Arithmer Seminar

"Arithmer Seminar" is a weekly seminar that aims to spread knowledge
in various fields to our employees by inviting speakers from outside of the company.

THE DATA SCIENCE OF PHYSICS

RIKEN　ENRICO RINALDI

2019/06/13

Arithmer Seminar

Arithmer Seminar」とは、週1回、弊社社員や外部から様々な分野の方を講師に招いて、社員の知見を広めることを目的としたセミナーです。
次頁以降のスライドは、講師を務めた外部の方の作成によるものであり、許可を得て公開しています。

ENRICO RINALDI

THE DATA SCIENCE OF PHYSICS

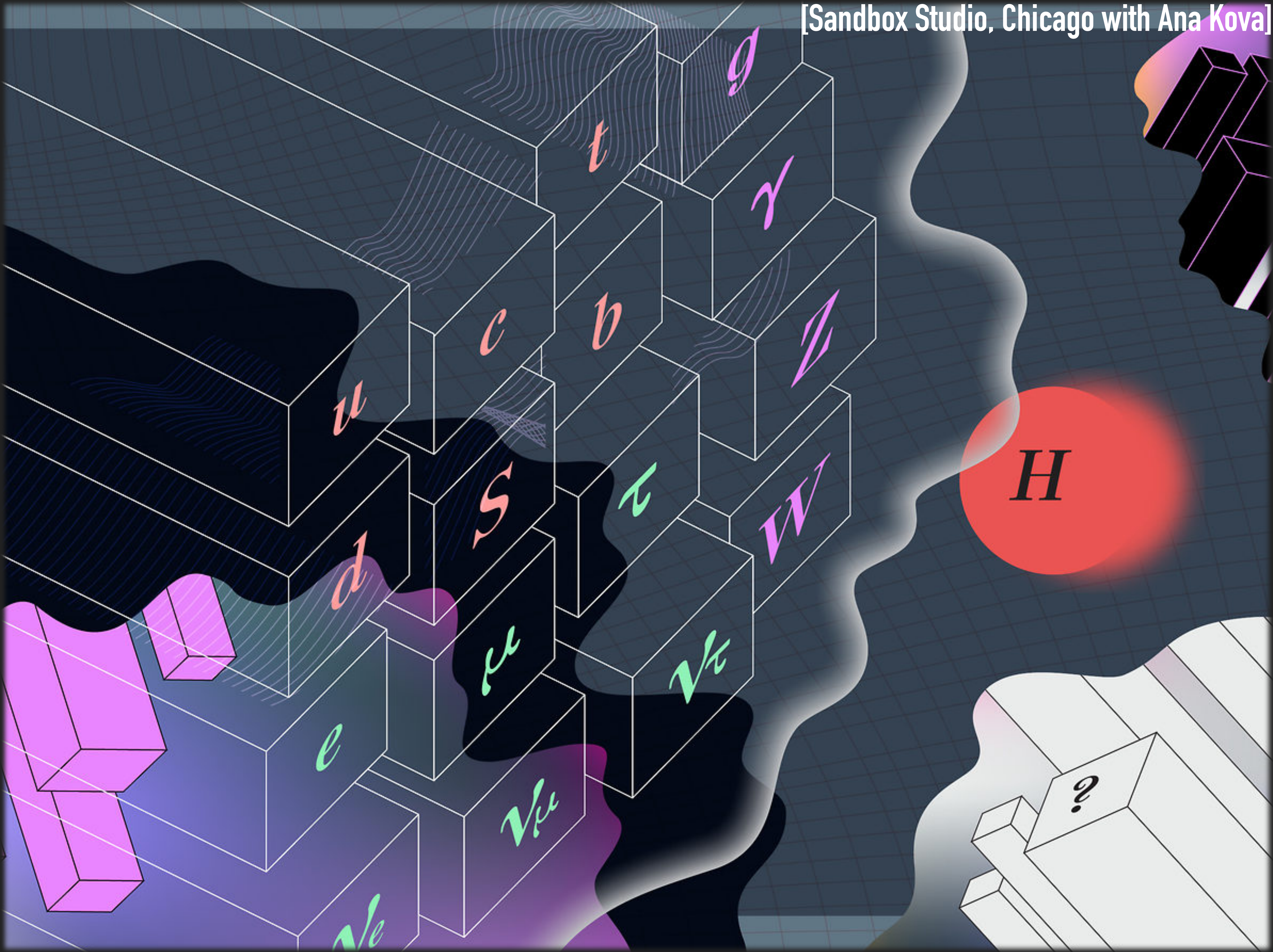
ENRICO RINALDI

THE DATA SCIENCE OF PHYSICS

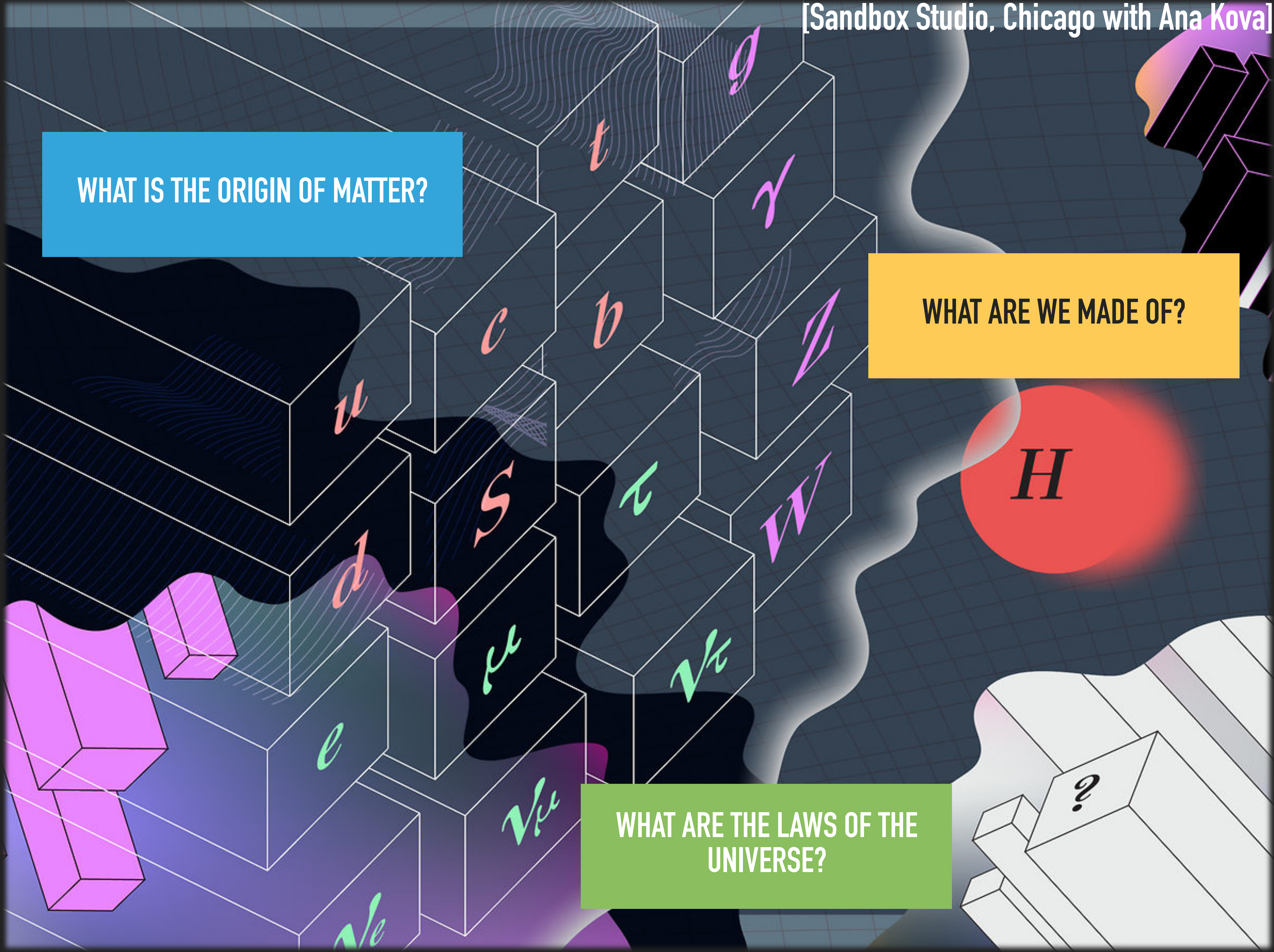
ACCELERATE PHYSICS DISCOVERIES WITH AI

WHO AM I?

- I am a theoretical particle physicist (High Energy and Nuclear)
- I am a computational physicist (High Performance Computing)
- I transform *abstract concepts* into *practical problems*:
  - from a mathematical theory
  - to an algorithm deployed on supercomputers
  - analyzing large amounts of data to test hypothesis
- Driven by curiosity…following the scientific method



[Sandbox Studio, Chicago with Ana Kova]



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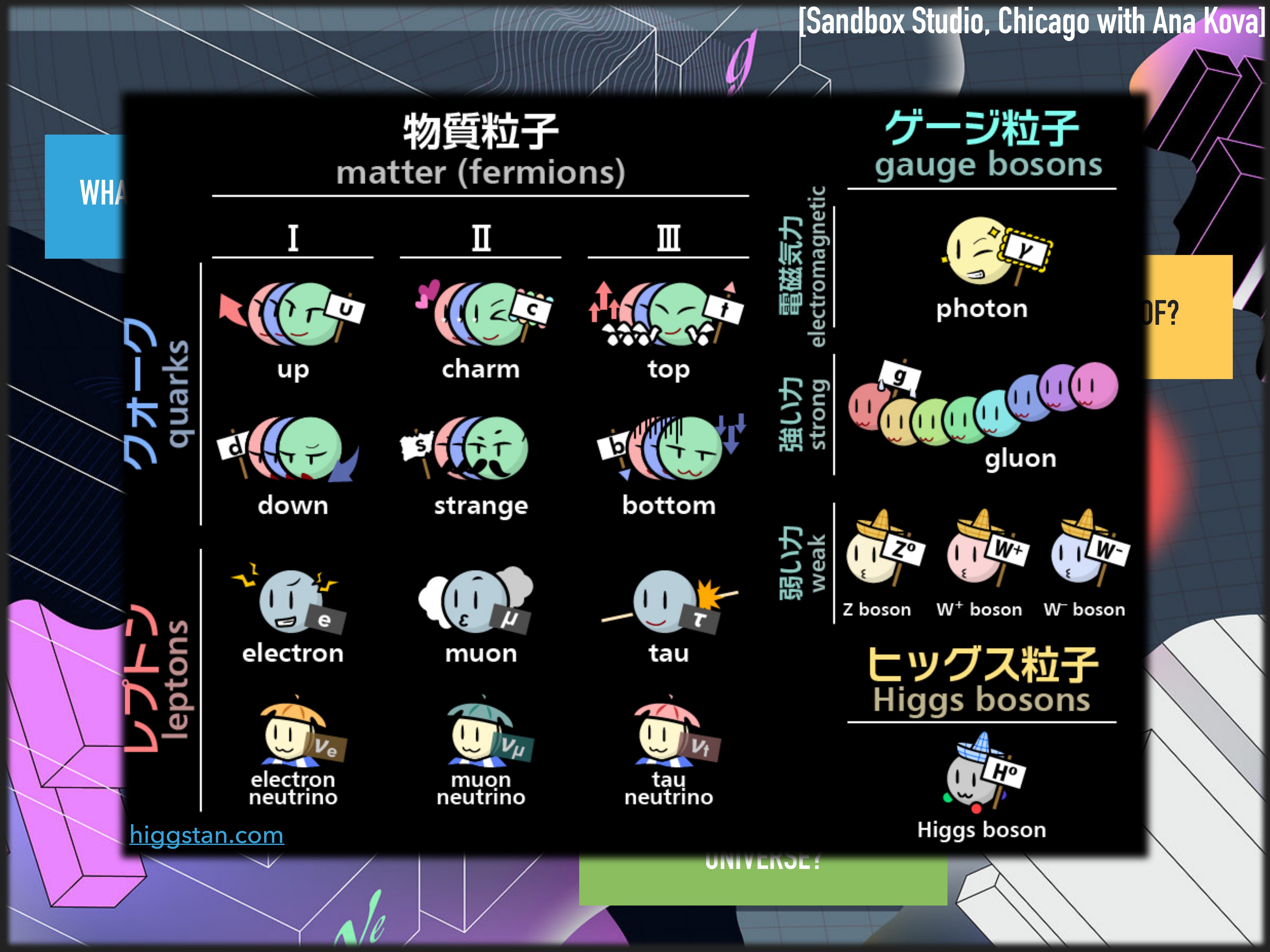

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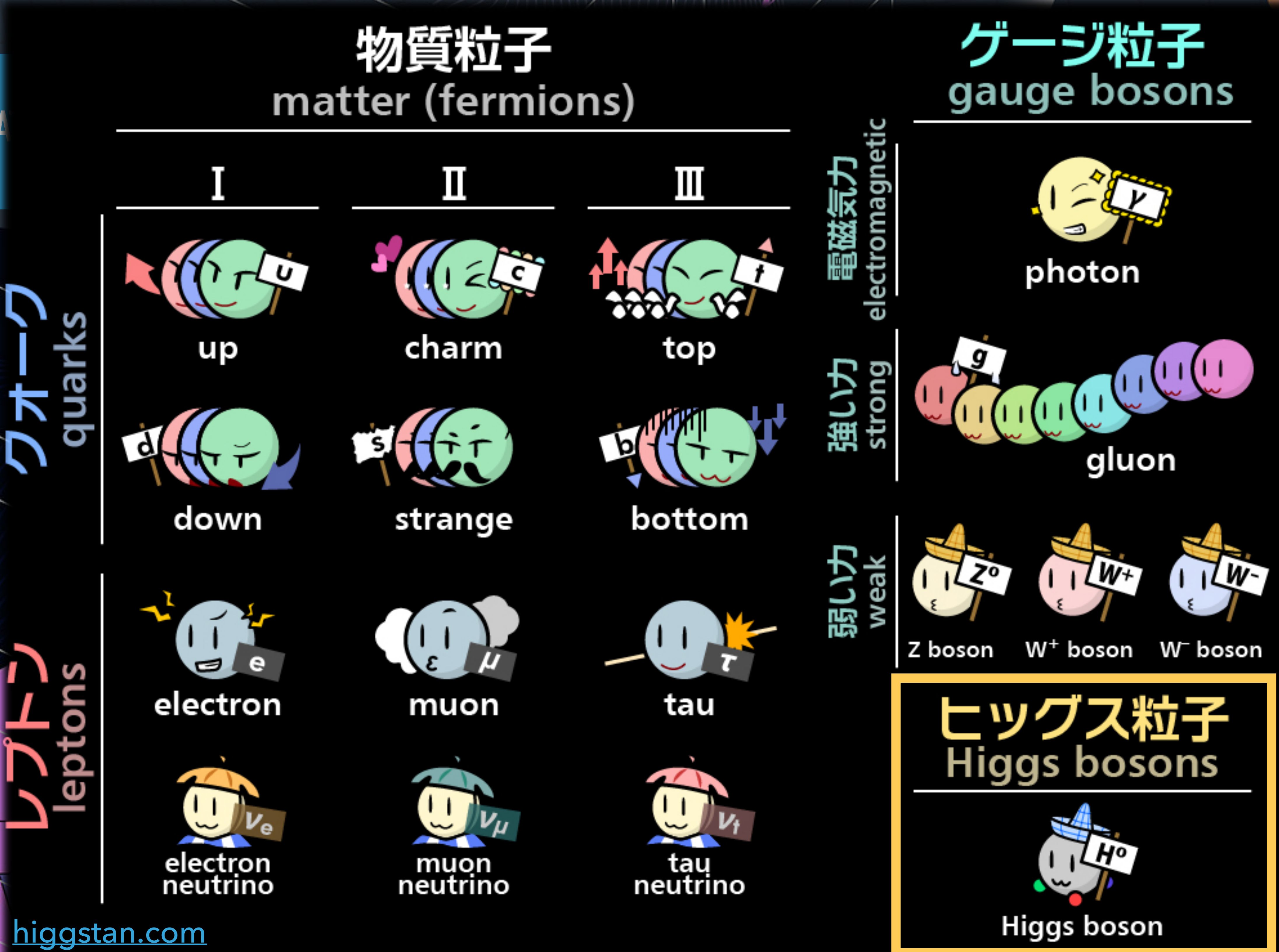
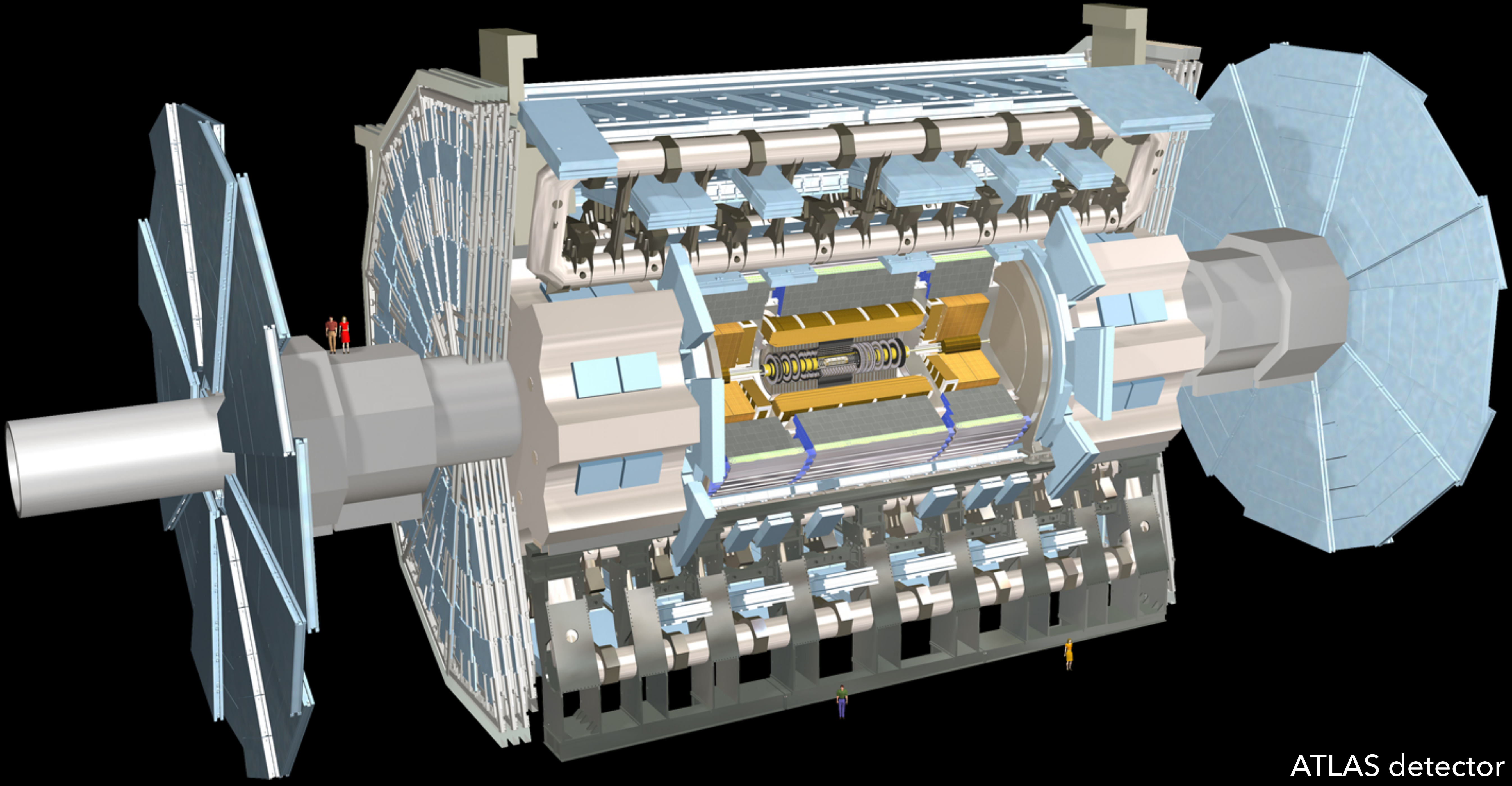
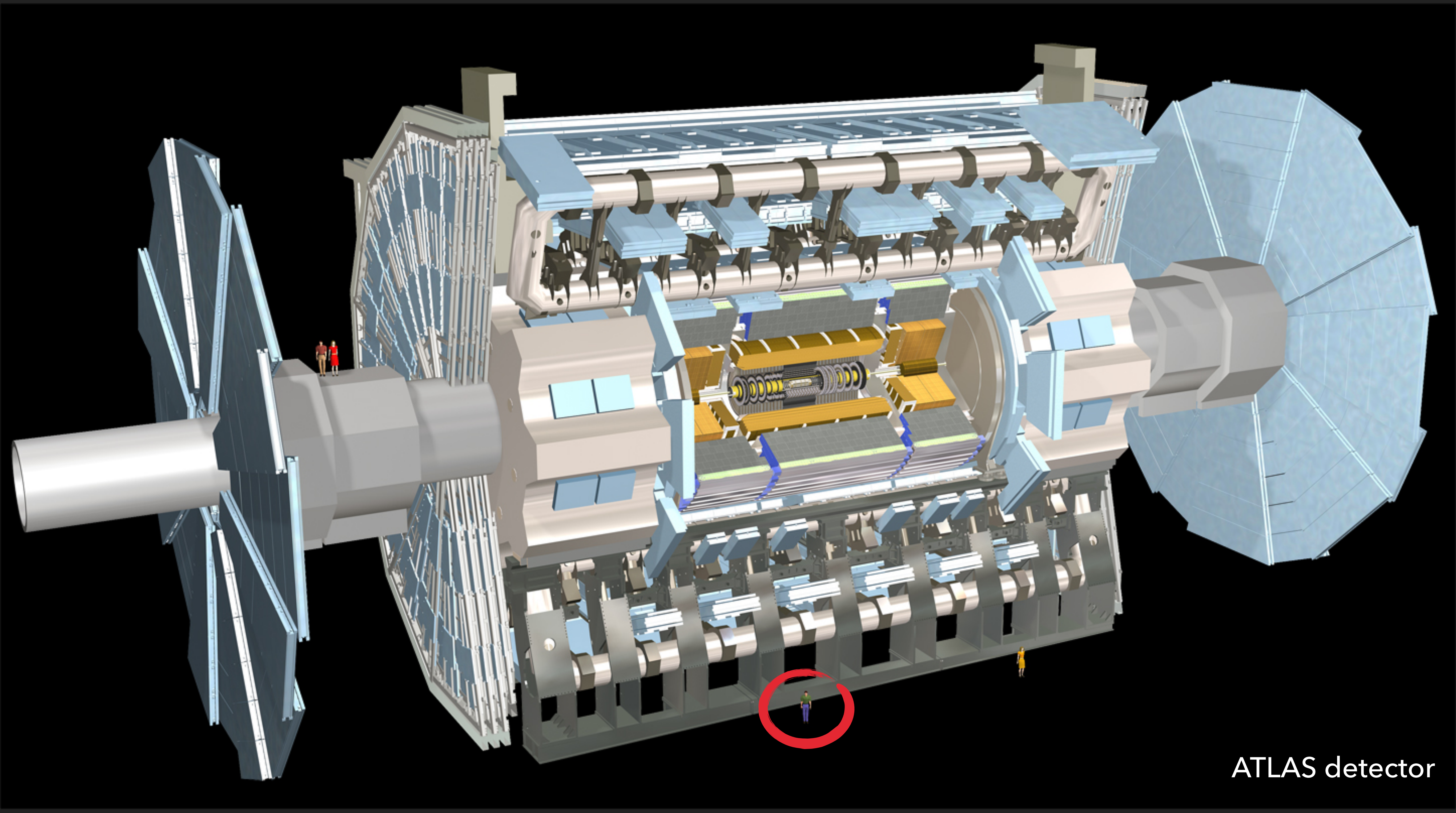
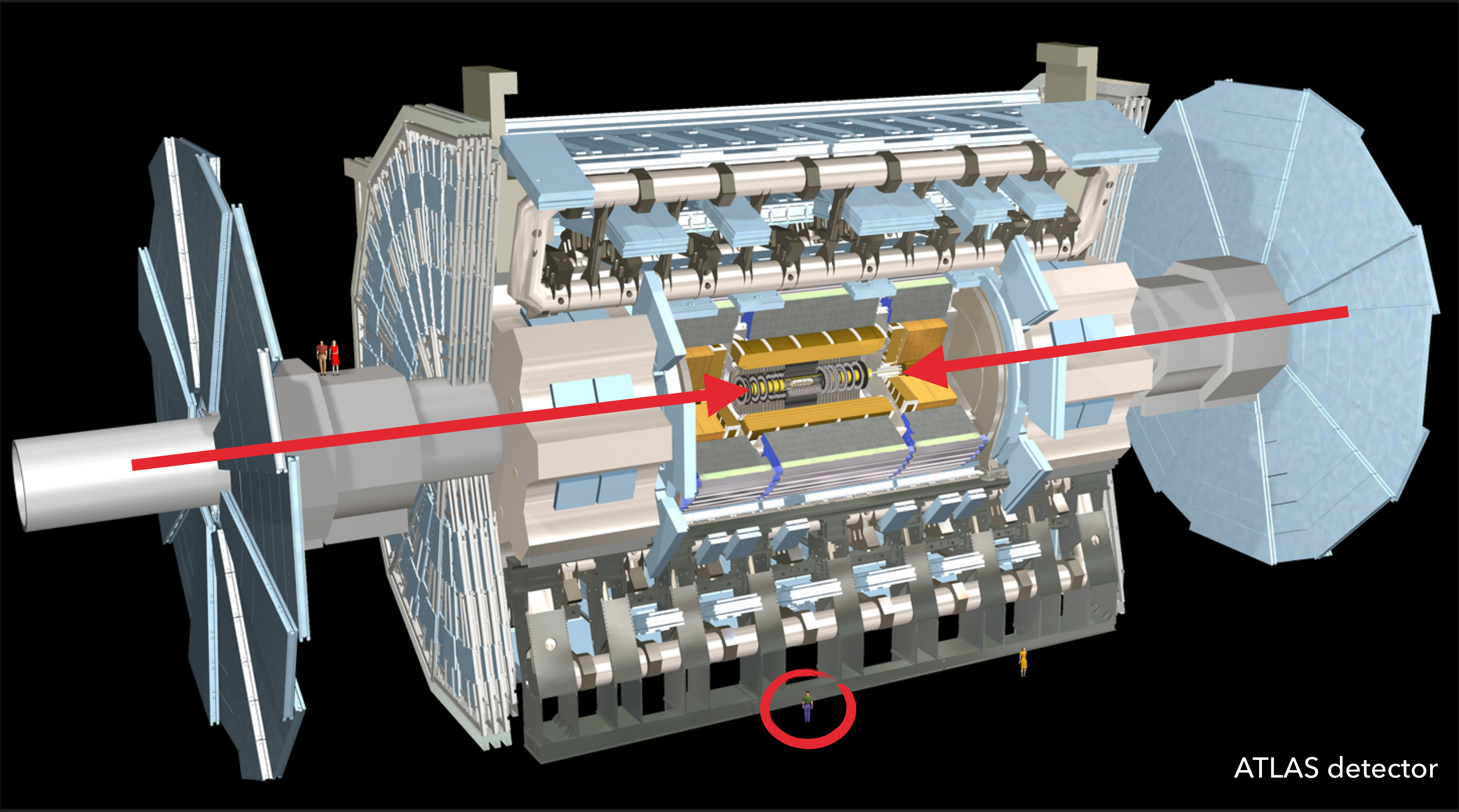




ATLAS detector


ATLAS detector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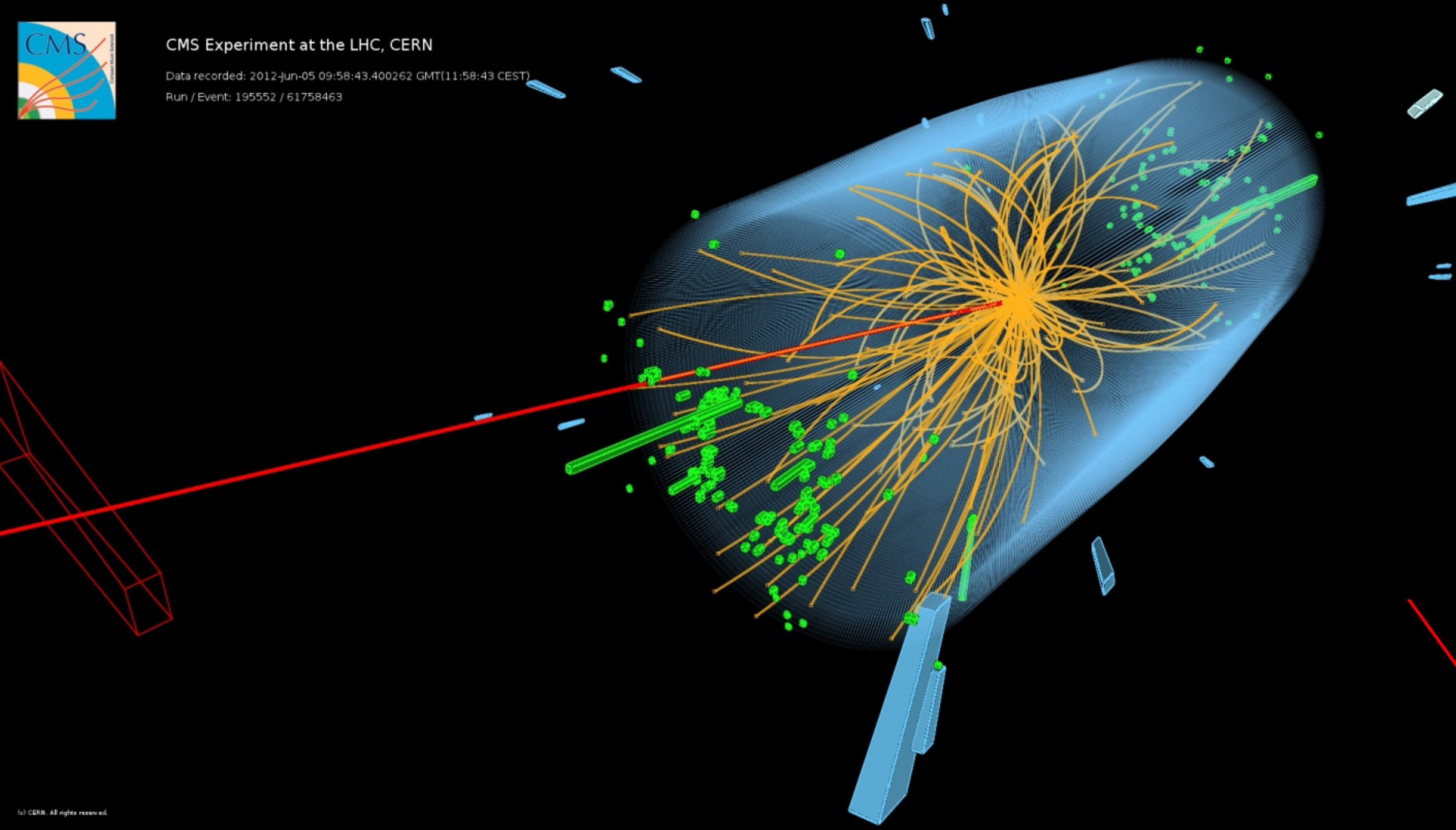
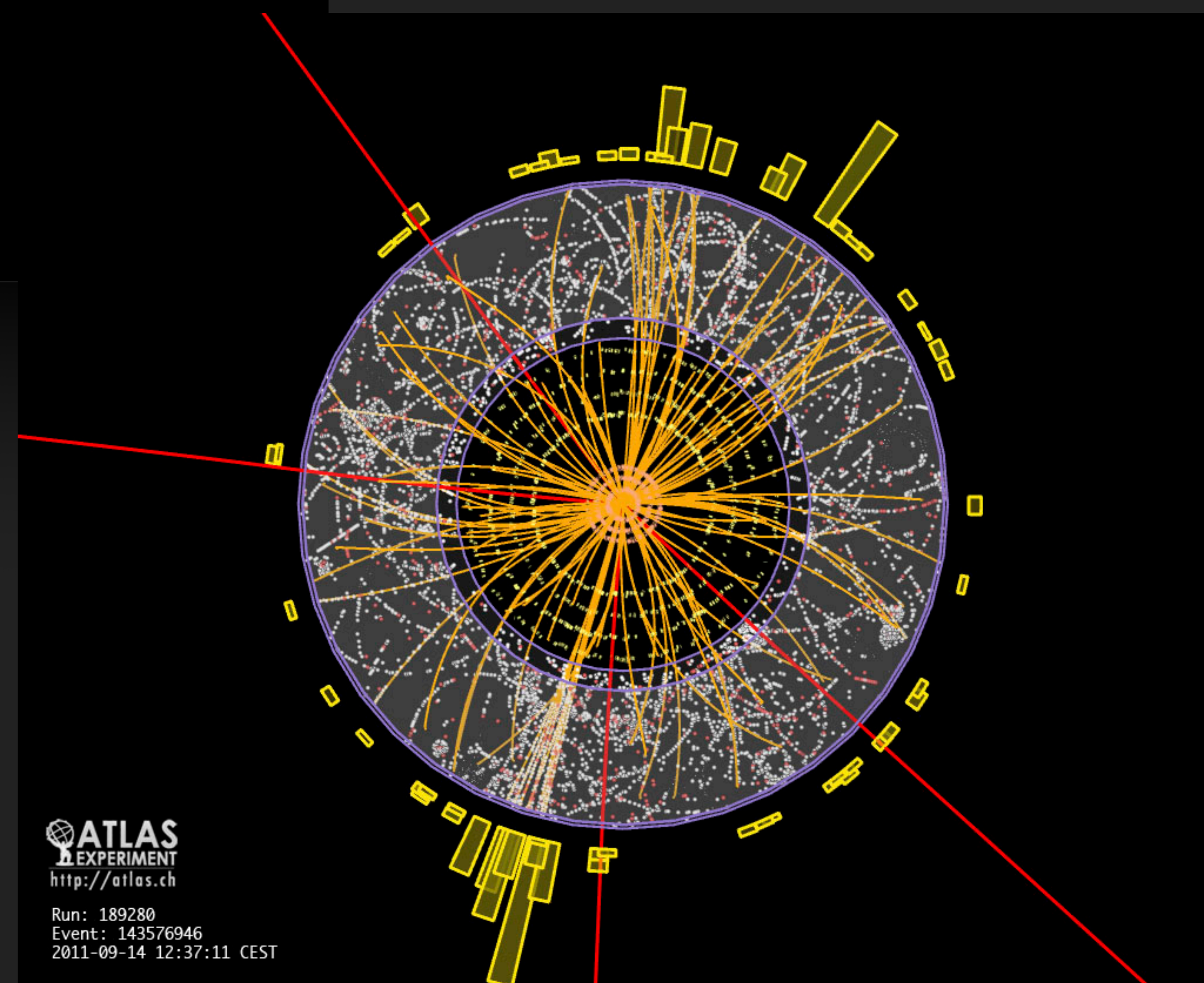
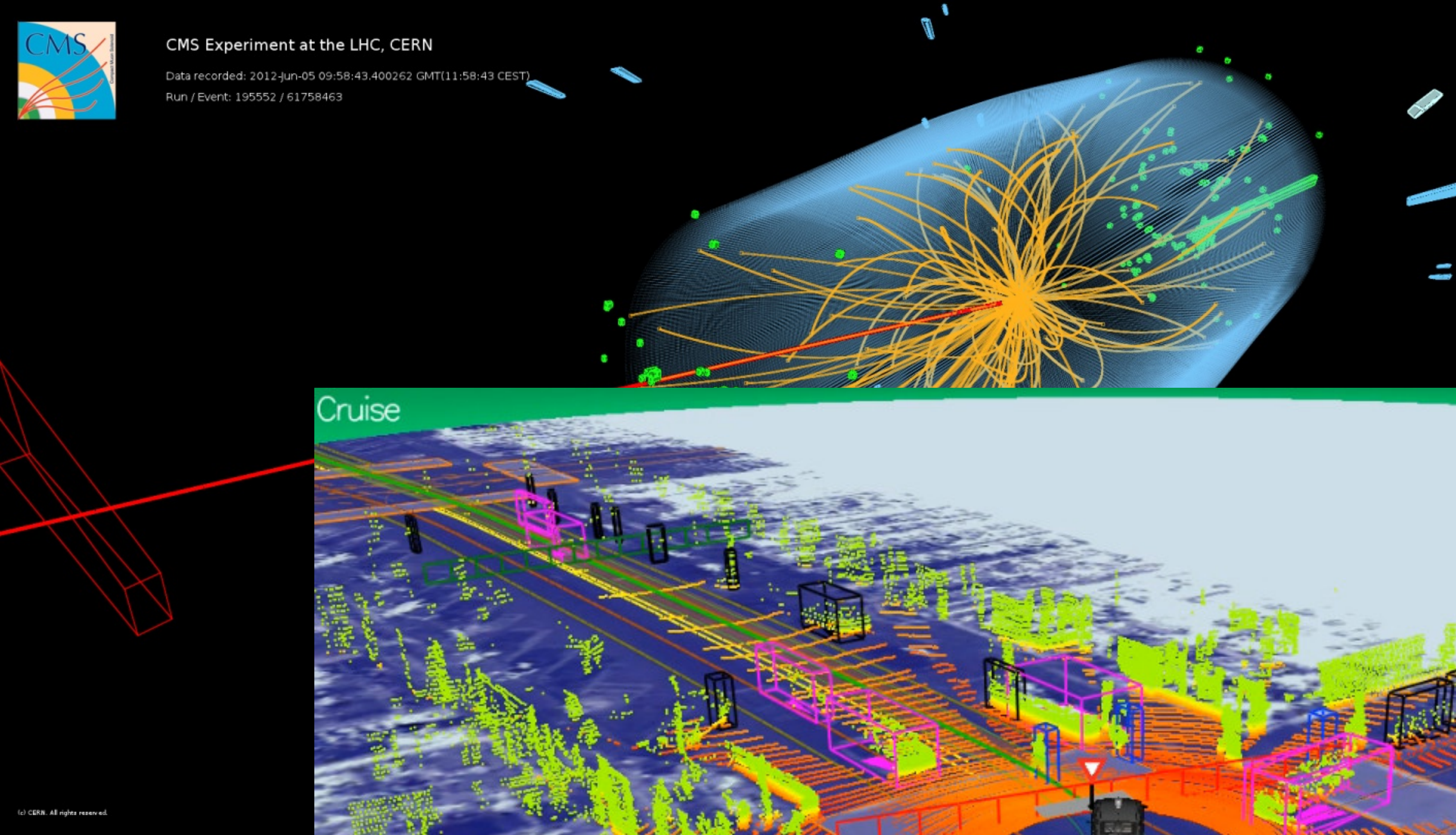
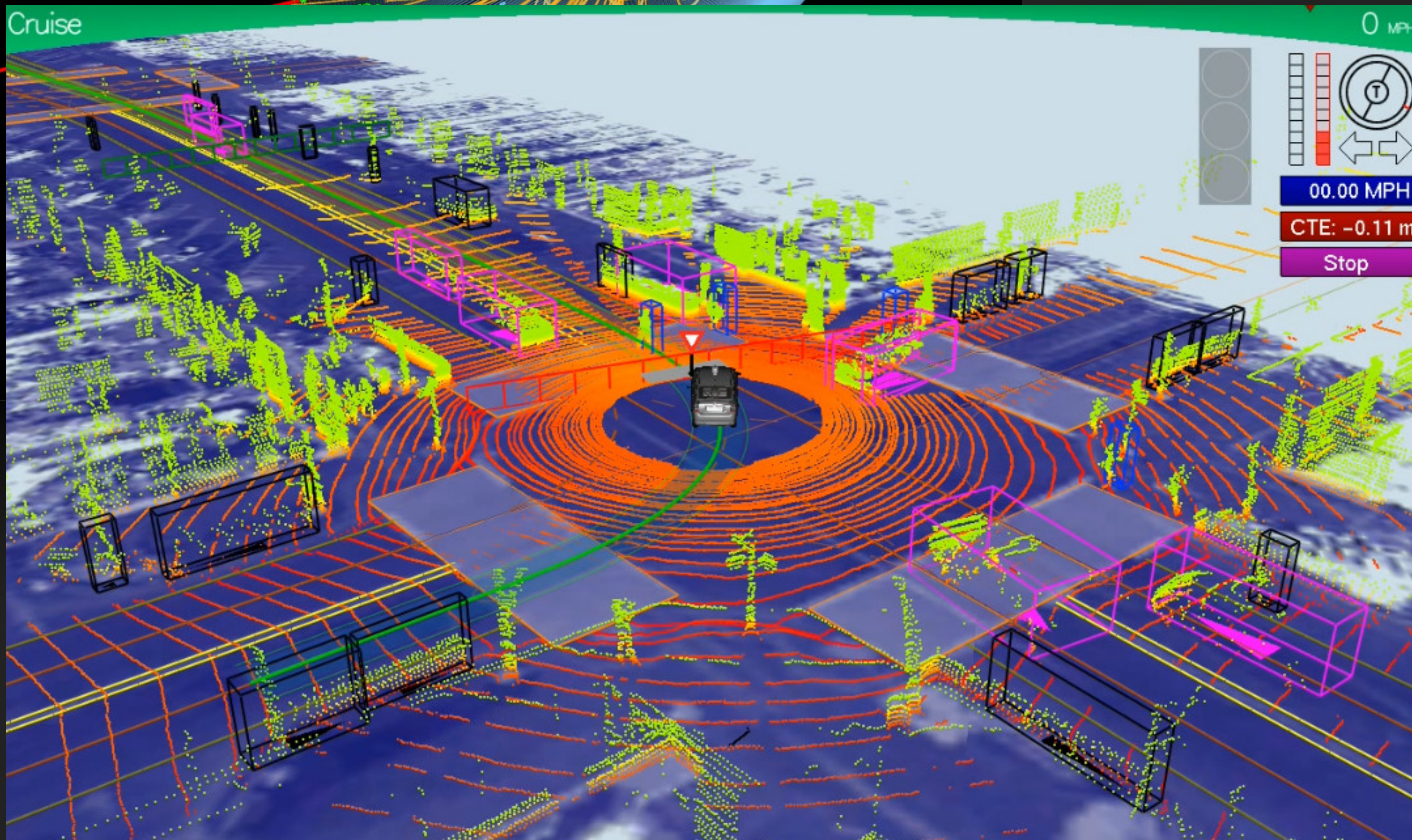


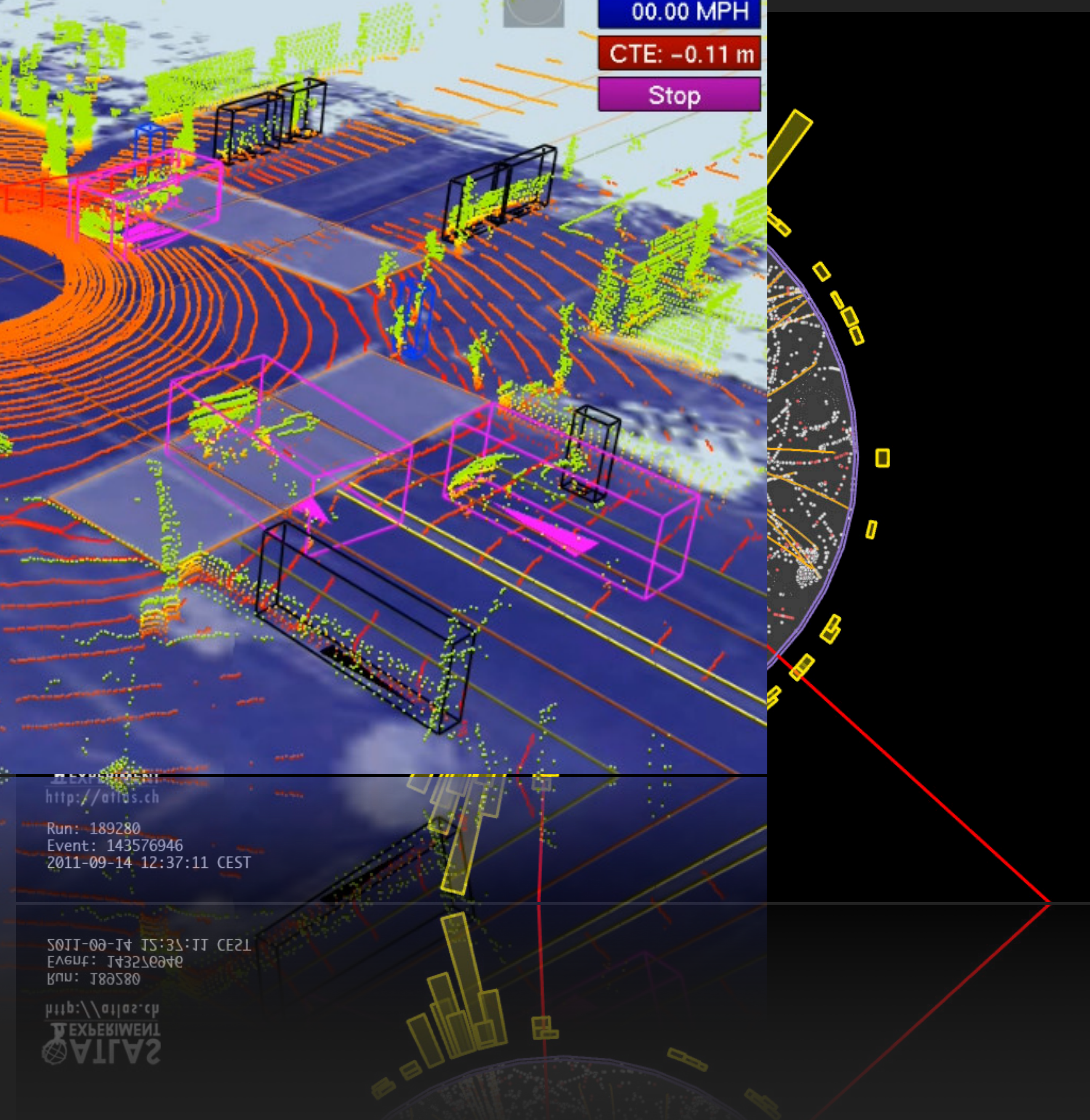


Particle Physics “events”

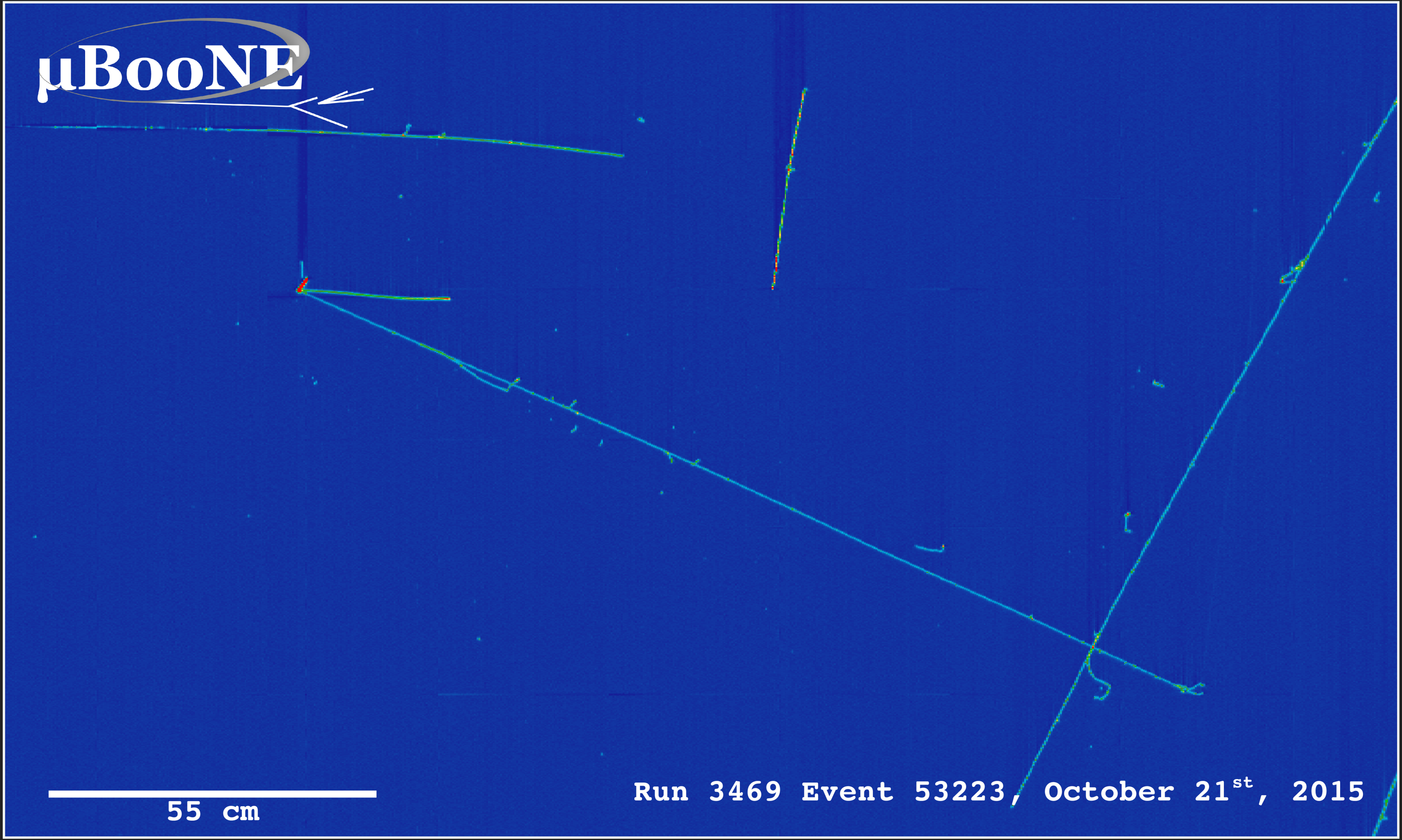
Self-driving “events”



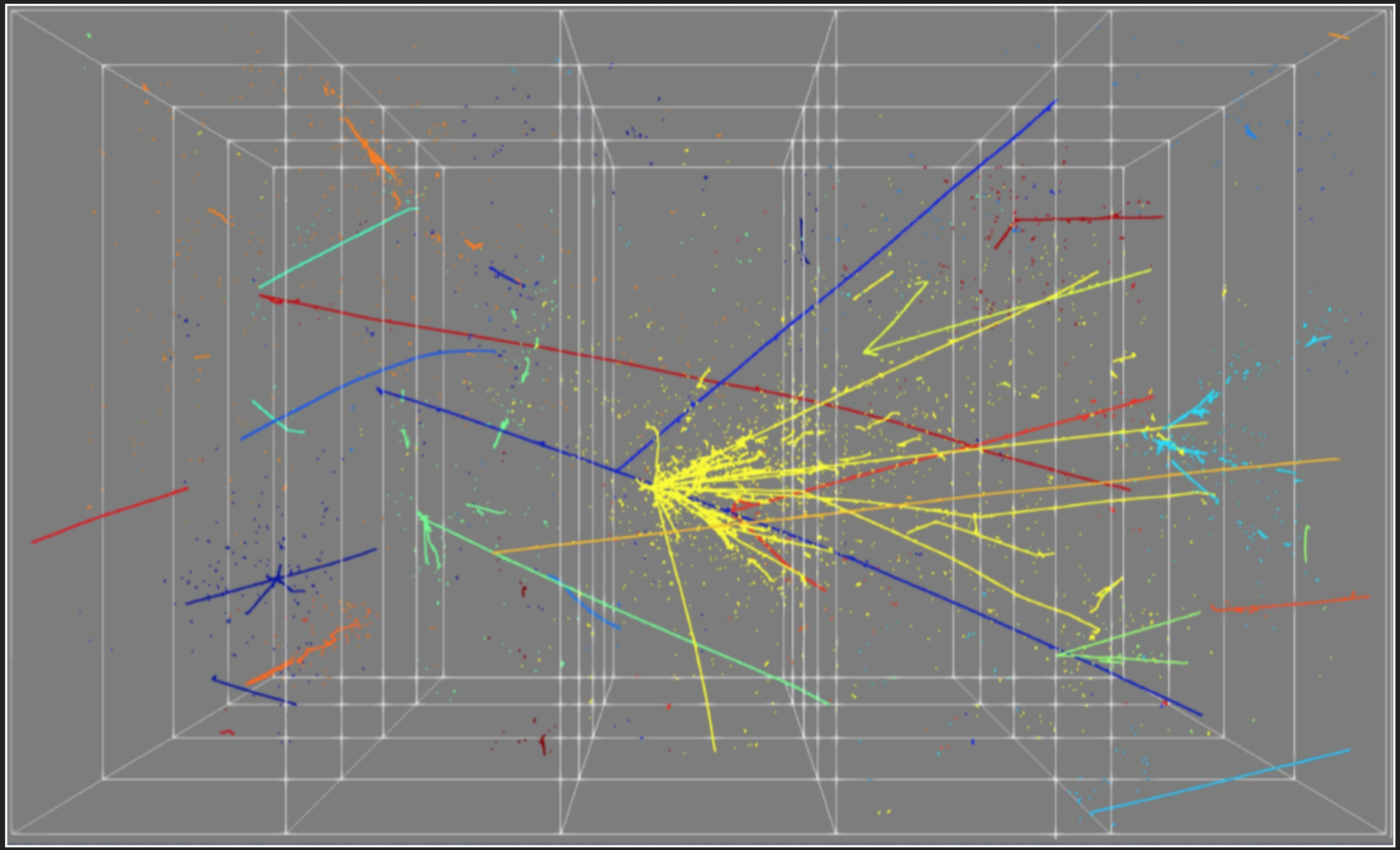




Particle Physics “events”



Particle “tracks” and “showers”



FUTURE UPGRADED EXPERIMENTS WILL PRODUCE ~10X MORE DATA!

HOW CAN WE MAKE SENSE OF IT AND HOW FAST?

Particle “tracks” and “showers”

"AI PROMISES TO SUPERCHARGE THE PROCESS OF DISCOVERY"

The scientists' apprentice - Tim Appenzeller

[KIYOSHI TAKAHASE SEGUNDO/ALAMY STOCK PHOTO]

MENU nature.com [web link]

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Alexander Radovic, Mike Williams [...] & Taritree Wongjirad

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Glider soaring via reinforcement learning in the field

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Gautam Reddy, Jerome Wong-Ng [...] & Massimo Vergassola

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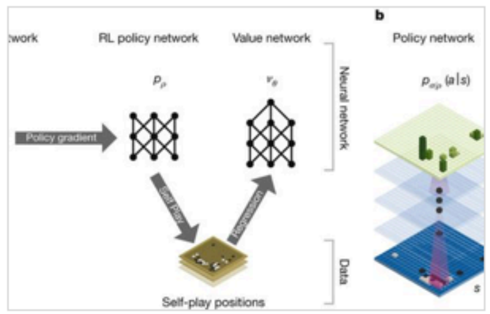

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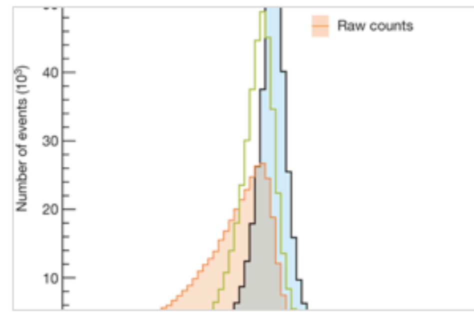

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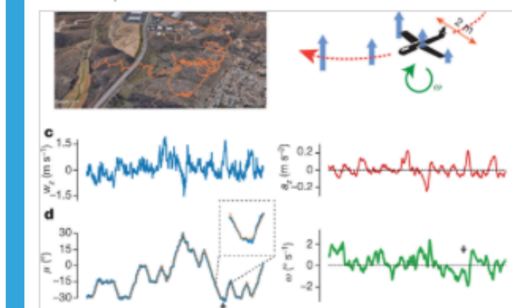

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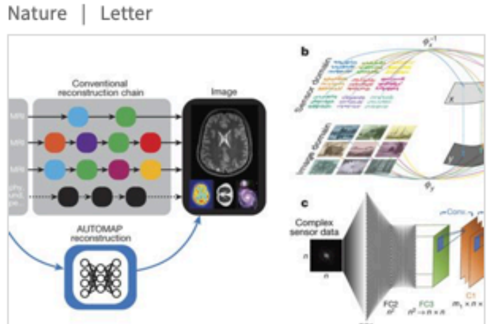

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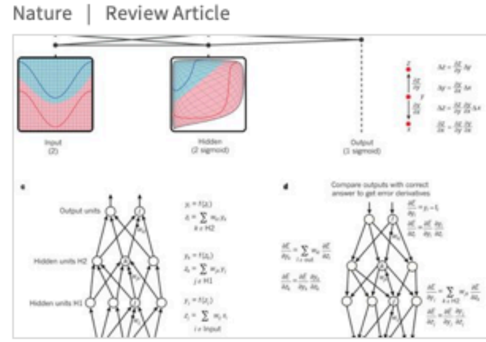

Deep learning

Yann LeCun, Yoshua Bengio & Geoffrey Hinton

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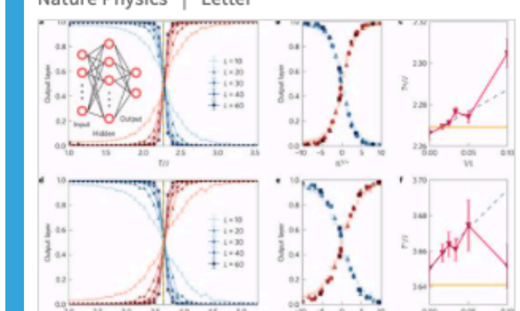

Machine learning phases of matter

The success of machine learning techniques in handling big data sets proves ideal for...
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"AI ... RGE
T... RY"

Appenzeller

[...AMY STOCK PHOTO]

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DIFFERENT LEARNING SCHEMES FOR A MACHINE

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Data → Labels

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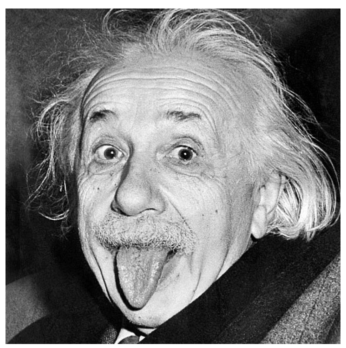
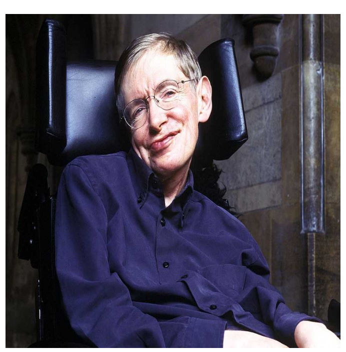


Albert Einstein



Stephen Hawking

DIFFERENT LEARNING SCHEMES FOR A MACHINE

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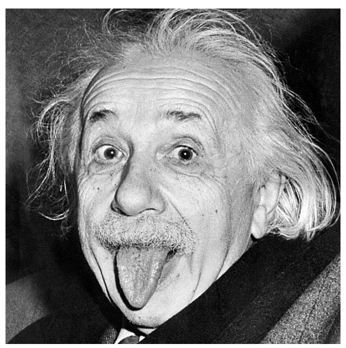

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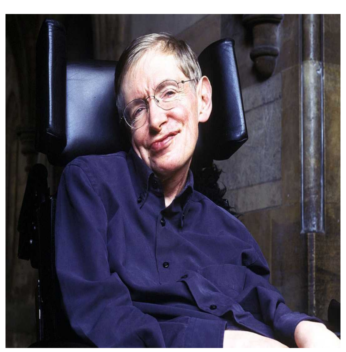

Stephen Hawking

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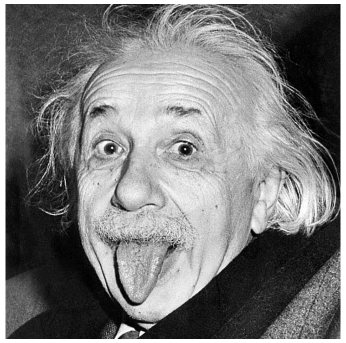
Data → Labels

Data → ??



Albert Einstein

Stephen Hawking

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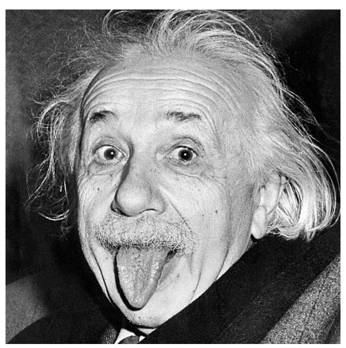
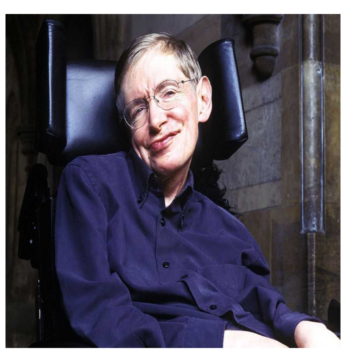
Data ⟶ Labels



Albert Einstein



Stephen Hawking

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Data ⟶ ??

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SUPERVISED

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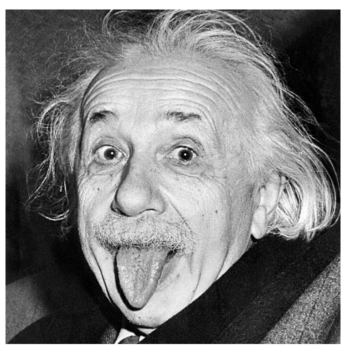
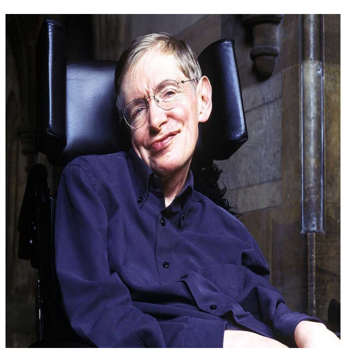
Data → Labels

Data → ??



Albert Einstein



Stephen Hawking

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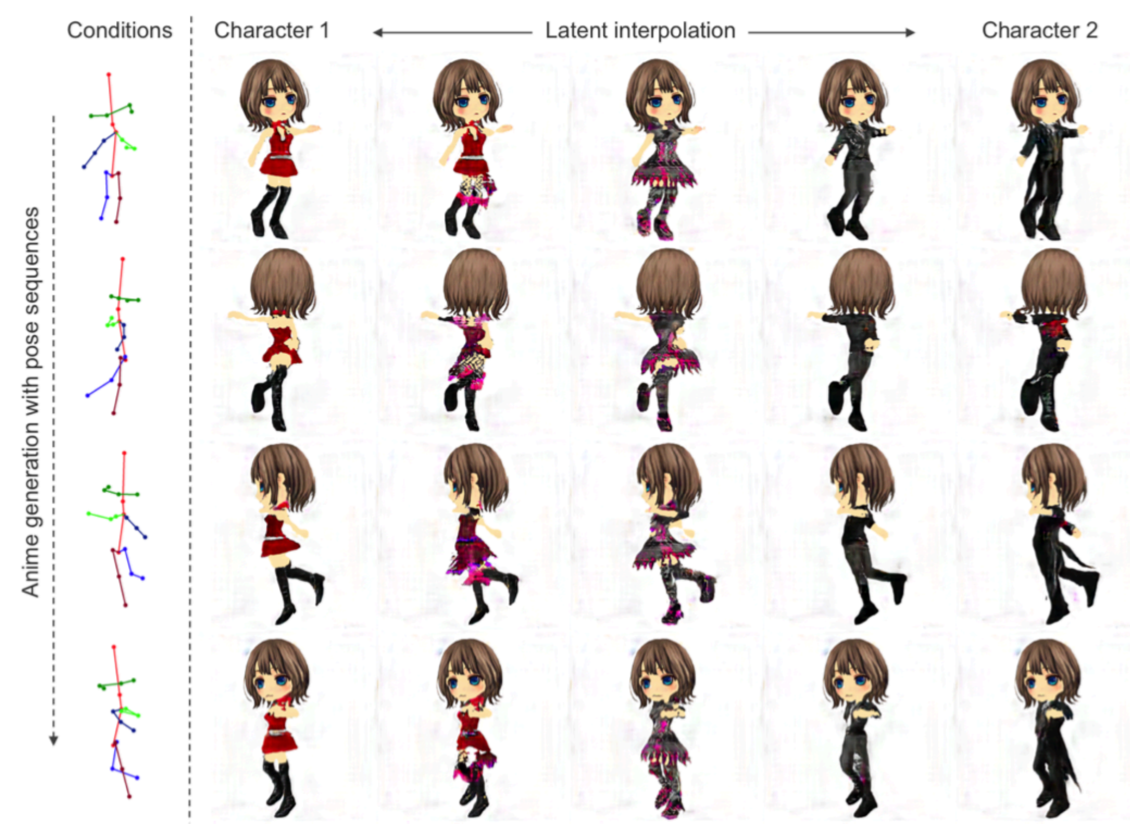

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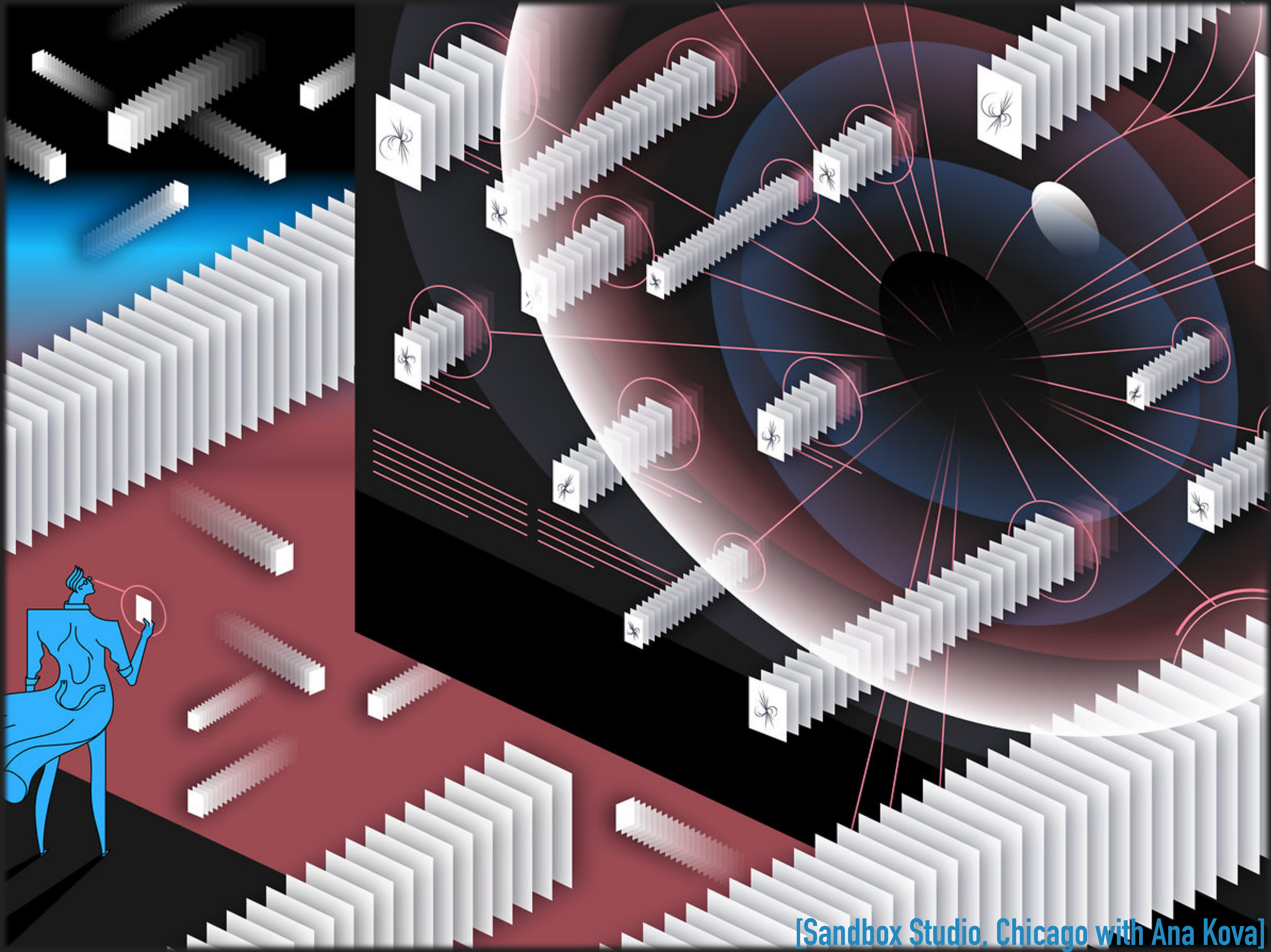
ability to recognize, classify and characterize complex sets of data



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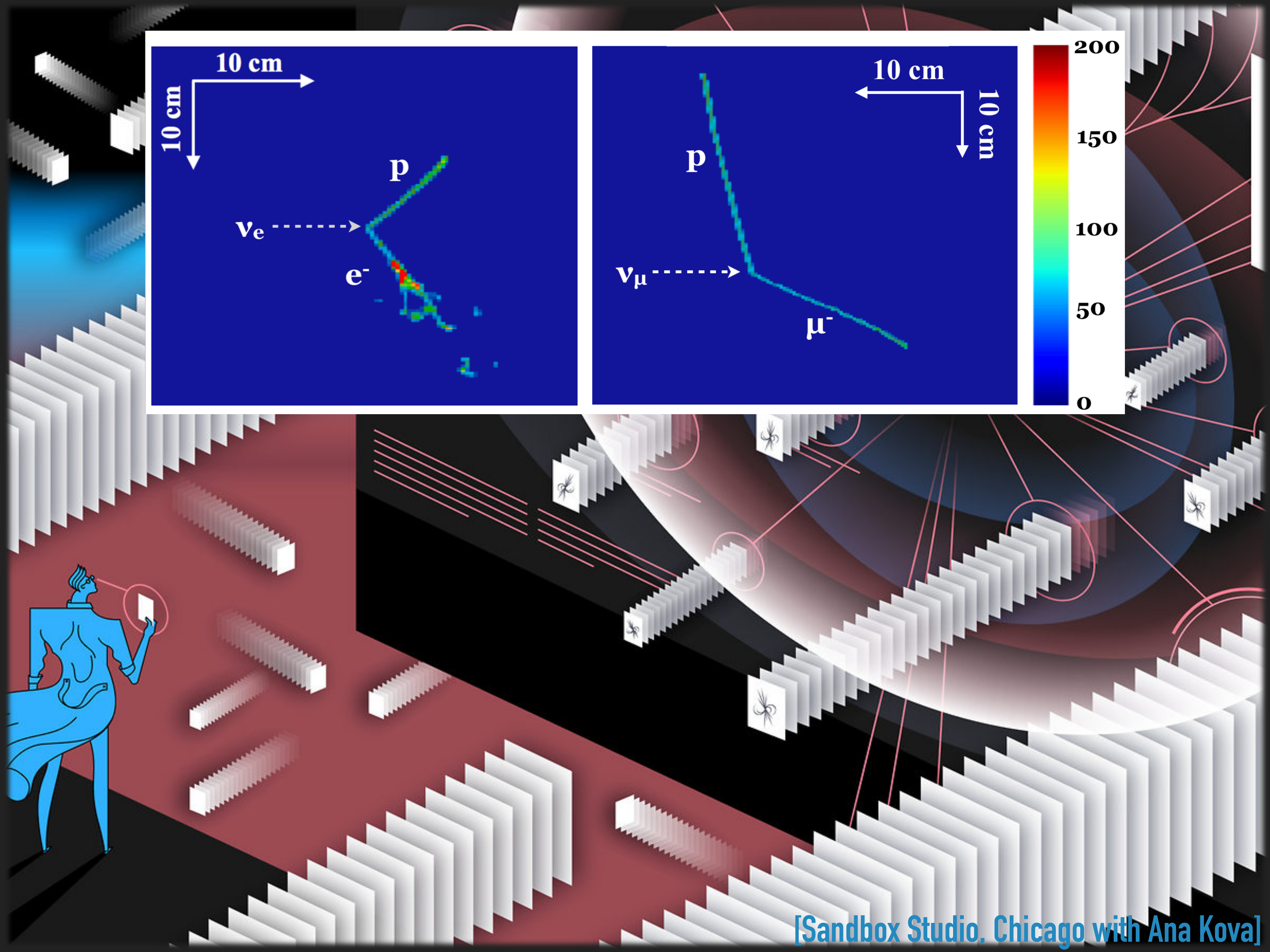
10 cm
10 cm
p
ν_e
e^-
p
10 cm
10 cm
ν_μ
μ^-
200
150
100
50
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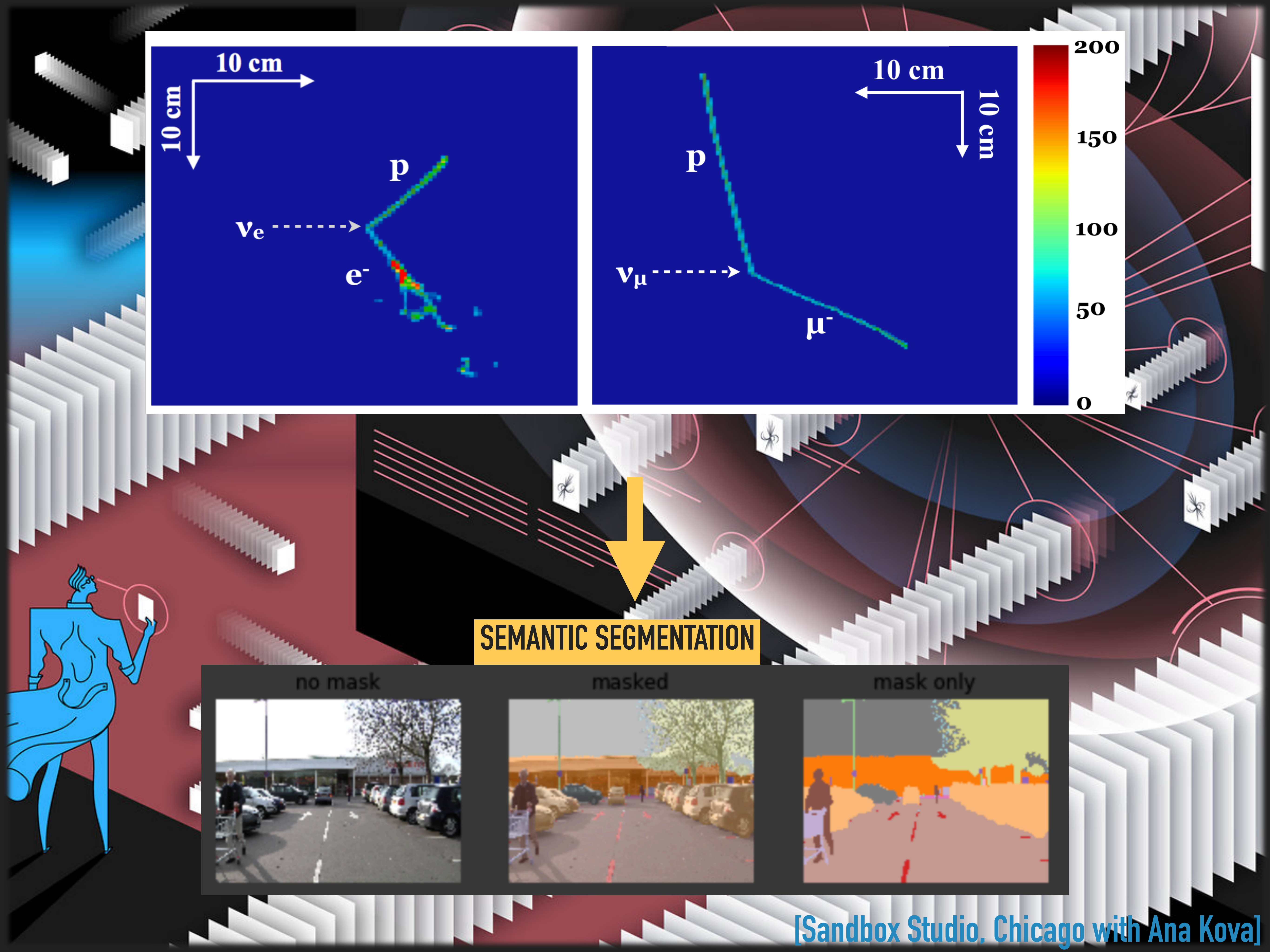
[Sandbox Studio, Chicago with Ana Kova]


10 cm
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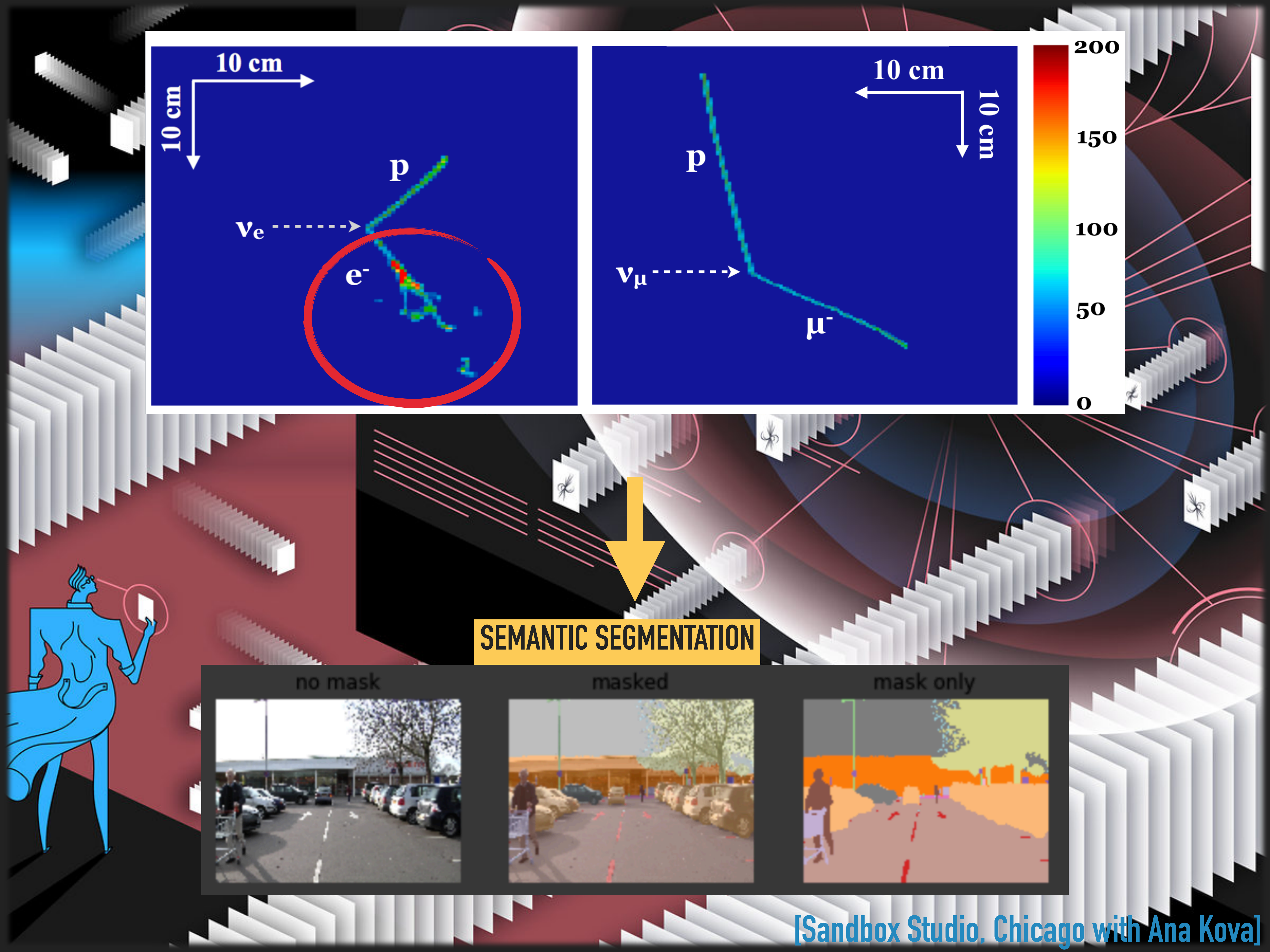
SEMANTIC SEGMENTATION
no mask
masked
mask only
[Sandbox Studio, Chicago with Ana Kova]



10 cm
10 cm
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SEMANTIC SEGMENTATION
no mask
masked
mask only
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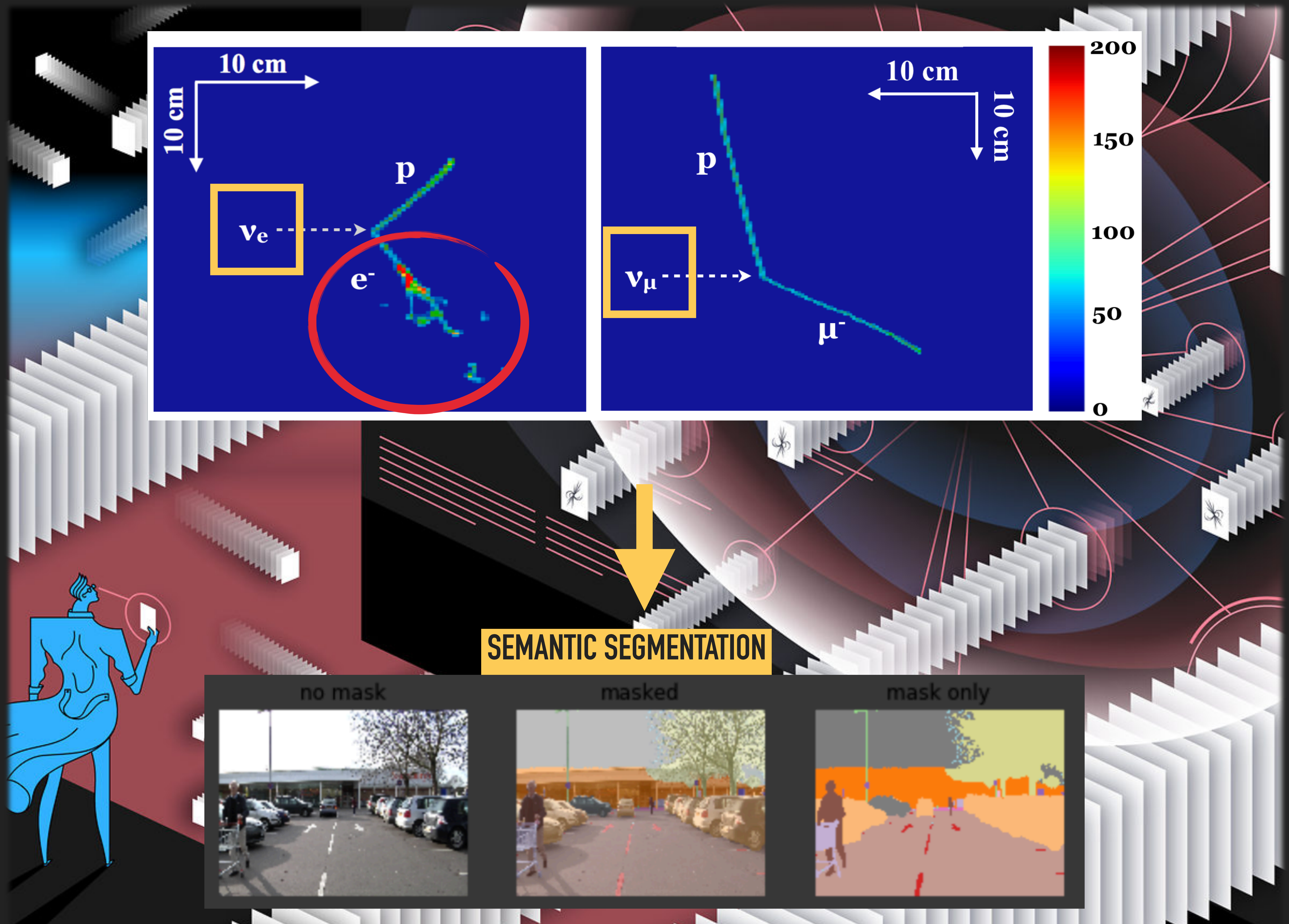

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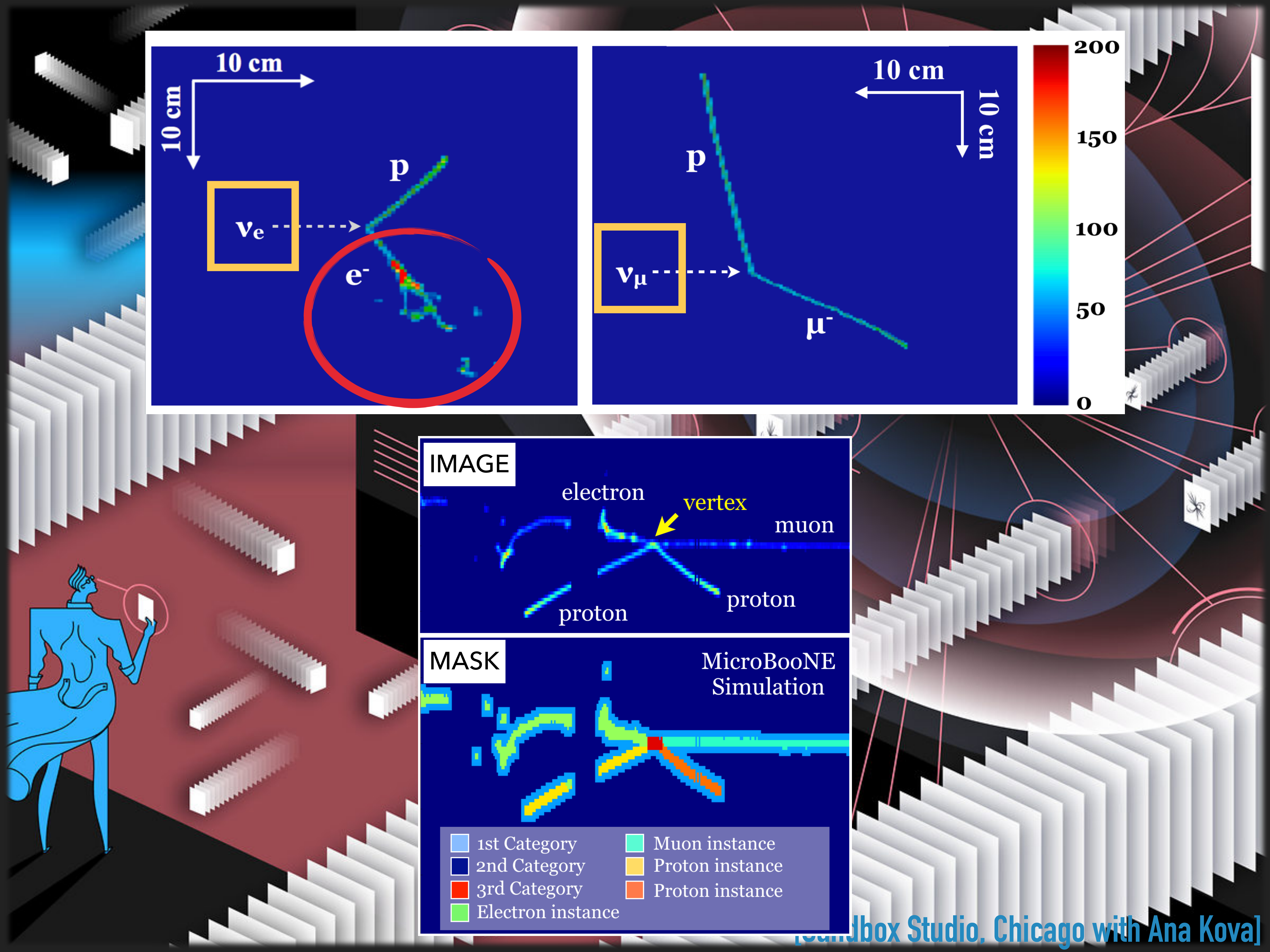
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IMAGE
electron
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muon
proton
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MASK
MicroBooNE
Simulation
1st Category
2nd Category
3rd Category
Electron instance
Muon instance
Proton instance
Proton instance
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[Scientific paper link](#)

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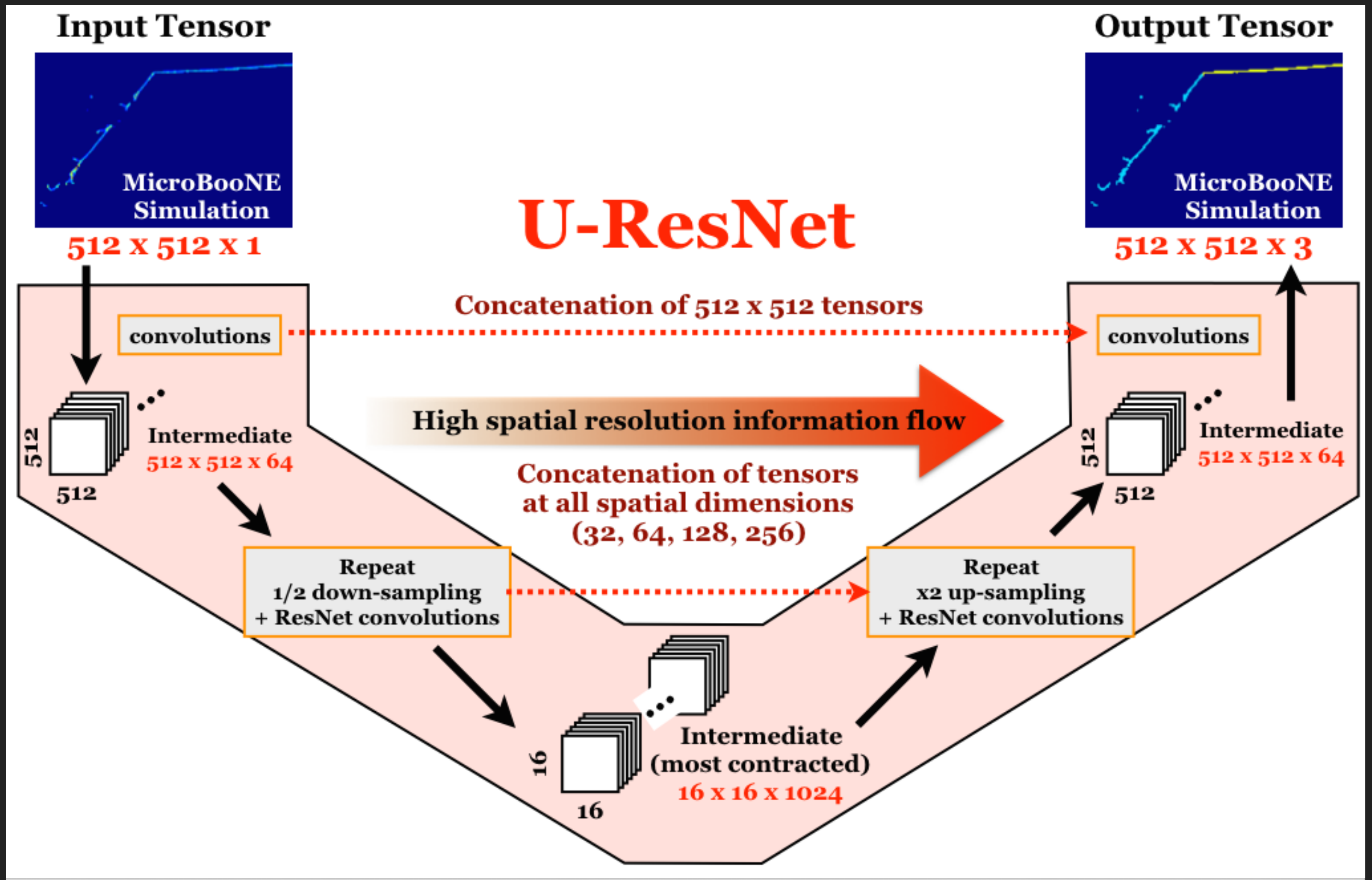
NETWORK ARCHITECTURE



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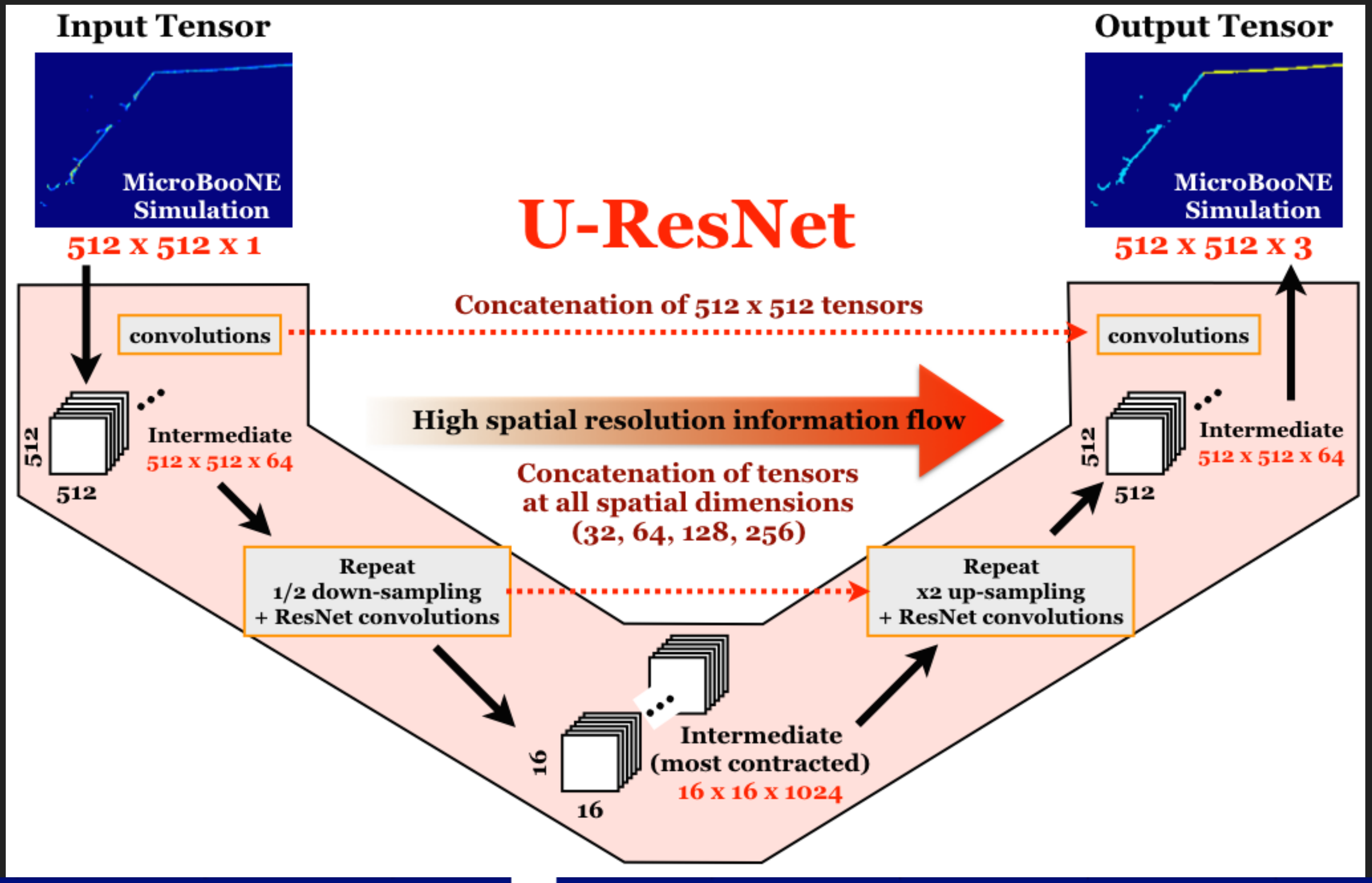

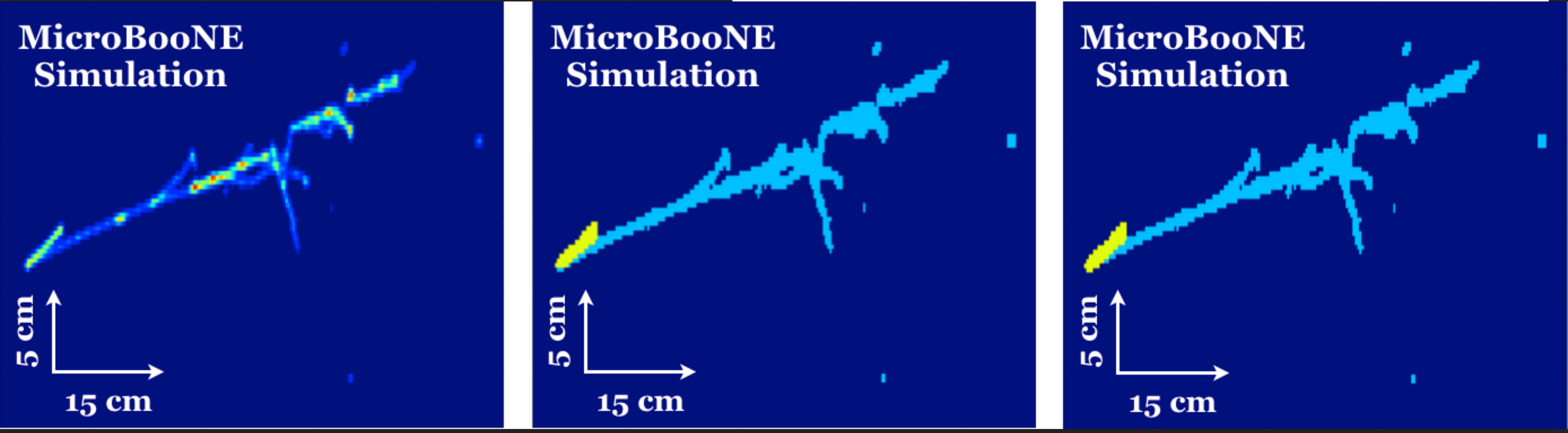

INPUT

“LABEL”

OUTPUT

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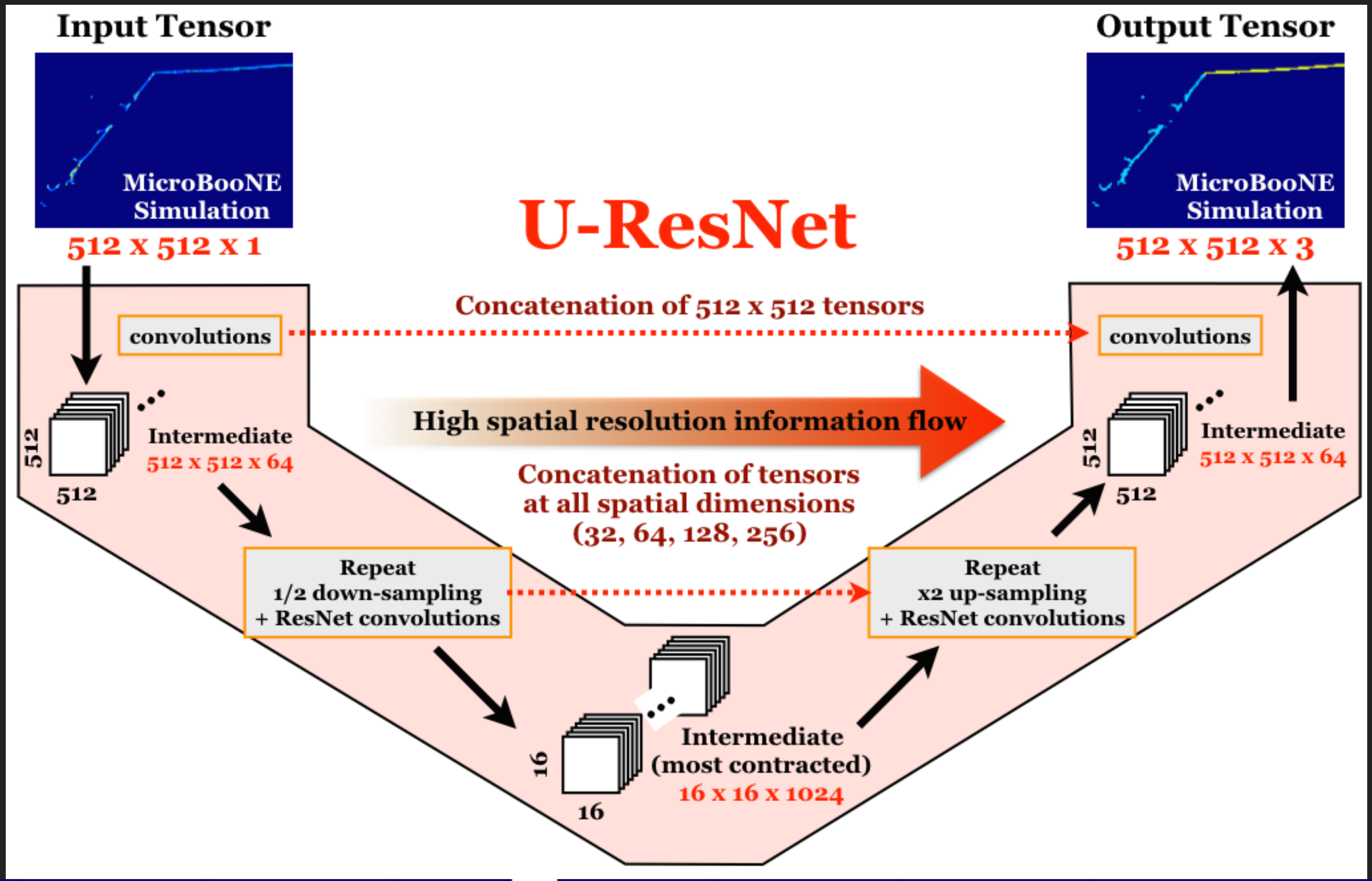
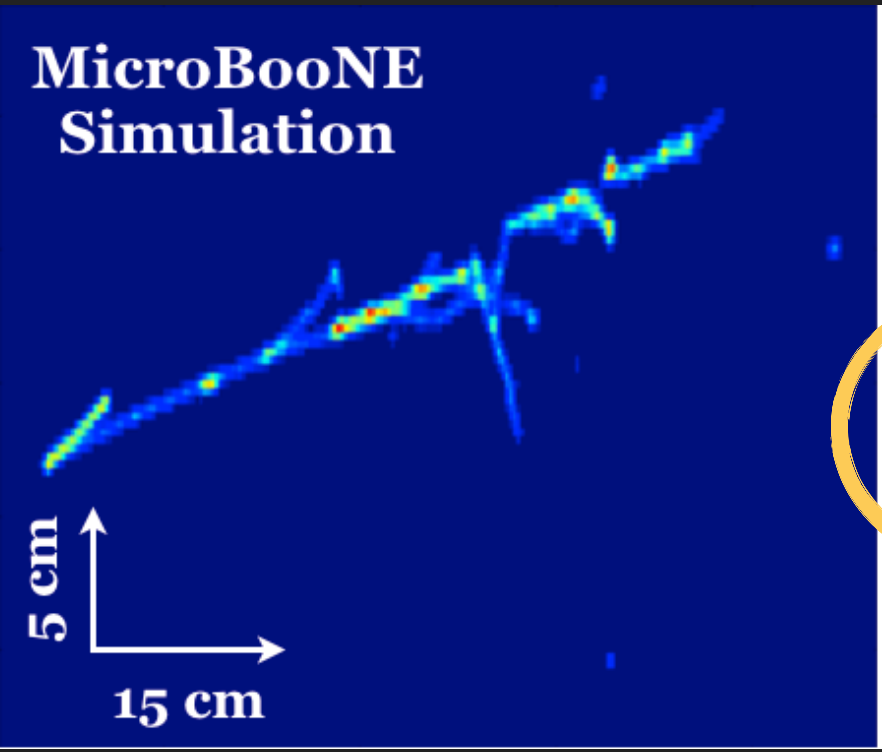
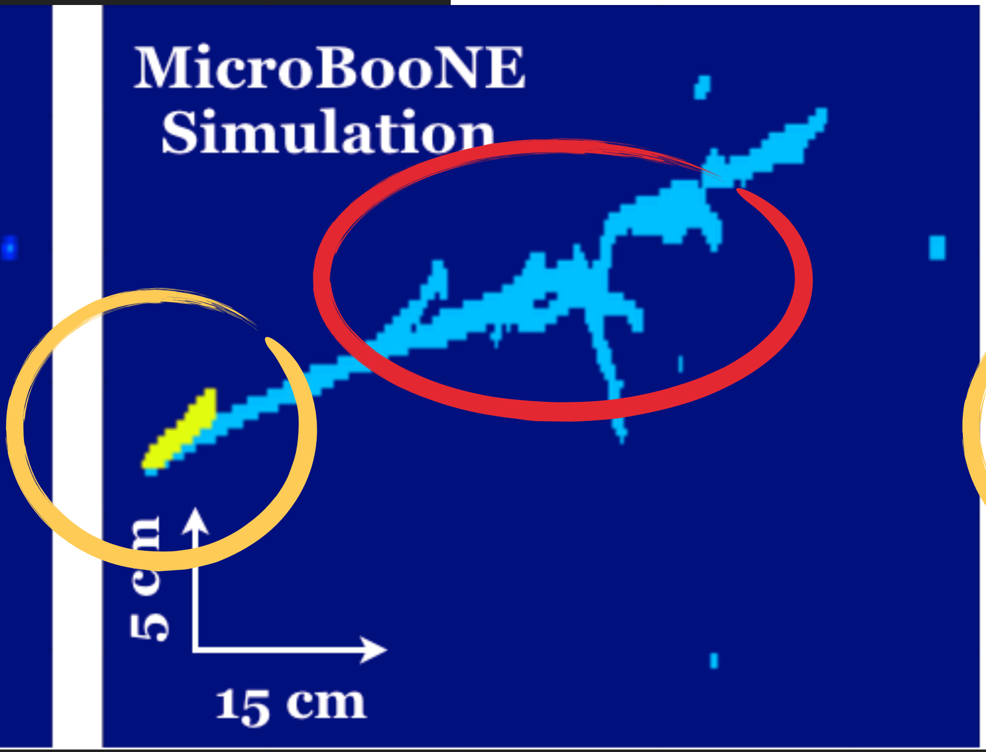
NETWORK ARCHITECTURE

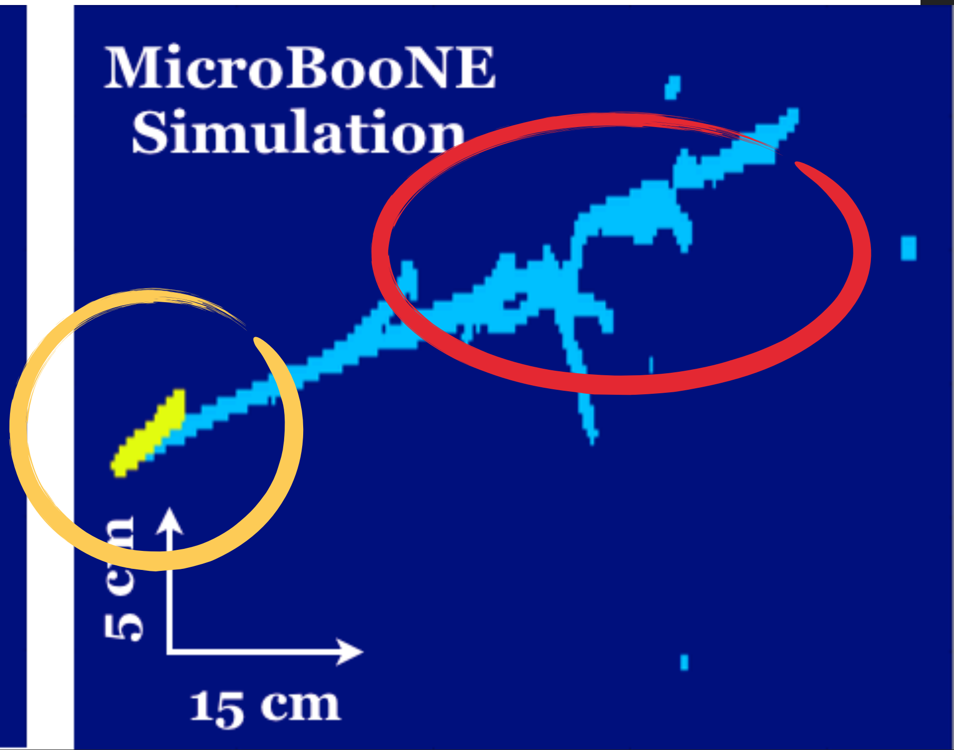




INPUT



"LABEL"



OUTPUT

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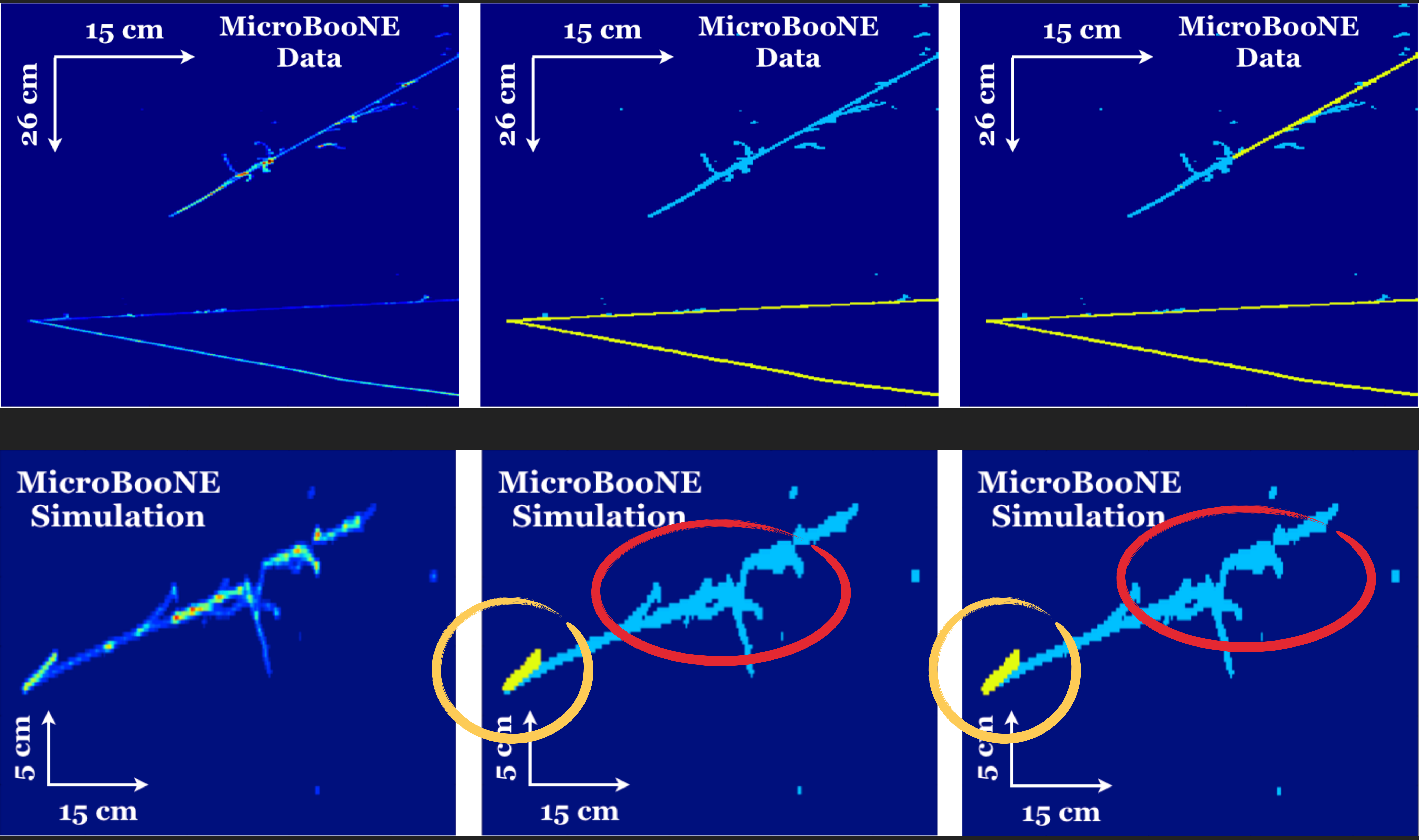
REAL DATA!



INPUT

"LABEL"

OUTPUT

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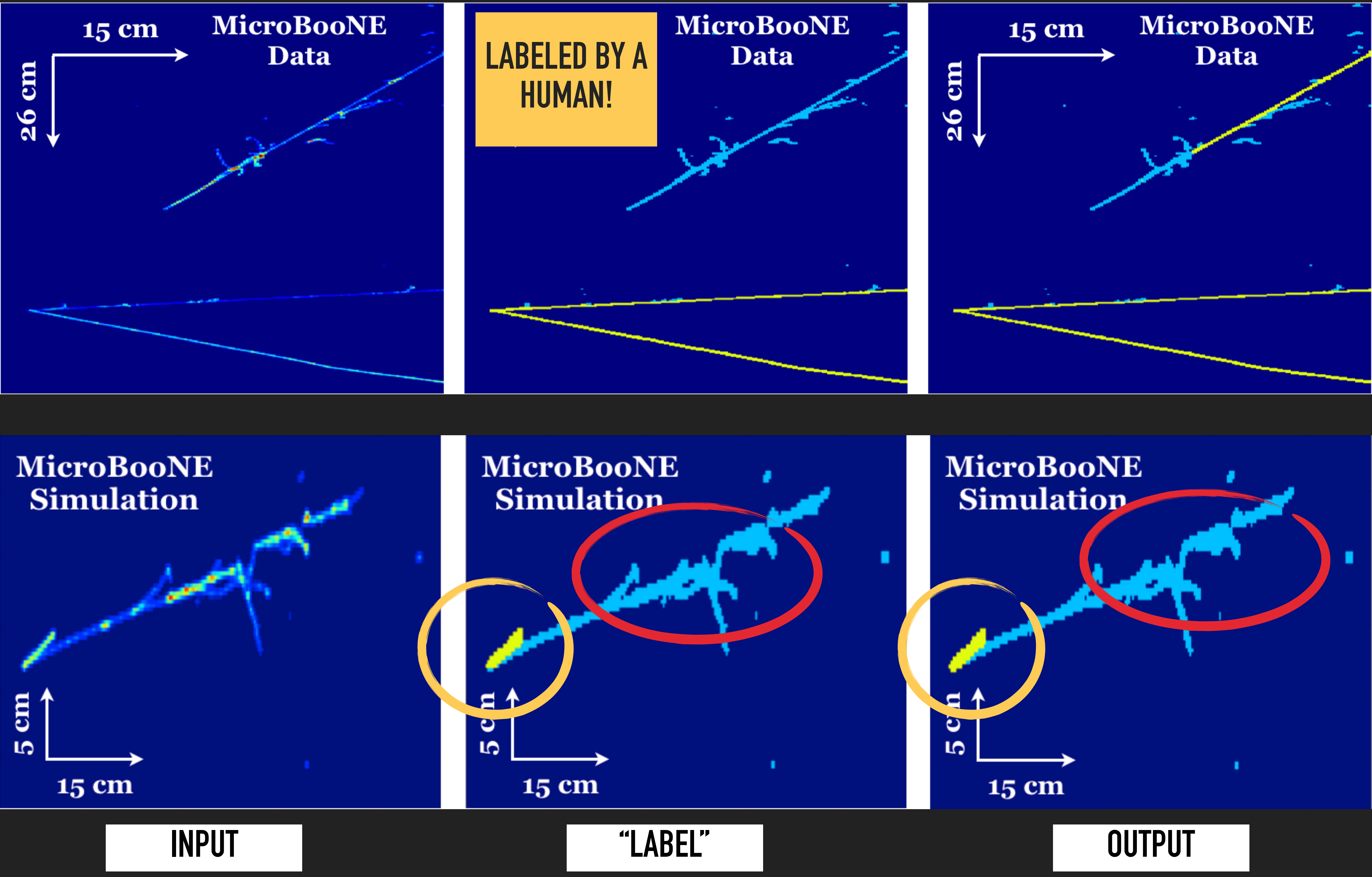
REAL DATA!



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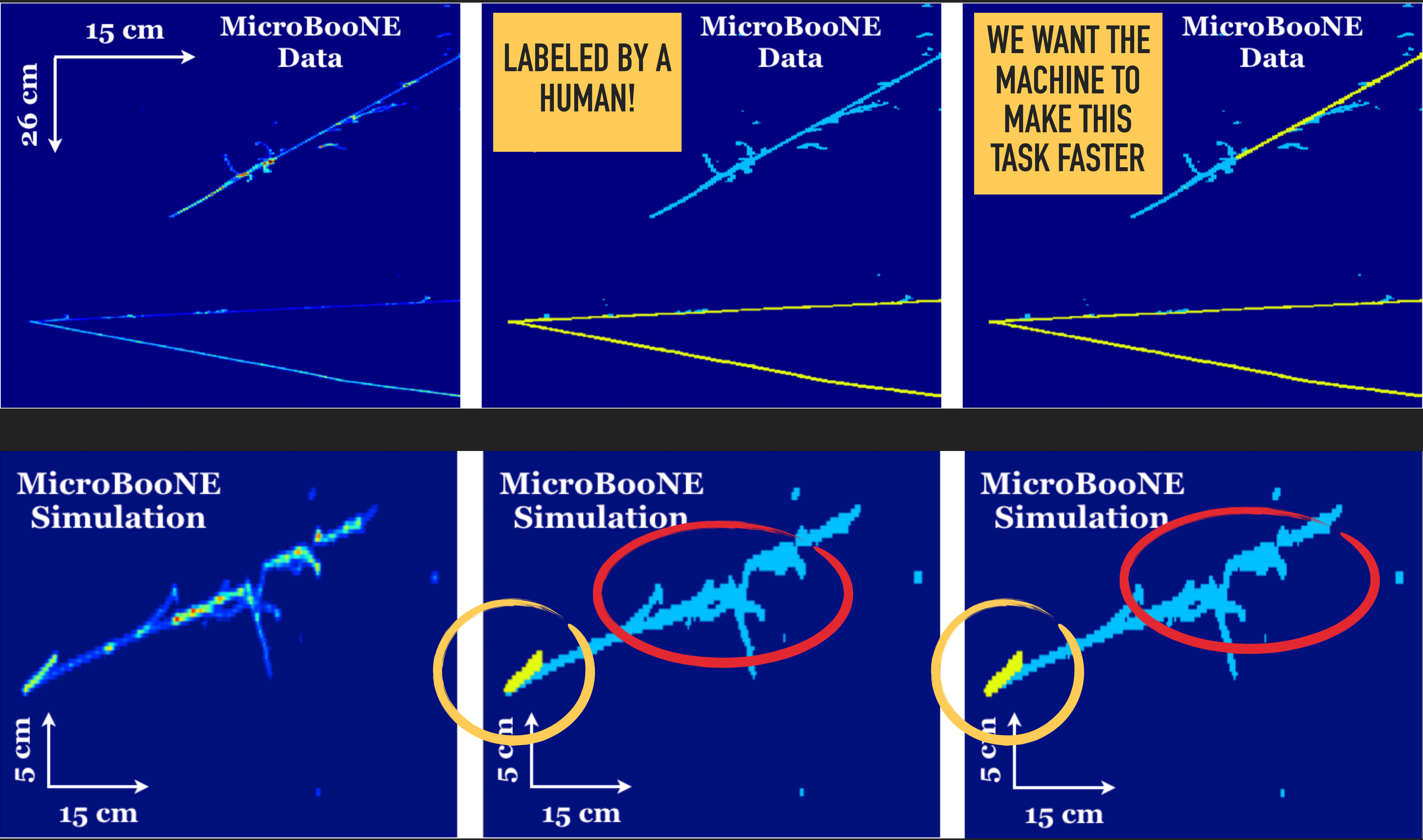
REAL DATA!



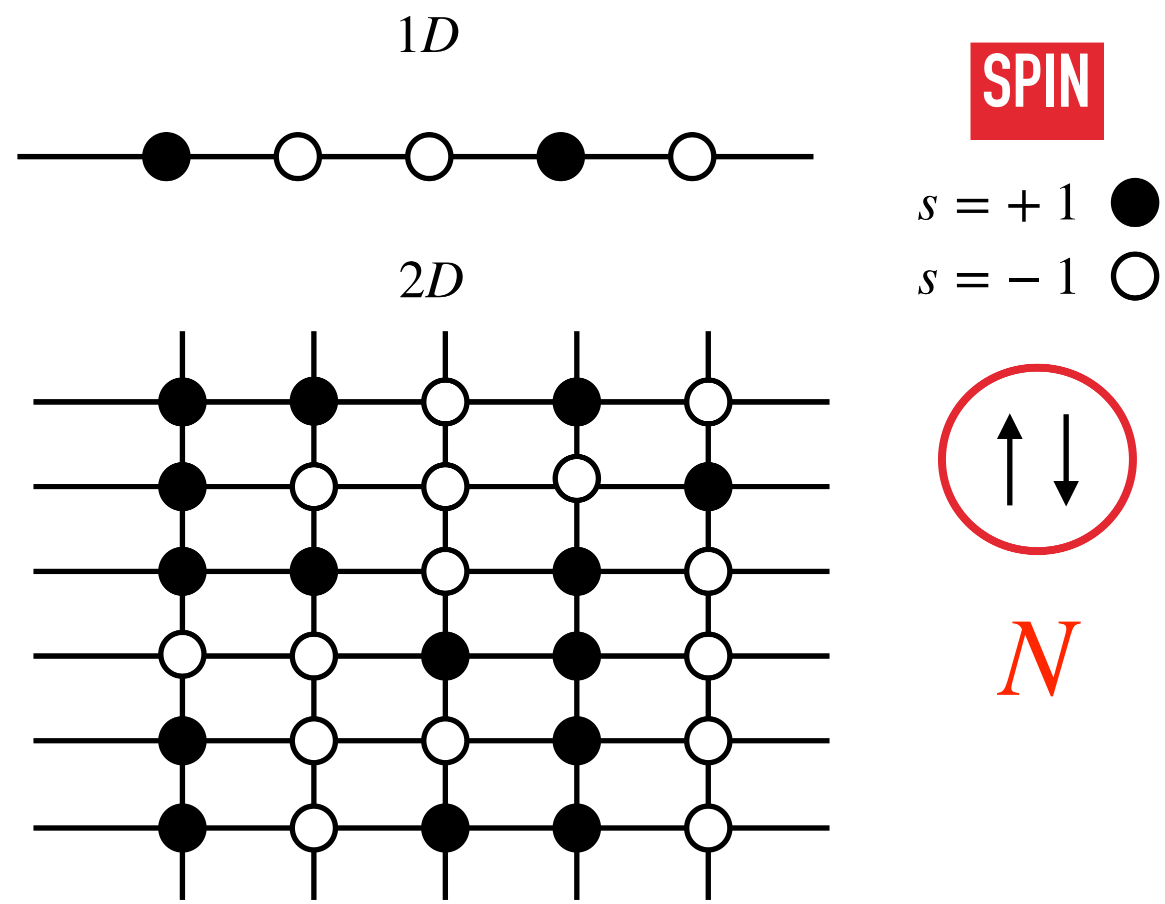
INPUT

“LABEL”

OUTPUT

$$E = \langle H \rangle = Z^{-1} \sum_{\{s_i\}} H\left(\{s_i\}\right) e^{-\beta H\left(\{s_i\}\right)}$$

THE ISING MODEL



Hamiltonian of spins with local interactions:

$$H\left(\{s_i\}\right) = -J \sum_{\langle i,j \rangle} s_i s_j - h \sum_i s_i$$

Probability of state:

$$p(\{s_i\}) = \frac{e^{-\beta H\left(\{s_i\}\right)}}{Z}$$

Inverse temperature

$$\beta = \frac{1}{k_B T}$$

Partition function:

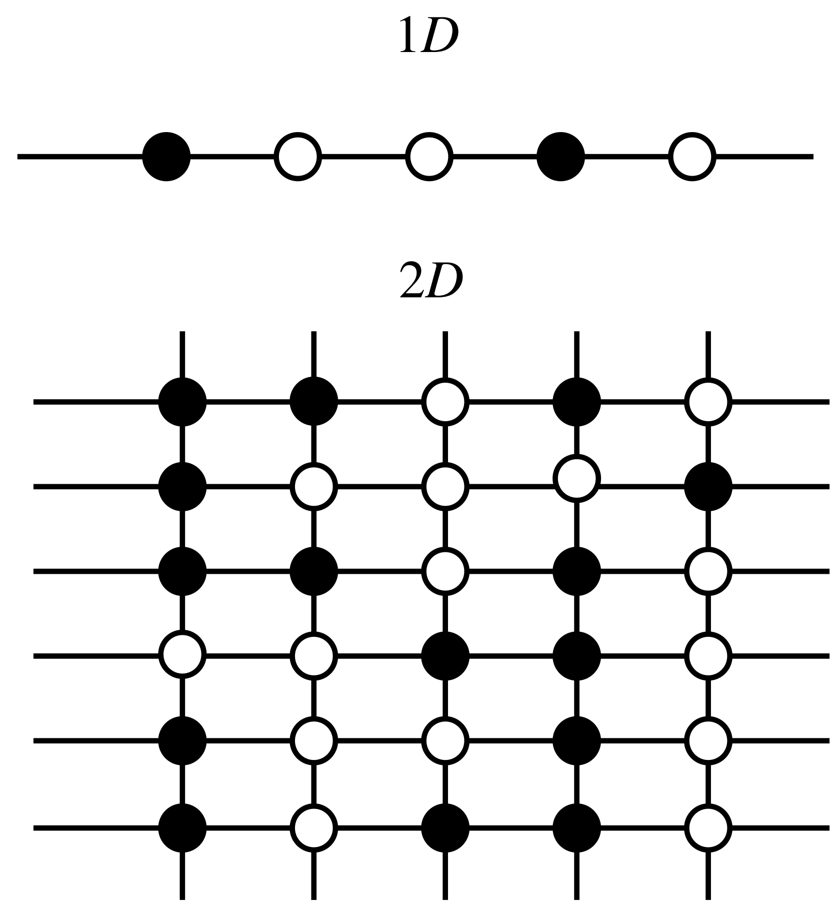
$$Z = \sum_{\{s_i\}} e^{-\beta H\left(\{s_i\}\right)}$$

Number of states:

$$\#\{s_i\} = 2^N$$

$$E = \langle H \rangle = Z^{-1} \sum_{\{s_i\}} H\left(\{s_i\}\right) e^{-\beta H(\{s_i\})}$$

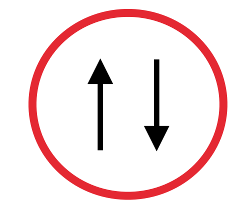
THE ISING MODEL



SPIN

$s = +1$ ●

$s = -1$ ○



N

Hamiltonian of spins with local interactions:

$$H\left(\{s_i\}\right) = -J \sum_{\langle i,j \rangle} s_i s_j - h \sum_i s_i$$

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$$p(\{s_i\}) = \frac{e^{-\beta H\left(\{s_i\}\right)}}{Z}$$

Inverse temperature

$$\beta = \frac{1}{k_B T}$$

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Number of states:

$$\#\{s_i\} = 2^N$$

Model for:

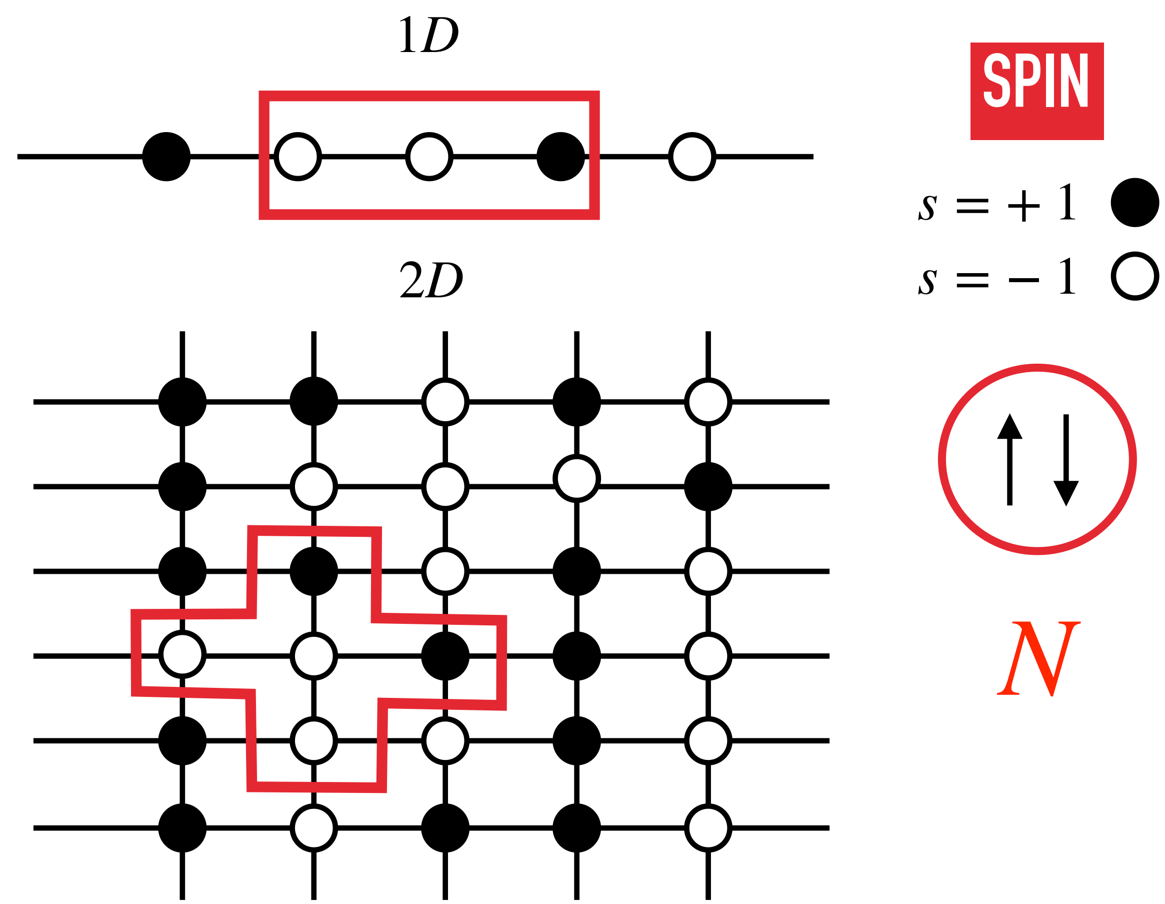
- Magnetic materials
- Neuronal activity
- Quantum computers

$$E = \langle H \rangle = Z^{-1} \sum_{\{s_i\}} H\left(\{s_i\}\right) e^{-\beta H(\{s_i\})}$$

THE ISING MODEL

Hamiltonian of spins with local interactions:

$$H\left(\{s_i\}\right) = -J \sum_{\boxed{\langle i,j \rangle}} s_i s_j - h \sum_i s_i$$



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Partition function:

$$Z = \sum_{\{s_i\}} e^{-\beta H(\{s_i\})}$$

Number of states:

$$\#\{s_i\} = 2^N$$

Model for:

- Magnetic materials
- Neuronal activity
- Quantum computers

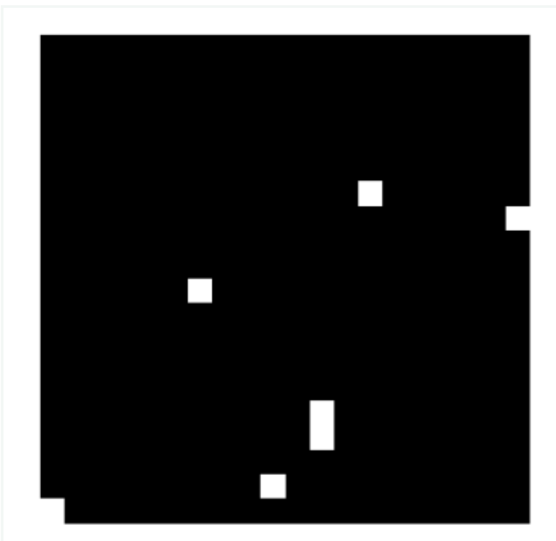
ORDERED AND DISORDERED PHASES

Ising

Water

ORDERED AND DISORDERED PHASES

Ising

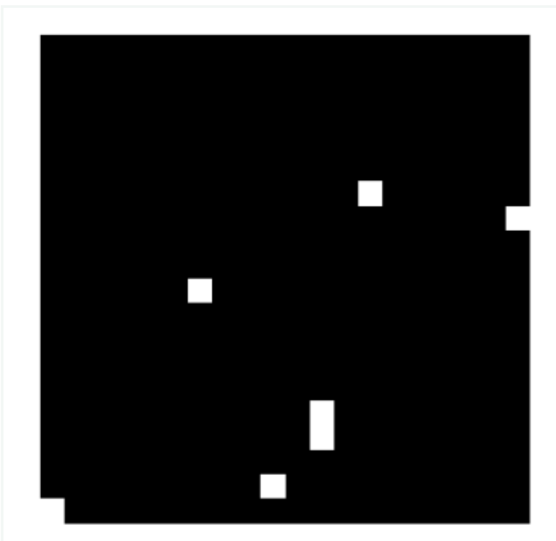


COLD HOT T

Water

ORDERED AND DISORDERED PHASES

Ising



COLD

HOT

T

ORDERED

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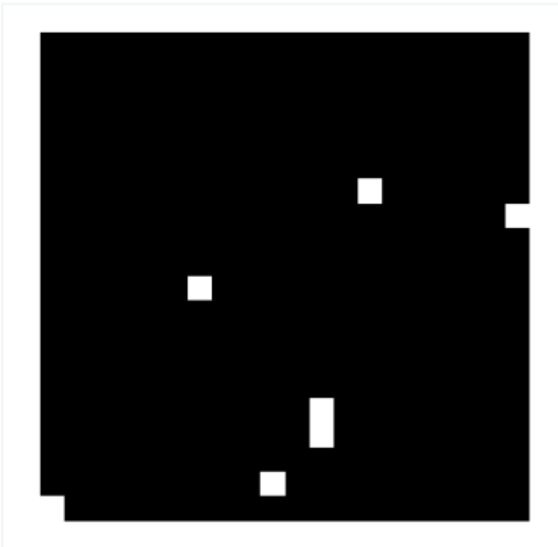

COLD

HOT

T

ORDERED

Water

ORDERED AND DISORDERED PHASES

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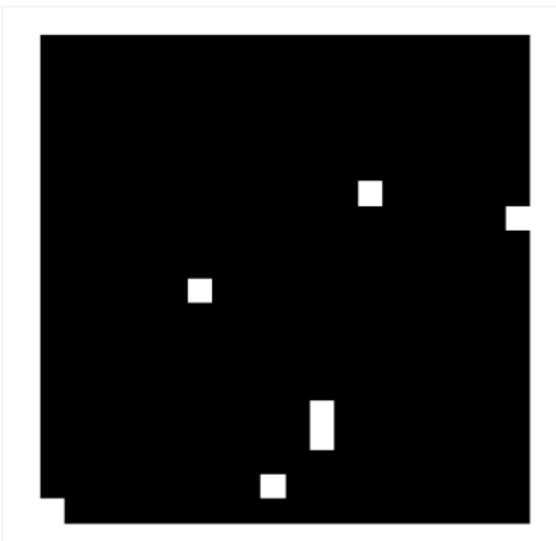


COLD → HOT → T

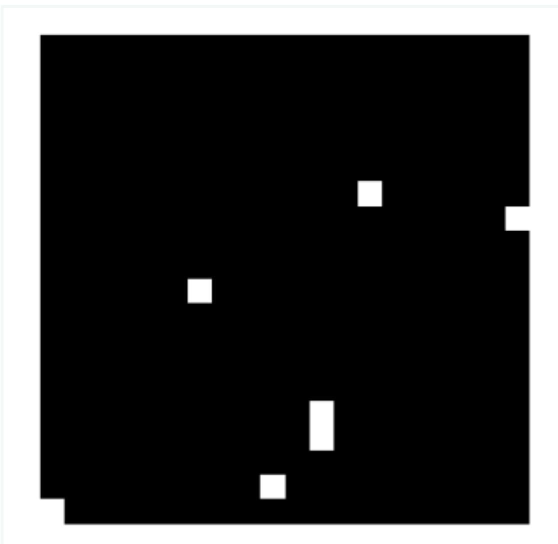
ORDERED

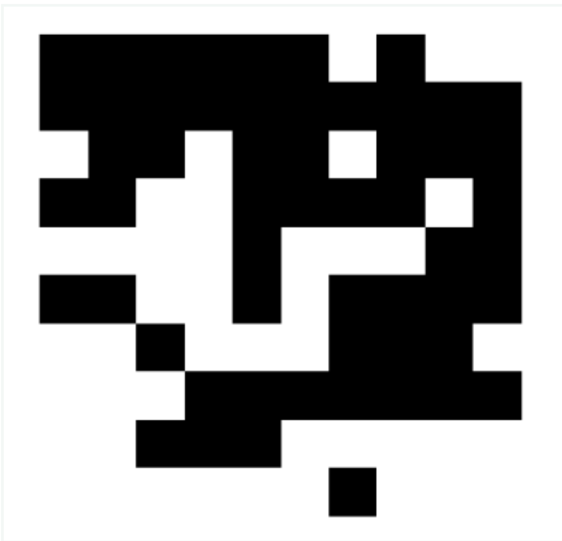
DISORDERED

Water

ORDERED AND DISORDERED PHASES

Ising





COLD — CRITICAL — HOT → T

ORDERED | PHASE TRANSITION | DISORDERED

Water

ORDERED AND DISORDERED PHASES

Ising

CAN WE PREDICT ANY OF THIS WITHOUT KNOWING THE MICROSCOPIC DETAILS?

DO WE NEED A FULL UNDERSTANDING OF THE COMPLEX DYNAMICS TO MAKE PREDICTIONS?

COLD — HOT → T

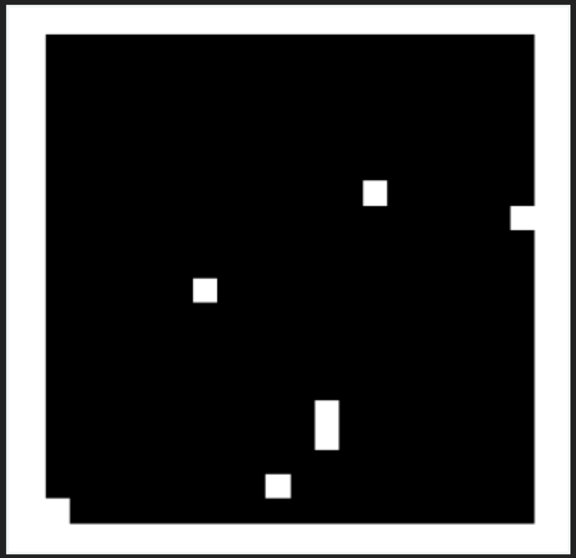
ORDERED | PHASE TRANSITION | DISORDERED

Water

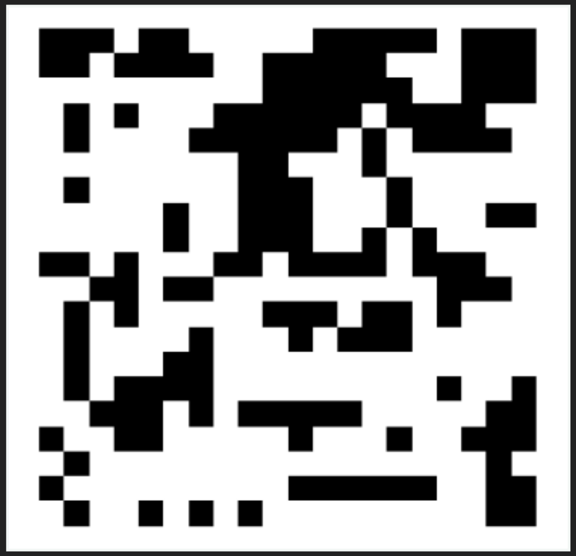
[Scientific paper link]

[Playground]

MACHINE LEARNING PHASES OF MATTER



→ COLD



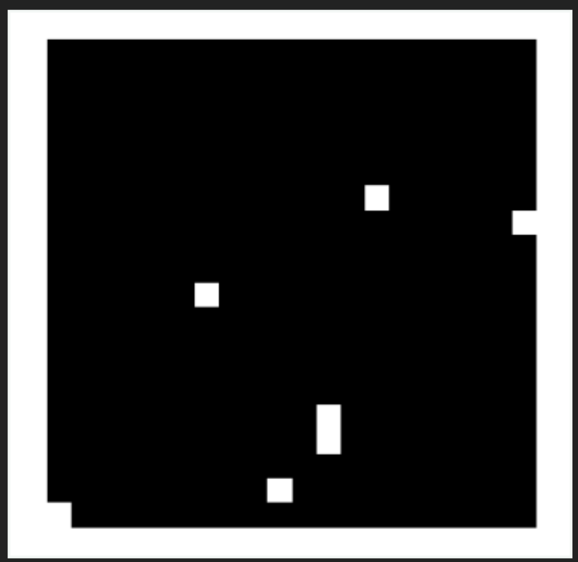
→ HOT

Scientific paper link

Playground

MACHINE LEARNING PHASES OF MATTER

IMAGE/Data → Labels



COLD

HOT

[Scientific paper link]

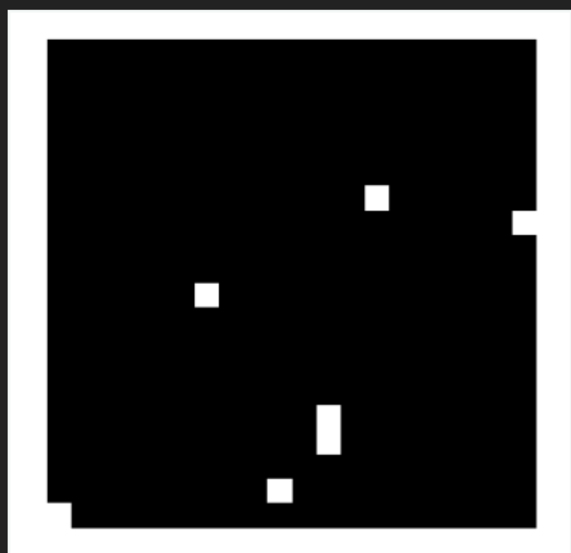
[Playground]

MACHINE LEARNING PHASES OF MATTER

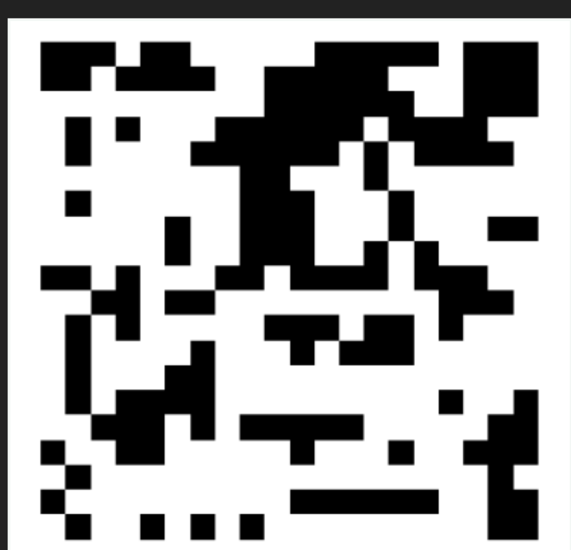
SUPERVISED CLASSIFICATION

SVM, MLP, CNN

IMAGE/Data → Labels



→ COLD



→ HOT

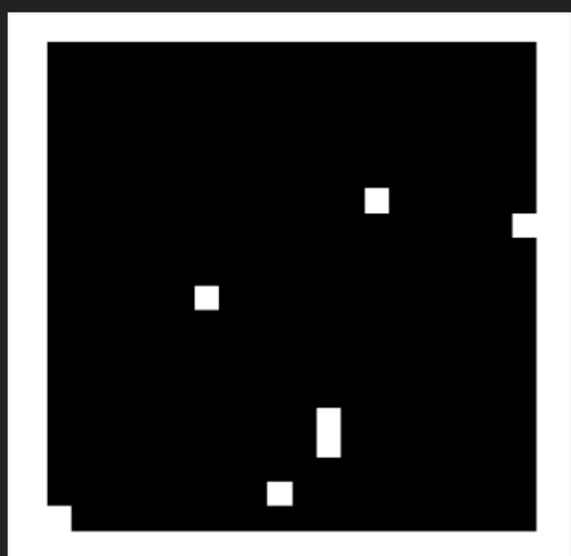
→ ??

MACHINE LEARNING PHASES OF MATTER

[Scientific paper link]

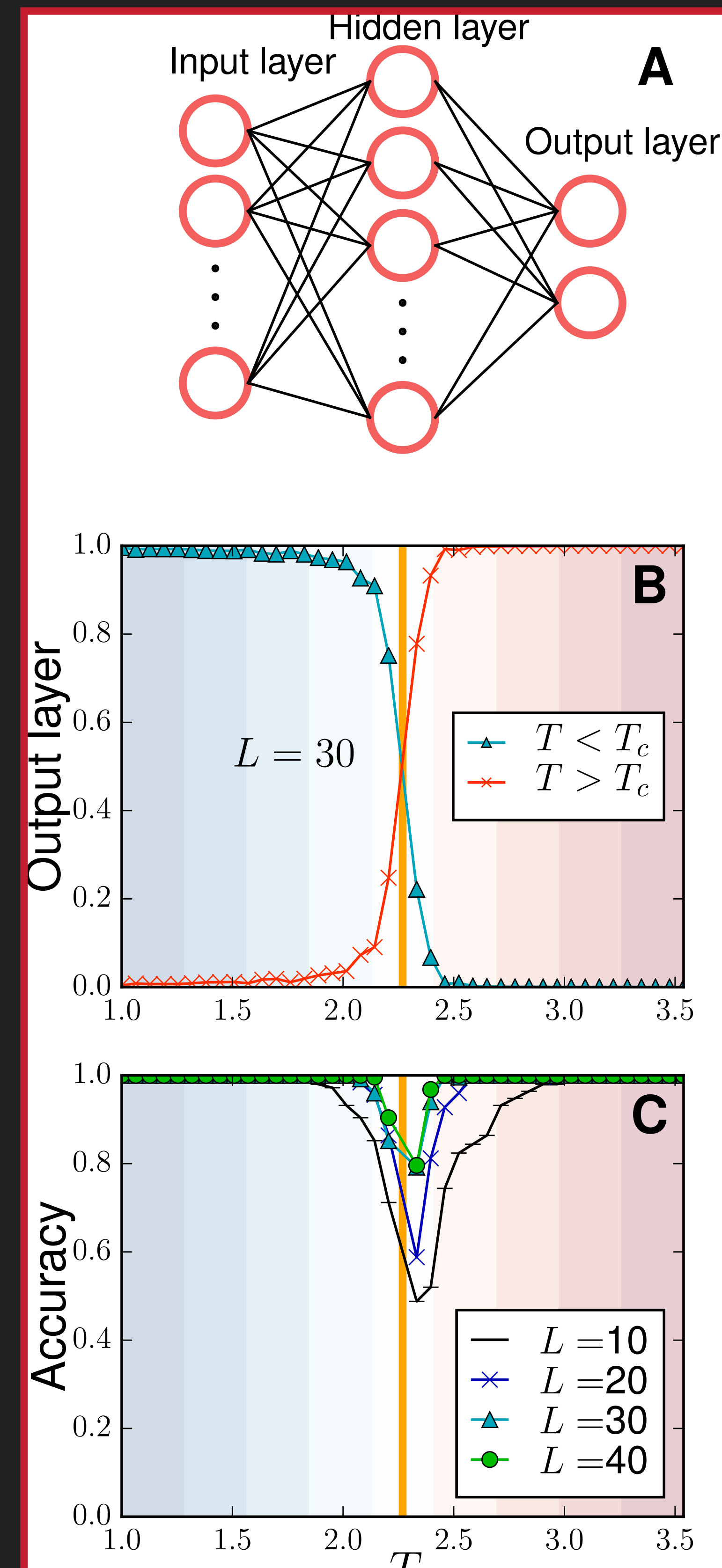
[Playground]

IMAGE/Data → Labels



→ COLD

→ HOT

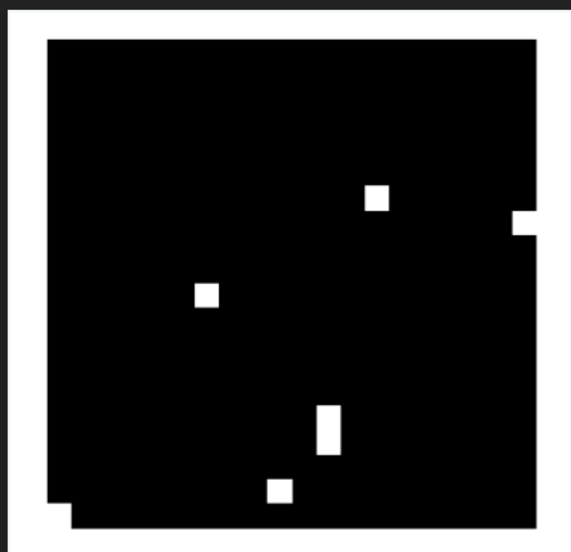


[Scientific paper link]

[Playground]

MACHINE LEARNING PHASES OF MATTER

IMAGE/Data → ??



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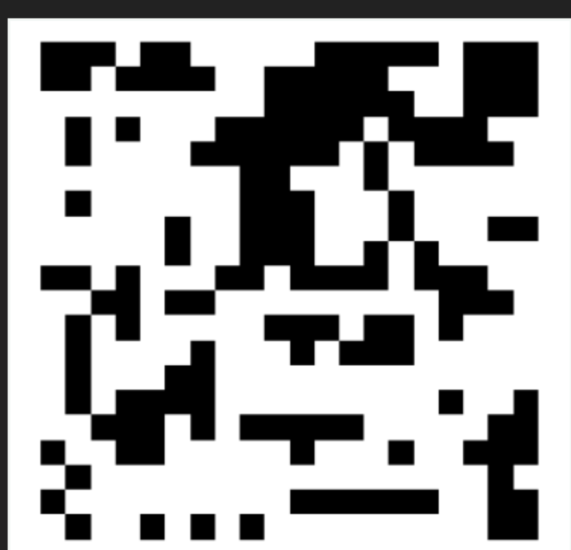


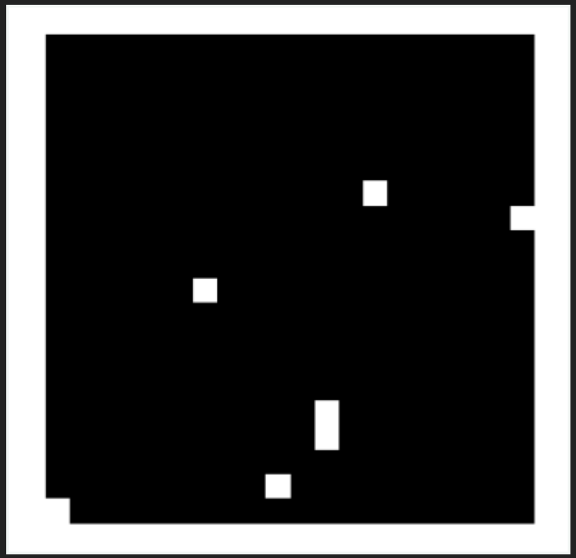
→ ??

[Scientific paper link](#)

[Playground](#)

MACHINE LEARNING PHASES OF MATTER

IMAGE/Data → ??



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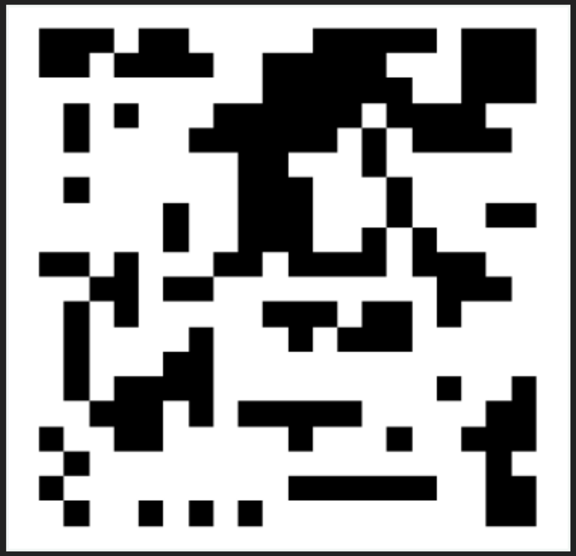

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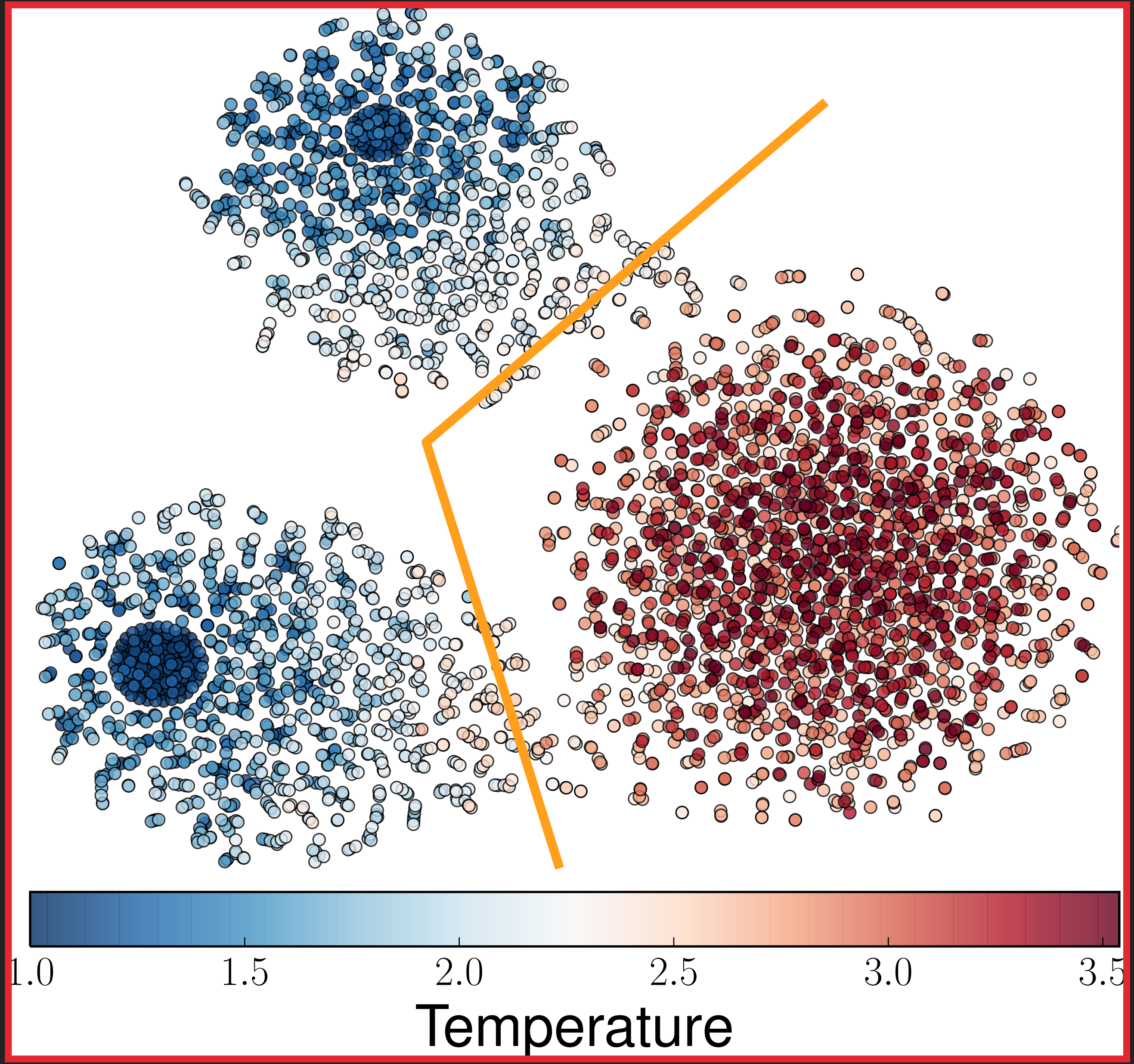
UNSUPERVISED CLUSTERING

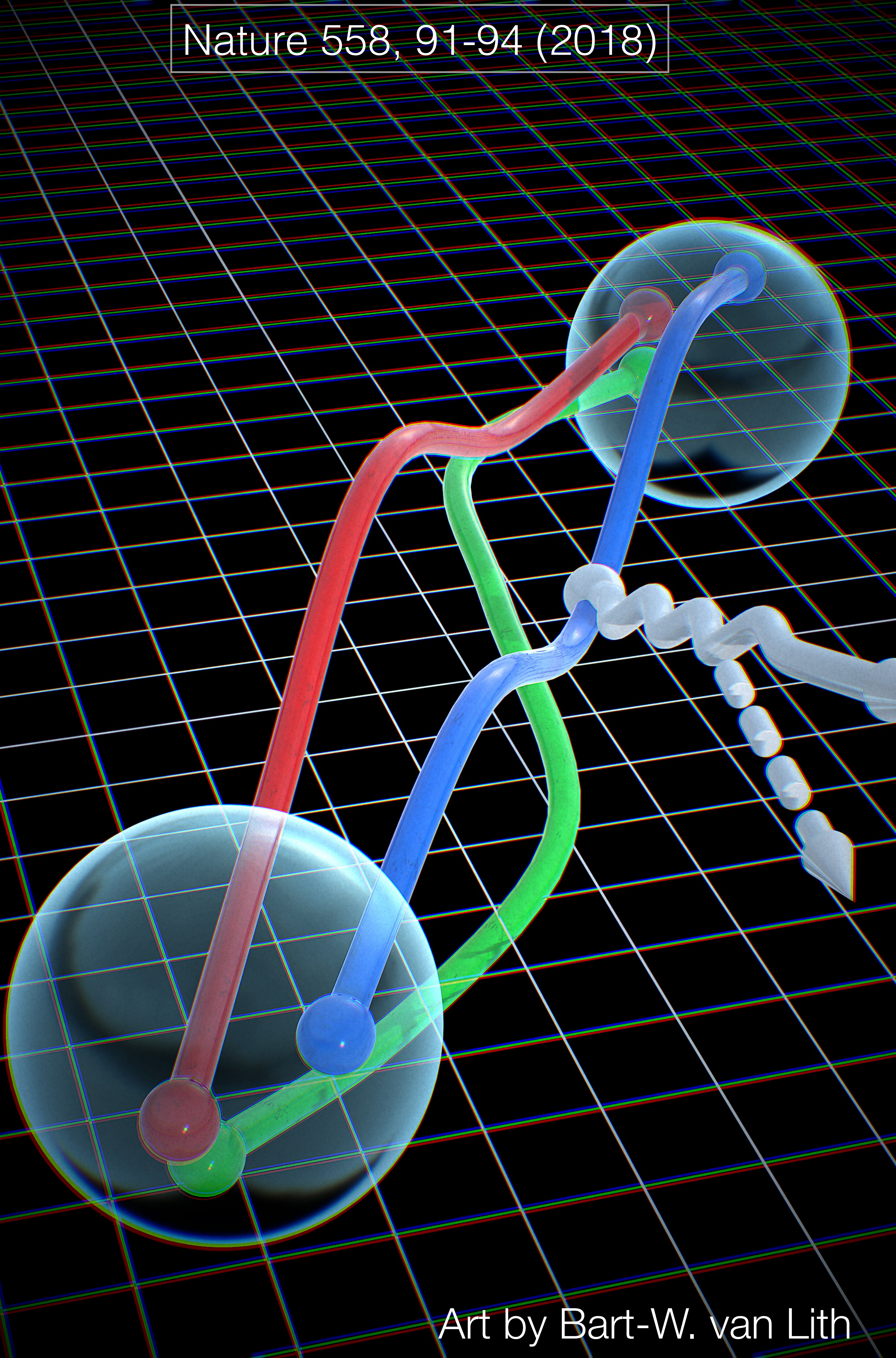
PCA, t-SNE, k-Means



CONCLUSIONS AND OUTLOOK

- ML is applied to several branches of physics: particle, statistical, astro…
- Physics is a complex problem with plenty of opportunities for Deep Learning algorithms
- Experimental and Computational physics provide a very large amount of data (sensors or simulations)
- Lead *top500* supercomputers have demonstrated amazing ML capabilities and applications
    - weather, earthquakes, etc…

EXTRA MATERIAL



nature
International journal of science

Letter | Published: 30 May 2018

A per-cent-level determination of the nucleon axial coupling from quantum chromodynamics

C. C. Chang, A. N. Nicholson, E. Rinaldi, E. Berkowitz, N. Garron, D. A. Brantley, H. Monge-Camacho, C. J. Monahan, C. Bouchard, M. A. Clark, B. Joó, T. Kurth, K. Orginos, P. Vranas & A. Walker-Loud

Nature **558**, 91–94 (2018) | Download Ci

Nuclear Scientists Calculate Value of Key Property that Drives Neutron Decay

Supercomputer simulations of neutrons' inner turmoil and a new method that filters out "noise" yield the highest-ever precision calculation of nucleon axial coupling, a property crucial to predicting neutron lifetime

May 30, 2018

UPTON, NY—Using some of the world's most powerful supercomputers, an international team including scientists from several U.S. Department of Energy (DOE) national laboratories has released the highest-precision calculation of a fundamental property of protons and neutrons known as nucleon axial coupling. This quantity determines the strength of the interaction that triggers neutrons to decay into protons—and can therefore be used to more accurately predict how long neutrons are expected to "live." The results appear in *Nature*.

"The fact that neutrons decay into protons is a very, very important fact in the universe," said Enrico Rinaldi, a special postdoctoral researcher at the RIKEN BNL Research Center at DOE's Brookhaven National Laboratory, who was involved in developing simulations essential to the new calculation. "It basically tells you how atomic nuclei—made of protons and neutrons—were created after the Big

理化学研究所

広報活動

Home > 広報活動 > プレスリリース（研究成果）

報道発表資料

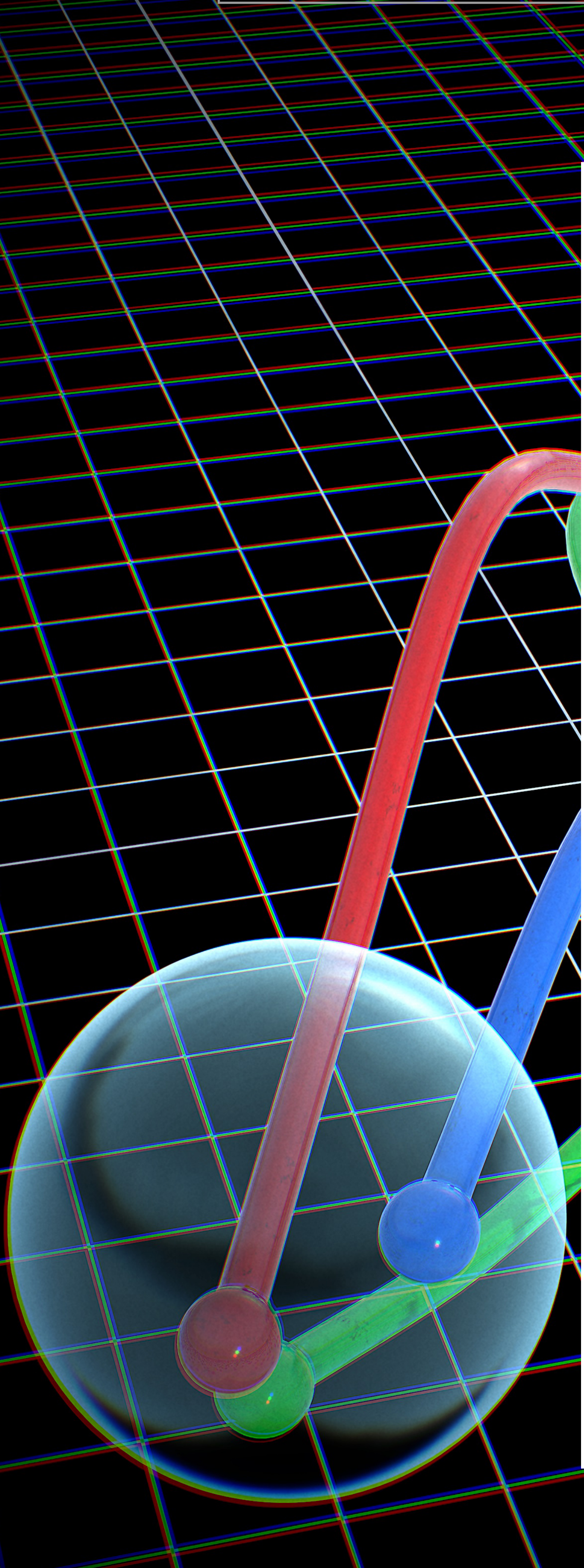
2018年5月31日
理化学研究所

中性子の寿命の仕組みを垣間見る

ー超高速計算による量子色力学方程式に基づいた中性子寿命計算ー

理化学研究所（理研）仁科加速器科学研究センター理研BNL研究センター計算物理研究グループのエンリコ・
特別研究員、数理創造プログラムのチアチェン・チャン研究員（ローレンス・バークレー国立研究所　研究員
グループ※は、世界最高性能のスーパーコンピュータを複数用いて、中性子の寿命[1]を決めている「軸性電荷
計算を実現し、これまでの実験値とほとんど矛盾しないことを示しました。

Nature 558, 91-94 (2018)



Art by Bart-W. van Lith

nature
International journal of science

ter | Published: 30 May 2018

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SCIENCE

AWARD FINALISTS DEMONSTRATE IMPROVED QCD CODE FOR SUPERCOMPUTING

BY KATIE ELYCE JONES

8 SHARE
3 LOVE

Modeling nuclei using fundamental quantum mechanics equations is a big job to manage, even for the world's fastest computers.

This article is part of a series covering the finalists for the 2018 Gordon Bell Prize that used the Summit supercomputer. The prize winner will be announced at SC18 in November in Dallas.

There is a fine line between particle physics and nuclear physics at which the subatomic particles quarks and gluons first join into protons and neutrons, then into atomic nuclei.

On one side of this line is the universe as it should be according to the Standard Model of particle physics: nearly devoid of matter and filled with leftover radiation from the mutual destruction of matter and antimatter. On the other side of this line is the universe as we observe it: space–time speckled with matter in the form of galaxies, suns, and planets.

To understand the asymmetry between matter and antimatter, scientists are using massive supercomputers in the search for new physics discoveries. Through a sophisticated numerical method known as lattice quantum chromodynamics (QCD), scientists calculate the interactions of quarks and gluons on a lattice of space–time to study the emergence of nuclei from the fundamental physics theory of QCD. By bridging the studies of particle interactions and atomic nuclei, lattice QCD simulations are also an entry point for learning much more about how the universe works.

One of the QCD research teams leading this charge is improving its ability to compute the precise duration of the neutron lifetime on the latest generation of US Department of Energy (DOE) supercomputers, including the 200-petaflop Summit supercomputer at DOE's Oak Ridge National Laboratory (ORNL) and the 125-petaflop Sierra supercomputer at DOE's Lawrence Livermore National Laboratory (LLNL).

Scientists Calculate Value of Key Property that Neutron Decay

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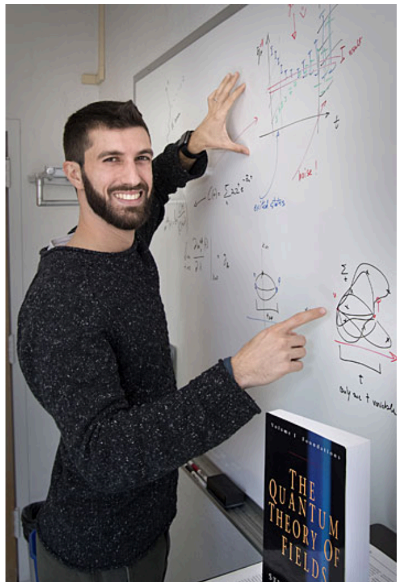
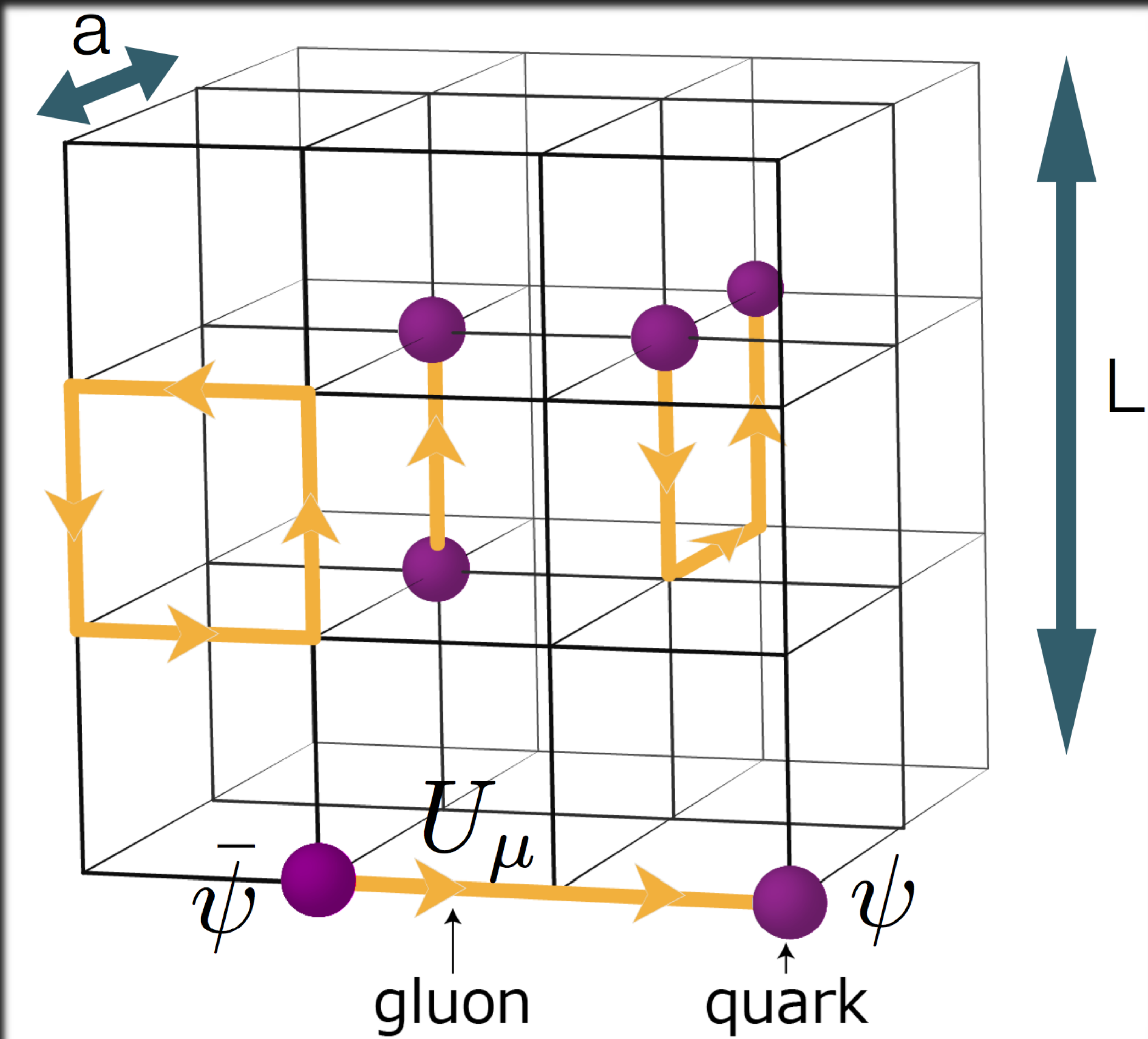


る
基づいた中性子寿命計算ー

理化学研究所（理研）仁科加速器科学研究センター理研BNL研究センター計算物理研究グループのエンリコ・特別研究員、数理創造プログラムのチアチェン・チャン研究員（ローレンス・バークレー国立研究所　研究員グループ※は、世界最高性能のスーパーコンピュータを複数用いて、中性子の寿命[1]を決めている「軸性電荷計算を実現し、これまでの実験値とほとんど矛盾しないことを示しました。

LATTICE QUANTUM FIELD THEORY - OVERVIEW



- DISCRETIZE SPACE AND TIME
  - LATTICE SPACING a
  - LATTICE SIZE L
- KEEP ALL D.O.F. OF THE THEORY
  - NOT A MODEL!
  - NO SIMPLIFICATIONS
- AMENABLE TO NUMERICAL METHODS
  - MONTE CARLO SAMPLING
  - USE SUPERCOMPUTERS
- PRECISELY QUANTIFIABLE AND IMPROVABLE UNCERTAINTIES
  - SYSTEMATIC: $L \to \infty$, $a \to 0$
  - STATISTICAL: $\sqrt{N}$

LATTICE QUANTUM FIELD THEORY - MATHEMATICS

$$\mathcal{L}_{QCD} = -\frac{1}{4}F^2 + \bar{\psi}(i\not{D} + m)\psi$$

MICROSCOPIC THEORY OF FIELDS

ψ: quark field

U: gauge field

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}\psi \, \mathcal{D}\bar{\psi} \, \mathcal{D}U \; e^{-S[\bar{\psi},\psi,U]} \mathcal{O}$$

QUANTUM FEYNMAN PATH INTEGRAL

Physical observable

DISCRETIZE

Makes integral finite dimens.

$$\{U_1, U_2, U_3, \ldots, U_N\}$$

MARKOV CHAIN MONTE CARLO

Sampling

$$\approx \frac{1}{N} \sum_{i=1}^{N} \mathcal{O}\left[U_i\right] + O\left(\frac{1}{\sqrt{N}}\right)$$

IMPORTANCE SAMPLING

Estimator

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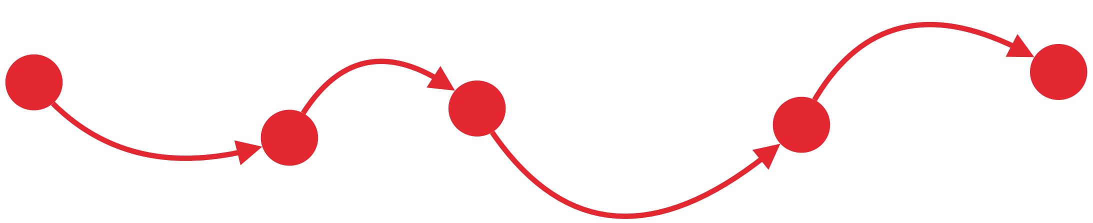

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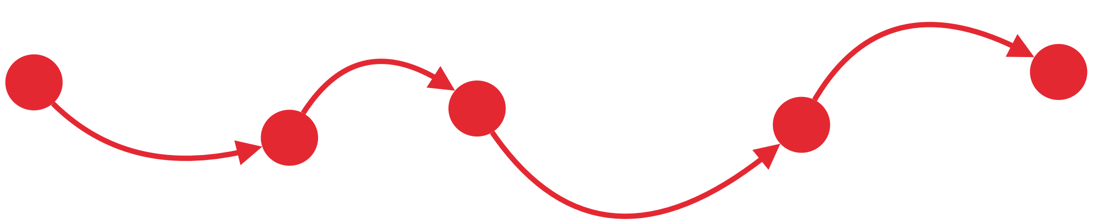

move in configuration space with prob.

MARKOV CHAIN MONTE CARLO

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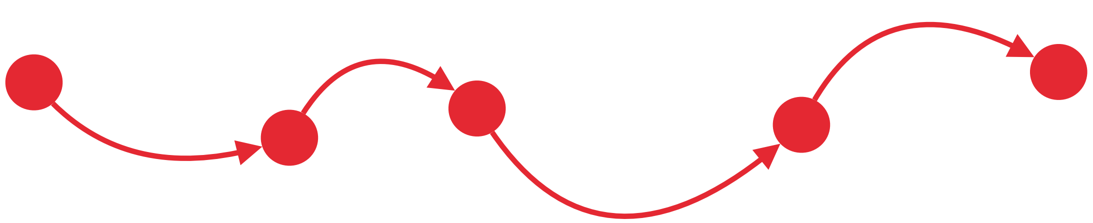

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MARKOV CHAIN MONTE CARLO

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IMPORTANCE SAMPLING

Estimator

MACHINE LEARNING IS INSPIRING NEW ALGORITHMS

GENERATION

- it is costly to generate configuration with MCMC in certain regimes
- accelerate sampling with generative models
- examples: RBMs, normalizing-flow models, GANs, self-learning

MEASURE

- unsupervised algorithms can be used to detect phase transitions in materials
- reconstruct microscopic parameters from macroscopic observations
- spectral inference can be used to find eigenfunctions of quantum systems

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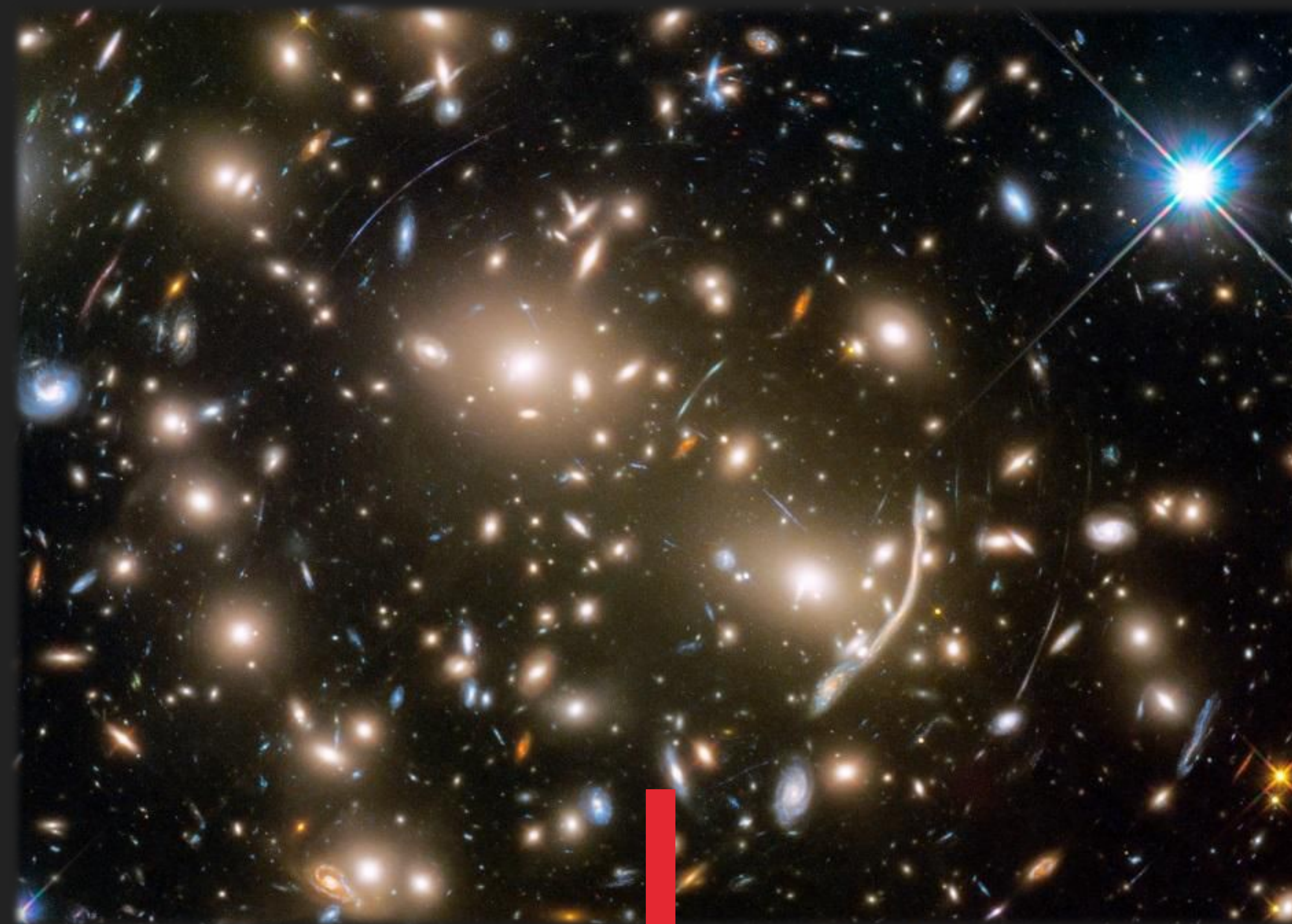
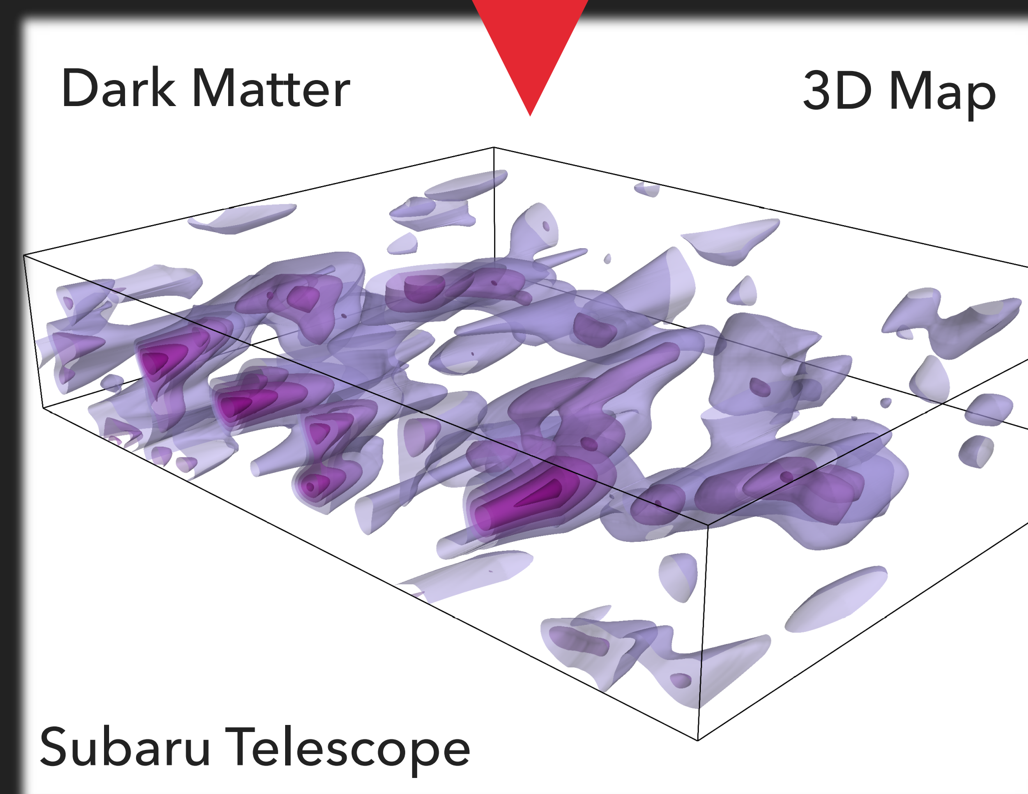
1. ORGANIZING (AI + LATTICE) WORKSHOPS
2. PAPERS IN PREPARATION ON USE CASES FOR GAN AND PHASE TRANSITIONS
3. SUPERCOMPUTERS ARE AI-READY

GRAVITATIONAL LENSING





GALACTIC ROTATION VELOCITY