastic Process



- **Reduce** frame rate. Multi-exposure images
- **Discrete**, Stochastic process
- Long sequence, **whole** spraying event
- Auto correlation analysis

Fuel Sprays: Stochastic Process



- Only 2D projections, **no 3D** structure
- **Idea**: Use **Deep Learning** to reconstruct **3D shape and temporal structure** from a series of 2D projections.
- Use computational fluid dynamics (CFD) simulations for training
- Neural Networks as **approximation** to solve Inverse problems

Evaluation and Benchmarking of algorithms

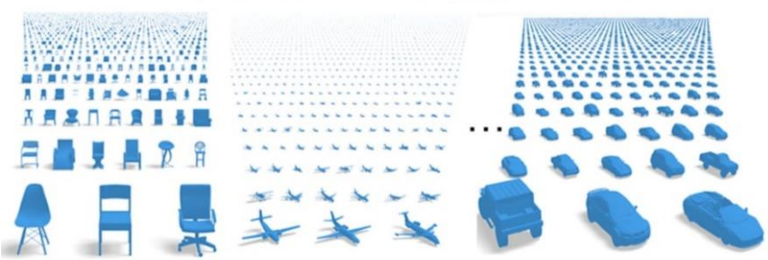
Large-scale Open Databases

Huge progress in Deep Learning is due to the establishment of **large**, **open** databases for training and benchmarking of ML algorithms.

- **ImageNet**: Visual Recognition Challenge evaluates algorithms for object detection and image classification. 20000 categories, 14M annotated images

- **ShapeNet**: large-scale dataset of 3D shape 55 object categories, 51,300 unique 3D models

and many others



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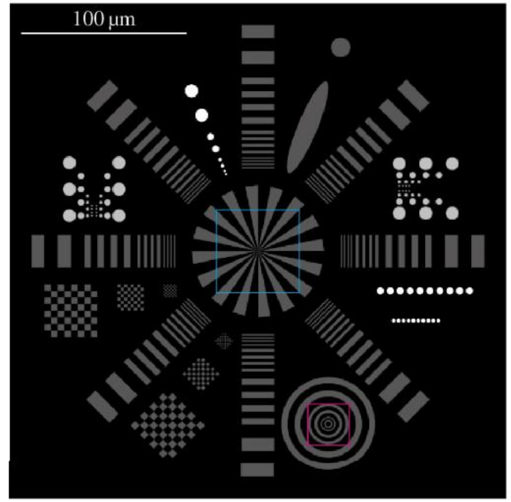
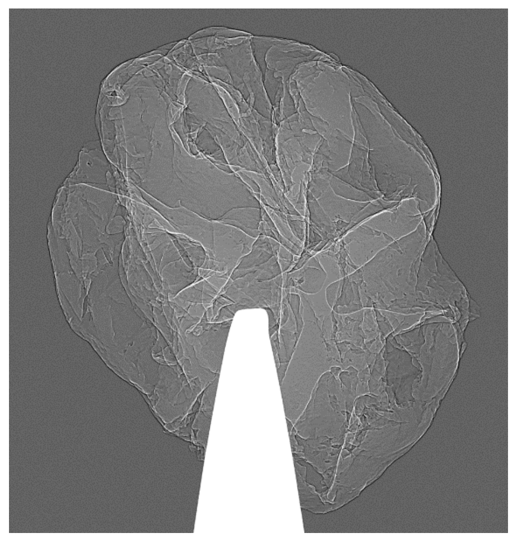
Database for X-ray Data

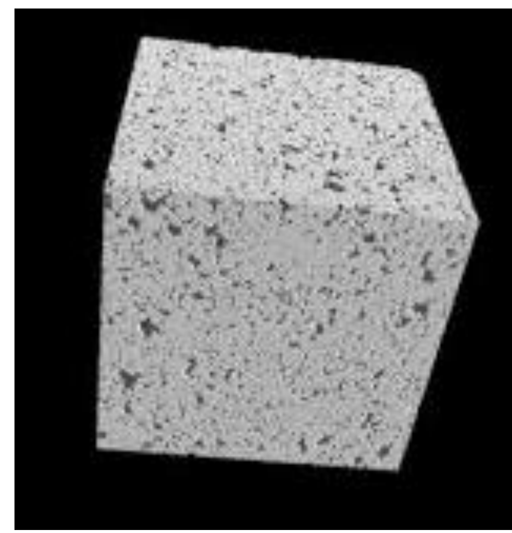
Data types:
- Real experimental data
  - Annotations
- Synthetic data
- Physical phantoms

X-ray sources:
- Synchrotrons
- Free-electron lasers
- X-ray tubes
- Liquid jets

Methods:
- 2D radiography
- 3D tomography
- 4D (3D+t) tomography







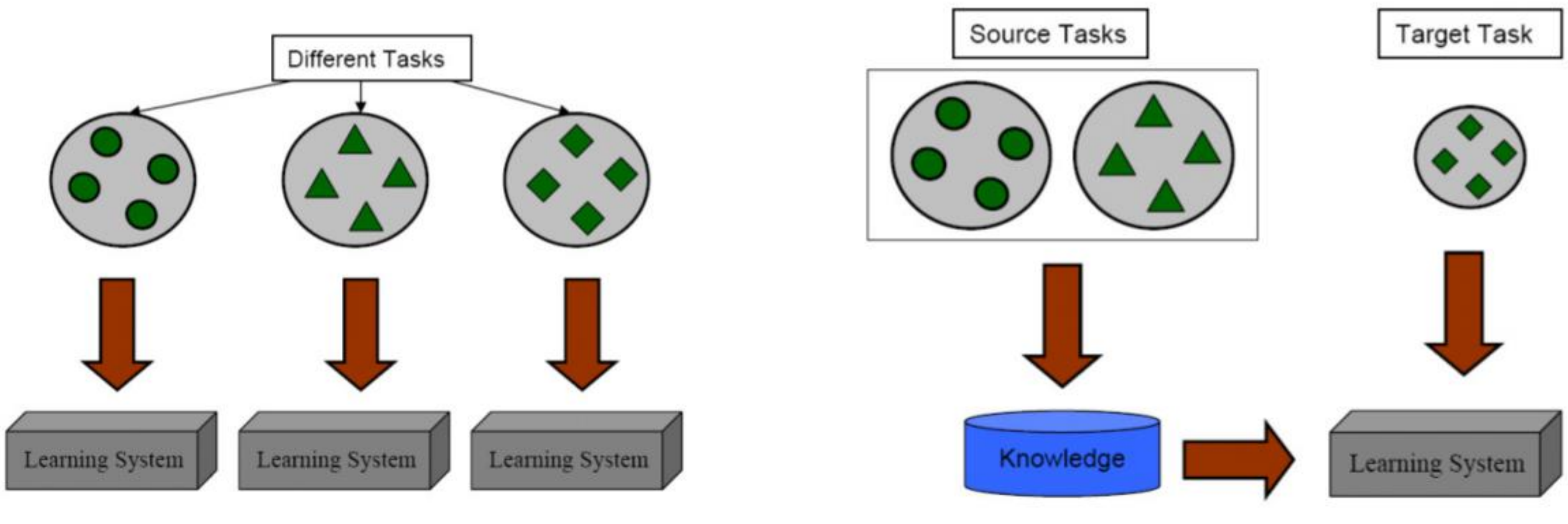
Transfer Learning and Domain adaptation

Transfer Learning / Knowledge Transfer

Problems

- Features of training and test (application) data are changing
- Lack of massive amount of labeled training data
- Expensive to perform re-training

Question: How to use previously trained models on new data?



(a) Traditional Machine Learning (b) Transfer Learning

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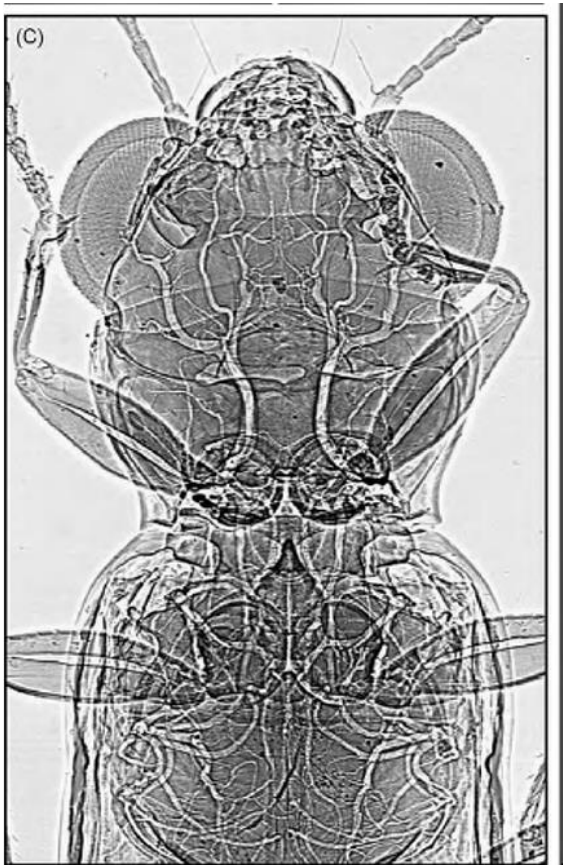
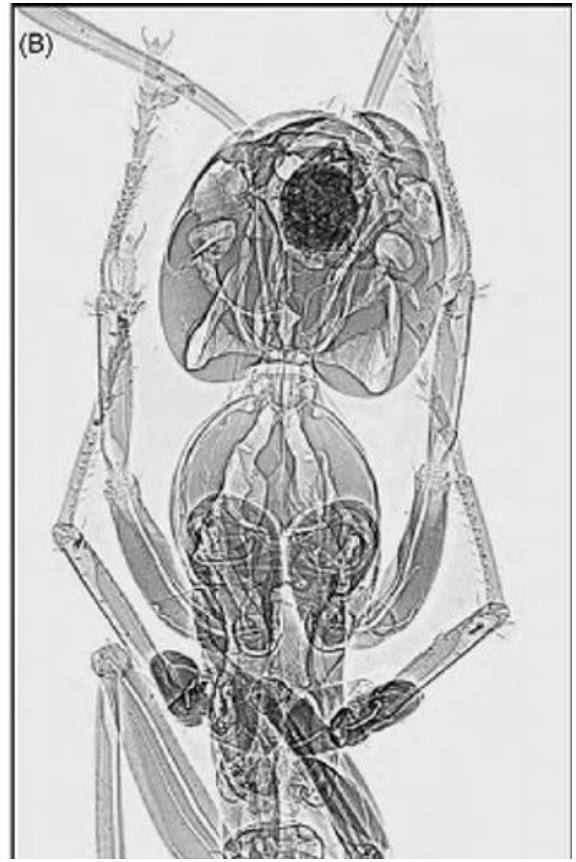
Transfer Learning

Different input distribution: e.g. different specimens



Ant worker
(*Camponotus pennsylvanicus*)

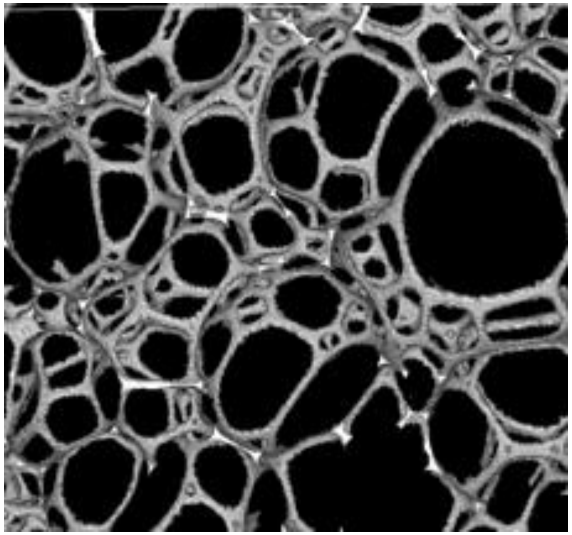


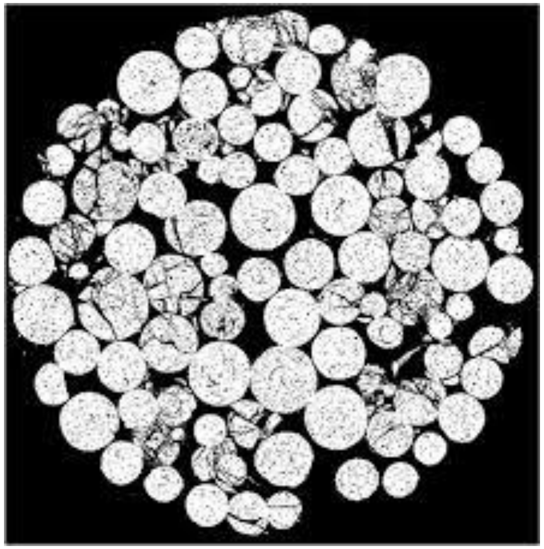
Carabid beetle
(*Notiophilus spp.*)

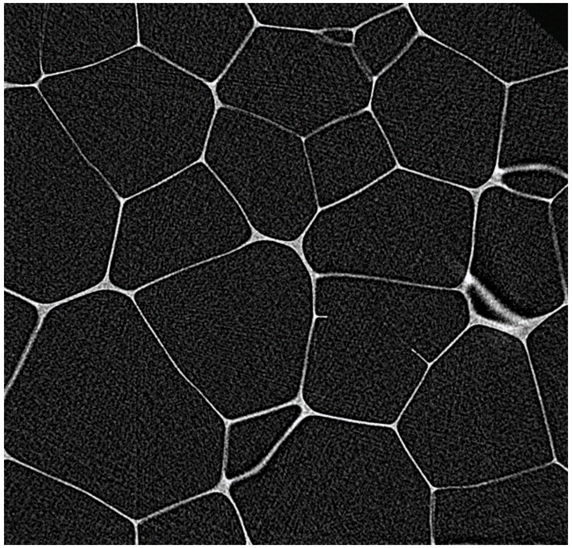
Socha, et al, 2010

Transfer Learning

Pre-training of Neural Networks on similar structures (features).
Example: cellular materials.







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Domain Adaptation

Question: Can we learn from other domains (experiments, methods)?

Problems

- Labeled data exists only in the **source** domain and absent in the **target**
- Data **distribution** is different, so we cannot directly apply ML methods.

Idea: Learn representation (model or features) which is both semantically meaningful and **domain invariant**.

Application examples:

- Train on synthetic data ⟺ Apply on real data
- 2D ⟺ 3D ⟺ 4D
- High resolution ⟺ Low resolution
- X-ray Tomography ⟺ MRI imaging ⟺ Ultrasound

Unsupervised Learning

Unsupervised Learning

All Machine learning techniques could be classified as:

- Fully supervised (Deep learning)
- Semi-supervised (Generative Models, Transfer Learning, Domain Adaptation)
- **Unsupervised**: Learn from unseen data or data without predefined labels

Different methods of Unsupervised Learning:

- Automated Machine Learning
- Anomaly Detection
- Model searching / Model Query
- Self-learning system, Meta-learning, Learning to learn

Data and Experiment Lifecycle

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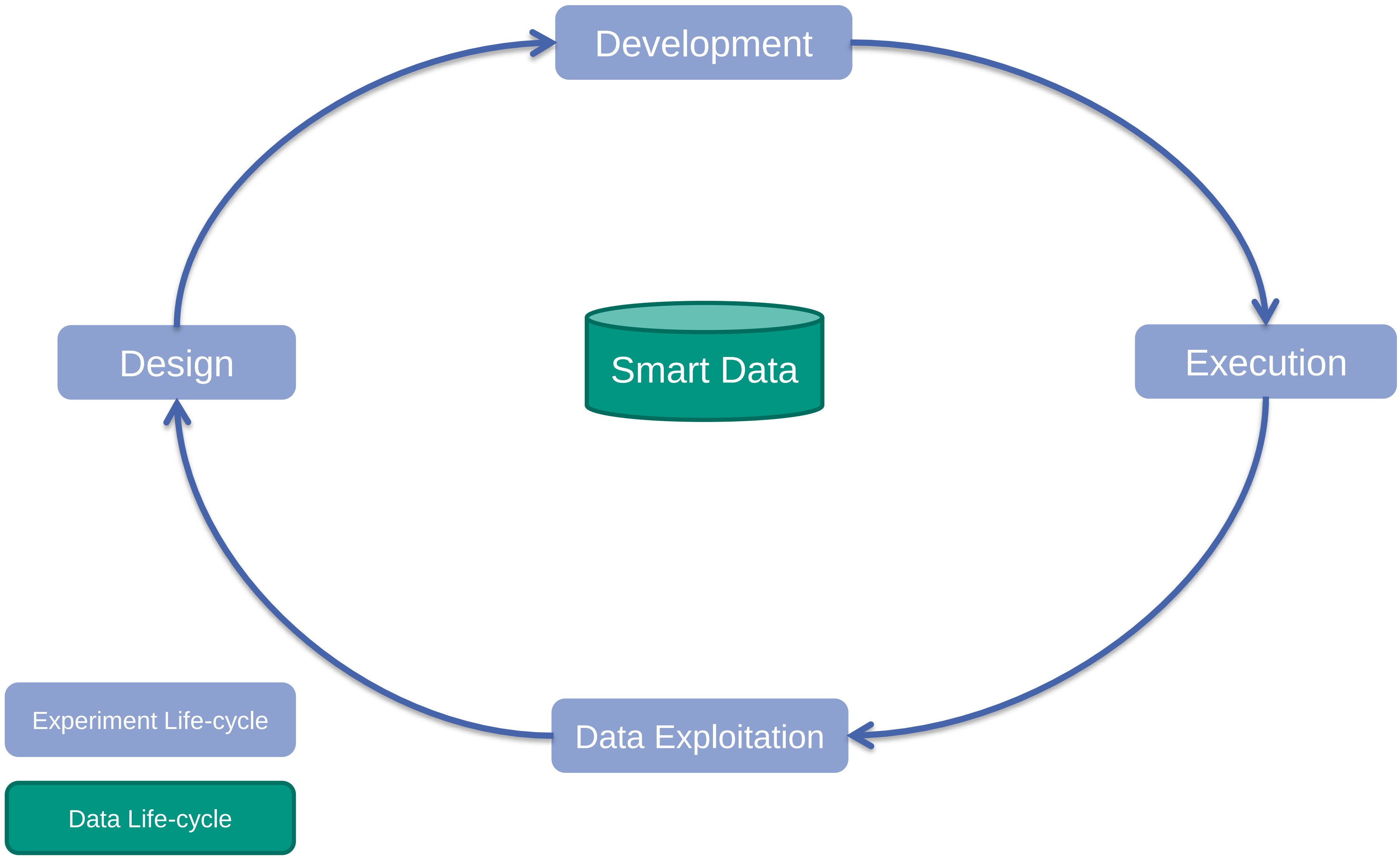
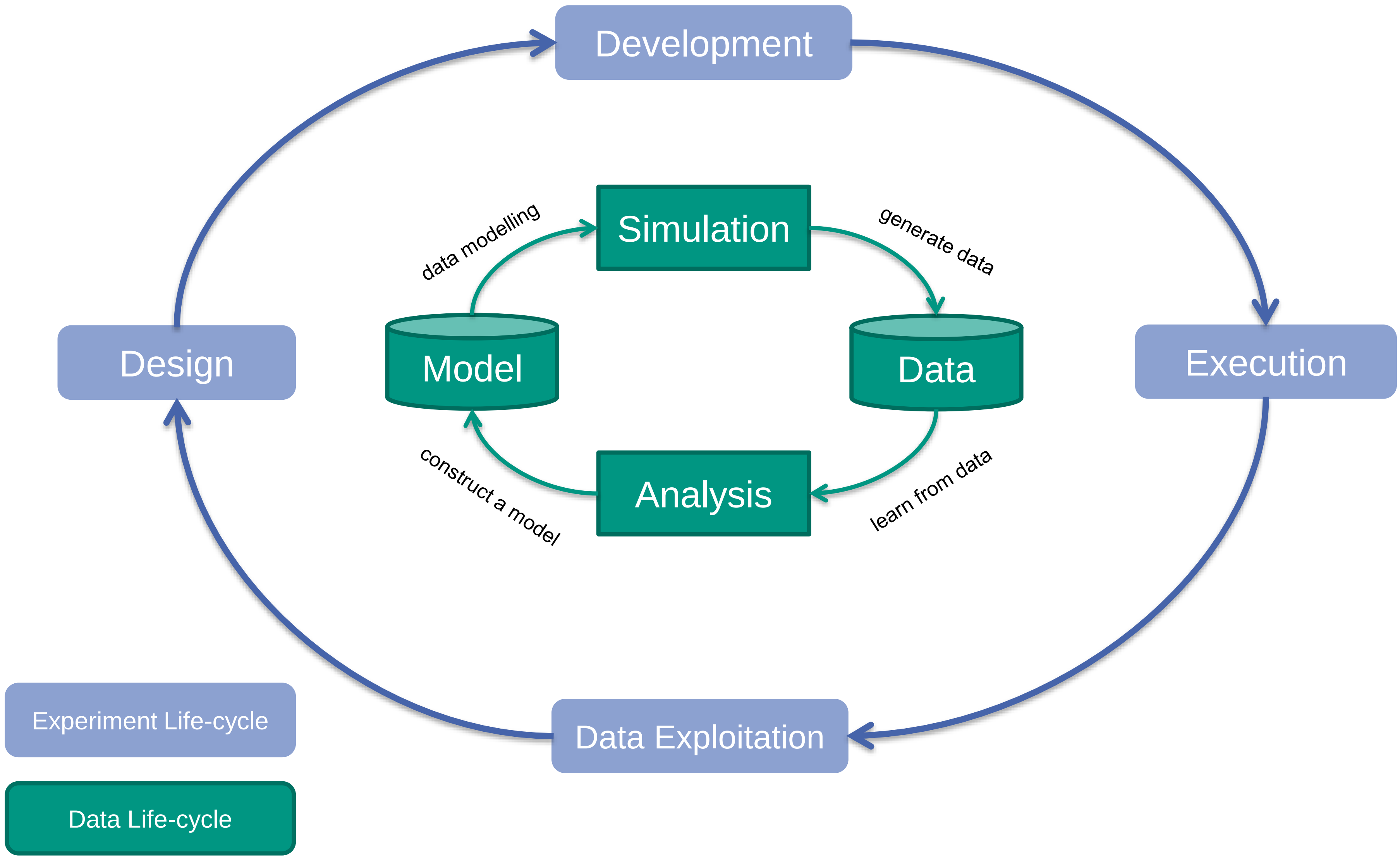
Experiment and Data Lifecycles



Experiment and Data Lifecycles



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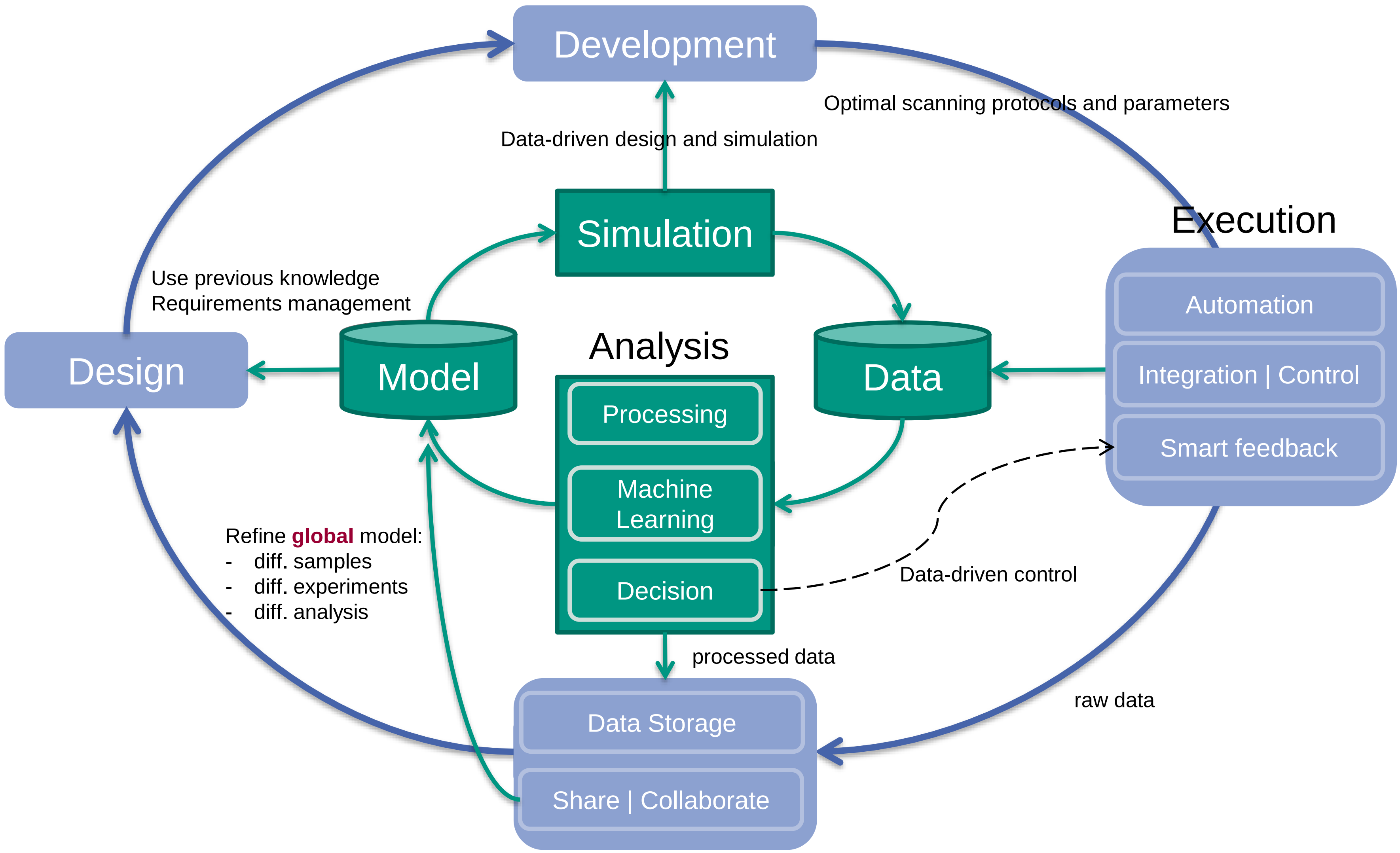
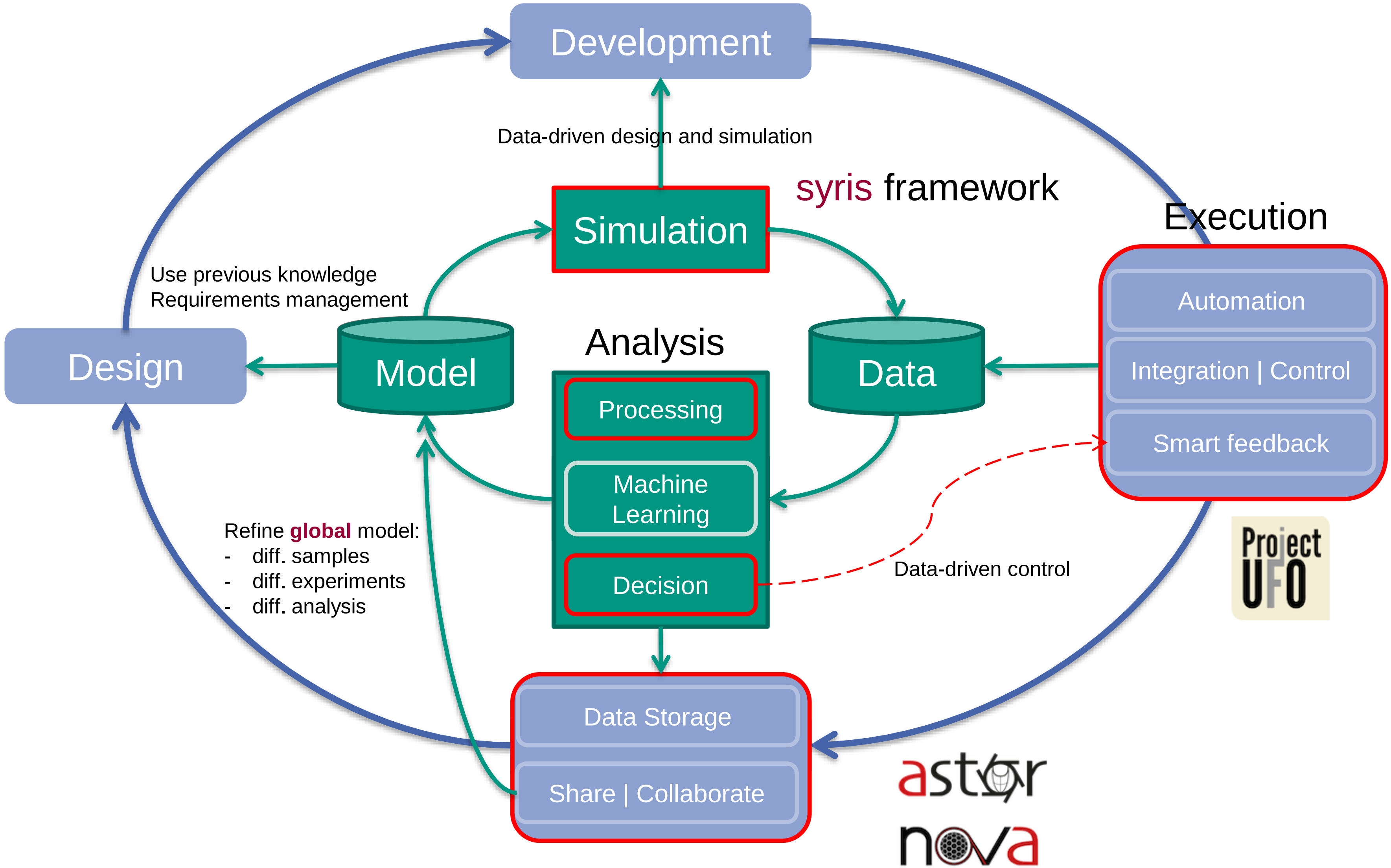
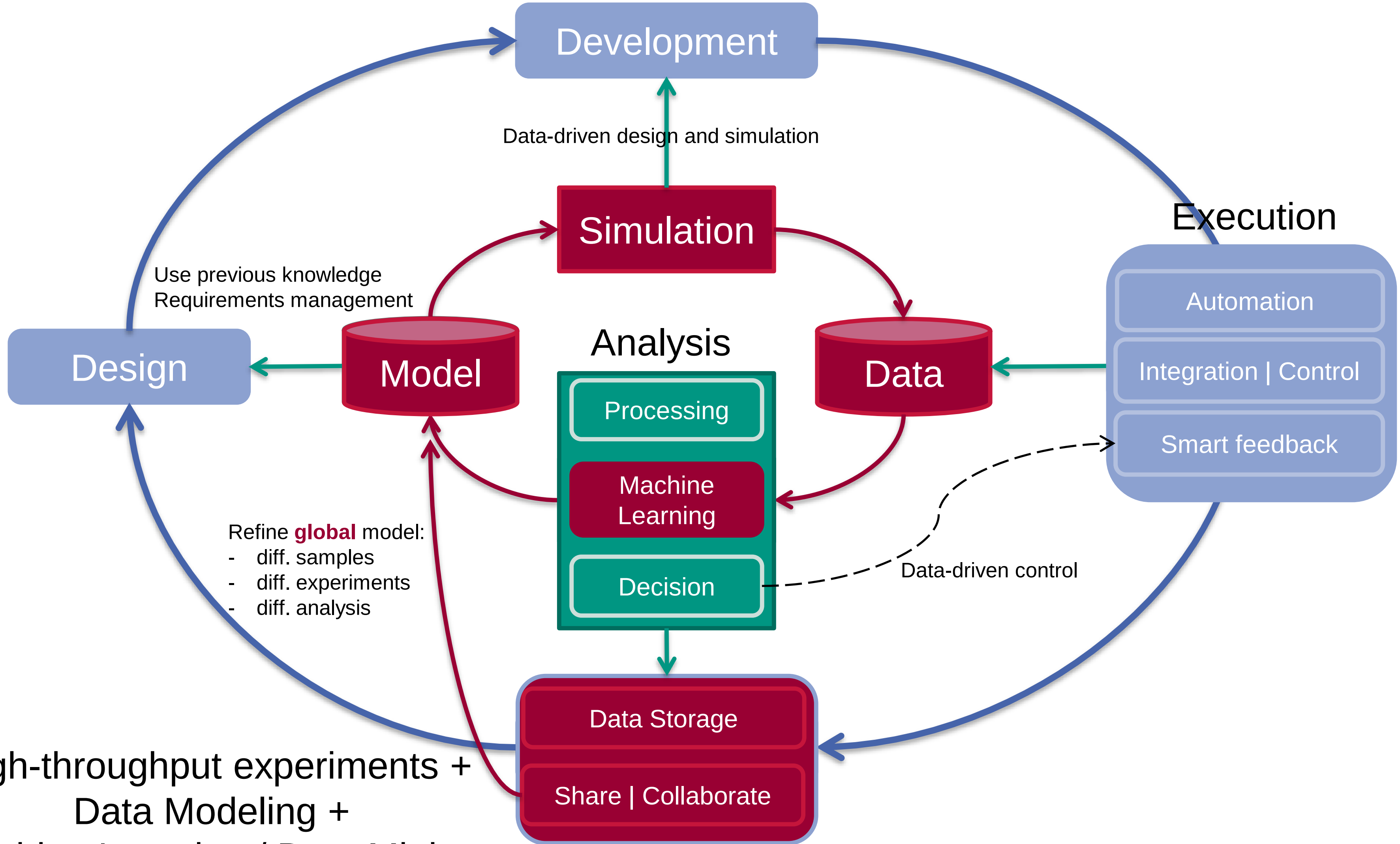
Experiment and Data Lifecycles



Experiment and Data Lifecycles



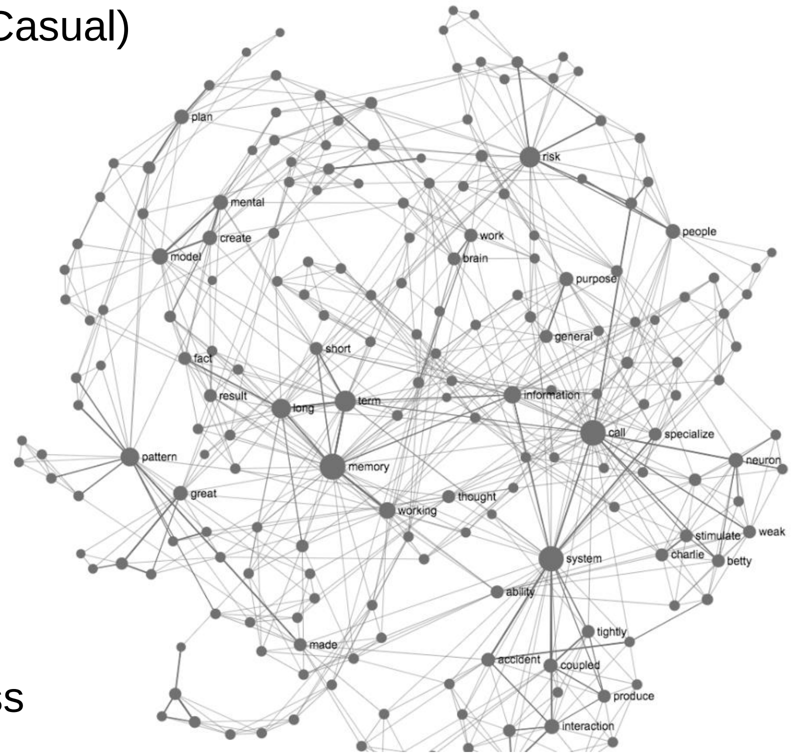
Crucial components for Digital Transformation



High-throughput experiments +
Data Modeling +
Machine Learning / Data Mining

Universal Knowledge Base

Contains:
- Descriptive models (Mathematical, Statistical, Casual)
- Experiments
- Simulation (generative models)
- Raw data, Simulated data
- Processing workflows and data views / states
- Machine learning algorithms
- Evaluations



Properties of Models:
- Abstract
- Unified
- Global
- Flexible
- Extensible
- Versioning (states)

Everything here is:
- Unified / Connected
- Online / Open Access
- Can be verified
- Can be build upon
- Explored (search)
- Modified
- Learned from

Summary

- Step-by-step approach for adoption of Machine Learning methods
- **Deep Learning** for high-throughput and most common tasks
  - Domain knowledge is crucial. Experts should learn to apply technology. Interdisciplinary research
  - Teaching within community: Courses, Workshops, Tutorials
- **Simulation**:
  - Best way to train Machine Lerning
  - Unified forward simulation framework for each community
- **Databases**: Large scale open databases, managed by consortium
- **Smart Data**: Models, Data, Algorithms -> Universal Knowledge Base
- Machine Learning:
  - **Transfer Learning and Domain Adaptation** – Extend ML to new data and applications
  - **Unsupervised Learning / Self-learning –** Ultimate goal

Thank you for your attention!