



Science3D - an open access project for 3D x-ray tomography

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- Origin of the Science3D project
- Synchrotron radiation tomography
- Applications
- Services
- Hurdles

Consortium of 13 Photon and Neutron RIs

- **Focus** entirely on topics around data management
- **Number of instruments** > 200
- **Number of users** >> 30.000 users/yr
- **Investment** > €4.000.000.000*
- **Running costs** > €500.000.000/yr*
- **Publications** > 10.000/yr*
- **RCosts/Publication** ~ €50.000*%
- **Data volume** >> 10PB/yr*

% ESRF: operation budget 80-100Mio
publications: ~1850

* wild guess



- Huge investment (tax money)
 - No access to data
 - Limited access to publication
 - Limited access to supplementary data
 - Useful meta-data only in the publication
 - Few tools for remote visualization, validation
- Quite limited return value (tax payer)



- PaNdata project tasks:
 - Demonstrator for a data catalogue integrating several services
- Drawback:
 - Projects don't last (this one ended 09/2014)
 - Demonstrators hardly ever survive beyond the end of a project
 - Unless there is a real use case
 - Frequently wasted time & effort
- Alternative:
 - Turn the demonstrator into something useful
 - Create the use case: Open Access Tomography Database

- Collect & make openly accessible
 - Raw data & meta-data
 - Derived data and any kind of supplement
 - Publications
 - Printable 3-D models
 - Tutorials & background information
- Provide services:
 - Visualization
 - Tools
 - Long term storage
- Why tomography
 - Applied science, comparably easy to capture the outcomes
 - Useful in a wide spectrum of applications; widely known technique

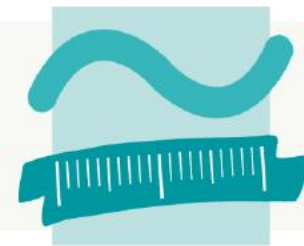




Tomography

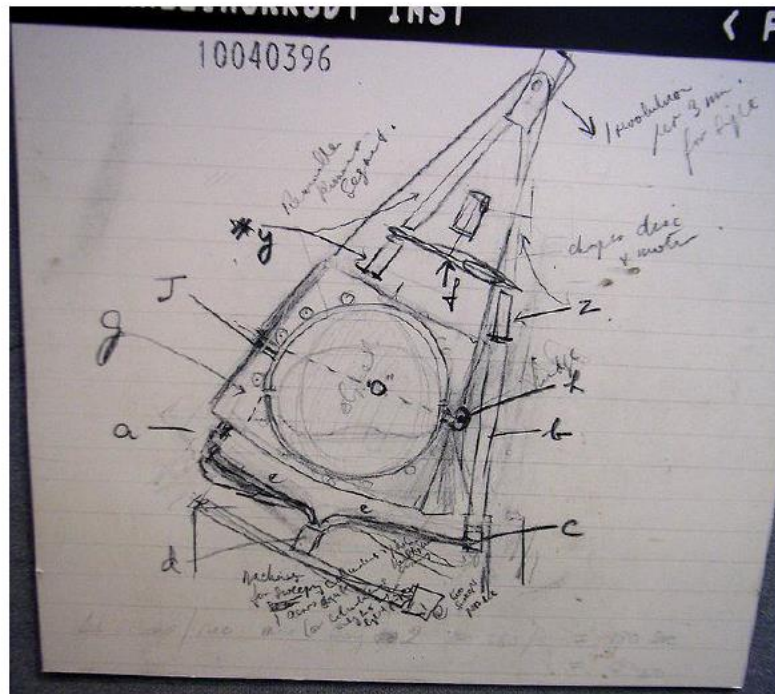


History: 2D \Rightarrow 3D

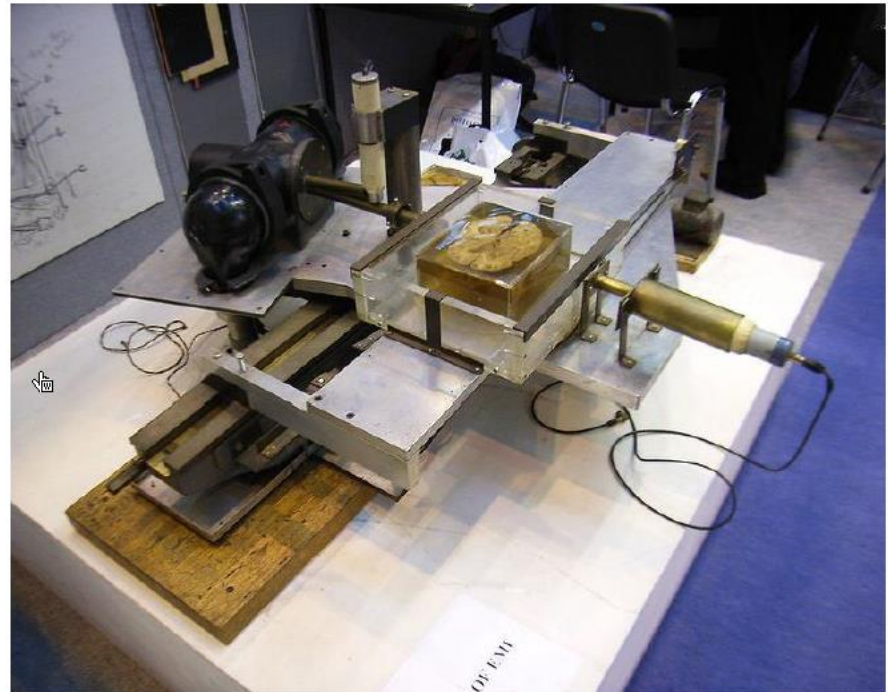


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- Medicine CT was developed in the late 1970s based on the idea of the British engineer **Godfrey Hounsfield** and the American physicist **Allan McLeod Cormack**
- Hounsfield and Cormack shared the 1979 Nobel Prize in Medicine



Original sketch from Hounsfield's notebook



The very first CT-scanner prototype invented by Hounsfield at EMI

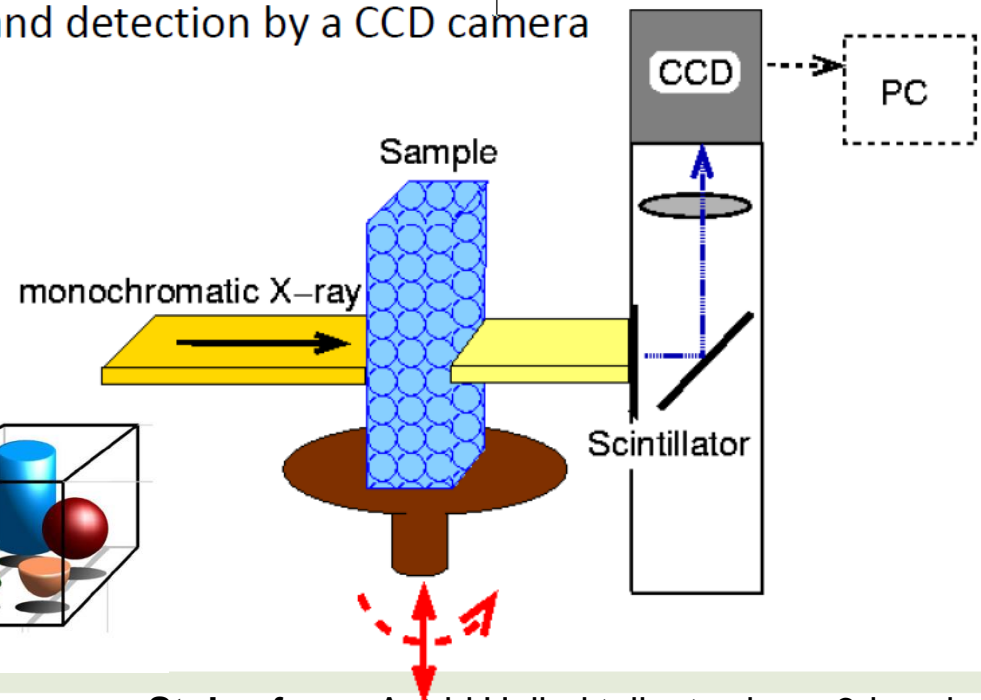
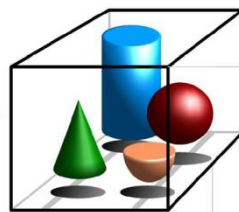
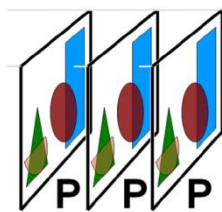
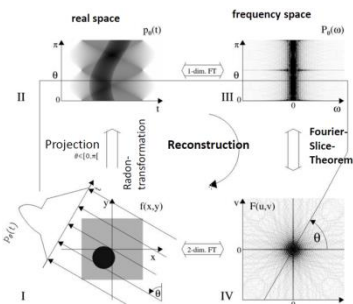
Synchrotron CT

- Measurement Principle -



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- **highly intensive**, (quasi-) **parallel**, **monochromatic**, **partially coherent beam** penetrates the sample
- local attenuation and/or phase shift depends on materials density, thickness and inner structures
- measuring of many different angular positions (0° - 180° , 900 -2400 images)
- conversion of the X-ray light into visible light by a scintillator screen
- magnification by a microscope optics and detection by a CCD camera
- reconstruction of the 3D image



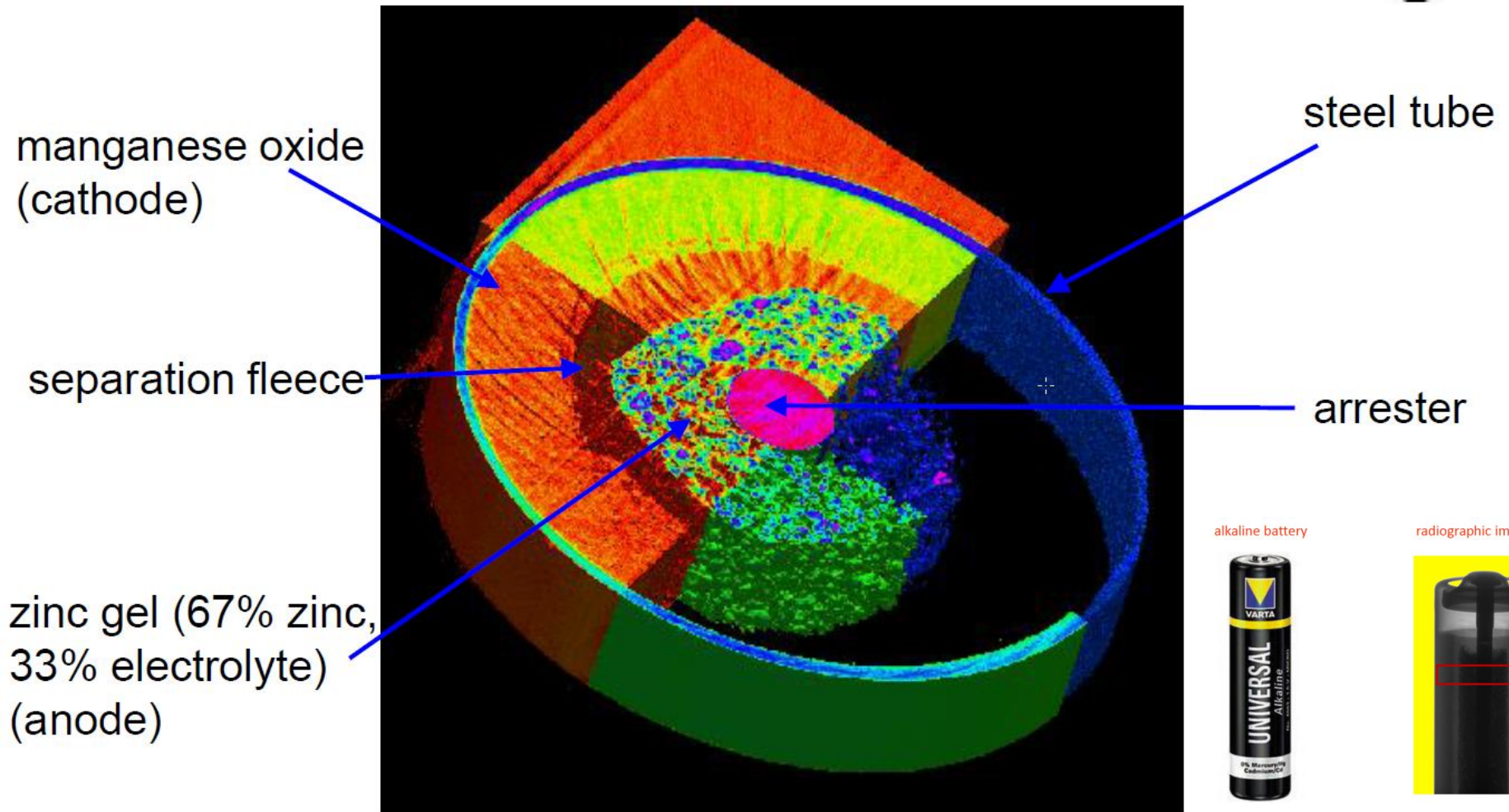
Applications





Application: In situ tomography at alkaline battery **LR61**

Investigation of zinc particle dissolution during discharging

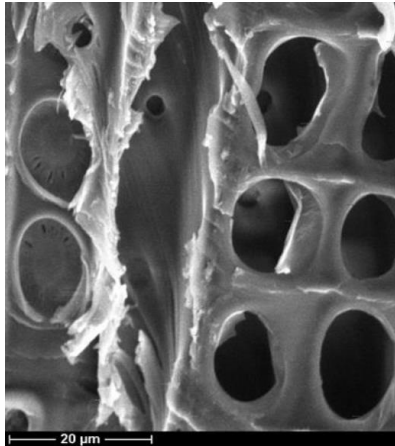


alkaline battery



radiographic image





Reconstruction of course of vessel by
light microscopy analysis (Zimmermann 1983)

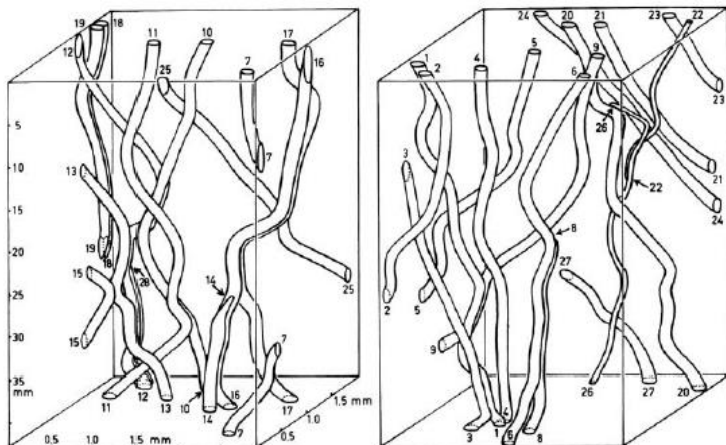
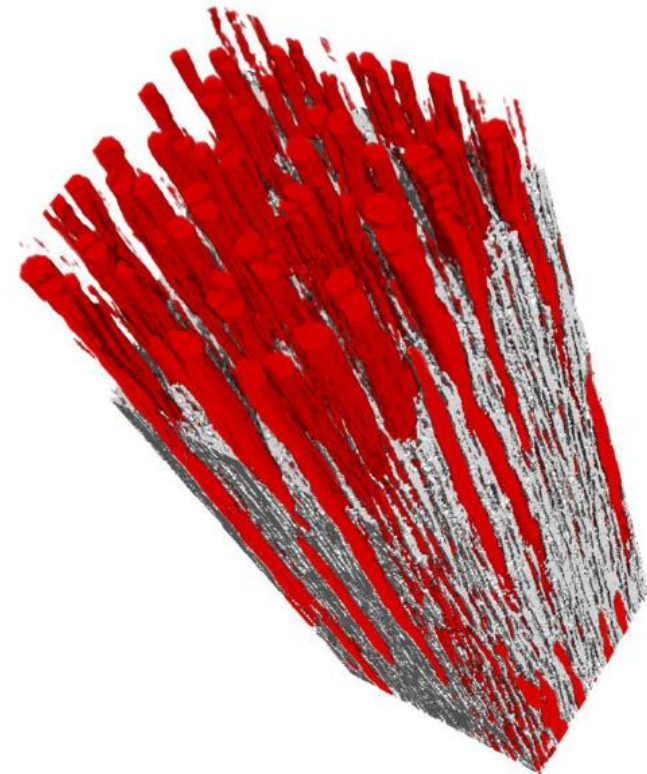
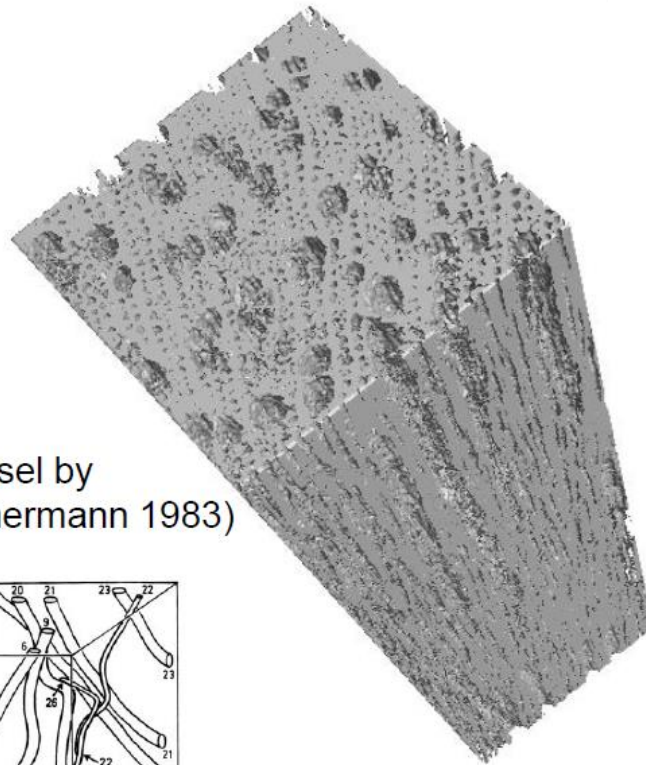


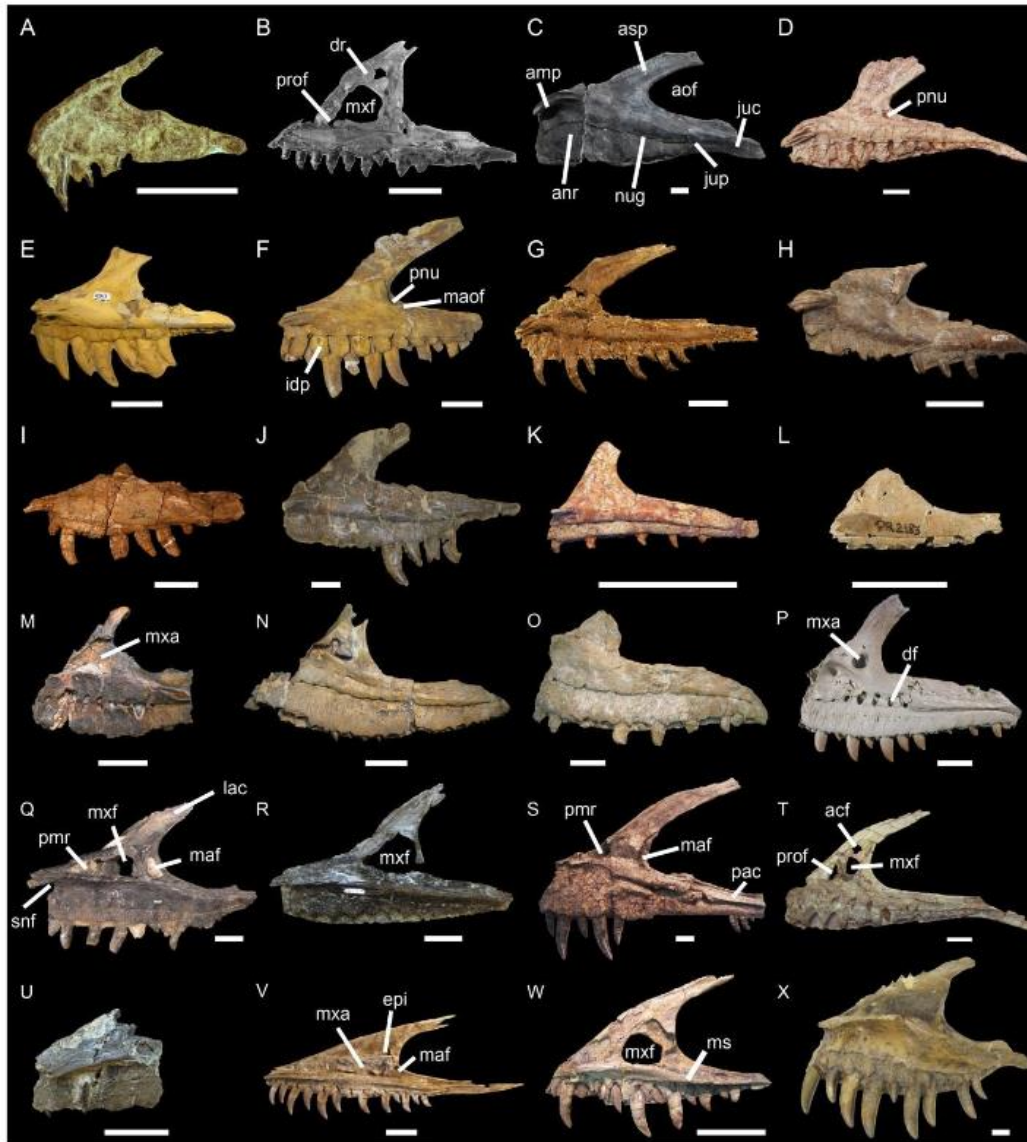
Fig. 2.2. Course of vessels in a piece of wood of *Cedrela fissilis*. Individual vessels have been arbitrarily separated into two blocks for clarity. Vessels are numbered where they exit from the block. Arrows show vessel ends. Note that the axial scale is foreshortened ten times. (Zimmermann and Brown 1971)



3D reconstruction of the vessel system



From chimpanzee over *Australopithecus africanus* to *Homo sapiens*



<http://www.nature.com/srep/2013/130530/srep01924/full/srep01924.html>



<http://felipe-elias-portfolio.blogspot.com>



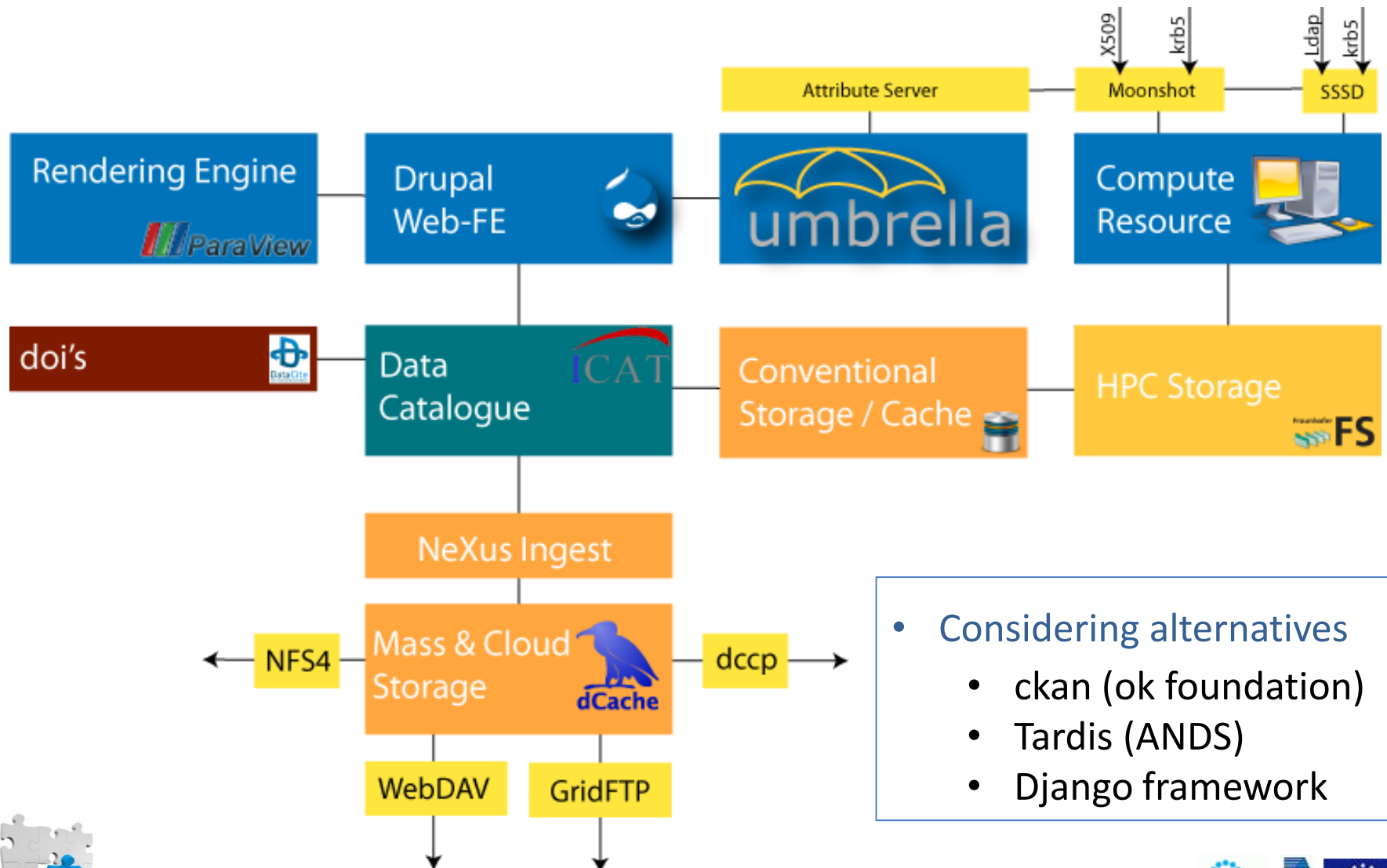
Note 3 – Maxillae of nonavian theropods in medial view. **A.** Embryo of *Torvosaurus* sp. (ML 1188, reconstructed). **B.** Hatchling of *Allosaurus* (IPFUB Gui Th 4; Rauhut &



- Not too far from topics typically taught in universities & schools
 - Comparative & evolutionary biology
 - 3-D models to look at on a sub- μm -scale – if you have the right tools
 - 3-D models to take to the classroom
 - 3-D printing the next revolution?
- Science3D workshop in June '14
 - <https://indico.desy.de/event/science3d>
 - Several teachers / educators
 - Presentations at a rather scholarly level
 - Have to see how it develops...








- Considering alternatives
 - ckan (ok foundation)
 - Tardis (ANDS)
 - Django framework



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About Science3D

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Science3D is an Open Access project to archive and curate scientific data and make them available to everyone interested in scientific endeavours. Science3D focusses mainly on 3D tomography data from biological samples, simply because these objects make it comparably easy to understand the concepts and techniques.

The data come primarily from the imaging beamlines of the Helmholtz Center Geesthacht (HZG), which make use of the uniquely bright and coherent X-rays of the **Petra3 synchrotron**. Petra3 - like many other photon and neutron sources in Europe and World-wide - is a fantastic instrument to investigate the microscopic detail of matter and organisms. The experiments at photon science beamlines hence provide unique insights into all kind of scientific fields, ranging from medical applications to plasma physics. The success of these experiments demands enormous efforts of the scientists and quite some investments. So it would be a shame to hide these valuable data in a drawer and not to make the data publicly available. The aim is to provide not only the original data, but also as much background information as possible both on the scientific results derived from the data as well as the techniques and tools used in this process.

The Science3D data catalog needs the support from the scientists providing data and background information and we'd like to invite and encourage the Photon Science users to contribute their expertise. Likewise, the Science3D data catalog aims to make information publicly available, so we'd love to hear from you any kind of feedback, critics and praise are equally welcome.

The data catalog is part of the **Helmholtz Open Access Initiative** and hosted by DESY and the HZG with support from the **Paldata OOI** project and the European commission.


Latest Publications

2014
Head morphology of *Tricholepidion gertschi* indicates monophyletic...



Latest datasets

Caeilian jaw-closing mechanics
Thomas Kleinteich, Alexander Haas, Adam P. Summers



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Publications

Sort by Year field_year Order Desc Apply

2014
Alexander Blanke, Markus Koch, Benjamin Wipfler, Fabian Wilde, Bernhard Misof
Head morphology of *Tricholepidion gertschi* indicates monophyletic Zygentoma

2014
Alexander Blanke, Thomas Westheide
Revival of forgotten characters and modern imaging techniques help to produce a robust phylogeny of the Diplopoda (Arthropoda, Myriapoda)

2014
B.M. von Reumont, A. Blanke, S. Richter, F. Alvarez, C. Bleidorn, R.A. Jenner
The first venomous crustacean revealed by transcriptomics and functional morphology: remiped venom glands express a unique toxin cocktail dominated by enzymes and a neurotoxin

2013
A. Blanke, C. Greve, R. Moko, F. Beckmann, B. Misof
An updated phylogeny of Anisoptera including formal convergence analysis of morphological characters

2013
R. Castanhinha, R. Araújo, L.C. Júnior, K.D. Angielczyk, G.G. Martins, R.M.S. Martins, C. Chaoiui, F. Beckmann, F. Wilde
Bringing dicynodonts back to life: paleobiology and anatomy of a new emydopoia genus from the Upper Permian of Mozambique

2013
R. Araújo, R. Castanhinha, R.M.S. Martins, O. Mateus, C. Hendrickx, F. Beckmann, N. Schell, L.C. Alves
Filling the gaps of dinosaur eggshell phylogeny: Late Jurassic Theropod clutch with epioles from Portugal

2013
F. Friedrich, H. Pohl, F. Beckmann, R.G. Beutel
The head of *Meropis tuber* (Meropidae) and the phylogeny of Mecoptera (Hexapoda)

2013
Alexander Blanke, Carola Greve, Benjamin Wipfler, Rolf G. Beutel, Barbara R. Holland, Bernhard Misof
The Identification of Concentrated Convergence in Insect Heads Corroborates Paleoptera

Latest Publications

2013
An updated phylogeny of Anisoptera including formal convergence analysis of morphological characters

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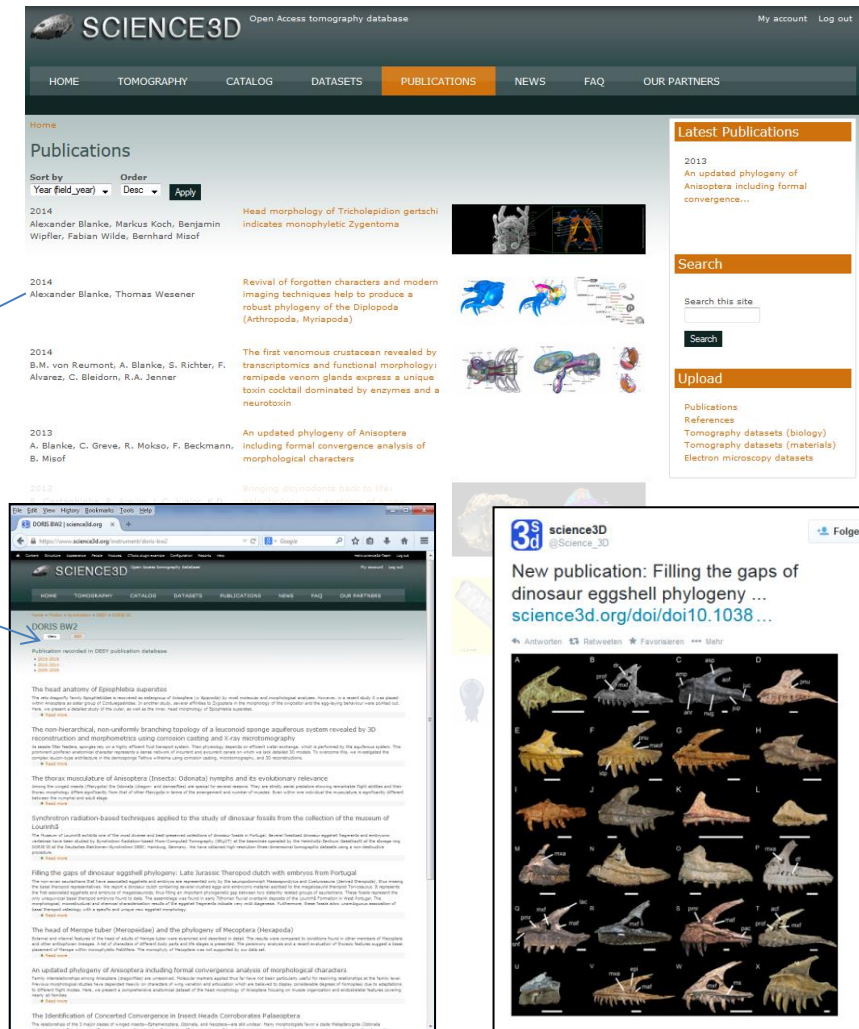
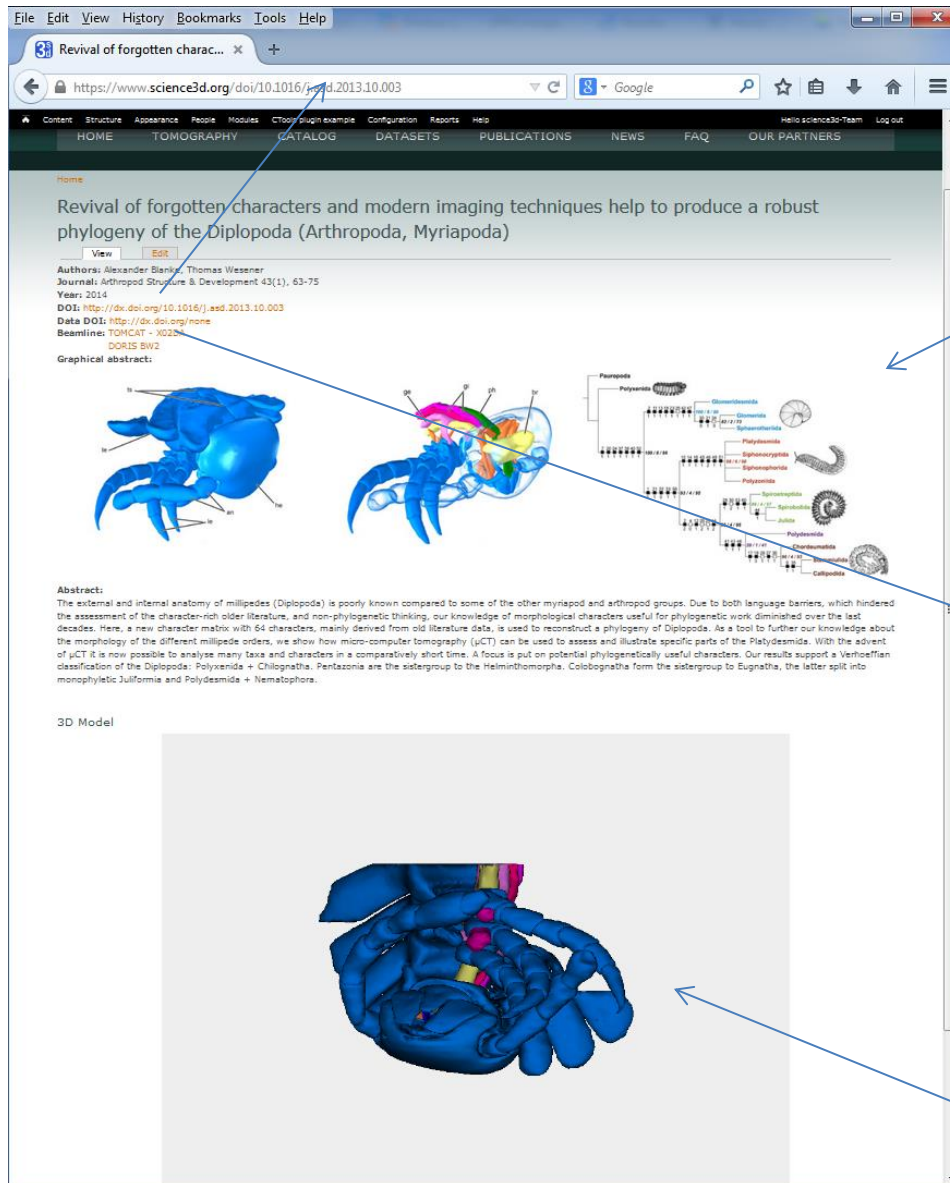
Publications
References
Tomography datasets (biology)
Tomography datasets (materials)
Electron microscopy datasets

- Simple mechanisms
 - Uploading any data
 - Highlighting input





web

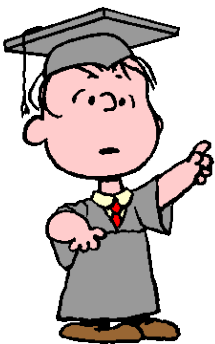


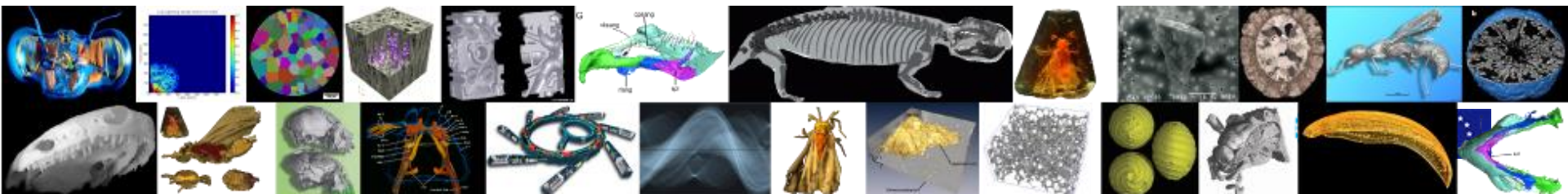
- 3-D models
 - Still primitive
 - Lacking 3-D pdf capabilities

- Data
 - Data upload/download
 - Long term mass storage dCache (unlimited)
 - Conventional storage for the catalog (secure, fast)
 - Fast cluster storage (for HPC wherever needed)
 - Register data with datacite
 - Convert / Provide data in maintainable formats
- Compute infrastructure
 - Work group server without access restrictions
 - Batch farm (~8000 cores); GRID farm (many more cores)
 - HPC cluster (~3000 cores) with fast interconnect (IB)
 - GPGPUS (nvidia M2050 → K20X) with slow/fast interconnect
 - Avizo, Matlab, IDL, Mathematica, Maple, etc
 - Fast remote graphical access
- Other Services
 - feeds/tweets/newsletters
 - 3D print (tbc)



- Tomography offers tremendous insights into evolution, anatomy, materials...
 - 3D models on the screen; 3D prints for the classroom
 - Still very difficult to harvest for pupils
 - Might well be completely unrealistic
- Science 3D might offer a platform
 - for scientists and teacher/pupils/students to make contacts and possibly bring science more into classrooms
- High hurdles
 - Physics, Mathematics, Biology, Language barriers
 - Even a challenge for teachers
- Considering making (very limited) experiment time available (Schülerlabor)

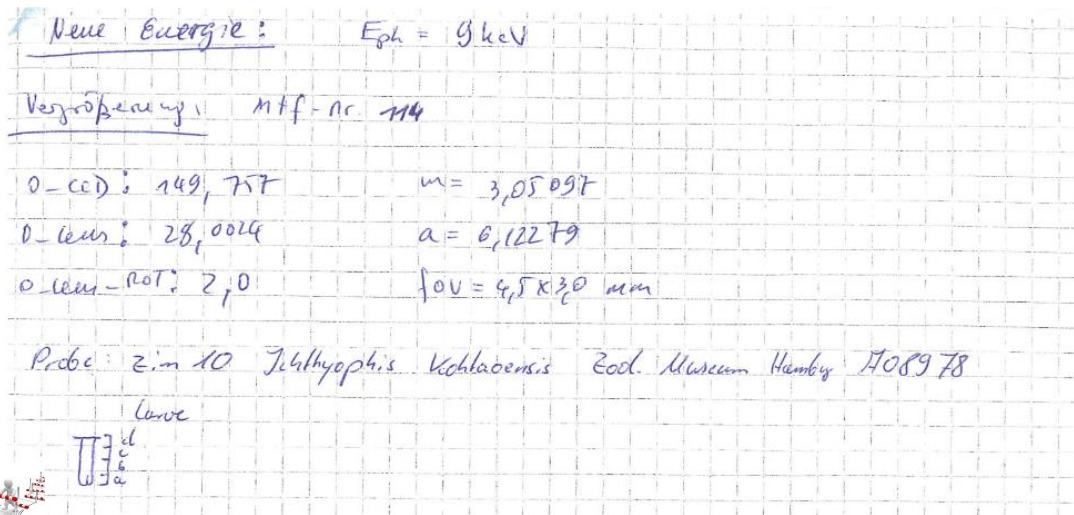




- **Hardware**
 - No problem at all
- **Chicken & egg**
 - But quite a bit of support from scientists
- **Manpower & Time**
 - Development of services (3D, workflows, platform)
 - Currently a very primitive setup
 - Data standardization & Content (background material)
 - HUGE problem – intend to apply for a H2020 grant
- **Knowledge**
 - We are lacking the information which data precisely where used
 - Sample preparation
 - Experiment parameters
 - We can't make data public; should be responsibility of the owner
 - Though ownership is an open debate
 - Name the sample correctly
 - Get taxonomies right



- Data formats & meta-data
 - NeXus/HDF5 as a standard
 - Evolving & insufficient
 - Software support limited
 - No data in standard format
 - Complex meta-data
 - Spread over various sources
 - No automatic workflow
 - Manual process



3.4.19. NXtomo

Status:

application definition, extends [NXobject](#), version 2.0

Description:

This is the application definition for x-ray or neutron tomography raw data. In t images and, of course the sample. In order to distinguish between them images

Symbols:

These symbols will be used below to coordinate datasets with the same shape.

nFrames: number of frames

xsize: number of pixels in X direction

ysize: number of pixels in Y direction

Groups cited:

[NXdata](#), [NXdetector](#), [NXentry](#), [NXinstrument](#), [NXmonitor](#), [NXsample](#), [NXsource](#)

Structure:

entry: [NXentry](#)

title: [NX_CHAR](#)

start_time: [NX_DATE_TIME](#)

end_time: [NX_DATE_TIME](#)

definition: [NX_CHAR](#)

Official NeXus NXDL schema to which this file conforms

Obligatory value: NXtomo

instrument: [NXinstrument](#)

(source): [NXsource](#)

type: [NX_CHAR](#)

name: [NX_CHAR](#)

probe: [NX_CHAR](#)

Any of these values: neutron | x-ray | electron

detector: [NXdetector](#)

data[nFrames, xsize, ysize]: [NX_INT](#)

image_key[nFrames]: [NX_INT](#)

- Publications & materials
 - Copyright situation almost always unclear
 - Providing resources on behalf of the author
 - Providing publications via the DESY-library services?
 - Re-use of images?
 - Re-use of supplemental materials?




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Title: Filling the gaps of dinosaur eggshell phylogeny: Late Jurassic Theropod clutch with embryos from Portugal

Author: Ricardo Araújo, Rui Castanhinha, Rui M. S. Martins, Octávio Mateus, Christophe Hendrickx, F. Beckmann

Publication: Scientific Reports

Publisher: Nature Publishing Group

Date: May 30, 2013

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