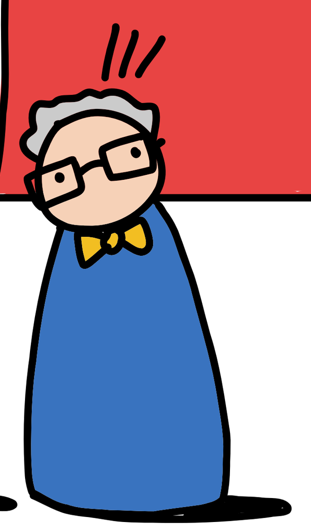
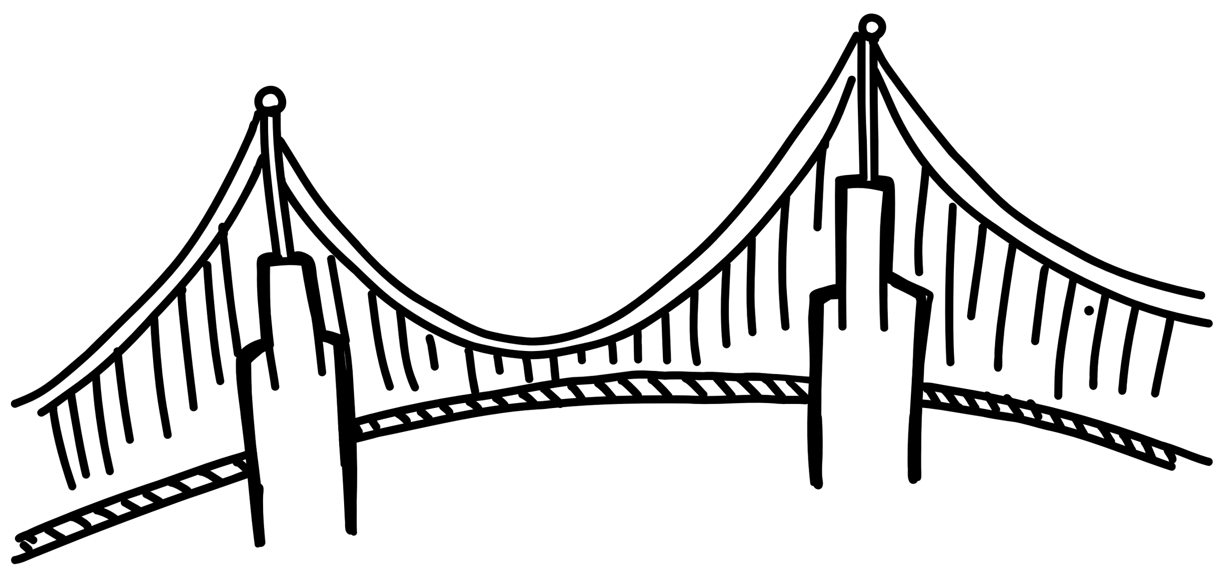
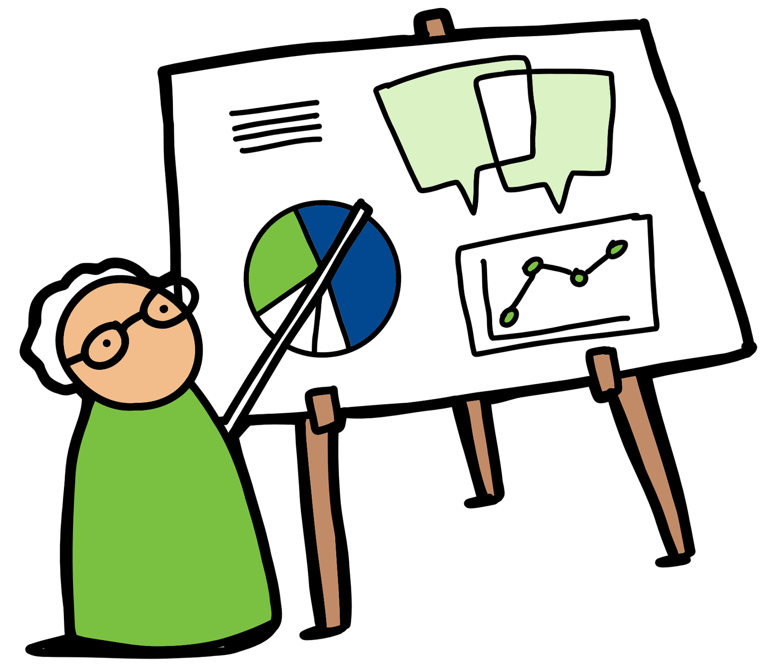
MACHINE LEARNING for SCIENCE



MATHEMATICS at the INTERFACE of DATA-DRIVEN & MECHANISTIC MODELLING

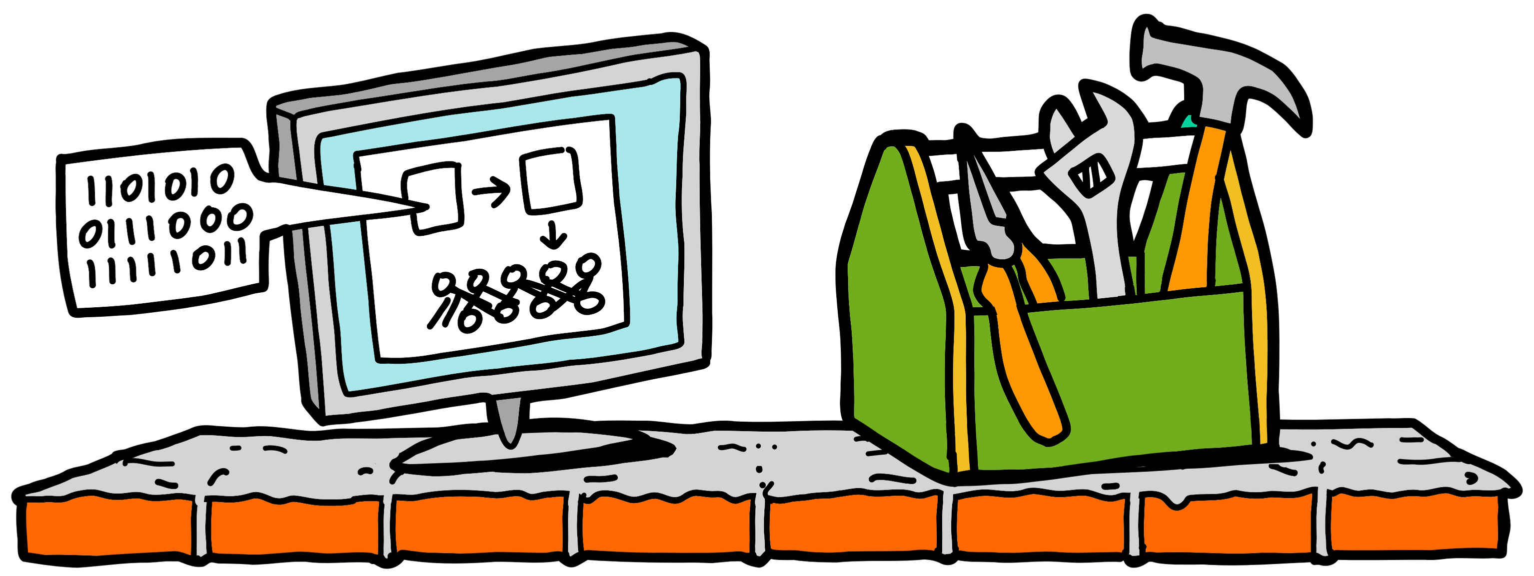


BRIDGING ML & SCIENCE: DIRECTIONS in MATHEMATICS



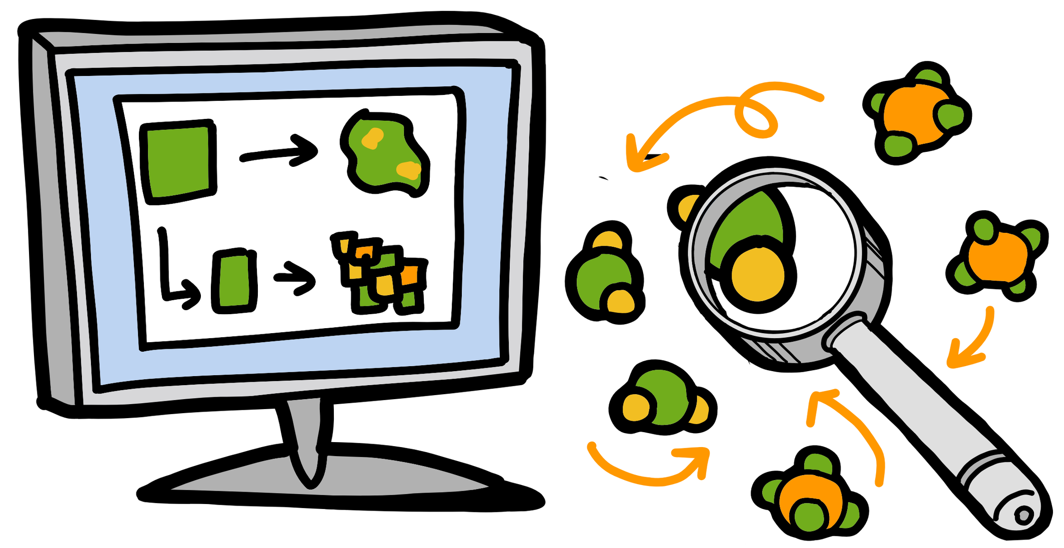
LESSONS from the APPLICATION of MACHINE LEARNING in SCIENCE

- MAREN BÜTTNER
- CHRISTIAN IGEL
- DINA MACHUVE
- CHALLENGER MISHRA
- KLAUS-ROBERT MÜLLER



FOUNDATIONAL CONCEPTS & EMERGING METHODS

- ROBERT C. WILLIAMSON
- PHILIPP HENNIG
- CARL-HENRIK EK
- RICHARD WILKINSON
- BUBACARR BAH
- BERT KAPPEN
- WILSON GREGORY
- SAMUEL KASKI
- JAKOB MACKE
- NIKI KILBERTUS



MACHINE LEARNING for EARTH & CLIMATE SCIENCES

- VERONIKA EYRING
- MARKUS REICHSTEIN
- GUSTAU CAMPS-VALLS
- CHRISTIAN REINERS, ALEXANDER WINKLER

THIS CONFERENCE was HELD at the MATHEMATISCHES FORSCHUNGSINSTITUT OBERWOLFACH on JULY 12-16, 2023

CLICK the SECTION TITLES/ SCIENTISTS' NAMES to GO to PAGE

ORGANISED by NEIL LAWRENCE, JESSICA MONTGOMERY, & BERNHARD SCHÖLKOPF

UNIVERSITY OF CAMBRIDGE

MAX PLANCK INSTITUTE FOR INTELLIGENT SYSTEMS

ACCELERATE PROGRAMME FOR SCIENTIFIC DISCOVERY

BRIDGING ML & SCIENCE: DIRECTIONS in MATHEMATICS

TODAY'S ML is USEFUL for...

- STITCHING TOGETHER DIFFERENT TYPES of DATA for a NUANCED VIEW.
- EXTRACTING INSIGHTS from DATA for MORE ACCURATE UNDERSTANDING of the PROPERTIES of a SYSTEM
- IDENTIFYING AREAS for EXPERIMENTATION & THEORIZING
- SPEEDING UP ANALYSIS
- SIMULATING COMPLEX SYSTEMS

BUT...

- HARD to ENGAGE BOTH ML & DOMAIN EXPERTISE TOGETHER
- TONS of DATA... BUT NO CLEAR WAY to TRACK SUCCESS
- we STILL LACK SOPHISTICATED TECHNIQUES for ESTABLISHING CAUSAL RELATIONSHIPS
- SYSTEMS NEED to be DEPLOYABLE & EASY to USE

LOWERING BARRIERS...

- PROVIDE ACCESSIBLE BENCHMARKS that REFLECT DOMAIN INTERESTS & EXISTING KNOWLEDGE
- SIMPLIFY USER INTERFACES
- ADDRESS a CLEAR NEED
- THEORIES of MIND for HUMAN INTERACTION
- NARRATIVES for SCIENTIFIC RESULTS

WHAT does "MATHEMATICAL FOUNDATIONS for ML" REALLY MEAN?

... ML'S FOUNDATIONAL INTERFACE with the WORLD?

MATHS HELPS US DESCRIBE RELATIONSHIPS

- ... to REPRESENT DOMAIN KNOWLEDGE to be EMBEDDED in ML SYSTEMS
- ... to EXPRESS CONCEPTS like FAIRNESS or INTERPRETABILITY
- ... to CREATE MODELS w/ UNCERTAINTY AWARENESS
- ... to HANDLE HIGH-DIMENSIONAL & SPARSE DATA
- ... to SUPPORT VALIDATION & BENCHMARKING
- ... to MODEL USERS
- ... to PRODUCE EFFICIENT METHODS

FOUNDATIONAL CONCEPTS & EMERGING MATHS can ACT as BRIDGES!

LIKE...

- ... STATISTICS & PROBABILITY
- ... RIEMANNIAN GEOMETRY
- ... LINEAR ALGEBRA
- ... OPTIMISM TECHNIQUES & CALCULUS

& ALSO...

- ... PROBABILISTIC NUMERICS
- ... IMPRECISE PROBABILITIES
- ... FINSLERIAN GEOMETRY
- ... ADJOINT LATENT FORCE MODELS
- ... EQUIVARIANCES

COULD we CREATE a SUITE of these AI TOOLS to DEPLOY ACROSS FIELDS?

RECENT CLIMATE CHANGE is UNPRECEDENTED

MODELS HELP us SIMULATE & ANALYSE the CLIMATE SYSTEM.

MODELS are VITAL, we NEED THEM to be TRUSTWORTHY

- STABLE
- PHYSICALLY-PLAUSIBLE
- BASED ON CAUSAL DRIVERS

CURRENT ML APPLICATIONS in CLIMATE SCIENCE HELP US...

- UNDERSTAND SYSTEMS for CO_2 EXCHANGE & CARBON DYNAMICS
- PREDICT LANDSCAPE & ECOSYSTEM CHANGES UNDER CHANGING CLIMATE CONDITIONS
- FORECAST EXTREME WEATHER EVENTS
- I.D. CAUSAL RELATIONSHIP THAT DRIVE THESE CHANGES

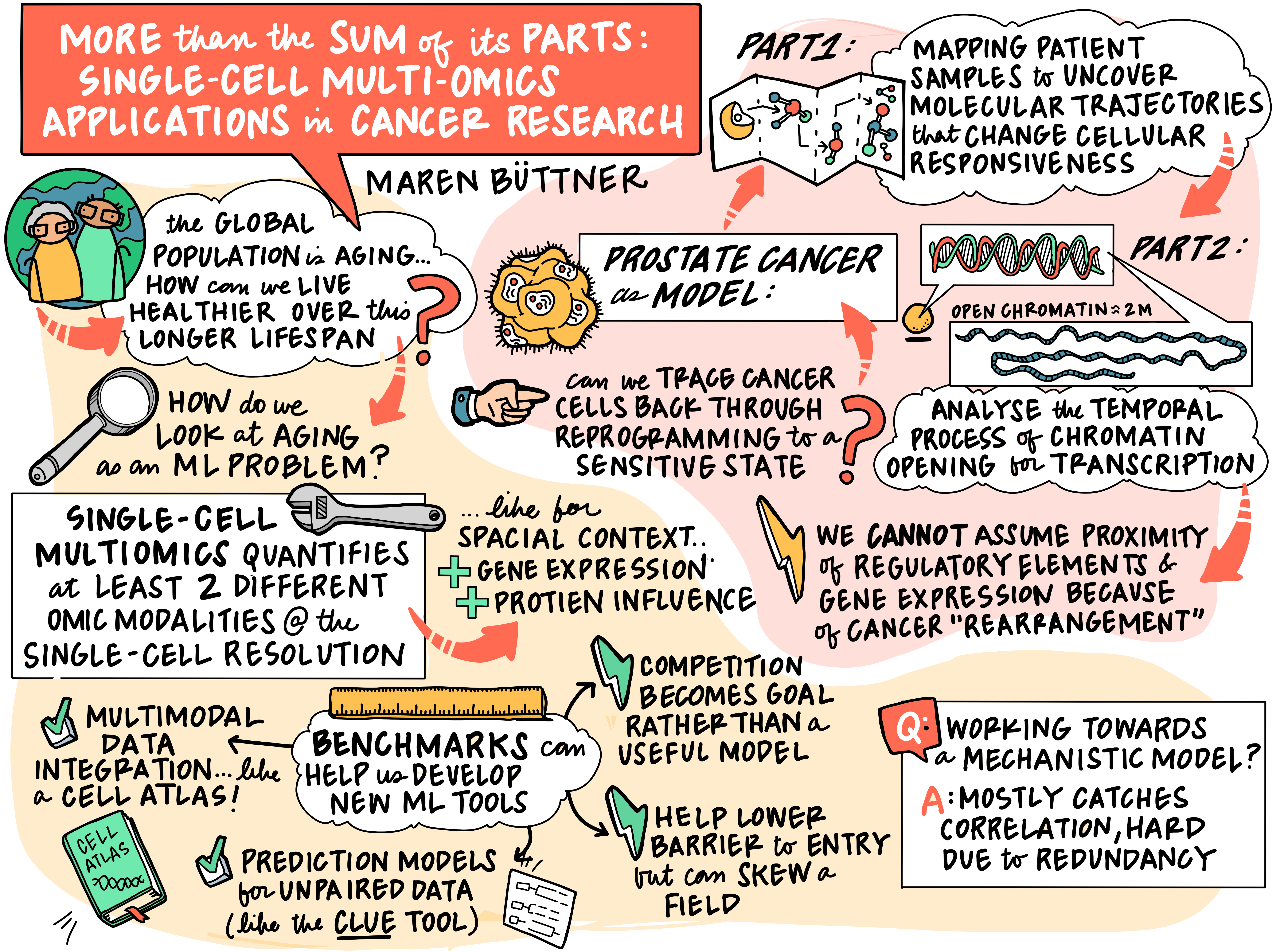
OPEN CHALLENGES...

- ... PARAMETER ESTIMATION & BAYESIAN INFERENCE
- ... EXPLAINABLE AI
- ... IMPROVED GENERALISATION ACROSS CHANGING DISTRIBUTIONS
- ... UNCERTAINTY QUANTIFICATION
- ... MANAGING HYBRID DATA-DRIVEN & MECHANISTIC MODELS

we NEED a COMMUNITY DEDICATED to DEVELOPING this WORK!

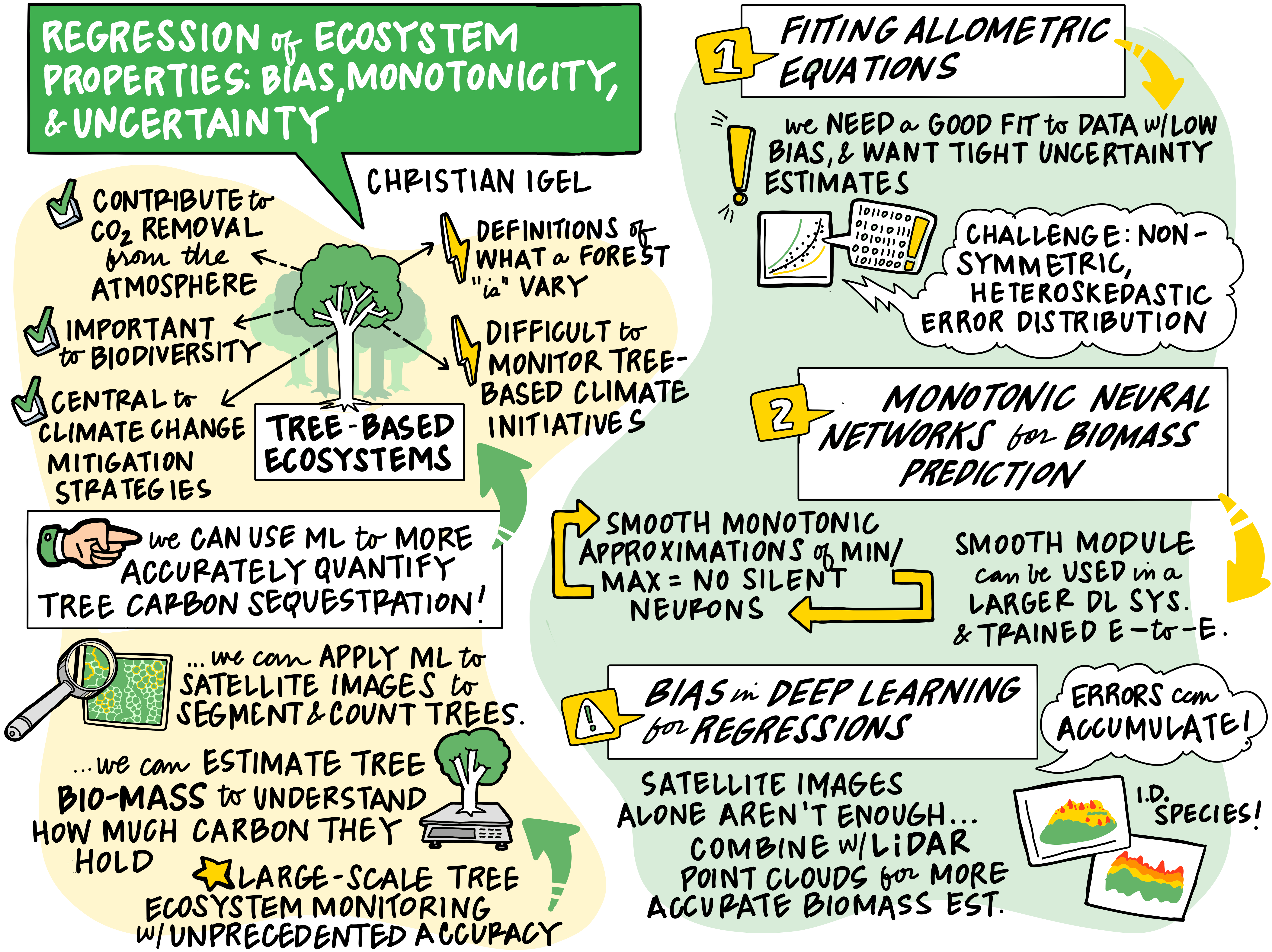
More than the Sum of it's Parts: Single-Cell Multi-omics Applications in Cancer Research

Maren Büttner
Calico Life Sciences
San Francisco, CA



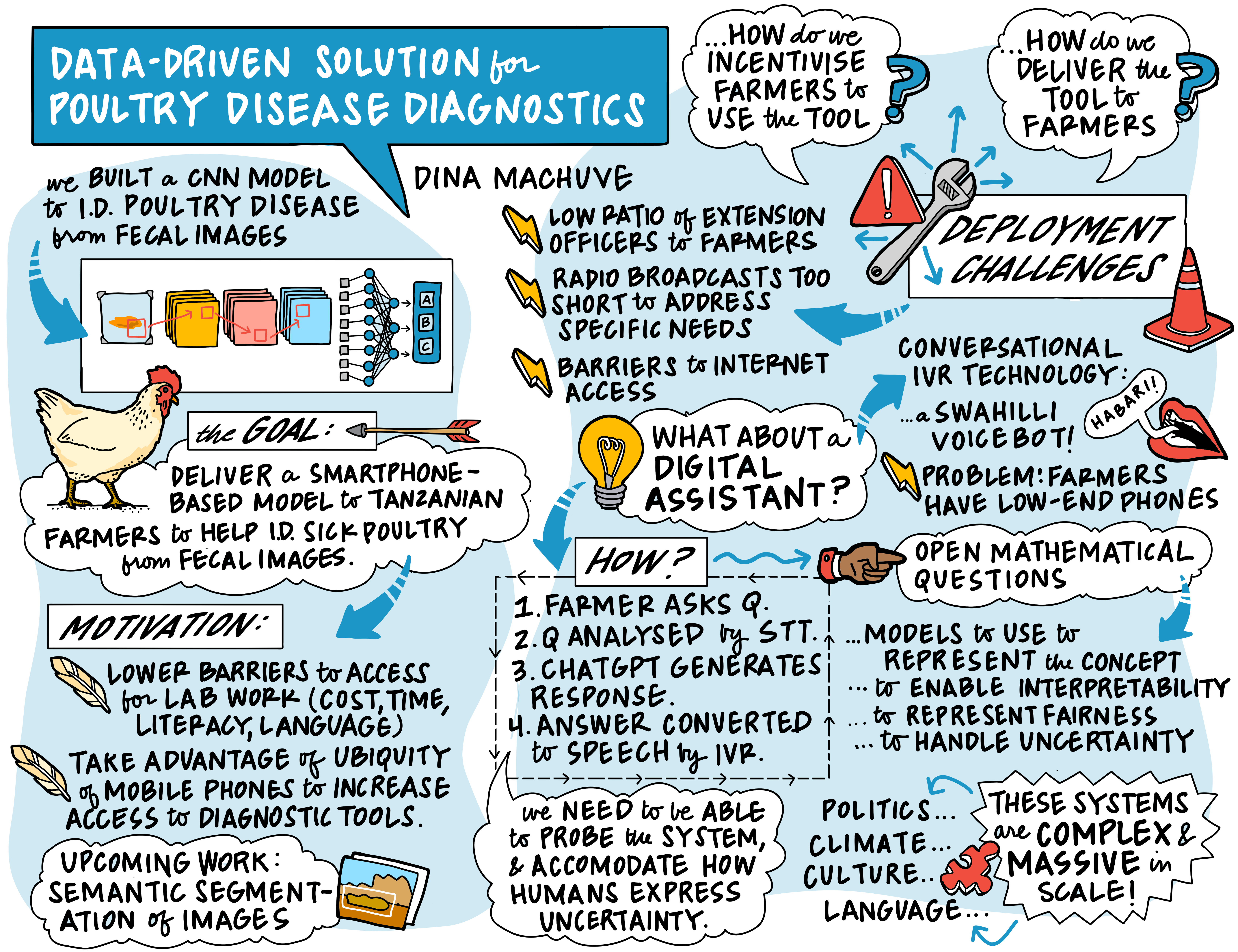
Regression of Ecosystem Properties: Bias, Monotonicity, & Uncertainty

Christian Igel
University of Copenhagen
Copenhagen, DN



Data-Driven Solution for Poultry Disease Diagnostics

Dina Machuve
DevData Analytics
Arusha, TZ



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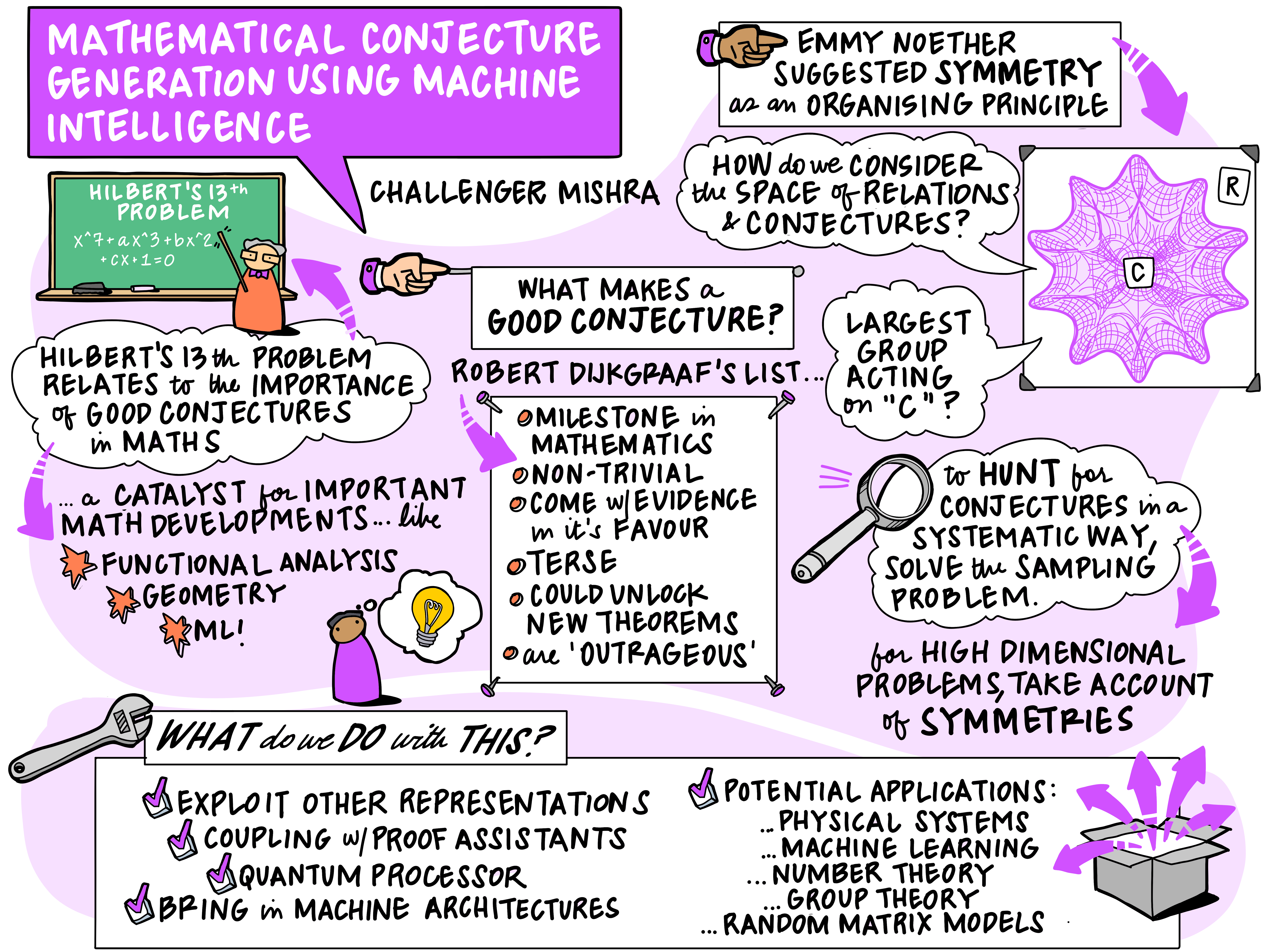
AP SCI ACCELERATE PROGRAMME FOR SCIENTIFIC DISCOVERY

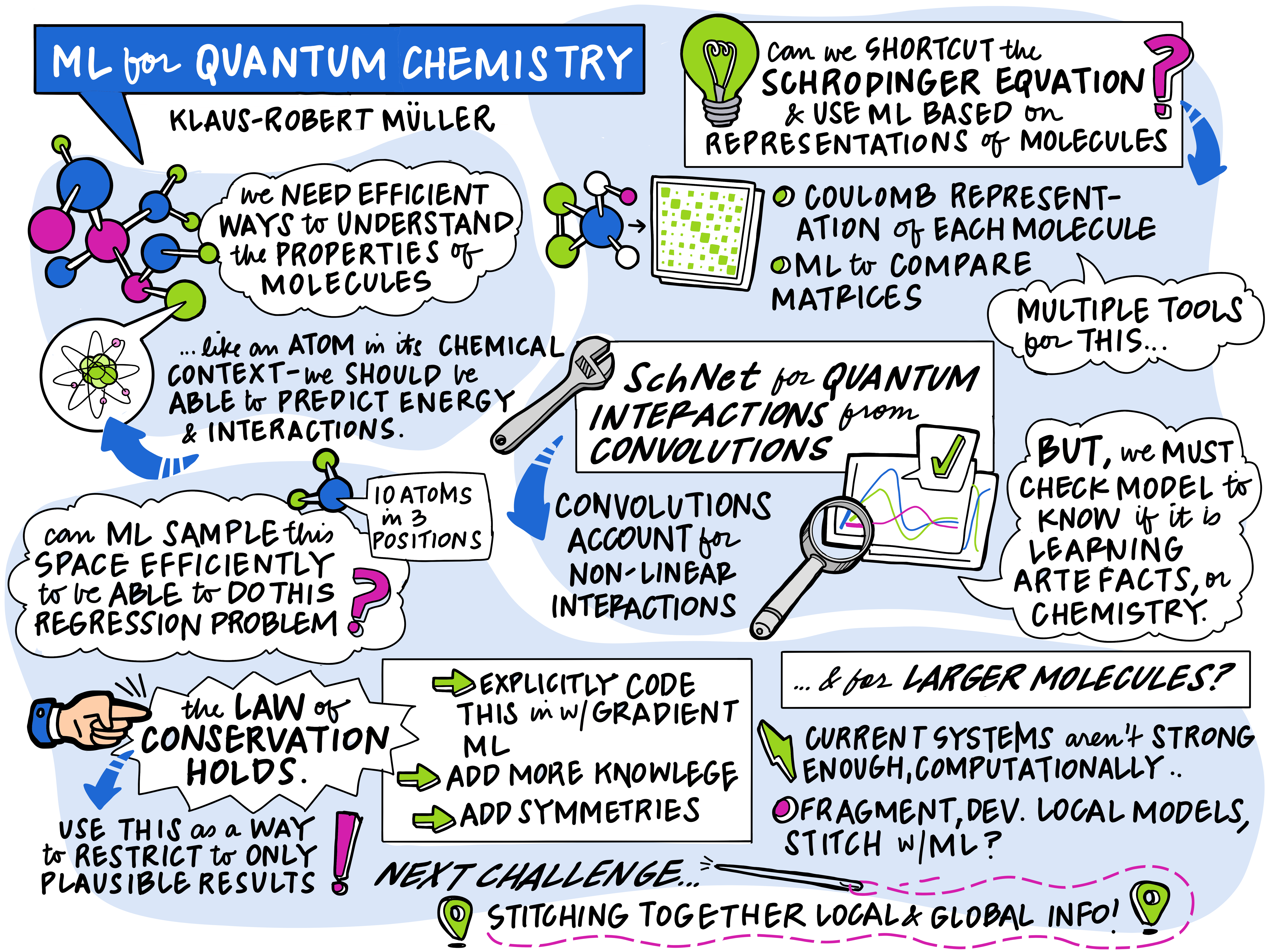
Mathematical Conjecture Generation using Machine Intelligence

Challenger Mishra
University of Cambridge
Cambridge, UK



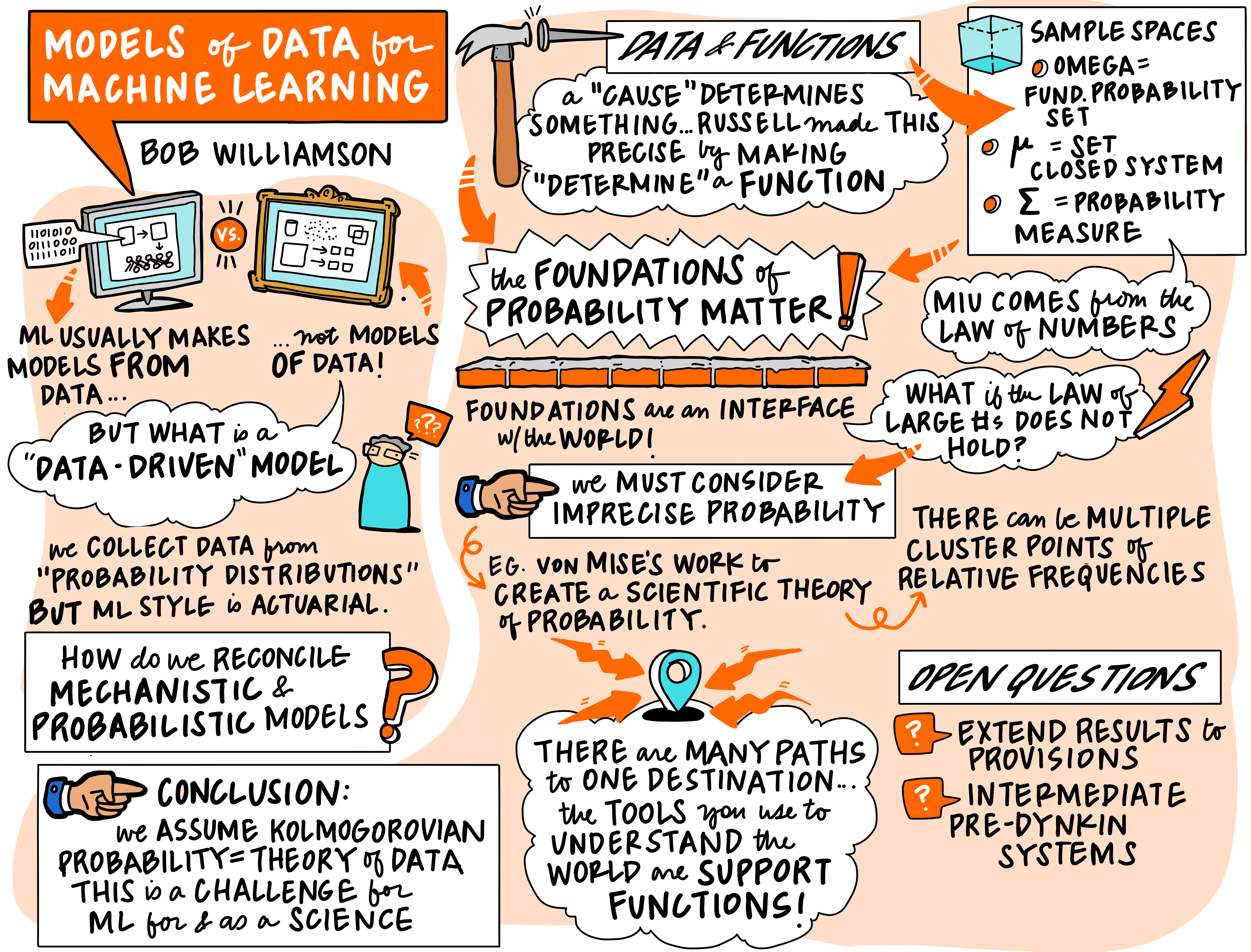
ML for Quantum Chemistry

Klaus-Robert Müller
Technical University Berlin
Berlin, DE



Models of Data for Machine Learning

Robert C. Williamson
University of Tübingen
Tübingen, DE

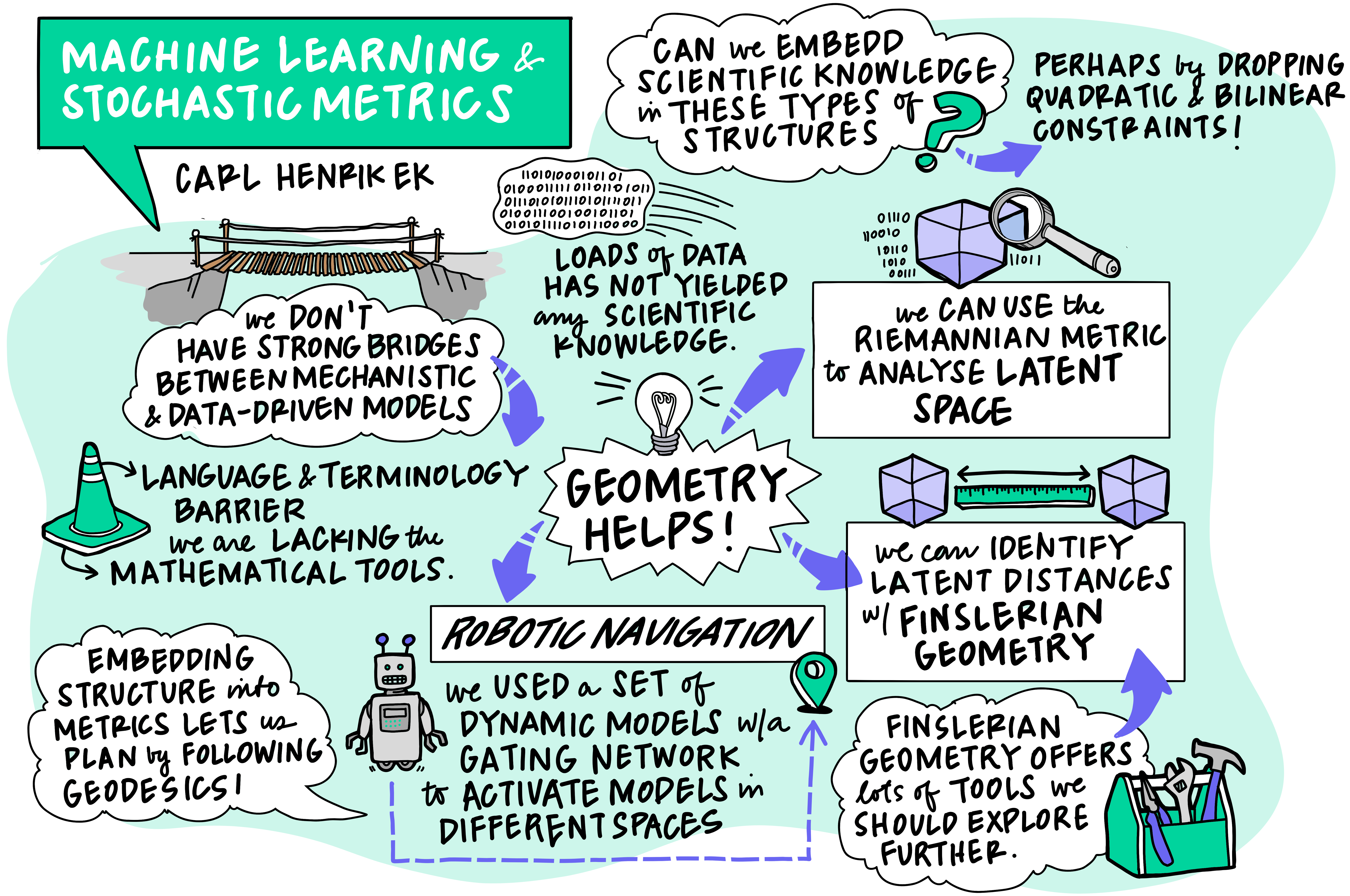


Deep Learning only works if its Bayesian, & Bayesian Deep Learning is Easy

Philipp Hennig
University of Tübingen,
Max Planck Institute for Intelligent Systems
Tübingen, DE

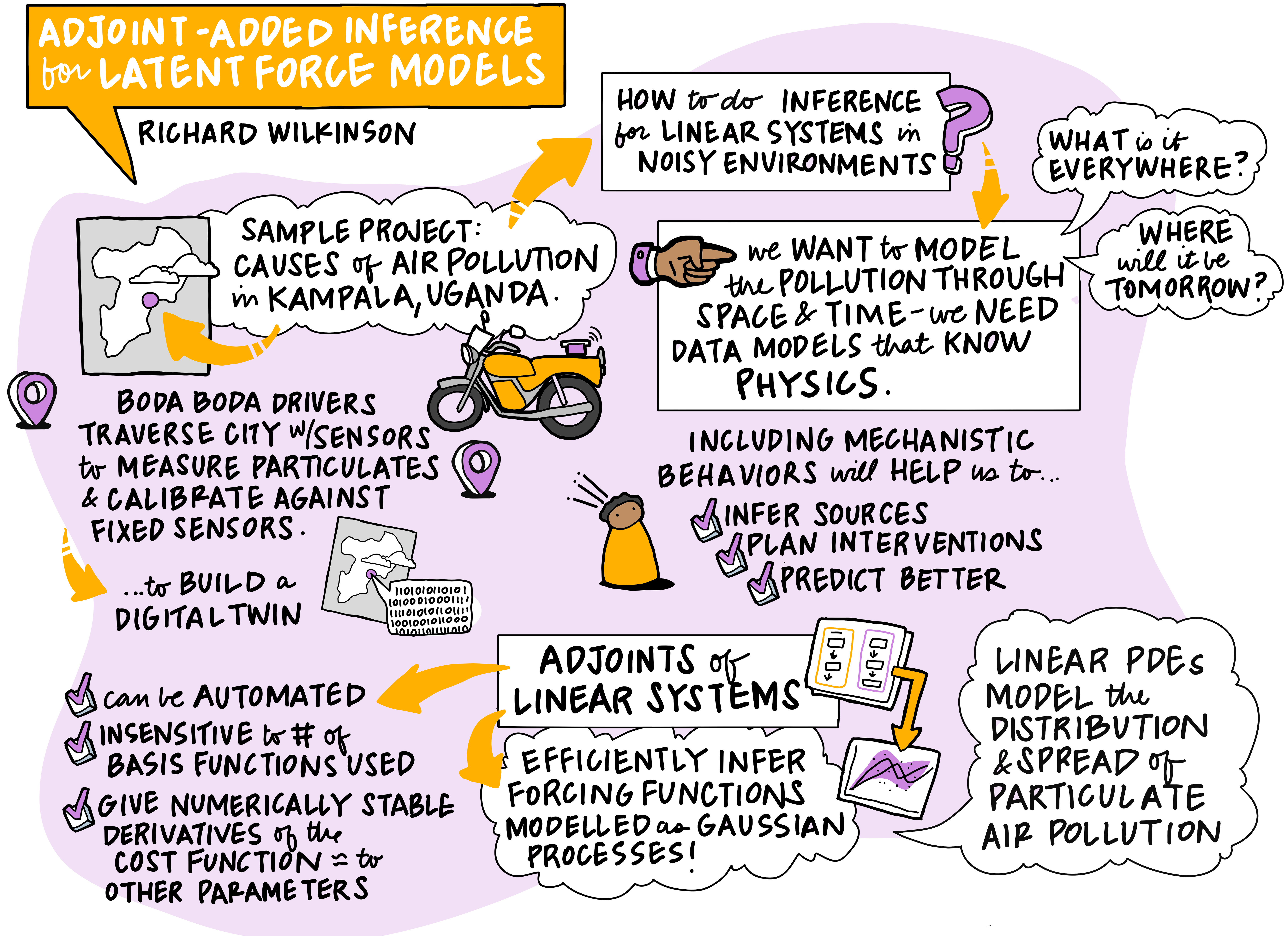
Machine Learning and Stochastic Models

Carl Henrik Ek
University of Cambridge, Cambridge, UK



Adjoint-added Inference for Latent Force Models

Richard Wilkinson
University of Nottingham
Nottingham, UK

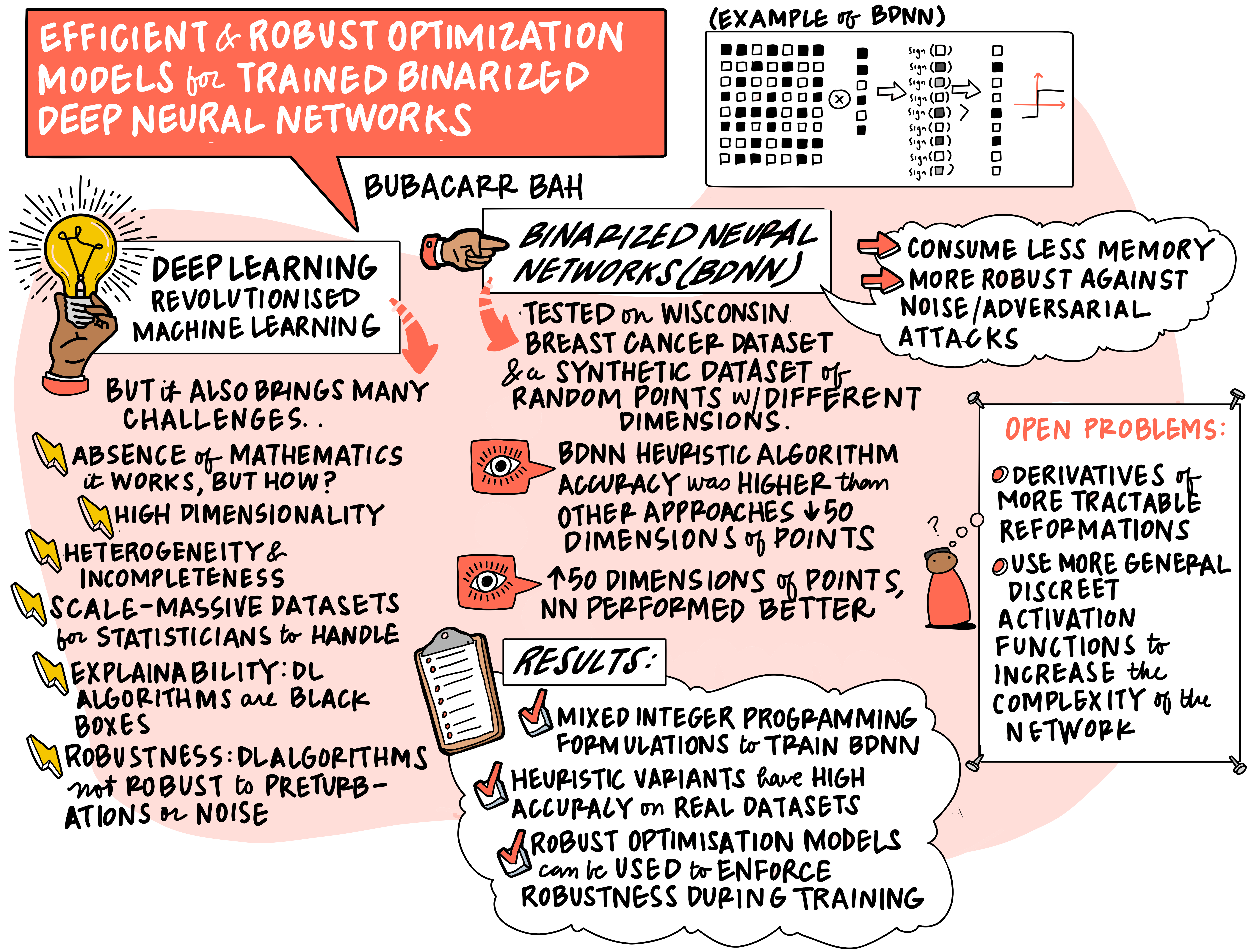


Efficient & Robust Optimization Models for Trained Binarized Deep Neural Networks

Bubacarr Bah

Medical Council Unit The Gambia, London School of Hygiene & Tropical Medicine

Serrekunda, GM



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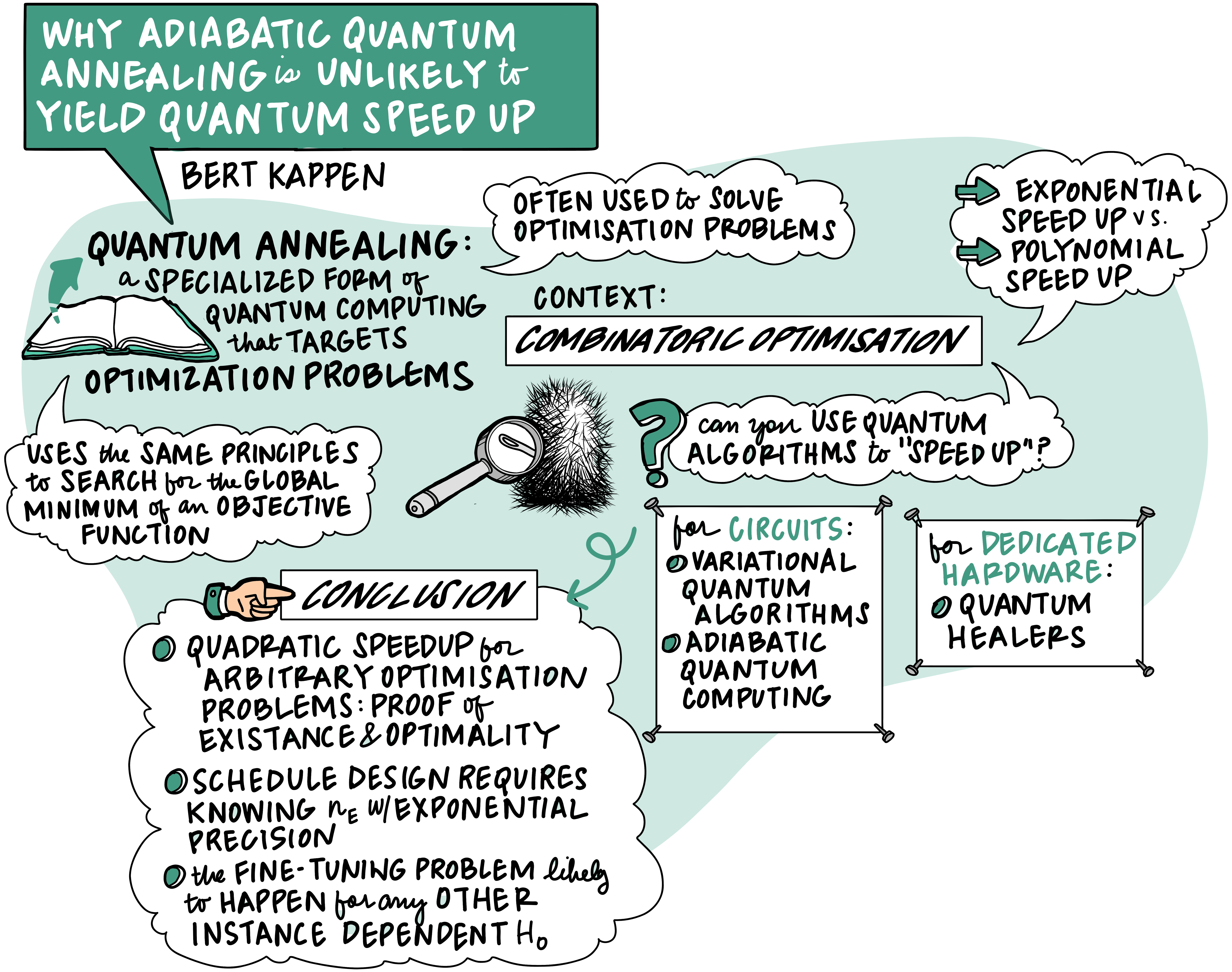
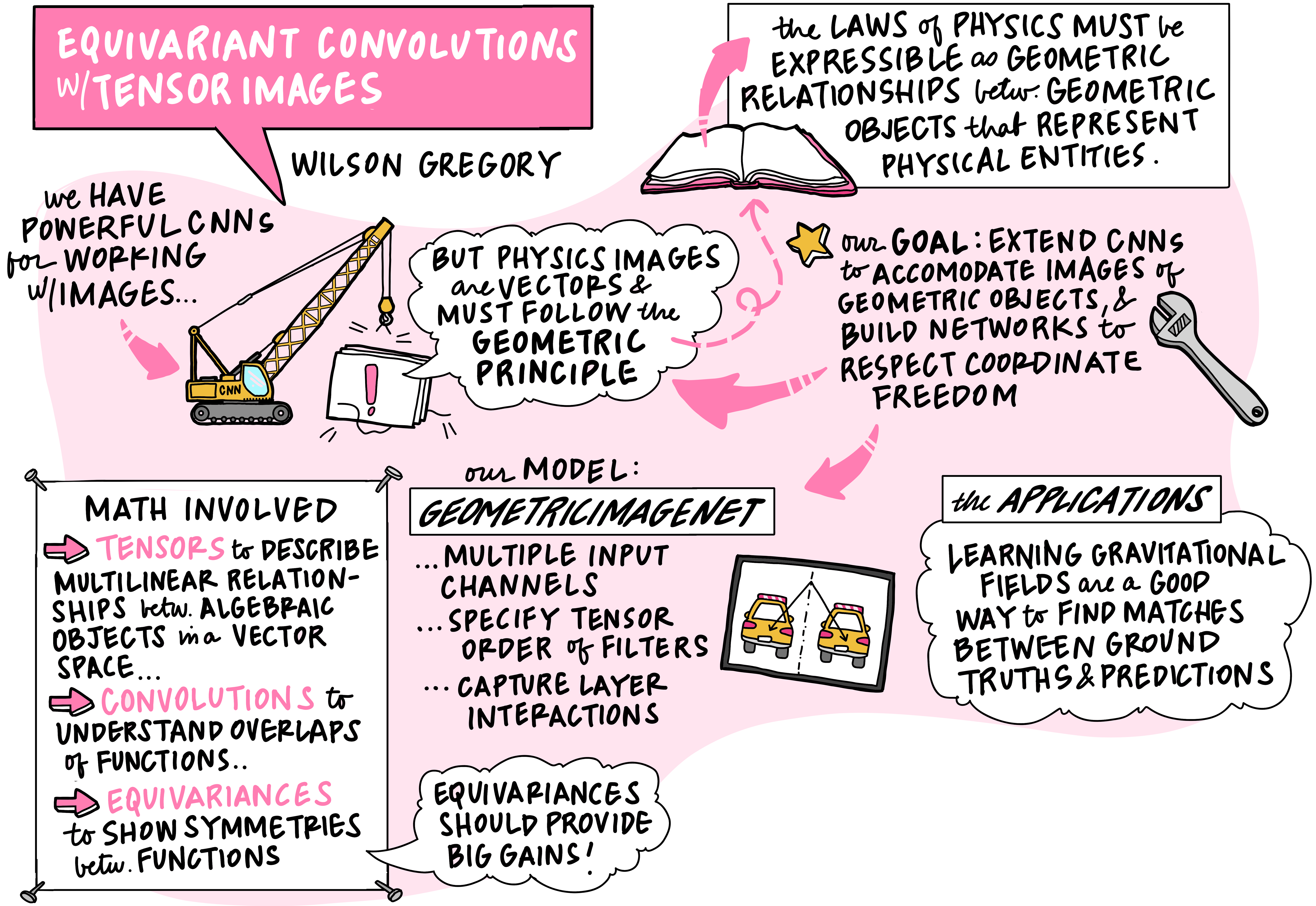
Why Adiabatic Quantum Annealing is Unlikely to Yield Quantum Speed Up

Bert Kappen
Radboud University
Nijmegen, NL



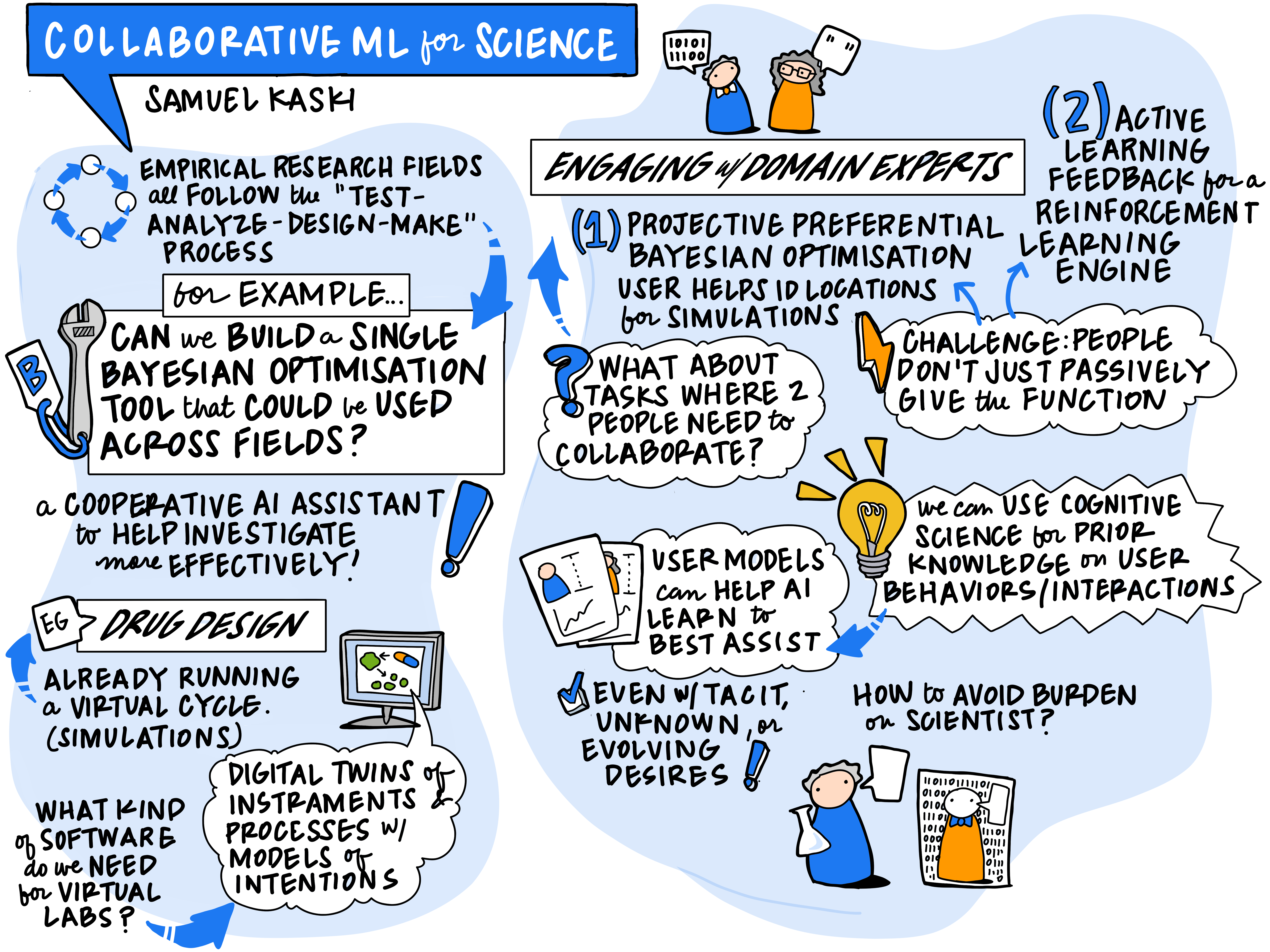
Equivariant Convolutions with Tensor Images

Wilson Gregory
Johns Hopkins University
Baltimore, US



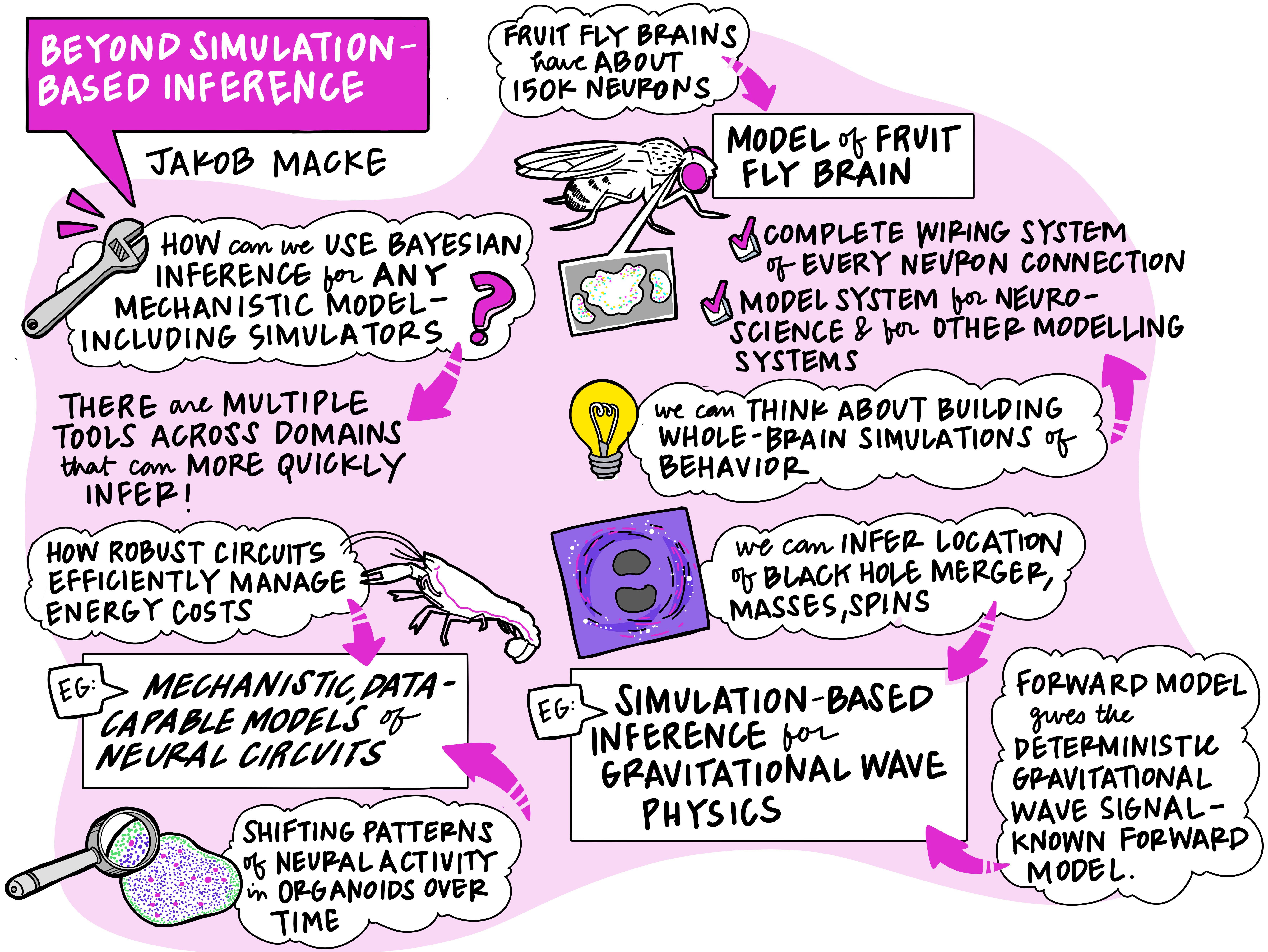
Collaborative ML for Science

Samuel Kaski
University of Manchester,
Aalto University
Manchester, UK,
Espoo, FI



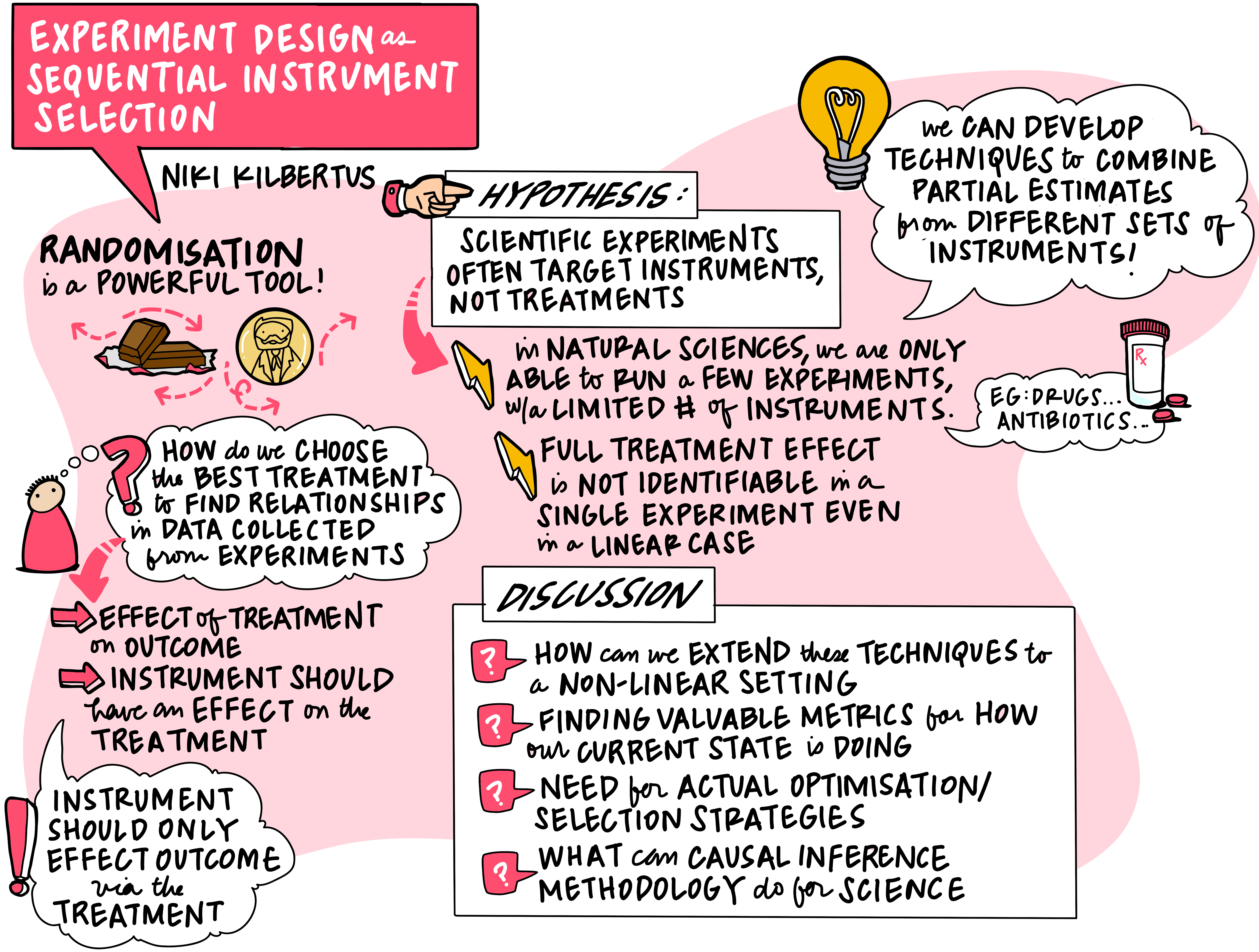
Beyond Simulation- Based Inference

Jakob Macke
University of Tübingen
Tübingen, DE



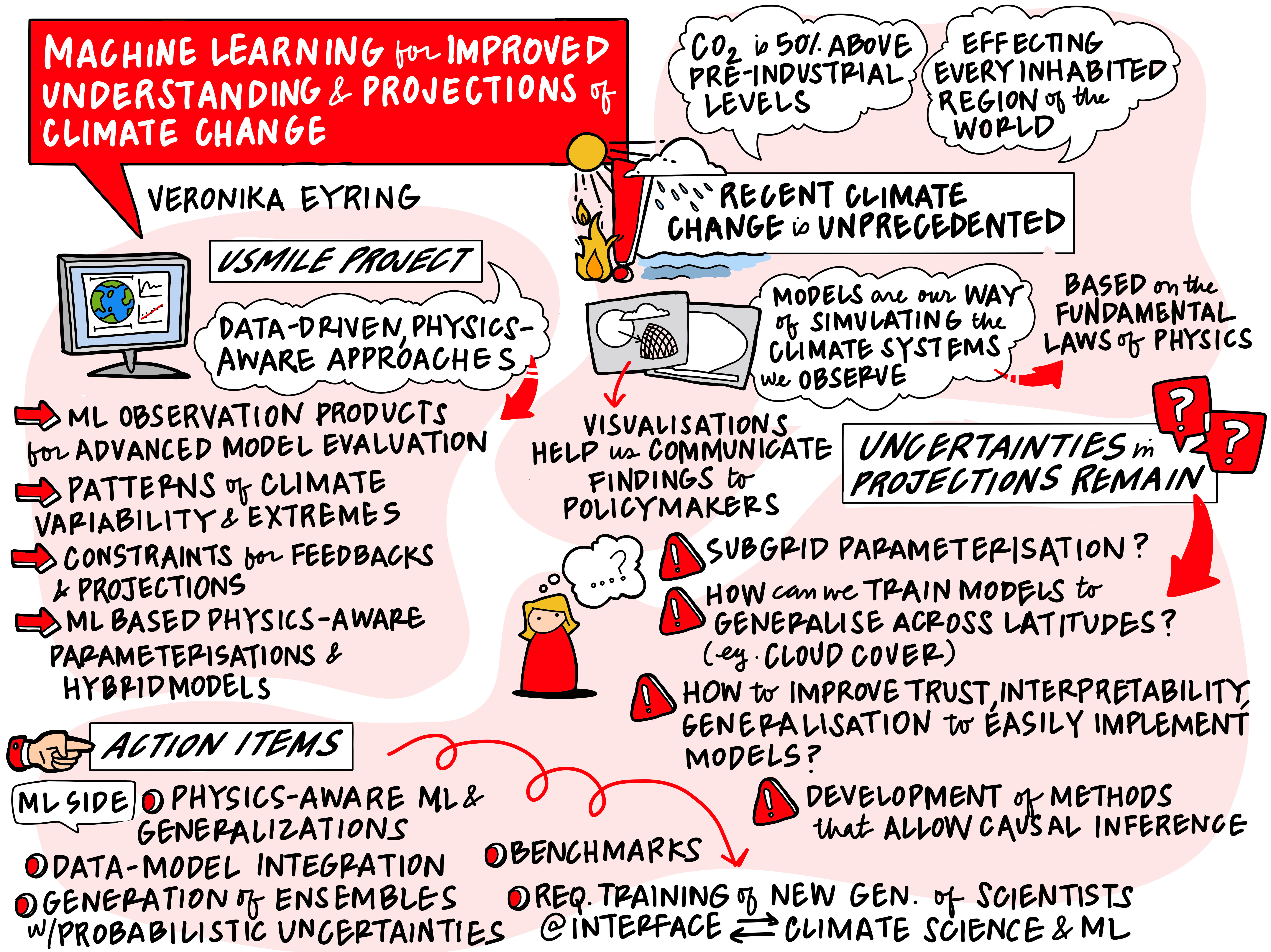
Experiment Design as Sequential Instrument Selection

Niki Kilbertus
Technical University of Munich
Munich, DE



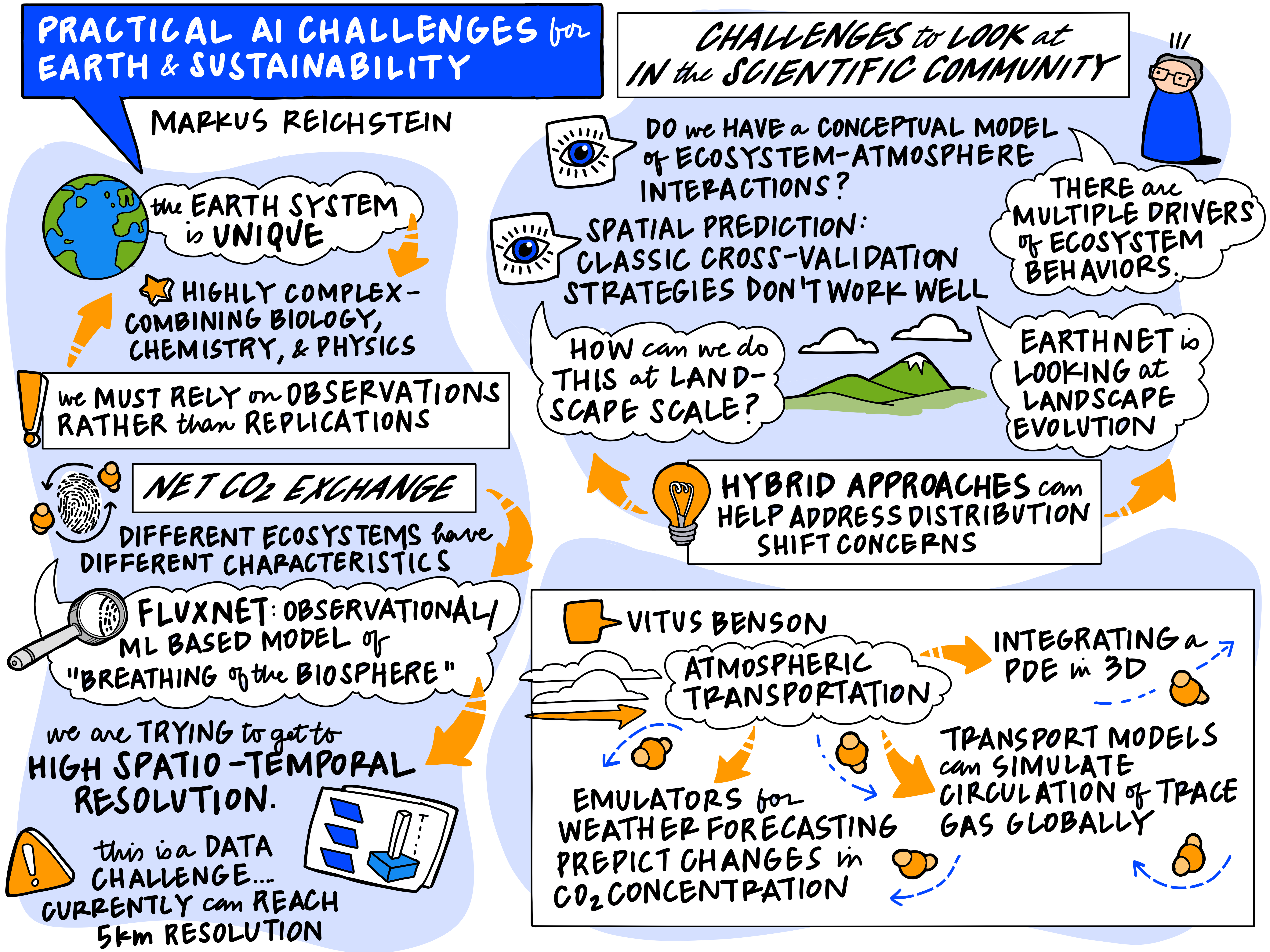
Machine Learning for Improved Understanding & Projections of Climate Change

Veronika Eyring
German Aerospace Center (DLR) Institute of Atmospheric Physics, University of Bremen
Bremen, DE



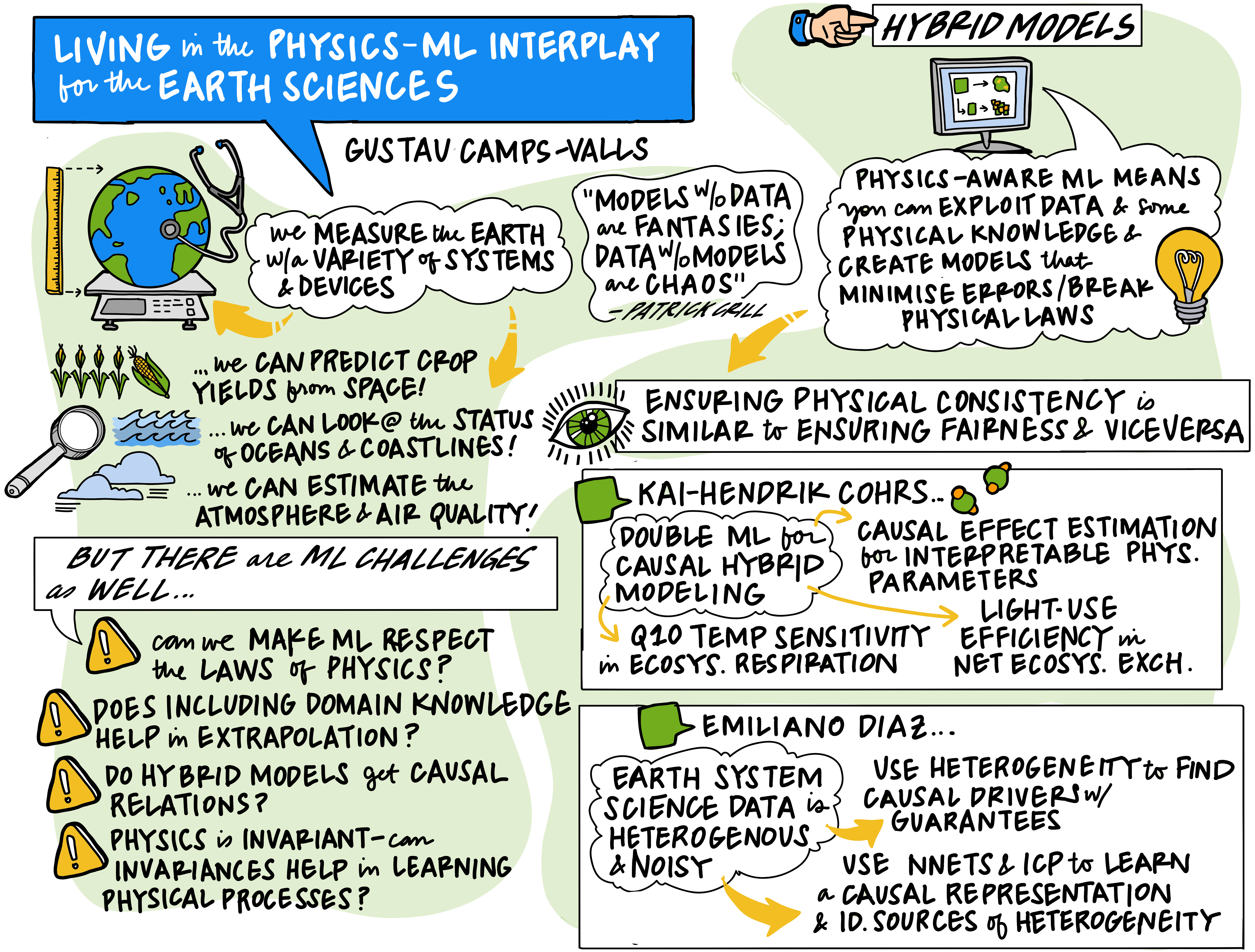
Practical AI Challenges for Earth and Sustainability

Markus Reichstein
Max Planck Institute for Biogeochemistry
Jena, DE



Living in the Physics-ML Interplay for the Earth Sciences

Gustau Camps-Valls
Universitat de València
València, ES



Machine Learning for Uncovering Hidden Relationships & Improving Predictions in the Couples Earth System Models

Christian Reimers & Alexander Winkler

Max Planck Institute for Biogeochemistry
Aachen University
Jena, DE
Aachen, DE