



Automated Analysis of X-ray Data

Alexey Ershov

INSTITUTE FOR PHOTON SCIENCE AND SYNCHROTRON RADIATION (IPS)



Outline



- Automated Analysis of X-ray Data
 - X-ray Imaging
 - Analysis of Dynamical X-ray Data
 - Application Examples
- Collaboration between TPU and KIT
 - Research Directions
 - Possibilities for Students
- Current Topics and Tasks
- Lecture: "Image Acquisition Methods and Image Analysis"



Automated Analysis of X-ray Data

X-Ray Imaging

X-rays are electromagnetic radiation:

- Wavelength in the range 0.01 to 10 nm
- Energies: 100 eV to 100 keV

Interaction of X-rays with the matter:

- Photoelectric absorption
- Scattering

More info on the lecture of Prof. Tilo Baumbach "Modern X-ray Physics"

X-ray application:

- X-ray crystallography
- X-ray astronomy
- X-ray microscopy
- X-ray fluorescence
- Radiography
- Computed Tomography (CT)
- Security systems





First X-ray radiograph. Source: Wikipedia



DNA structure. Source: Wikipedia

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CT of the neck region

ANKA Synchrotron





Time-resolved X-Ray Imaging



X-ray imaging allow to investigate internal structure of time-varying processes.

Study examples:

- Evolution of structures
- Fabrication processes
- Living organisms
- Liquid flows, Diffusion processes and many more...

Time-resolved X-ray data analysis:

- Study of the dynamics
- Motion analysis and Object tracking
- Motion-based segmentation



Metal foaming process. Source: TU Berlin



Crack growth in flip-chips.



Moving bug. Source: State Museum of National History, Karlsruhe

We aim to extract dynamical information using **optical flow** methods.

Optical Flow



Optical flow problem is related to the field of **Computer Vision**.

Given: Two images $\mathbf{f} = (f_{1,1}, ..., f_{N,M})^{\top}$ and $\mathbf{g} = (g_{1,1}, ..., g_{N,M})^{\top}$ **Task:** Displacement field $\mathbf{u} = (\mathbf{u}_{1,1}^{\top}, ..., \mathbf{u}_{N,M}^{\top})^{\top}$ which maps all the pixel from the first frame to their new positions on the second frame



chewing cockroach sequence

vector visualization

motion field using color coding

A number of well-established optical flow methods exists. **Our choose**: Variational optical flow methods

Optical Flow Model



General idea: Use assumptions about image data and motion model.

First idea: brightness constancy assumption

f(x, y, t) - color of a pixel on the first image f(x, y, t+1) - color of a pixel on the second image f(x, y, t) - f(x+u, y+v, t+1) = 0 u, v - unknown displacements

Second idea: Assume the smoothness of the flow field.

$$\Box u = \Box u_x \Box = - \text{spatial gradient} \qquad |\Box u| = \sqrt{u_x^2 + u_y^2} - \text{magnitude of gradient} \qquad |\Box u|^2 \rightarrow 0$$

The variational methods compute the **displacement field** as a minimiser of the energy functional:

$$E(u,v) = \int_{\Omega} \underbrace{\left(f(x,y,t) - f(x+u,y+v,t+1)\right)^2}_{\text{data term}} + \alpha \underbrace{\left(|\nabla u|^2 + |\nabla v|^2\right)}_{\text{smoothness term}} dx \, dy \, .$$

Many advanced models and model assumptions are developed for state-of-the-art optical flow methods...

Solution



convex function

global minimum

How to find the minimizer for the constructed energy functional?

$$F(u,v) = \int_{\Omega} \underbrace{\left(f(x,y,t) - f(x+u,y+v,t+1)\right)^2}_{\text{data term}} + \alpha \underbrace{\left(|\nabla u|^2 + |\nabla v|^2\right)}_{\text{smoothness term}} dx \, dy \, .$$

Idea: Use tricks from mathematics

If functional is **convex** a unique, global minimum exists and can be derived directly using **Euler-Lagrange equations**:

$$0 \stackrel{!}{=} F_u - \frac{\partial}{\partial x} F_{ux} - \frac{\partial}{\partial y} F_{uy}, \quad \text{with (reflecting) Neumann boundary conditions:}
0 \stackrel{!}{=} F_v - \frac{\partial}{\partial x} F_{vx} - \frac{\partial}{\partial y} F_{vy}, \quad \mathbf{n}^\top \nabla u = 0 \\ \mathbf{n}^\top \nabla v = 0.$$

Next step: Discretize the Euler-Lagrange equations on rectangular grid. Solve system of equations $A\mathbf{x} = \mathbf{b}$, by using an approximation and **iterative** scheme $\mathbf{x}^{k+1} = A_1^{-1}(\mathbf{b} - A_2 \mathbf{x}^k)$ (Gauss –Seidel method)

We use state-of-the-art, highly accurate and robust optical flow methods.

Developmental Biology



African Clawed Frog (Xenopus laevis) - Vertebrate model organism



adult African clawed frog

embryo development of Xenopus laevis.

- Unlimited availability
- \rightarrow over 1000 eggs per day
- Homogeneous population
- \rightarrow no individual factors

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- Manipulation
- \rightarrow injections, transplantations,...
- Experiments within the embryo
- (*in vivo*) and in petri dish (*in vitro*)



In-vivo X-ray Study of Embryo Development



Application: Analyze morphogenetic movements during embryogenesis. Imaged by *in-vivo* phase-contrast 4D X-ray microtomography.



Problem: Complexity of movements and many interconnected events **Solution**: Use multi-scale (**hierarchical**) motion analysis approach

Data Processing Pipeline



Aim: Correct image artifacts and enhance data quality



3D Rendering of Entire Embryo





Differential motion



Aim: Distinguish collective and individual cells motion; passive and active movements



 $ec{v}$ - motion field v_x, v_y, v_z - components $ec{
abla}$ - spatial gradient

Measures

 $|\vec{v}|$ - motion magnitude

 $G \equiv |\vec{\nabla} v_x| + |\vec{\nabla} v_y| + |\vec{\nabla} v_z|$

- motion non-uniformity

Analyzing individual cells



Aim: Track individual cells, analyze their dynamics to study interaction mechanisms.



J. Moosmann, A. Ershov, V. Altapova, T. Baumbach, M. Prasad, C. LaBonne, X. Xiao, J. Kashef, and R. Hofmann *X-ray phase-contrast in vivo microtomography probes new aspects of Xenopus gastrulation* **Nature 497** (7449), 374–377 (2013)

Moosmann, J.; Ershov, A.; Weinhardt, V.; Baumbach, T.; Prasad, M. S.; LaBonne, C.; Xiao, X.; Kashef, J. & Hofmann, R. *Time-lapse X-ray phase-contrast microtomography for in vivo imaging and analysis of morphogenesis*, **Nature Protocols 9** (2), 294—304 (2014)

Changes in internal structures



Aim: Analyze changes in internal structures to get insights about embryo morphogenesis.



J. Moosmann, A. Ershov, V. Altapova, T. Baumbach, M. Prasad, C. LaBonne, X. Xiao, J. Kashef, and R. Hofmann *X-ray phase-contrast in vivo microtomography probes new aspects of Xenopus gastrulation* **Nature** 2013

In-vivo X-ray 4D Cinetomography

Application: Analyze function of hip joints in living insect.

In-vivo X-ray Cinetomography = Ultra-fast 4D X-ray Imaging + Automated Data Analysis



experimental setup



radiographic projection





biological screw



volume rendering



photon energy: 9.6–24 keV pixel size: 1.2 µm imaging rate: 1500 projection / sec projections / tomogram: 200 tomograms / sec: 7.5 volumes



Problem: The data quality is not sufficient to compute reliable motion field

Robust method to extract kinematics:

- Distribute landmarks for both parts
- Track landmarks in forw. and back. directions
- Filter only reliable landmarks
- Register landmarks from frame i and i+1
- Obtain global transformation M_t
- Decompose M_t into

translational and rotational components

Confidence measure: Forward-backward cross-check



Morphodynamics



Aim: In-vivo study of morphological dynamics of a screw joint system.



In vivo X-ray 4D Cinetomography for Tracking Morphological Dynamics T. dos Santos Rolo, A. Ershov, T. van de Kamp, and T. Baumbach **Proceedings of the National Academy of Sciences** 2014

In-vivo X-ray 4D Cinetomography









In vivo X-ray 4D Cinetomography for Tracking Morphological Dynamics T. dos Santos Rolo, A. Ershov, T. van de Kamp, and T. Baumbach **PNAS** 2014



Collaboration between TPU and KIT

TPU & KIT: Current Activities

Main research fields:

- Physics
- Informatics

Visiting students (2011 - 2014):

- 7 Bachelor students
- 5 Master/Specialist students
- 4 Guest scientists (PhD)

Current students and scientists:

- 3 Master/Specialist students
- 2 PhD students at KIT
- 1 Guest scientist from TPU

Collaboration projects:

- UFO: Ultra fast X-ray imaging of scientific processes with on-line assessment and data-driven process control
- ASTOR: Arthropod structure revealed by ultra-fast tomography and online reconstruction
- STROBOS-CODE: Stroboscopic and correlative diffraction imaging



Andrey Shkarin PhD students at KIT





Dr. Sergey Lazarev, DESY, Hamburg, Germany



Roman Shkarin PhD student at KIT

Dr. Venera Weinhardt (Altapova), University of Heidelberg, Germany



TPU & KIT: Proposals



To strengthen scientific collaboration between TPU and KIT we propose:

Scientific collaboration in 2 research direction:

- Image Processing and Data Analysis for Medicine and Visual Inspection Systems
- Motion Analysis and Tracking for Video Processing, Monitoring and Intelligent Systems
- Internships / student practice in KIT, Karlsruhe, Germany
- Topics for scientific projects for students
- Topics and co-supervision of Bachelor/Master thesis
- Scientific collaboration with TPU doctorands
- Joint scientific projects with Institute of Cybernetics



Current Topics and Tasks



Task: Automated segmentation of structures in materials and biological specimens.



Institute for Photon Science and Synchrotron Radiation, Imaging Group



Task: Automated segmentation of structures in materials and biological specimens.





Task: Automated segmentation of structures in materials and biological specimens.



Automated segmentation is required for high throughput data analysis!

Automated segmentation methods:

- Grey value thresholding
- Clustering methods
- Edge detection
- Region-growing methods
- Graph partitioning methods
- Watershed segmentation
- Trainable segmentation (NN)

Approaches:

- Automated segmentation
- Semi-automated segmentation
- Multi-level approach

Applications:

- Morphological analysis
- Object detection





Topic: Morphological Analysis



Task: Morphological analysis of porous and fiber materials.



MAVI: A modular system for the quantitative analysis of volume images, <u>www.mavi-3d.de</u> Fraunhofer-Institut für Techno- und Wirtschaftsmathematik ITWM, Kaiserslautern

Topic: Morphological Analysis





tomographic 2D slice

bubbles volume



Baker, D. R.; Brun, F.; O'Shaughnessy, C.; Mancini, L.; Fife, J. L. & Rivers, M. (2012), 'A four-dimensional X-ray tomographic microscopy study of bubble growth in basaltic foam', Nat Commun 3



Task: Create digital atlases of model organisms (*Xenopus*, *Medaka*) to study anatomy, pathology, phenotypes and many biological questions.

Examples of successful projects:



The e-Mouse Atlas Project

Mouse embryo

Chicken embryo



2D tomographic slice

3D volume rendering

The e-Chick Atlas of Anatomy



Task: Create digital atlases of model organisms (*Xenopus*, *Medaka*) to study anatomy, pathology, phenotypes and many biological questions.



African Clawed Frog (Xenopus laevis)



Embryo development of *Xenopus laevis*.



Aus Purves/Sadava/Orians/Heller, Biologie, 7. Aufl., © 2006 Elsevier GmbH



Current Xenopus atlas on the xenbase.org website



Task: Create digital atlases of model organisms (*Xenopus*, *Medaka*) to study anatomy, pathology, phenotypes and many biological questions.





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Current *Xenopus* atlas on the Xenbase website



Inspiration: Human Immunodeficiency Virus (HIV) model visual-science.com, Russia

Topic: Tomographic Reconstruction



Task: Reconstruct a 3D object from a series of radiographic images taken at different angles.



parallel beam geometry line integrals of rays



Example of reconstruction using: 1,2,3,10,45,180 projections

Attenuation: $I = I_0 \exp\left(-\int \mu(x, y) \, ds\right)$ Example of reconstructions Total attenuation along the ray: $p(r, \theta) = \ln(I/I_0) = -\int \mu(x, y) \, ds$

For coordinate system position is given : $x \cos \theta + y \sin \theta = r$

Radon transform: $p(r,\theta) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x,y) \delta(x\cos\theta + y\sin\theta - r) \, dx \, dy$ Reconstruct original object f(x,y)

Topic: Tomographic Reconstruction



Task: Reconstruct a 3D object from a series of radiographic images taken at different angles.



Fourier based methods



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Algebraic reconstruction techniques (ART)

Aims for reconstruction algorithms:

- Improve quality of reconstruction:
 - Robust to noise and artifacts
 - Take into account additional information
- **Reconstruction of dynamical data:**
 - Reduction of motion artifacts
- **Reduce number of projections:**
 - Reduce dose for biological specimens
 - Decrease acquisition time



Topic: Computing on GPUs



Task: High-performance image processing algorithms on graphics processing units (GPU).



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cuBLAS Linear Algebra



NPP Image Processing Primitives

GPU accelerated software in IPS and IPE:

- UFO framework
- Filtered-back projection
- Laminographic reconstruction
- Simulation of X-ray Data (SYRIS)



cuSover Direct Solvers





cuFFT Fast Fourier Transform



Neural Networks

Current developments:

- Segmentation algorithms
- ART reconstruction to reduce dose
- 3D Optical flow methods



Lecture "Image Acquisition Methods and Image Analysis"

"Методы получения и анализа изображений"

Image Acquisition Methods and Image Analysis



- For Bachelor students of Institute of Cybernetics (IC)
- As the discipline on student's choice
- Online course from KIT (Germany) to TPU
- Language: Russian or English?
- Requirements:
 - Mathematics
 - Programming
 - No previous knowledge of algorithms or image processing is required!
- Practical exercises
- Final exam

Image Acquisition Methods

- Imaging with Visible Light
 - Electromagnetic Spectrum
 - Optics, Sensors
 - Photography
 - Telescopes, Microscopy
- 2D X-ray and Gamma-ray Imaging
- X-Ray Computed Tomography (CT)
 - Principles
 - Reconstruction: FBP, ART
 - Artifacts
 - Visualization
- Magnetic Resonance Imaging (MRI)
- Electron Microscopy
- Light-sheet Microscopy
- Ultrasound (US)















Image Processing and Computer Vision



- Foundations
- Image Transformations
 - Fourier Transform
 - Wavelet Transform
- Image Compression and Interpolation
- Linear Filters
- Non-linear Filters
- Morphological operations
- Image Segmentation
- Sequence Analysis
 - Optical Flow
 - Image registration
 - Object Tracking
- 3D Image Reconstruction
- Object Recognition









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Phase retrieval



Tomy dos Santos Rolo

Fast tomography



Jubin Kashef Developmental biology



Thomas van de Kamp

Zoology (arthropods)

Summary

If you are interested in:

- Work on topics of Bachelor/Master thesis (will be available soon)
- Make an internships / student practice in KIT, Karlsruhe, Germany
- Participate in lecture: "Image Acquisition Methods and Image Analysis".
- Scientific collaboration with our group

Lecture will be organized **only** if there will be interest from students!

Take a short poll and give your feedback! http://simpoll.ru/run/survey/39a97383



Thank you for your attention!

Questions?

