Artificial intelligence in the analysis of time-resolved (4D) micro-computed tomography data
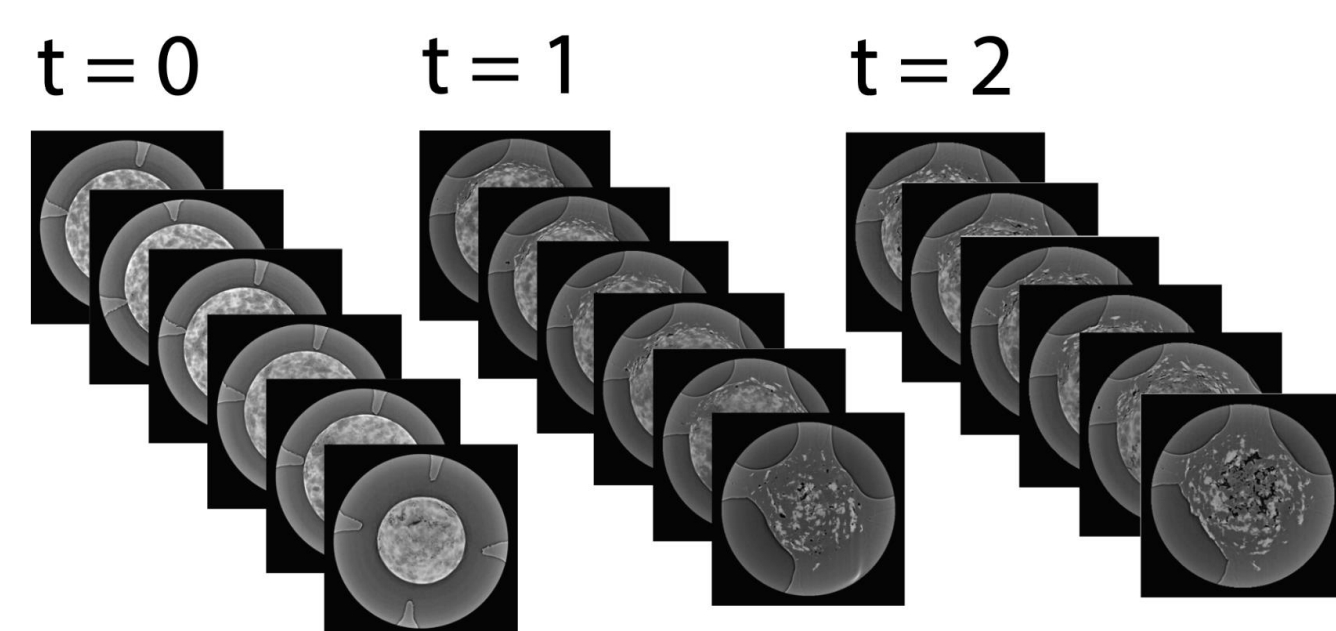
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AIMS

- Provide reconstruction and analysis pipeline for 4D-µCT data
- Demonstrate the potential of artificial intelligence for the analysis of large amounts of very heterogenous data
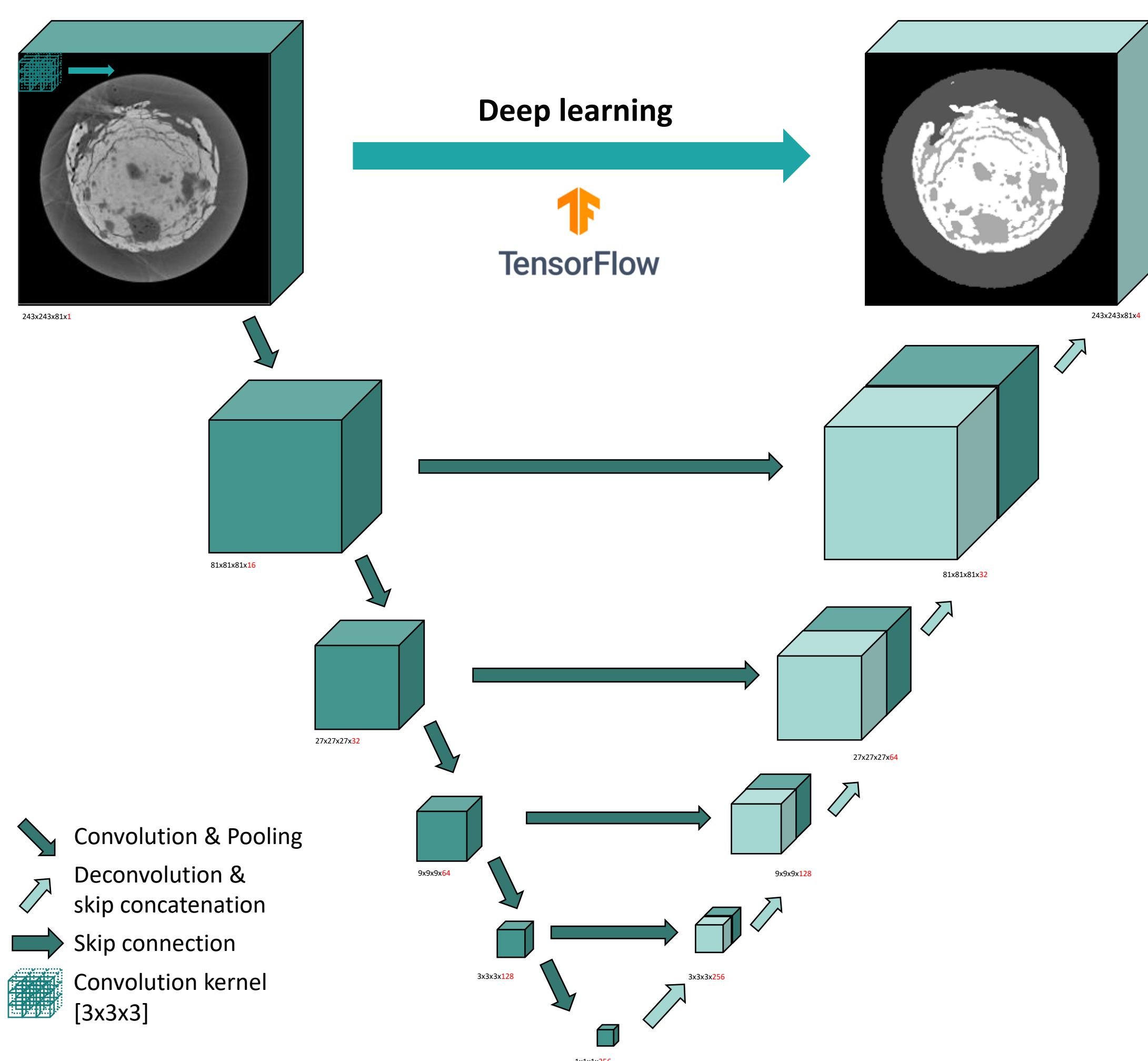- Gain new insights into tablet disintegration and similar dynamic systems

DATA ACQUISITION

Paul Scherrer Institute
Swiss Light Source (SLS) Synchrotron

4D projection raw data

- Time-resolved (4D) µCT image acquisition of disintegrating mini-tablets
- 64 different tablet formulations according to design of experiment → API, disintegrant, lubricant, filler are varied
- 1 to 10 scans per second for up to 30 seconds
- 23 TB of raw projection data

IMAGE RECONSTRUCTION

t = 0   t = 1   t = 2

4D reconstructed data

- Custom raw data reconstruction software
- Uses filtered backprojection algorithm
- Phase contrast extraction using Paganin filter
- Written in Python and CUDA-C++
- Runs massively parallelized on GPUs
- Reconstruction quadruples file size, only done as needed

COMPUTATION

- Software runs on the sciCORE high-performance computing facility
- Data storage handled by sciCORE
- Unsupervised operation of configurable computing instances

IMAGE SEGMENTATION

Deep learning
TensorFlow

- Convolution & Pooling
- Deconvolution & skip concatenation
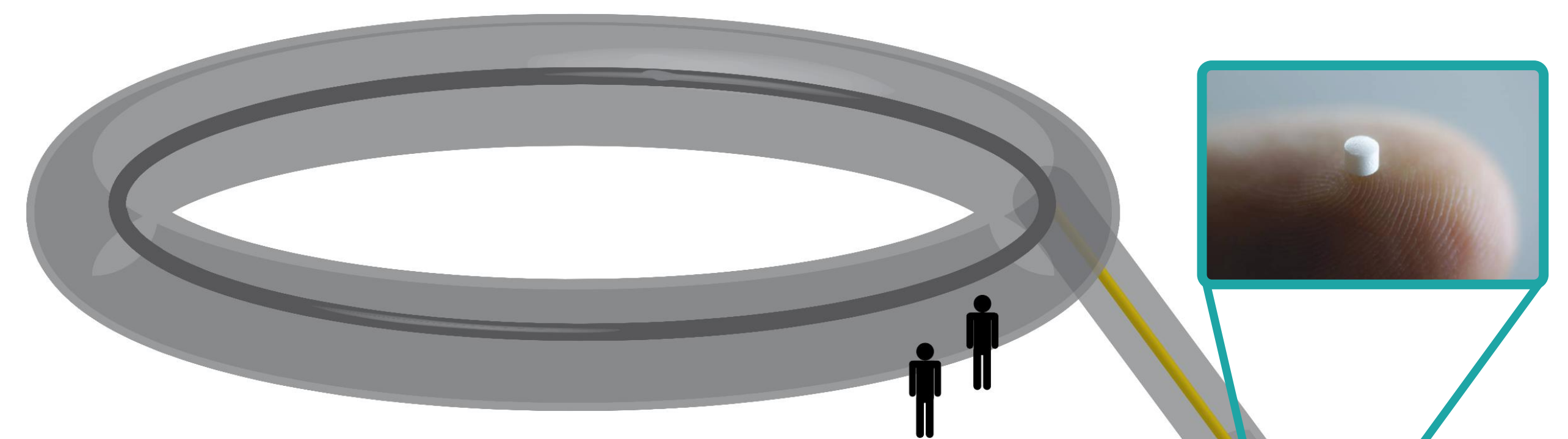- Skip connection
- Convolution kernel [3x3x3]

- Image segmentation using convolutional neural net (UNet) architecture
- Algorithm trains autonomously on a large sample dataset
- Training dataset generated in Ilastik using supervised machine learning
- Realization in Tensorflow and Python
- Runs parallelized on GPUs
- Trained neural net can be applied to the entirety of the image data for rapid unsupervised image segmentation

OUTCOME

- Complete data handling pipeline which processes CT raw data all the way to segmented, reconstructed image stacks without supervision
- Image segmentation which is quick and very consistent thanks to deep learning → 'one ruleset for all data' enables and facilitates data analysis
- Dataset of 4D CT scans of different tablet formulations dissolving in water to enable research into the mechanism of tablet disintegration

CONCLUSION

- The deep learning approach works extremely well for the segmentation of CT-images.
- The Convolutional neural network outperforms humans in speed and consistency
- This method demonstrates the huge potential of deep learning in all kinds of pharmaceutical applications
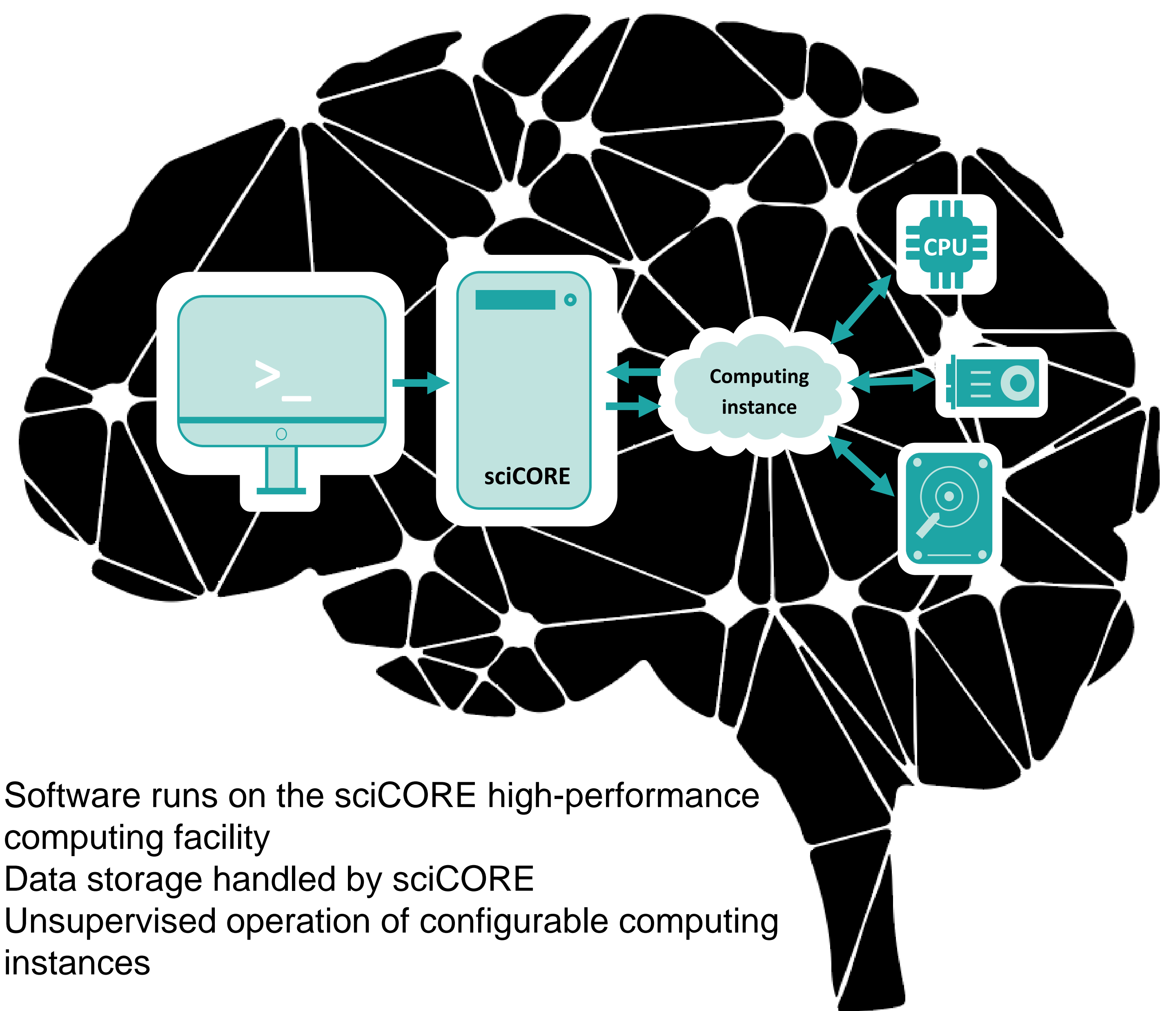- 4D µCT provides direct insight into the complex process of tablet disintegration

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