Data Science and Scientific Computing

presented by Christoph Lampert

IST AUSTRIA
Institute of Science and Technology

Data Science and Scientific Computing (DSSC)

Interdisciplinary Track in the Graduate School, combining aspects of:

- data analysis
- information processing
- modelling
- numerical simulation

Dan Alistarh

DISTRIBUTED ALGORITHMS AND SYSTEMS

Nick Barton

EVOLUTIONARY GENETICS

Bernd Bickel

COMPUTER GRAPHICS AND DIGITAL FABRICATION

Calin Guet

SYSTEMS AND SYNTHETIC BIOLOGY

Edouard Hannezo

PHYSICAL PRINCIPLES IN BIOLOGY

Marco Mondelli

INFORMATION-THEORETIC VIEW OF DATA SCIENCE

Tim Vogels

COMPUTATIONAL NEUROSCIENCE

Sandra Siegert

NEURO-IMMUNOLOGY

Beatriz Vicoso

SEX-CHROMOSOME BIOLOGY AND EVOLUTION

Christoph Lampert

MACHINE LEARNING AND COMPUTER VISION

Matt Robinson

MEDICAL GENOMICS

Chris Wojtan

COMPUTER GRAPHICS AND PHYSICS SIMULATION

Gasper Tkacik

THEORETICAL BIOPHYSICS AND NEUROSCIENCE

Caroline Muller

ATMOSPHERE AND OCEAN DYAMICS

Carl Goodrich

COMPUTATIONAL SOFT-MATTER PHYSICS

future professors

Dan Alistarh

Distributed Algorithms and Systems

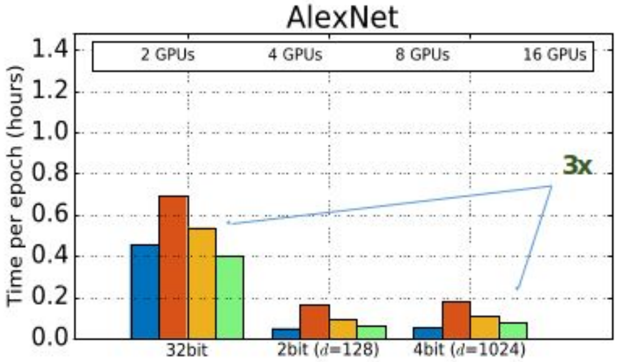
Christoph Lampert

Machine Learning and Computer Vision

Algorithms, data structures, and architectures for *scalable* **distributed computation.**

Theory ↔ Software ↔ Hardware

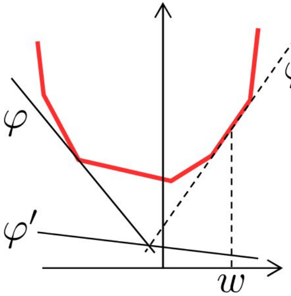
Example:



Scalable Deep Learning

Statistical machine learning:

- transfer learning, continual learning, trustworthy learning, theory of deep learning



Applications in Computer Vision:

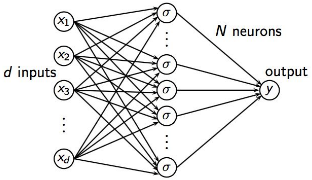
- scene understanding
- generative models of dynamic scenes

Marco Mondelli

Information Theoretic View of Data Science

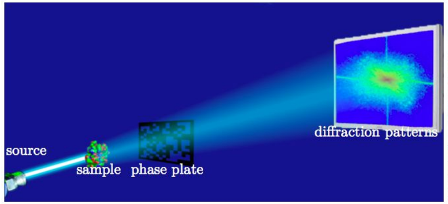
Given data, develop principled solutions to inference problems

- communication, phase retrieval, neural networks



Consider:

- minimum information necessary, low-complexity algorithms, parameter trade-offs



Nick Barton

Evolutionary Genetics

Hybrid zones:

- study selection, gene flow, random fluctuations

Genetics of complex traits:

- theory, experimental evolution, data analysis

Making sense of DNA sequence:

- how can we infer population history, and detect selection

Beatriz Vicoso

Sex-Chromosome Biology and Evolution

Example:
How do sex chromosomes evolve?

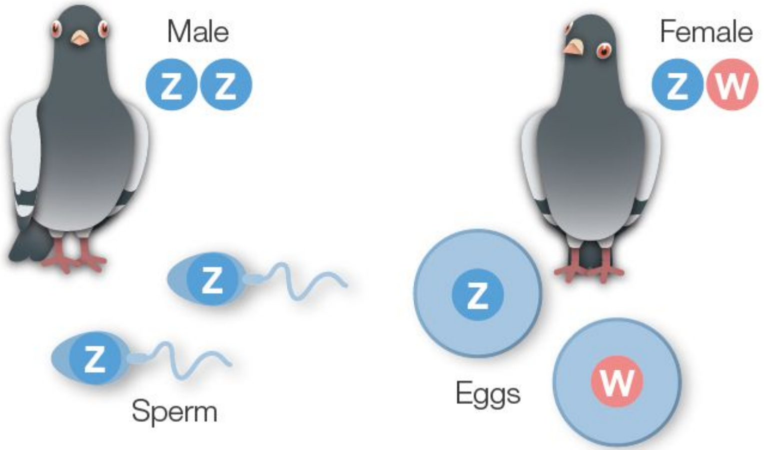
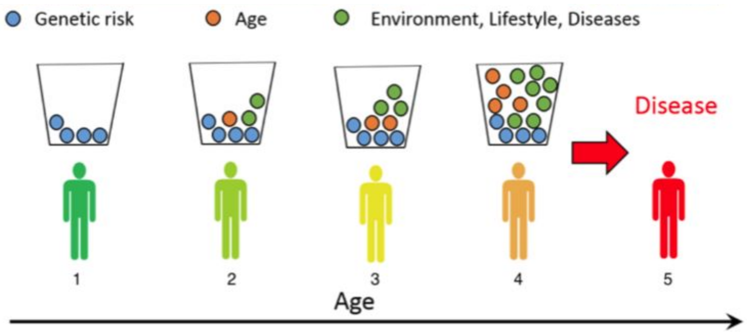


Image: Wikipedia

Matt Robinson

Medical Genomics

Statistical models and computational tools for models of very large-scale human medical record data.



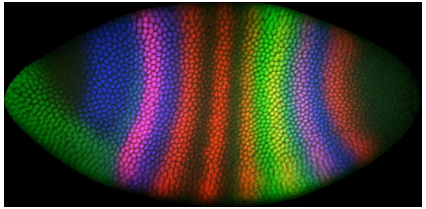
How do genetics and our lifestyles shape our risk of disease?

Gasper Tkacik

Information Processing in Biological Systems

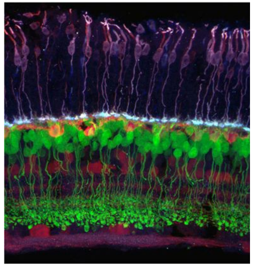
How do biological networks

- evolve?
- learn?
- process information?



Natural science group (biophysics, systems biology), but ~50% project are data-driven, using

- statistics
- information theory
- numerical simulation
- optimization
- ...



Edouard Hannezo

Physical Principles in Biology

Example: how do cells “know” how to make the right decisions?

Bernd Bickel

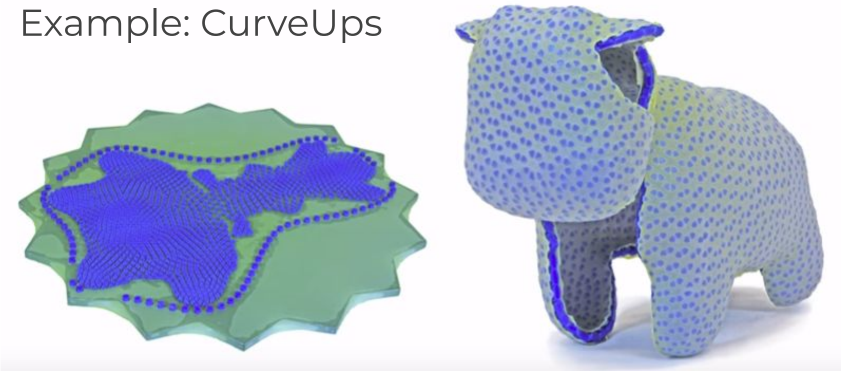
Computer Graphics and Digital Fabrication

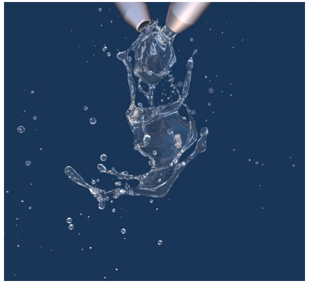
Chris Wojtan

Physics Simulation and Geometry Processing

Methods for modeling, simulating and optimizing (printable) 3D objects

Example: CurveUps





Numerical algorithms for solving differential equations

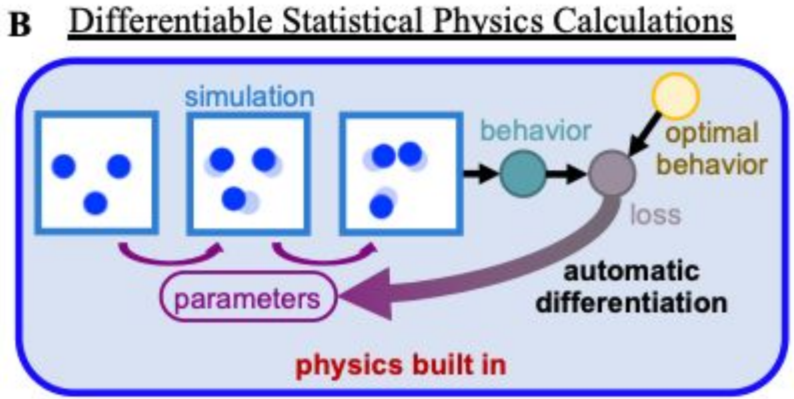
Efficient and robust methods for animating physics

Create tools for manipulating shapes

Carl Goodrich

Theoretical and Computational Soft Matter

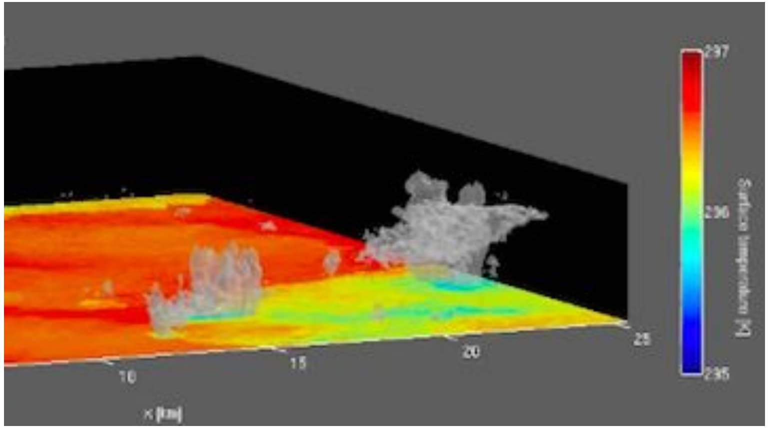
Discovering basic soft matter principles using computational and theoretical tools, such as artificial neural networks



Caroline Muller

Atmosphere and Ocean Dynamics

Fundamental understanding of small-scale processes, such as ocean waves, on our climate, using theoretical and numerical tools, as well as in-situ and satellite measurements.



Tim Vogels

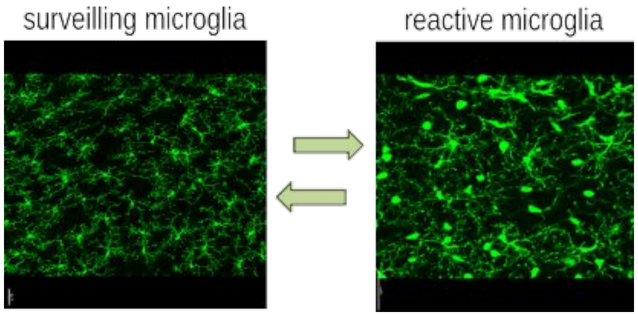
Computational Neuroscience and Neurotheory

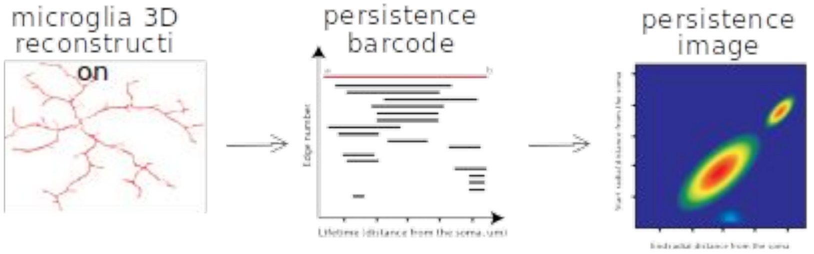
Models of neurons and neuronal networks that distill and re-articulate the current knowledge of how nervous systems compute at a mechanistic level.

Sandra Siegert

Neuroimmunology in Health and Disease

(Topological) data analysis to classify immune cells' morphology and function.



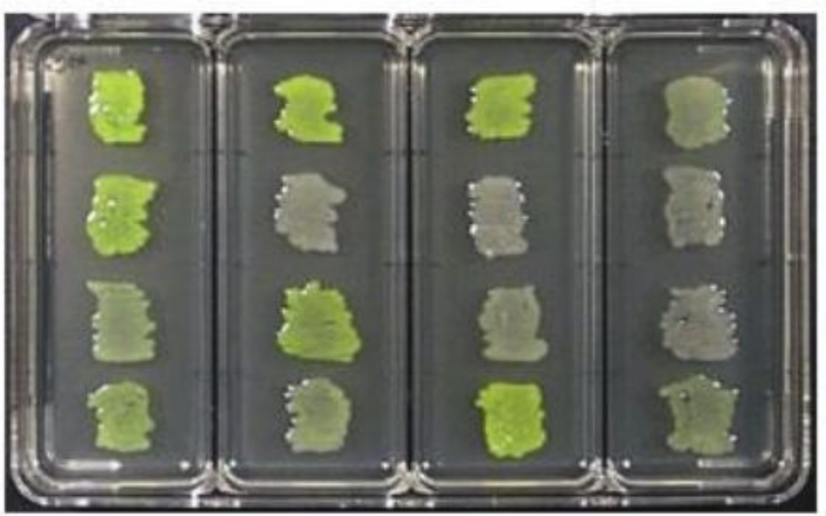


Calin Guet

Systems and Synthetic Biology

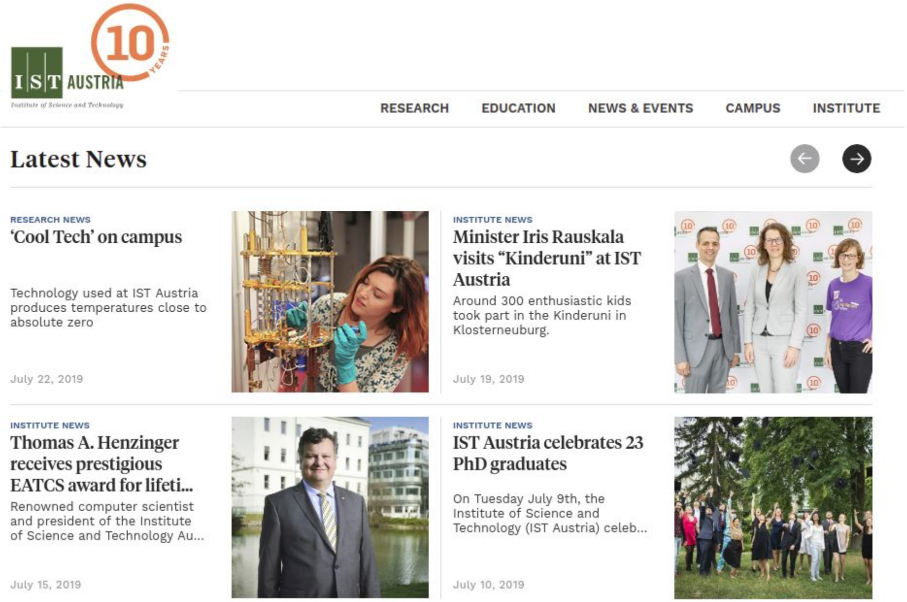
future professor(s)

Example: synthetic genetic networks



Colonies of Escherichia coli performing Boolean logic computations with two chemical inputs and green fluorescent protein (GFP) as the output state.

… regularly check IST Austria homepage …



Data Science and Scientific Computing Track Core Course

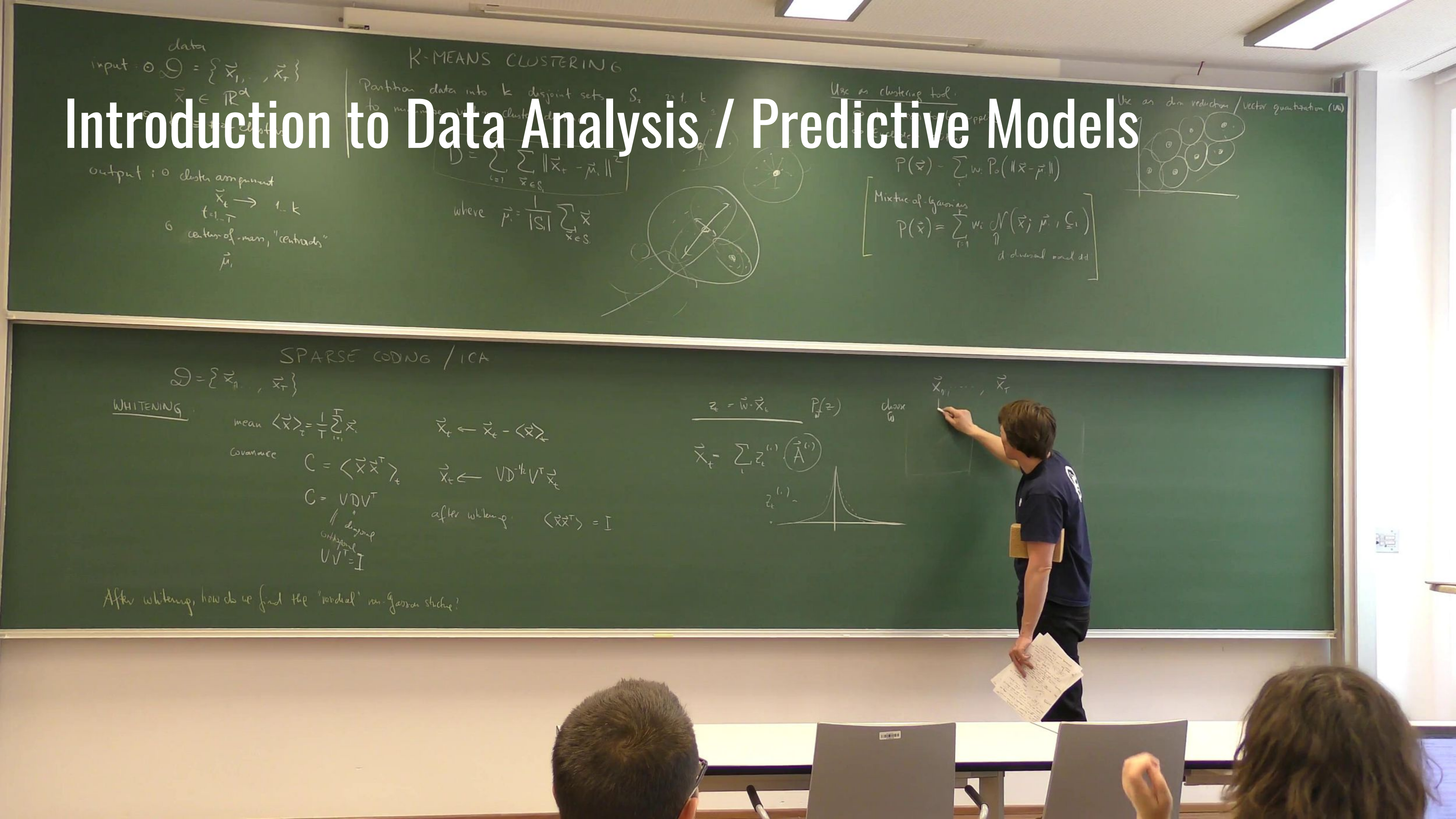
Track Core Course (6 ECTS, spring semester)

- introduction to data analysis / predictive models
- introduction to numerical simulation / optimization
- individual projects that combine both aspects

Prerequisites

- programming skills (preferably Python)
- strong mathematical skills (linear algebra, calculus)
- good understanding of statistics / probabilities

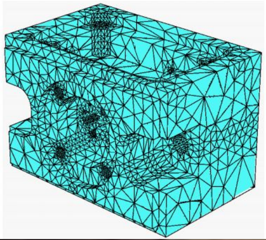
Introduction to Data Analysis / Predictive Models



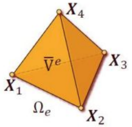
Introduction to Numerical Simulation/Optimization

Overview of Finite Elements

3. Compute forces acting on each element



Finite Elements: Deformation



- Point inside the undeformed tetrahedron (let's assume X_4 is at 0):

$$X = [X_1 - X_4, X_2 - X_4, X_3 - X_4]\lambda$$

$$\lambda = [X_1 - X_4, X_2 - X_4, X_3 - X_4]^{-1}X$$
$$\phi(X) = [x_1 - x_4, x_2 - x_4, x_3 - x_4]\lambda$$

Individual Project

- simulating neuron firing together and developing patterns
- simulating molecular dynamics of chiral proteins to learn group behaviors
- simulating/animating ant colonies
- N-body simulator to study evaporation of star clusters
- study of pattern formation in reaction-diffusion equations
- simulating a "turbidostat" - a lab tool in the Kondrashov group for growing bacteria and studying mutations
- study of data set compression for machine learning models
- game theory simulation to find stable population behaviors
- study of stable/unstable balances between predator/prey interactions on a graph


QUESTIONS
ANSWERS

Following: Meet and Greet in the Courtyard

Reka Borbely
(Tkacik group)

Bernd Prach
(Lampert group)

Manas Borbely
(Tkacik group)