

# AI for HEP



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**CHACAL, Johannesburg, Jan 2024**



# Outline

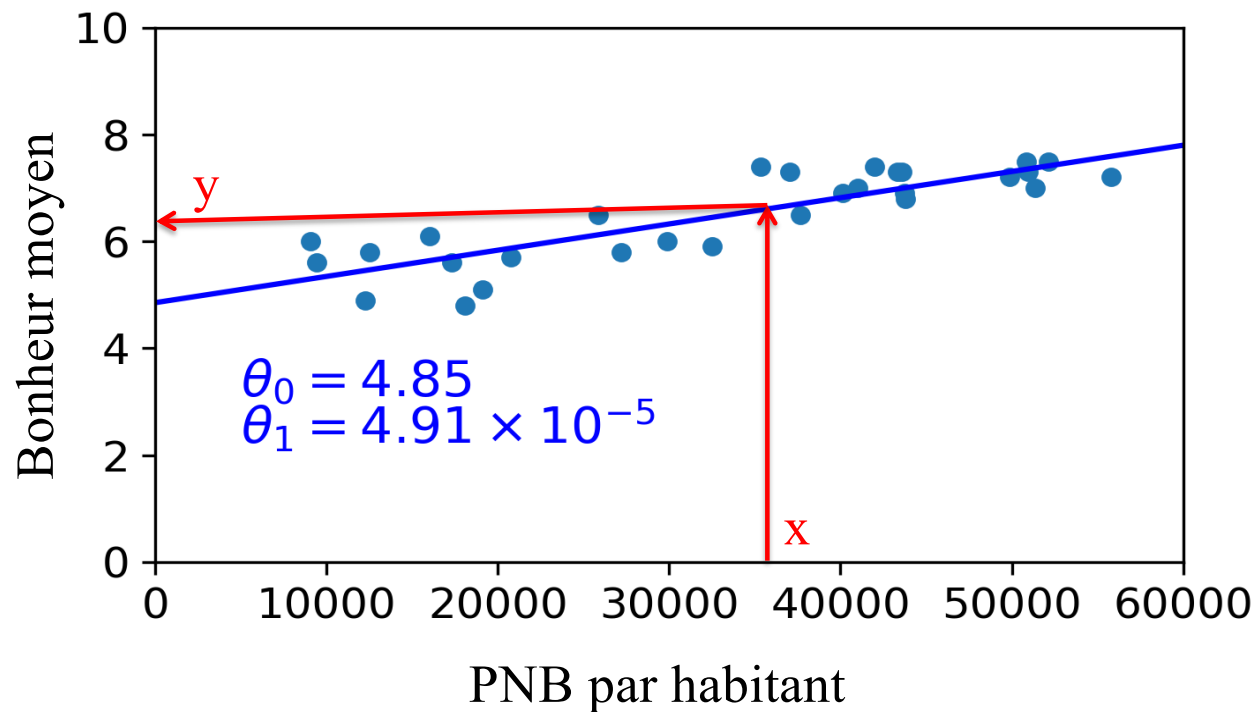
- Broad overview of AI for science : now
- Basics of AI for physics + BDT tutorial : now and this PM
- Neural Networks course and tutorial : friday
- Advance ML for HEP : saturday

# AI for science



# Linear Regression

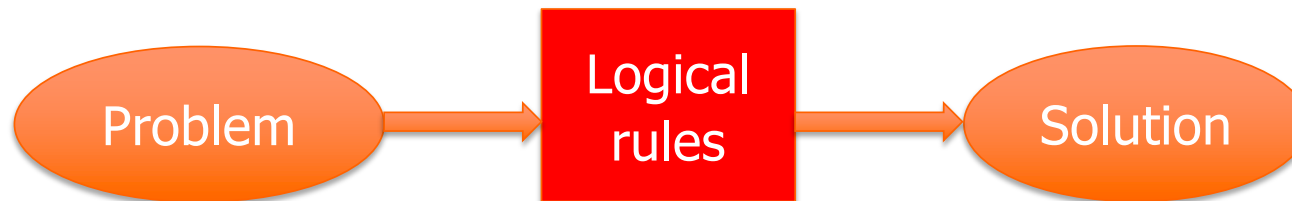
Boskovic, Legendre, Laplace, Gauss



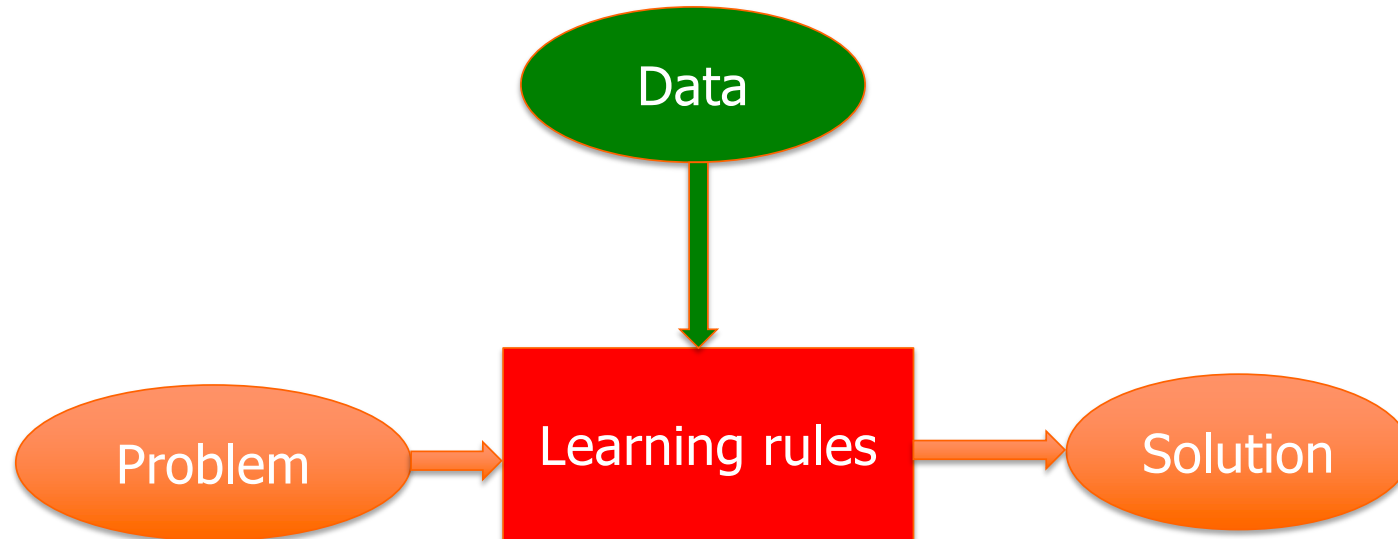
Given  $x$ , we want  $y \rightarrow$  how to build  $f$  ?

- Written text  $\xrightarrow{f}$  text  $y$
- Image  $\rightarrow$  cat or dog ? Mom ?
- « Comment ça va ? »  $\rightarrow$  «Unjani? »
- Speach  $\rightarrow$  text
- Facebook account.  $\rightarrow$  ads
- Chess diagram  $\rightarrow$  next move
- Camera+GPS  $\rightarrow$  steering wheel action
- « write an essay on AI and science »  $\rightarrow$  essay

# Traditional computing



# Machine Learning



Learning = = optimising algorithm internal parameters:  $n=2$  à  $10^{12}$

# Scientific inference





# Discovery of the positron

☐ Cloud chamber



Carl Anderson  
Nobel 1936

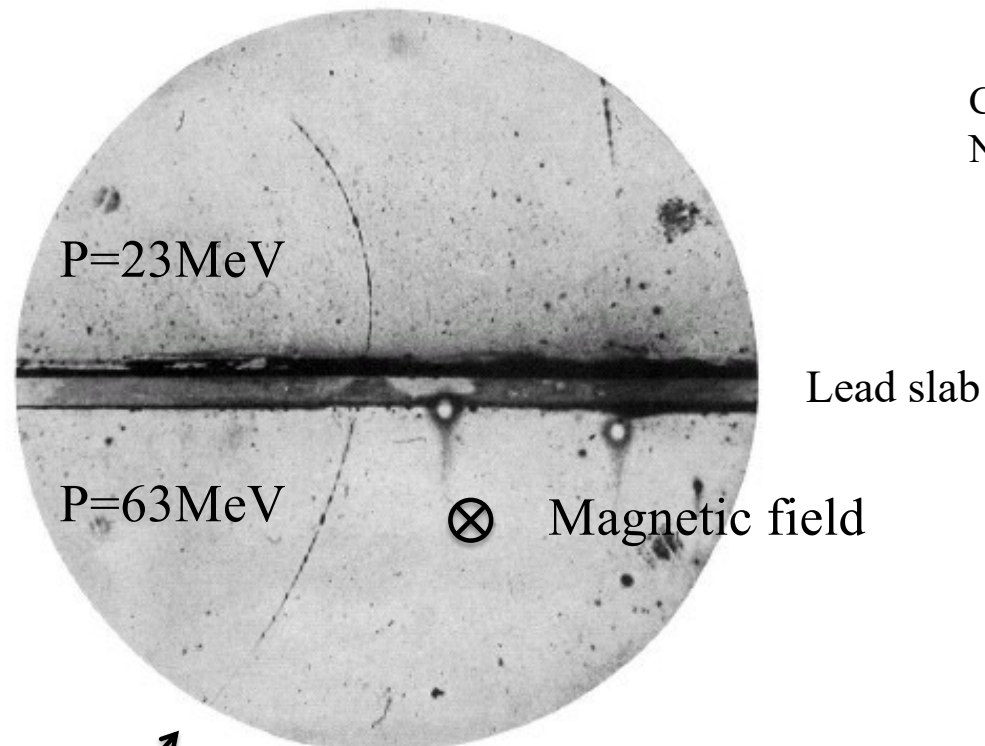
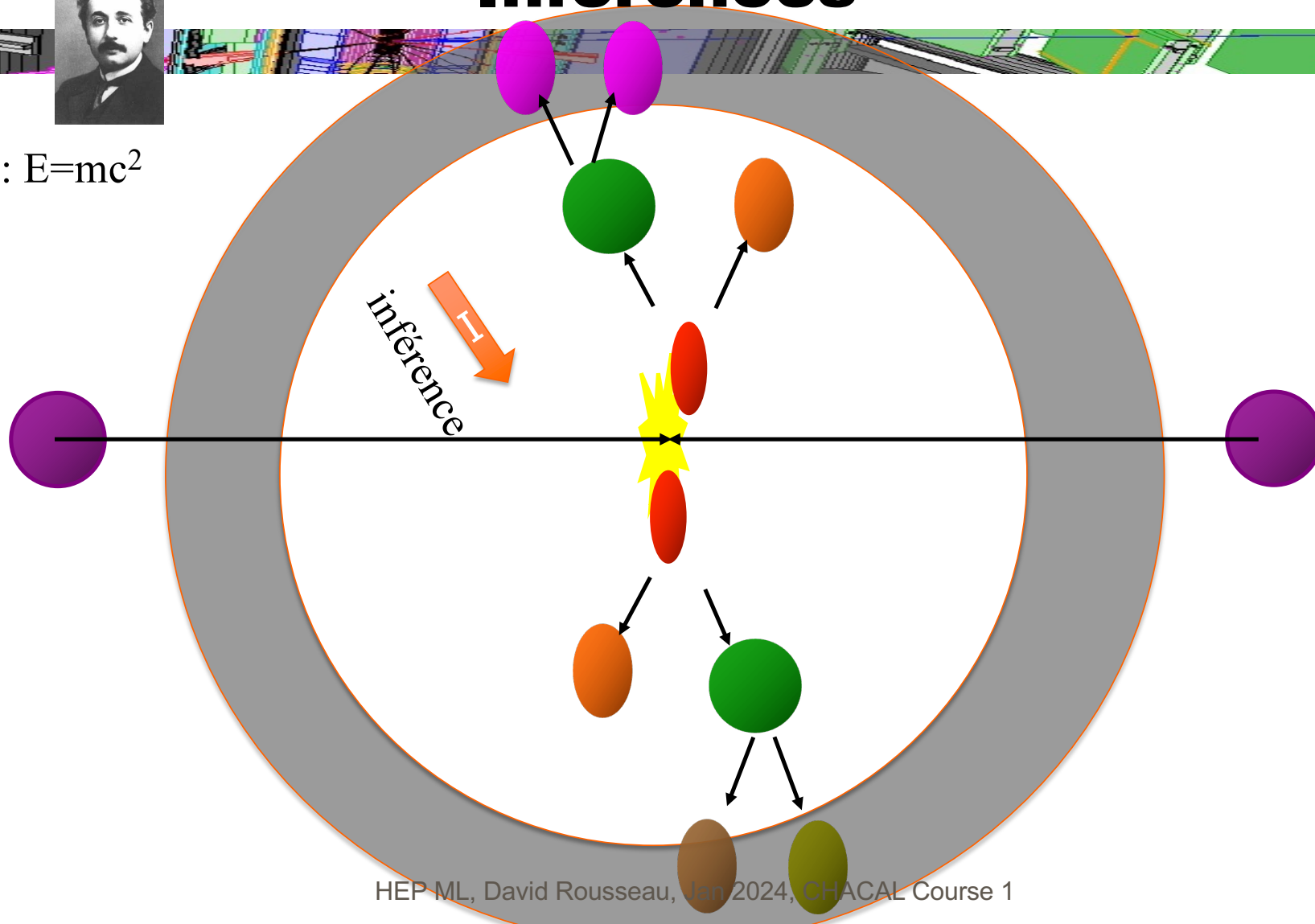


FIG. 1. A 63 million volt positron ( $H_p = 2.1 \times 10^9$  gauss-cm) passing through a 6 mm lead plate and emerging as a 23 million volt positron ( $H_p = 7.5 \times 10^4$  gauss-cm). The length of this latter path is at least 100 times greater than the possible length of a proton path of this curvature.

# Inferences



Einstein:  $E=mc^2$





# ATLAS EXPERIMENT

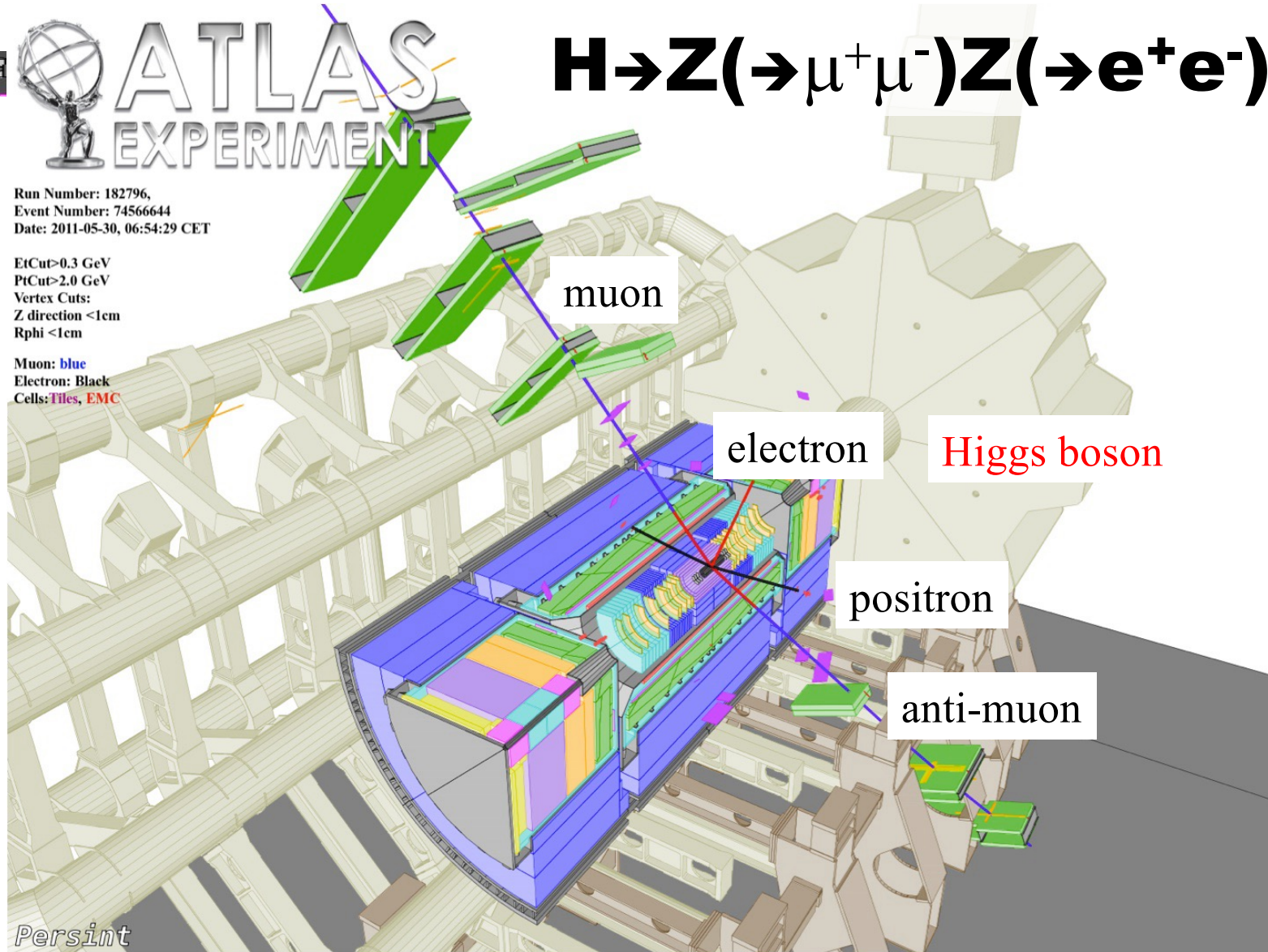
$$H \rightarrow Z (\rightarrow \mu^+ \mu^-) Z (\rightarrow e^+ e^-)$$



Run Number: 182796,  
Event Number: 74566644  
Date: 2011-05-30, 06:54:29 CET

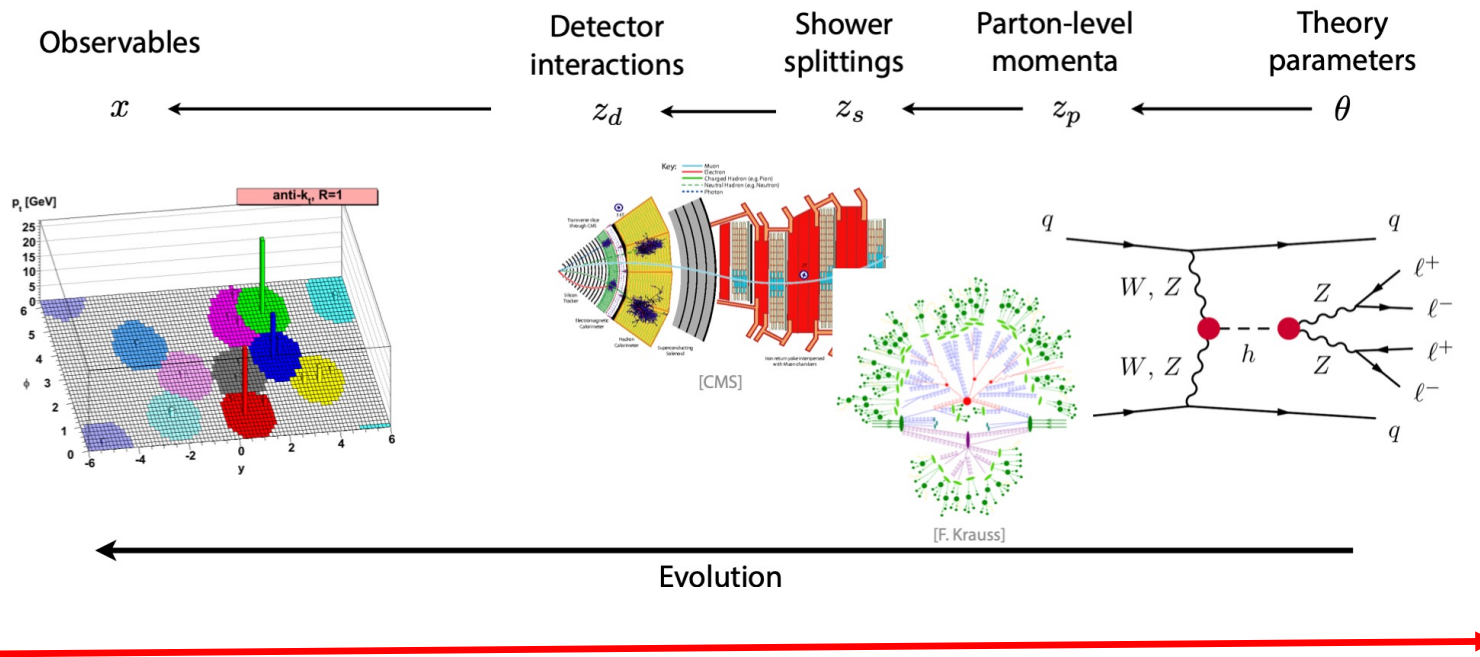
EtCut > 0.3 GeV  
PtCut > 2.0 GeV  
Vertex Cuts:  
Z direction < 1cm  
Rphi < 1cm

Muon: blue  
Electron: Black  
Cells: Tiles, EMC



Persint

# Modeling and Inference

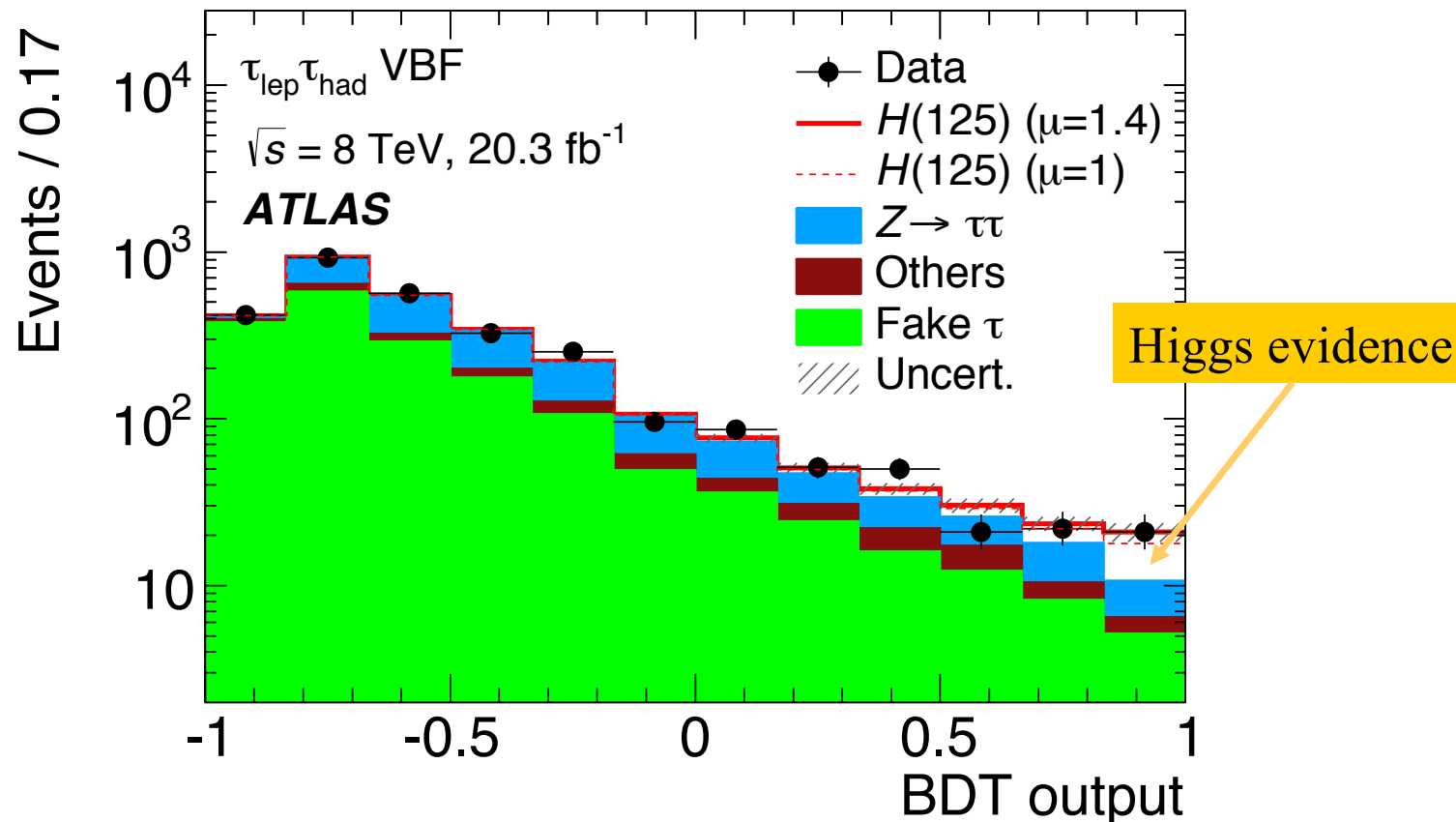


Inference

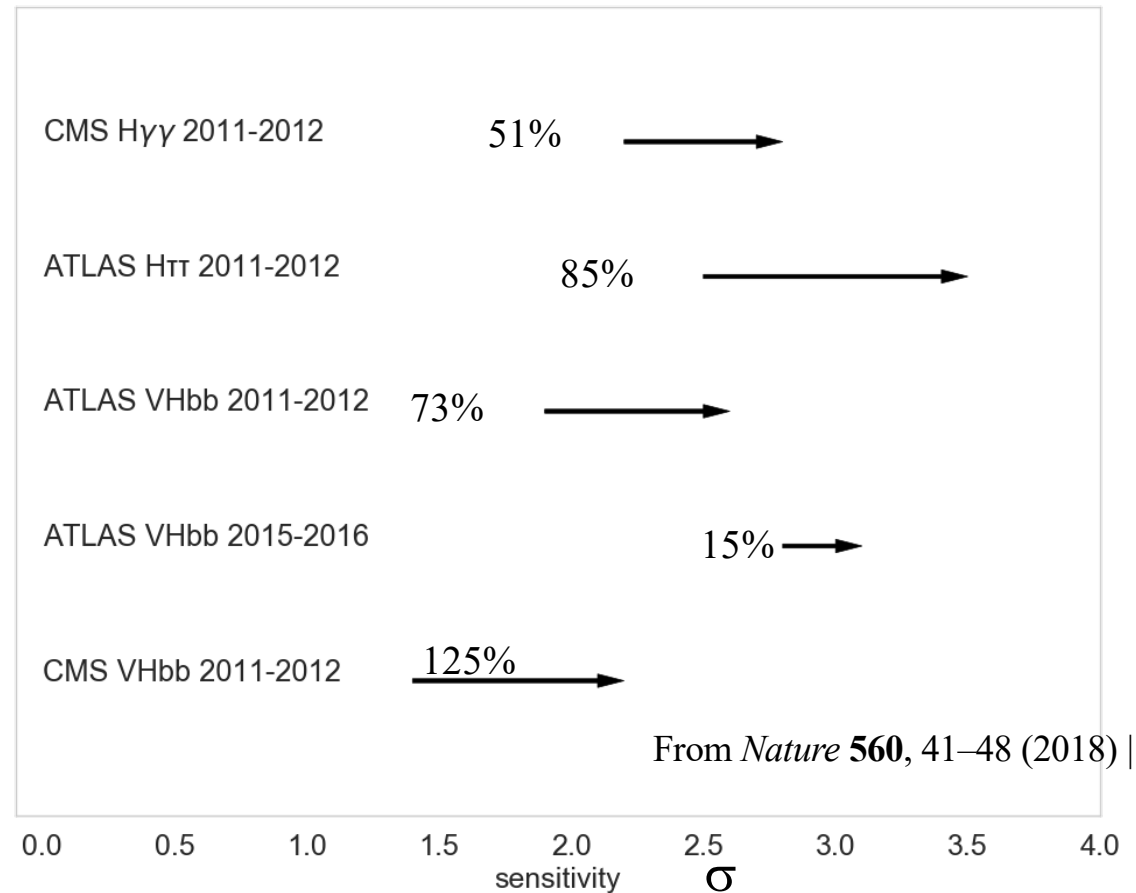
# Higgs Boson at LHC with a classifier

JHEP 04, 117 (2015) 1501.04943

Boosted Decision Tree on a dozen features



# Impact of ML on Higgs Physics

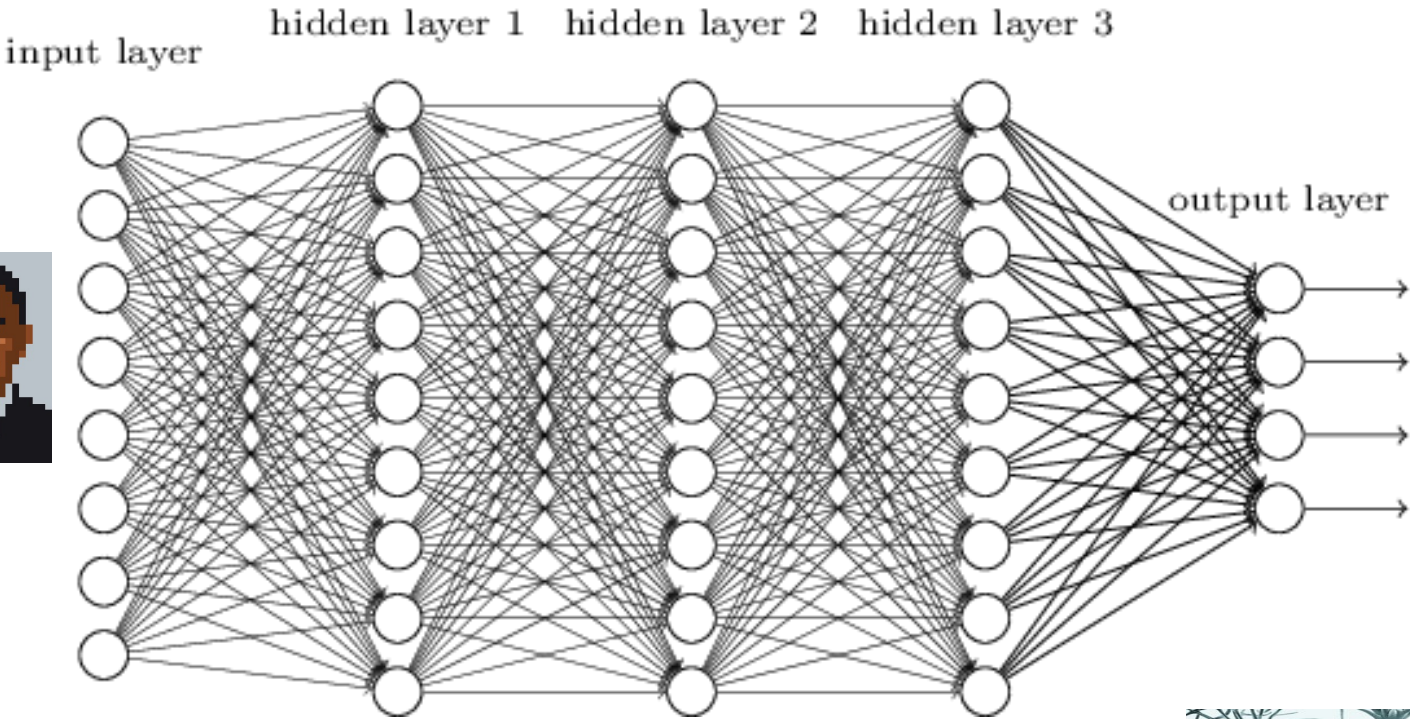


→ ~ 50% gain on LHC data!

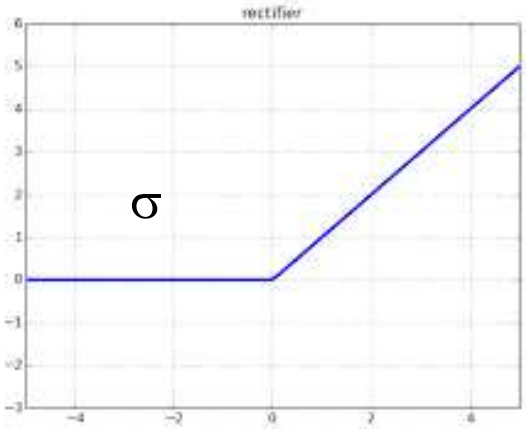
# Neural Network sur des images



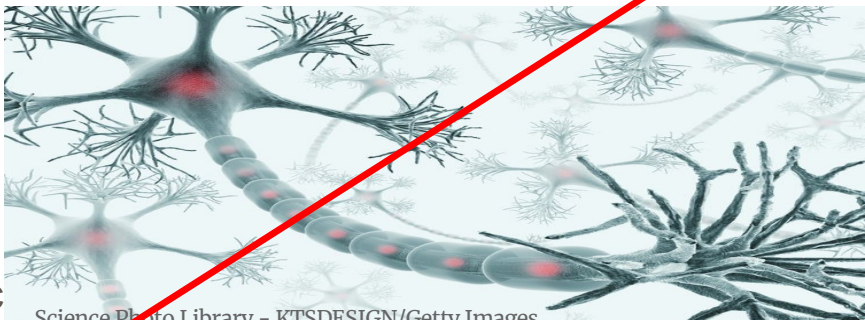
# Neural Network



activation function (non linear!)



$$\text{Node}_j = \sigma(b_j + \sum w_{ij}x_i)$$

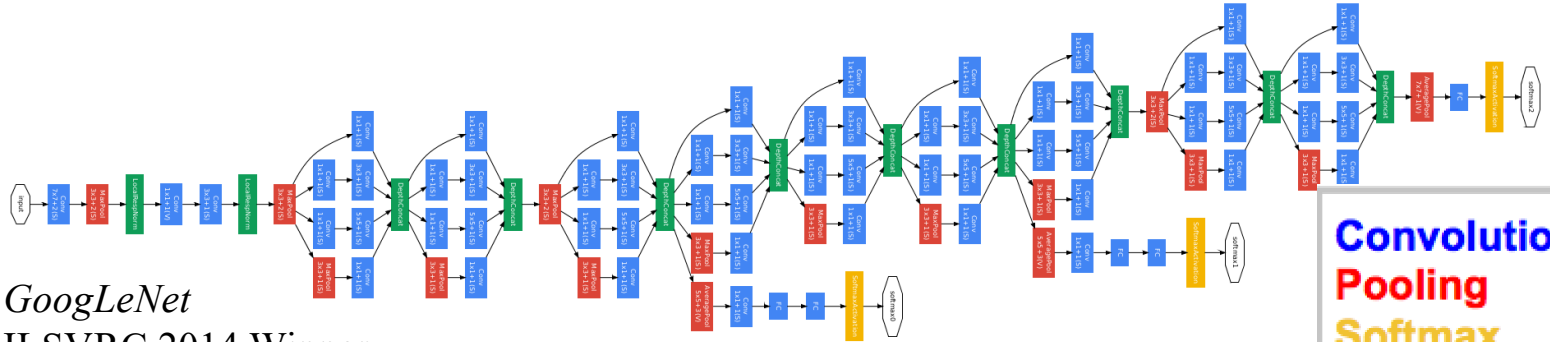
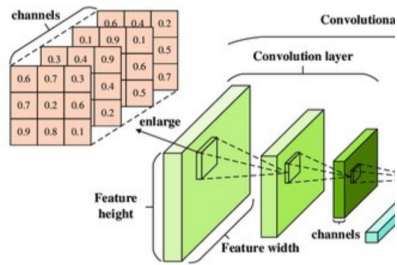
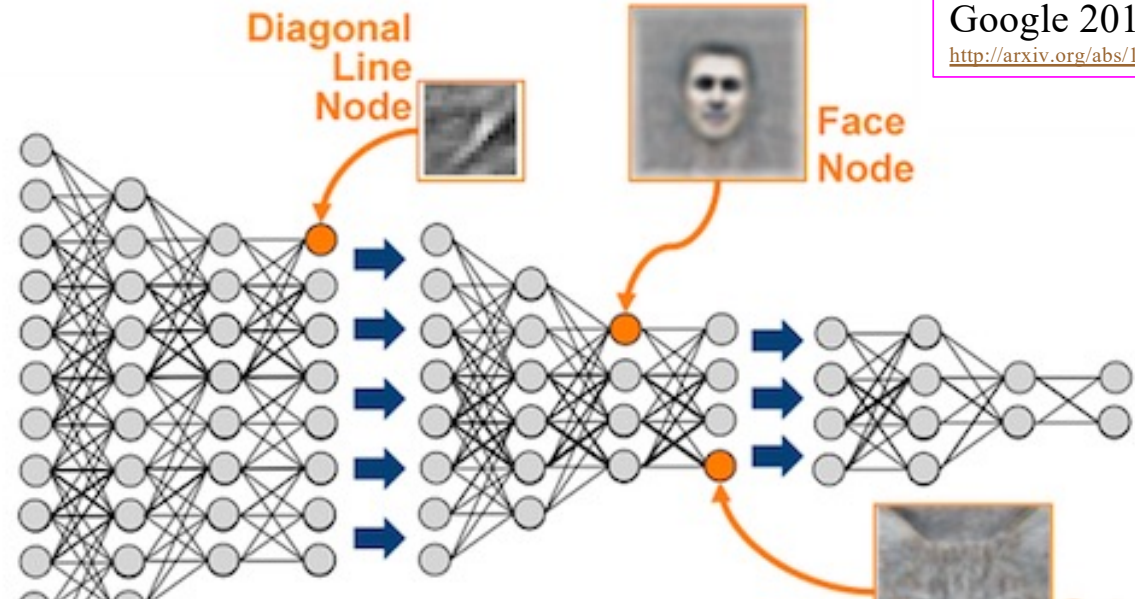




# Convolutional Neural Network



Google 2012  
<http://arxiv.org/abs/1112.6209>

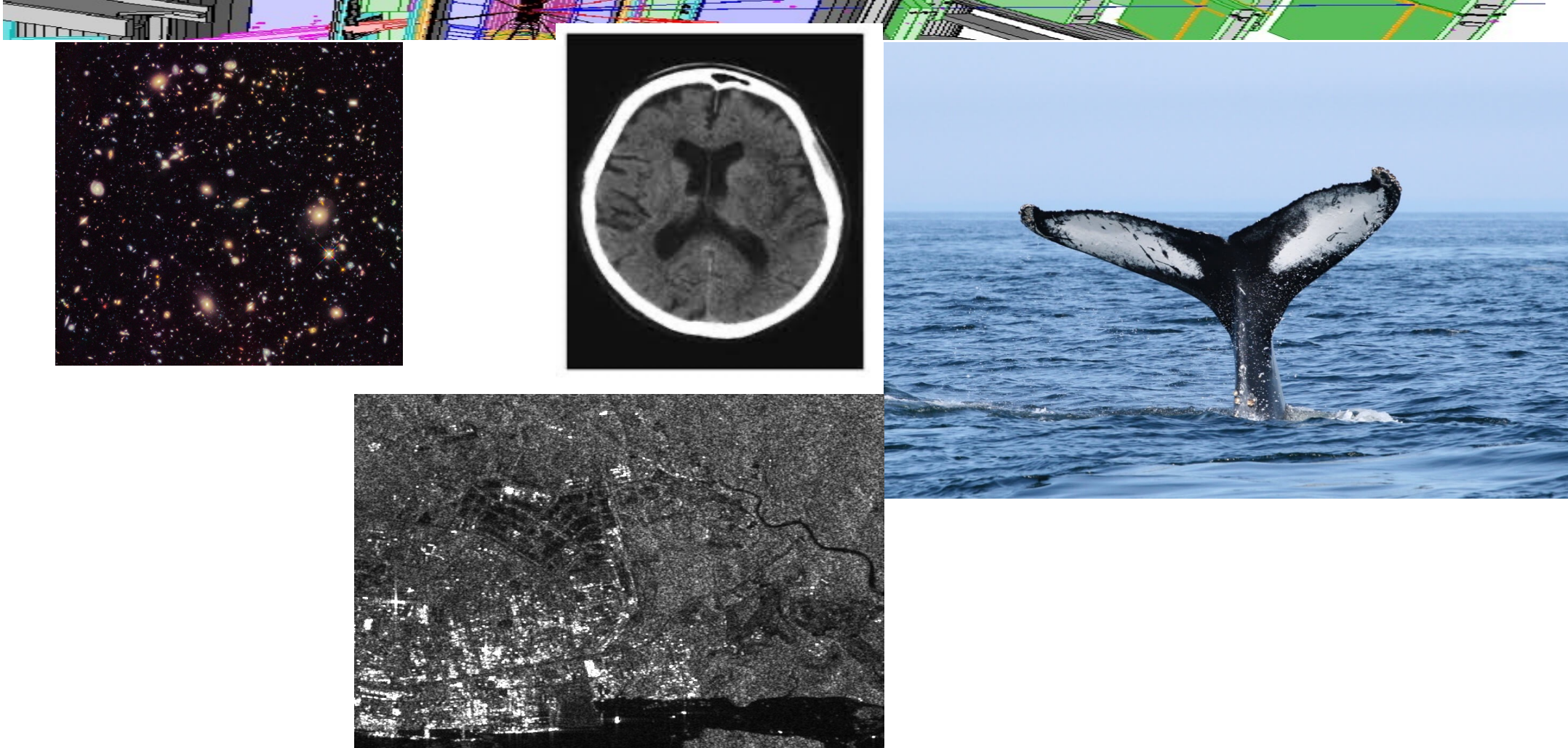


GoogLeNet  
 ILSVRC 2014 Winner  
 4M parameters

HEP ML, David Rousseau, Jan 2024, CHACAL Course 1

Convolution  
 Pooling  
 Softmax  
 Other

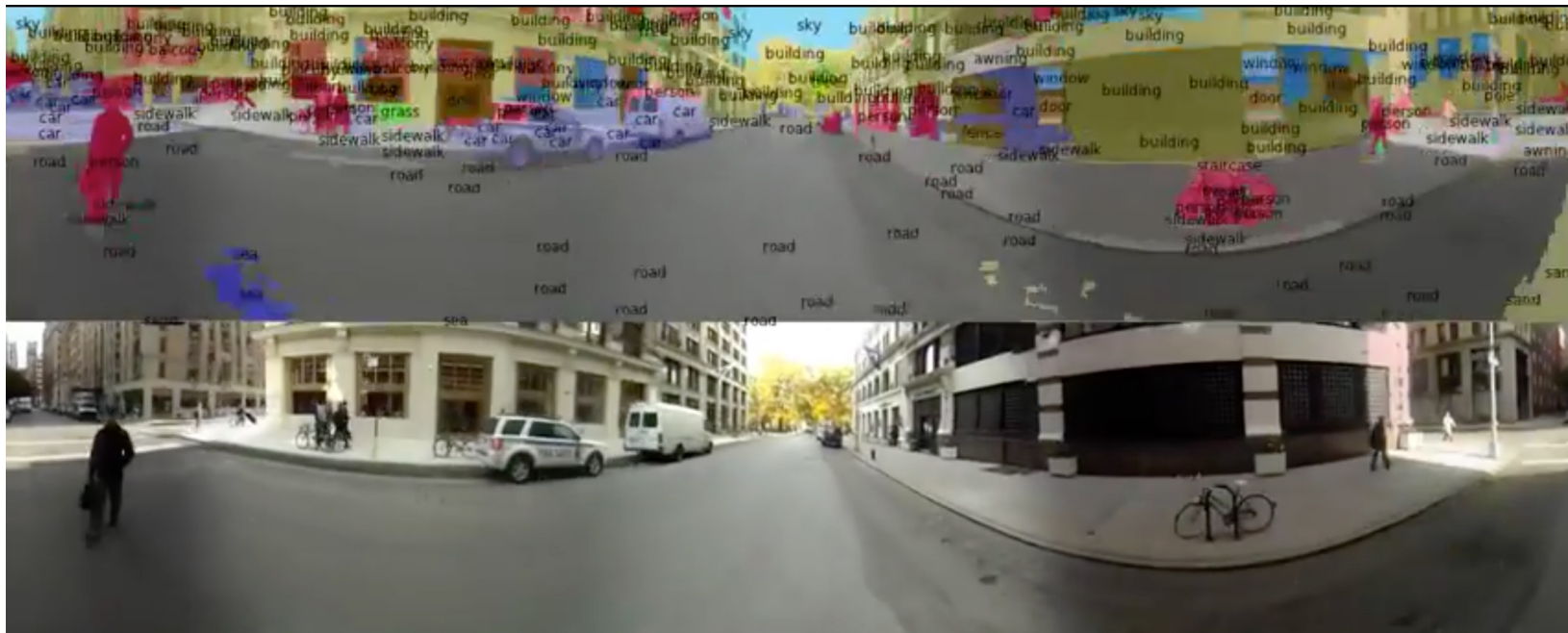
# Many Applications



**Scientific data are often not images**

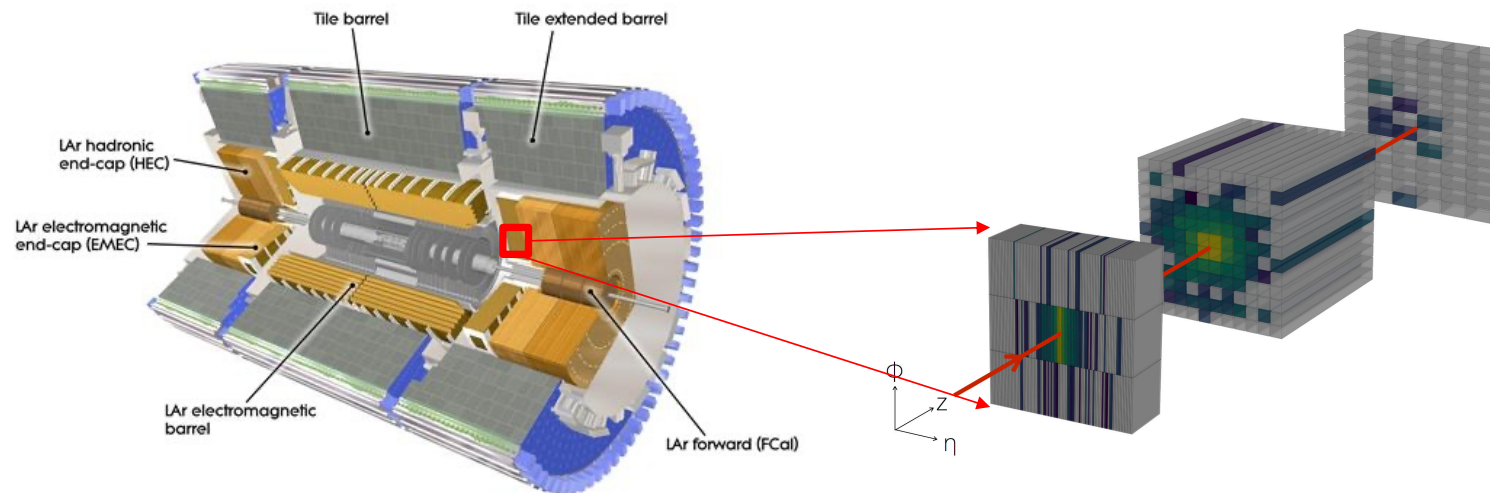


# Typical Deep Learning application



(supervised) learning needs labeled data → accurate simulator are very useful!

# Scientific instruments are complex 3D objects



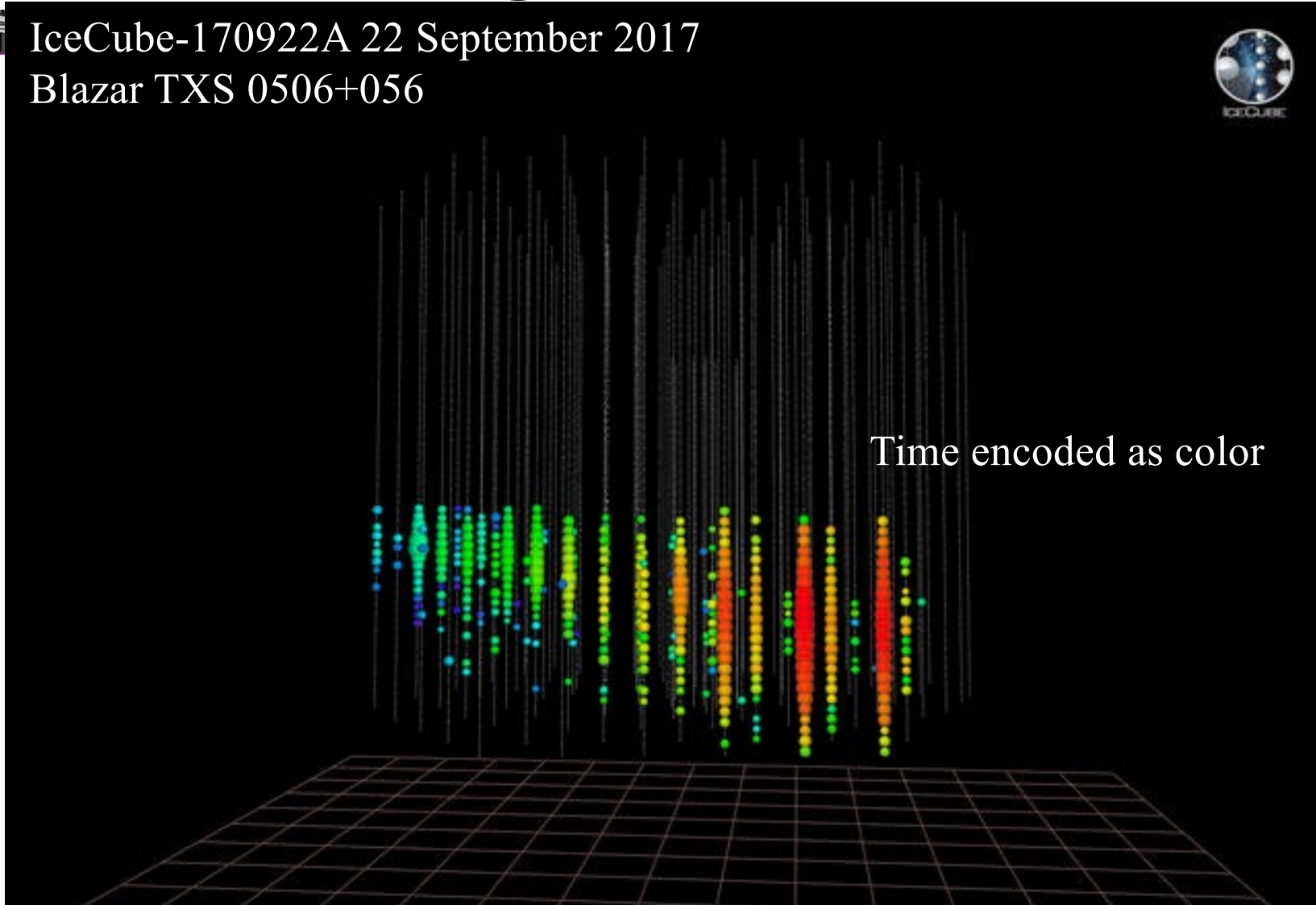
# An image, not the data

IceCube-170922A 22 September 2017

Blazar TXS 0506+056

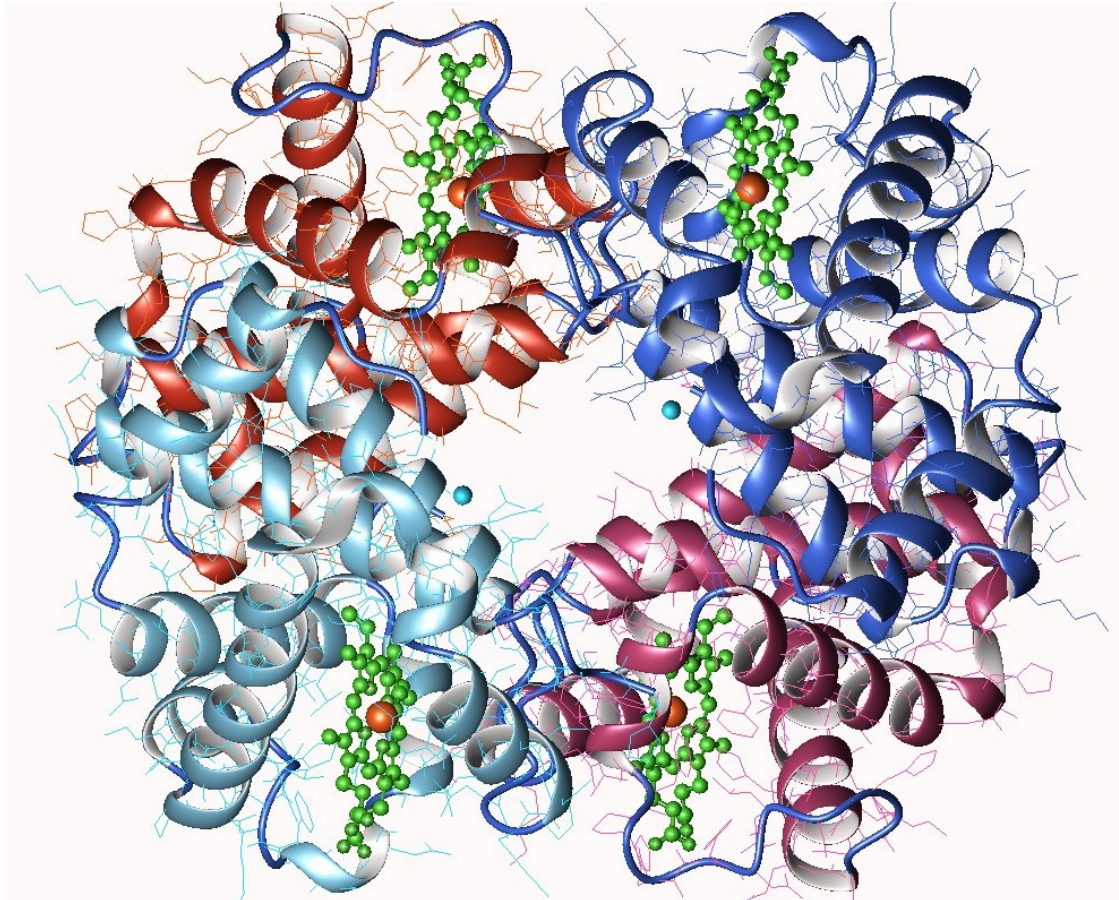


Time encoded as color



# An image, not the data

hemoglobin  
structure



Par Deposition authors: Fermi, G., Perutz, M.F.;  
visualization author: User: Astrojan —  
<https://www.rcsb.org/structure/3hhb>,  
CC BY-SA 4.0,  
<https://commons.wikimedia.org/w/index.php?curid=48714519>

# Specialised architecture



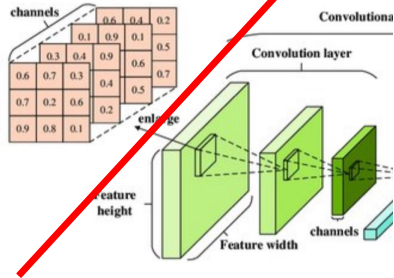


# Graph Neural Network

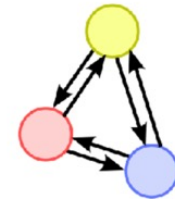
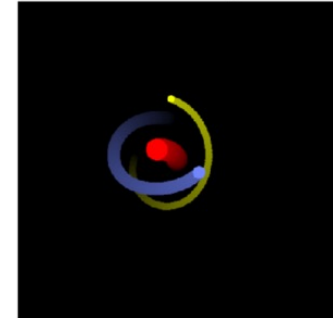


## □ Structure définie

- $v_i$  : noeud
- $e_k$  : arête
- $u$  : global



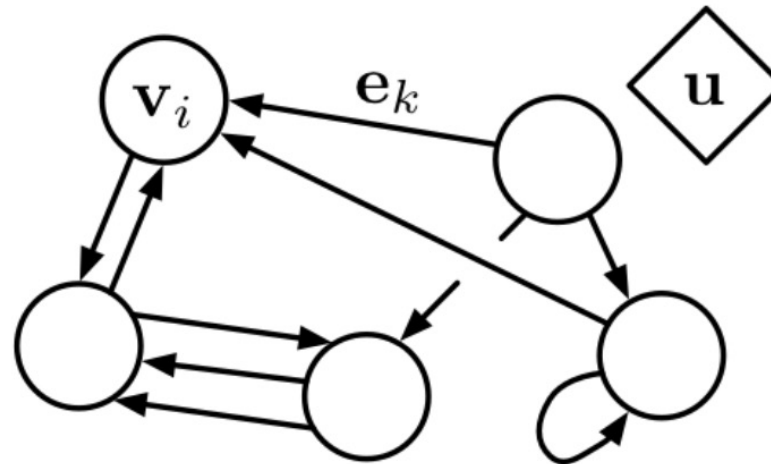
n-body



Nodes: bodies

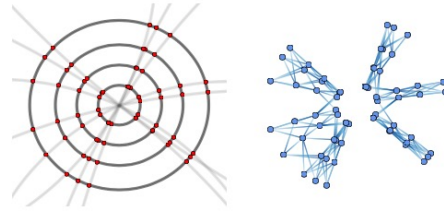
Edges: gravitational forces

Global : potential energy

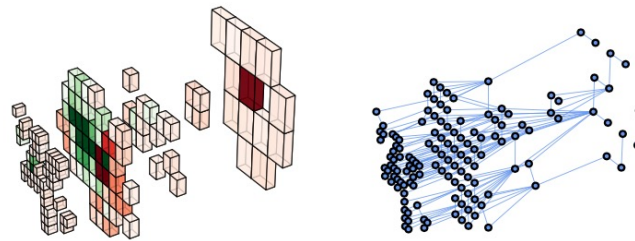


# Graph on HEP data

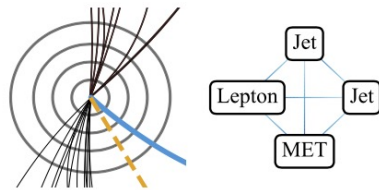
from 2007.13681



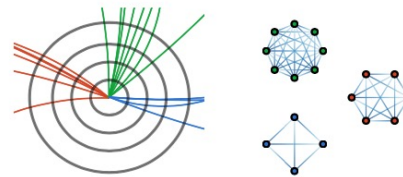
(a)



(b)



(c)

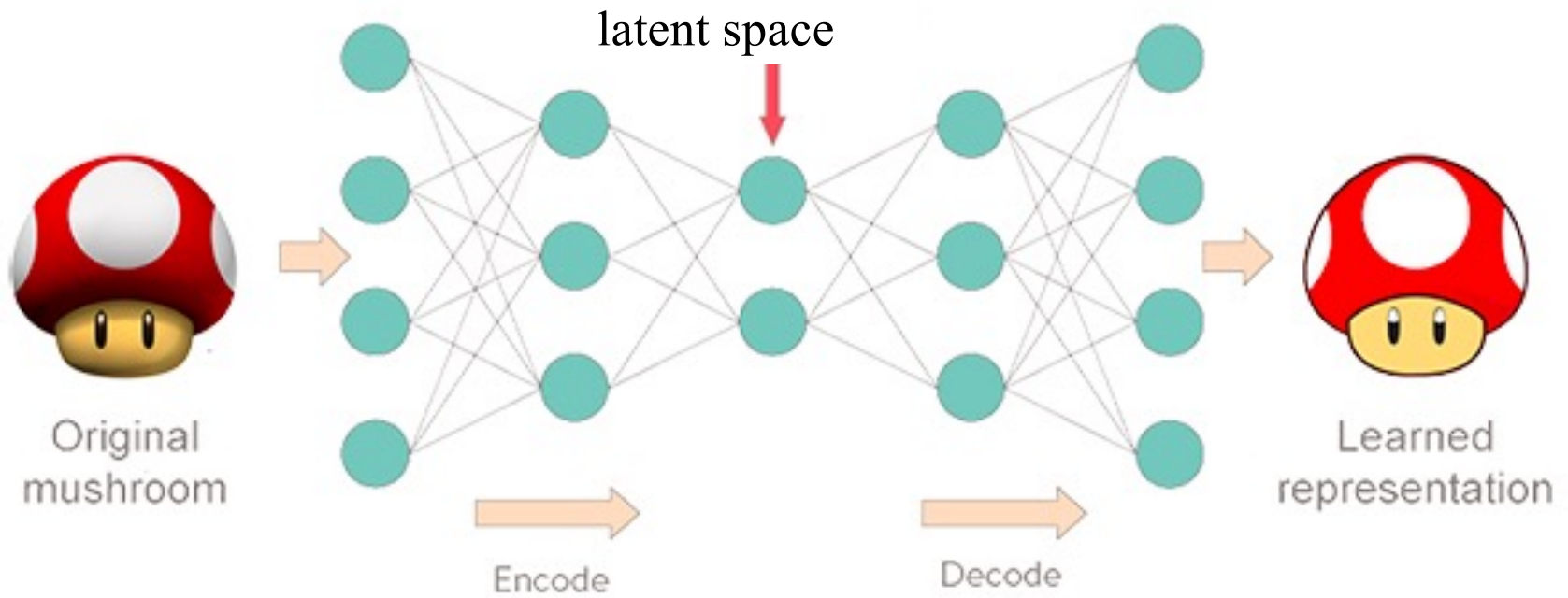


(d)

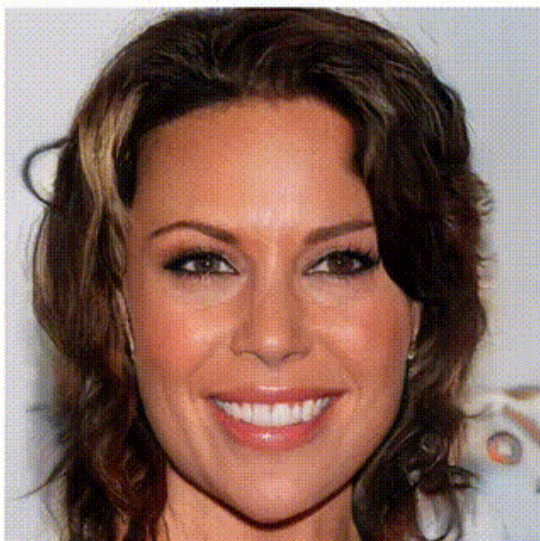
# Latent Variables



# Auto encoders



INSTRUCTION: press +/- to adjust feature, toggle feature name to lock the feature

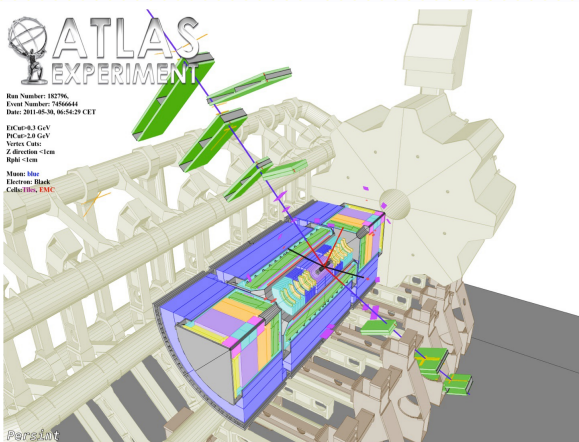


random face		
Male	Age	Skin_Tone
- +	- +	- +
Bangs	Hairline	Bald
- +	- +	- +
Big_Nose	Pointy_Nose	Makeup
- +	- +	- +
Smiling	Mouth_Open	Wavy_Hair
- +	- +	- +
Beard	Goatee	Sideburns
- +	- +	- +
Blond_Hair	Black_Hair	Gray_Hair
- +	- +	- +
Eyeglasses	Earrings	Necktie
- +	- +	- +

□ latent variables == (few) abstract variables summarising differences between images

□ Applications:

- Classification/evaluation
- Fast Generation
- Explicability → relation between latent variable latente and scientific concept
- Inverse problem
- Anomaly detection



# Surrogate models



When AI does not better, but as well and much faster

# Universality theorem

- Mathematical Theorem 1991

[https://en.wikipedia.org/wiki/Universal\\_approximation\\_theorem](https://en.wikipedia.org/wiki/Universal_approximation_theorem)

- Any continuous function  $R^n \rightarrow R^p$

- ... can be approximate sufficiently well

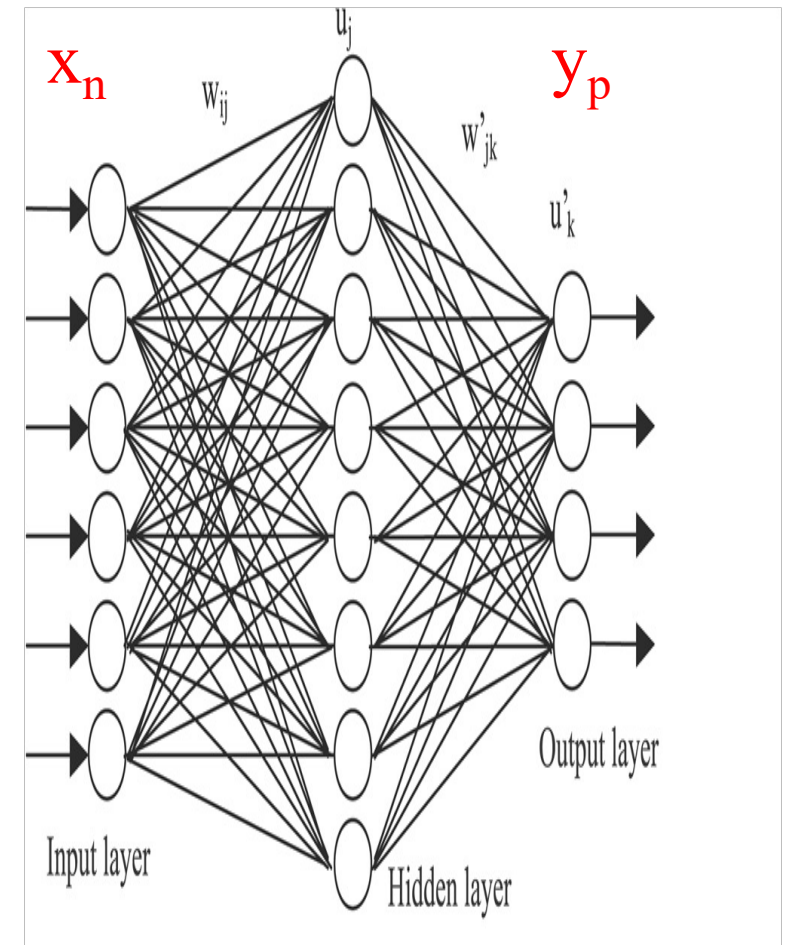
- ... with a NN with one hidden layer and enough node

- (does not say how to build this NN)

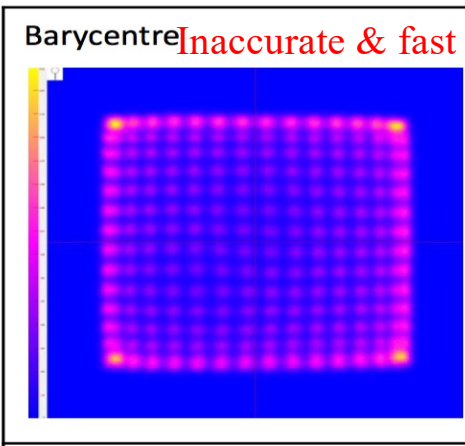
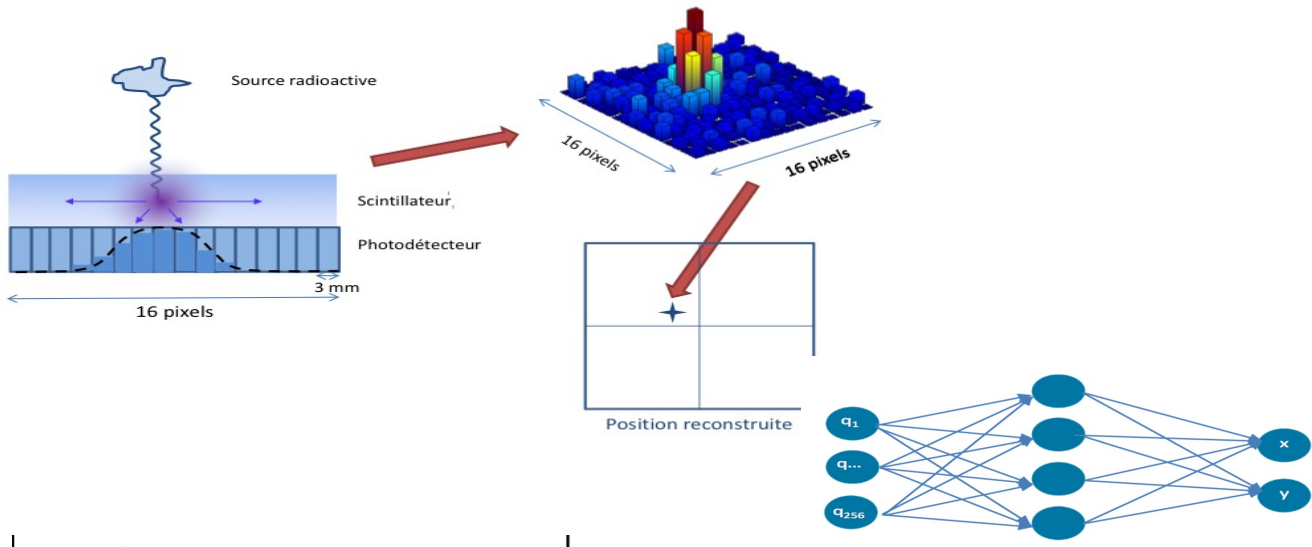
- → one can train a NN to emulate an existing simulator

- → speed gain x10... x100000

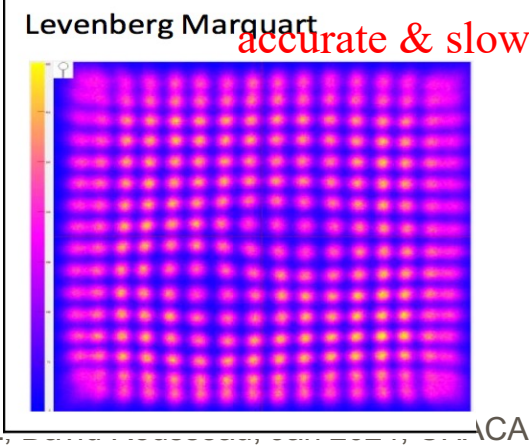
- (however precision...extrapolation...)



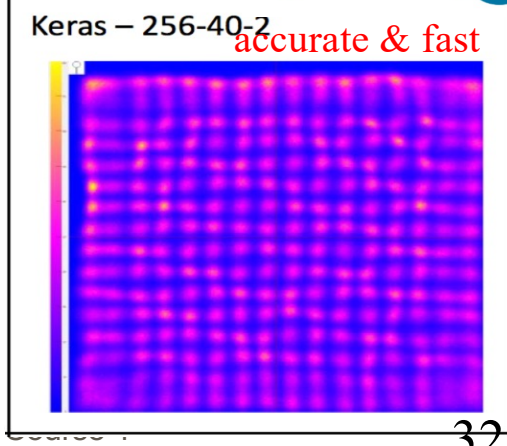
# Exemple : $\beta, \gamma$ camera for surgical



EP ML



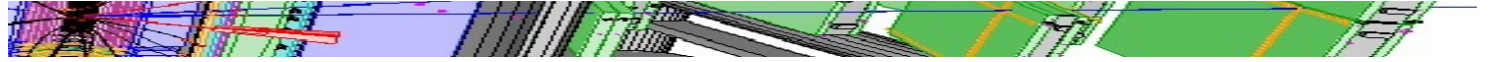
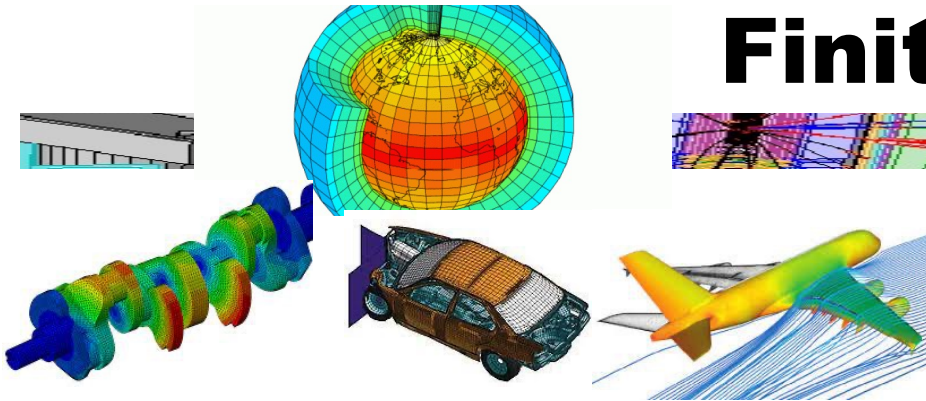
CAL



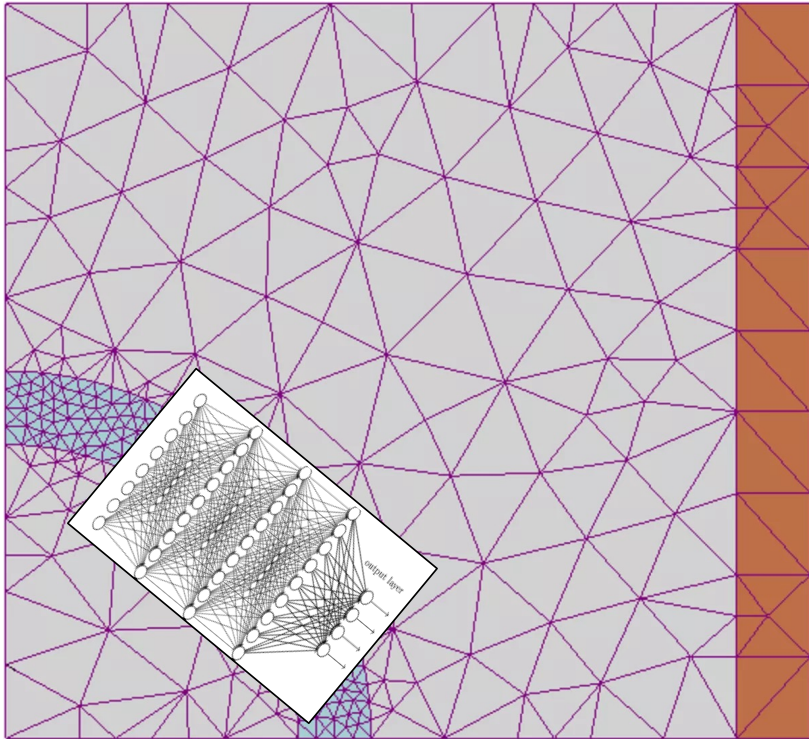
32



# Finite Elements

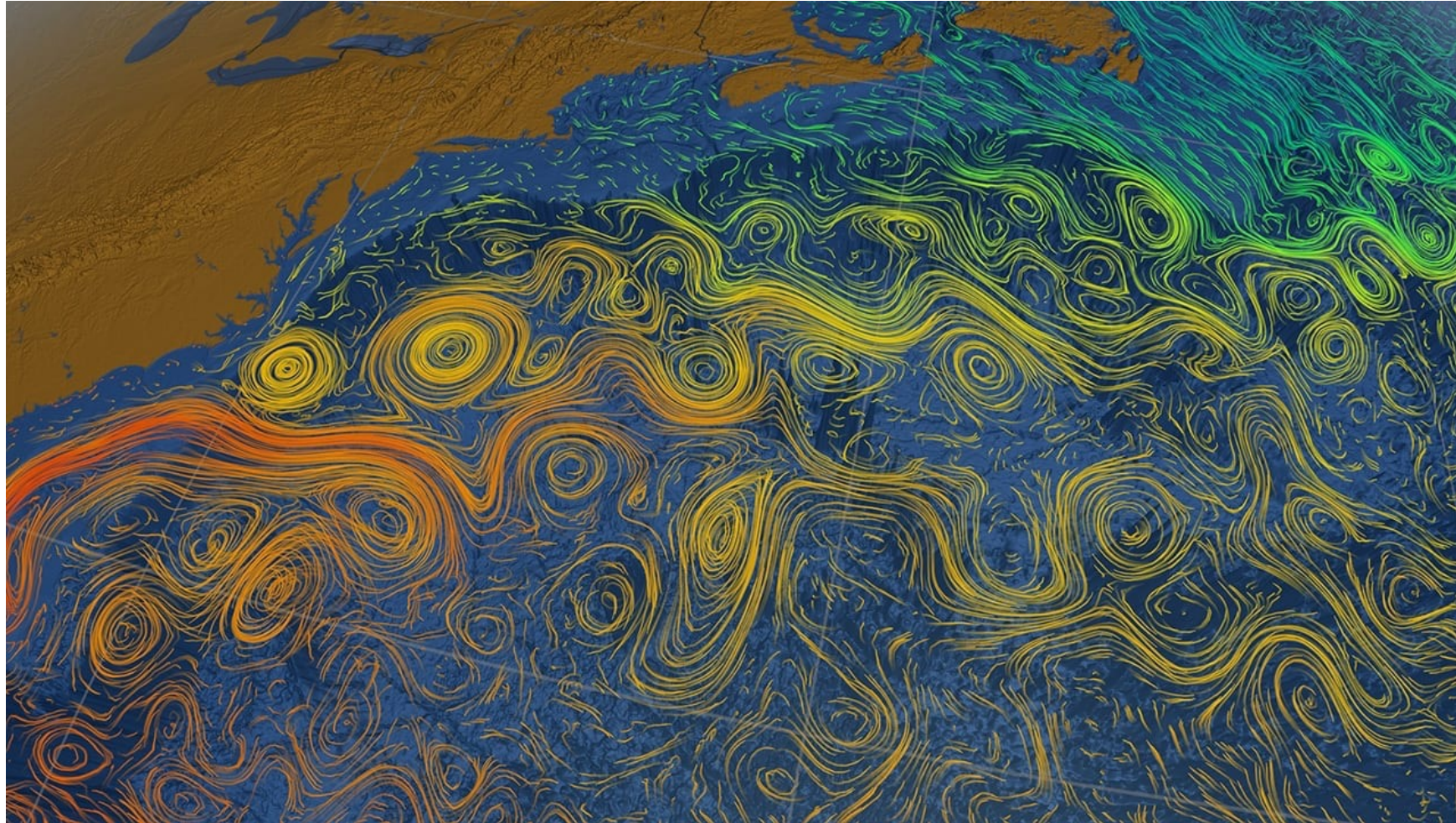


- ❑ Fundamental techniques
- ❑ Limited by mesh size
- ❑  $\text{maillage} / 2 \rightarrow \text{resources} \times 8$  (memory, speed)
- ❑ Instead of reducing mesh size, train an NN to emulate the behavior of a set of small meshes



# Application oceanography

NASA



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# Modeling the unknown



If a phenomenon cannot be modelled, emulate it with an NN

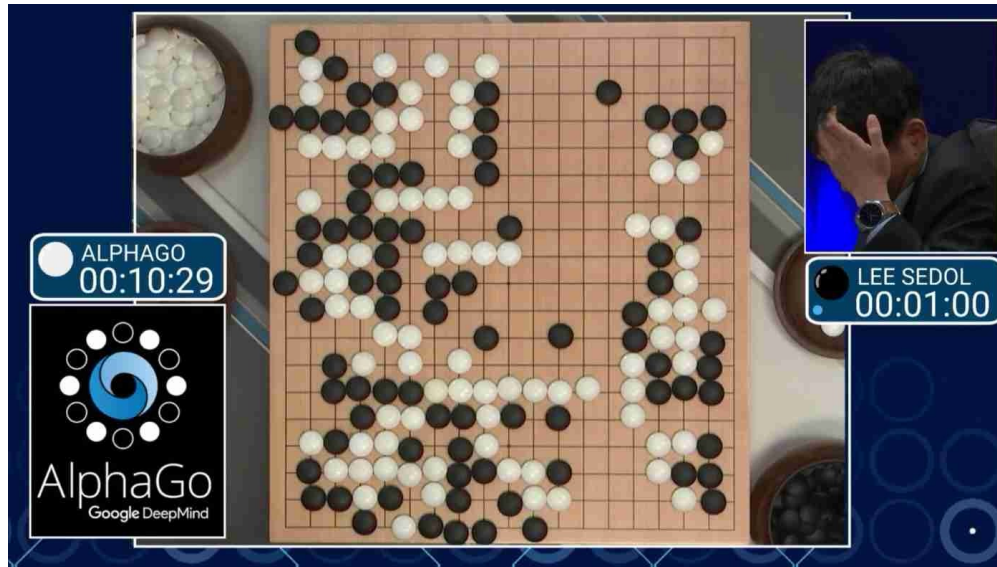
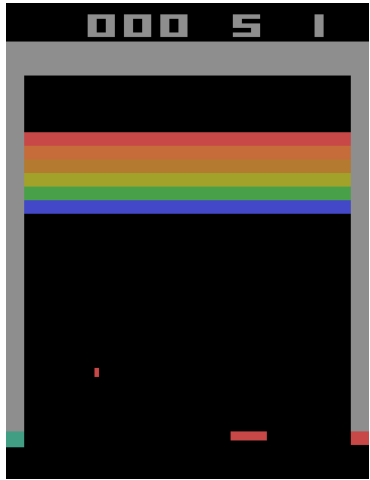
Ex: study of rogue wave  
Hokusai

# Reinforcement Learning (RL)

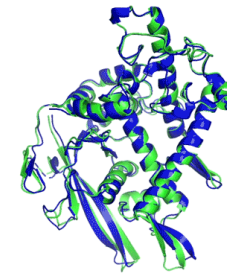


“It's not the destination, it's the journey”  
Ralph Waldo Emerson

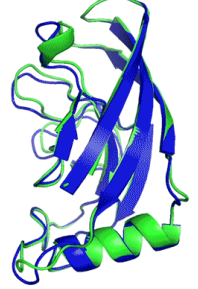
# RL works better if



## Alpha-Fold

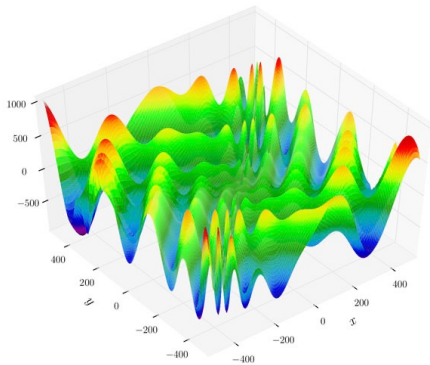


T1037 / 6vr4  
90.7 GDT  
(RNA polymerase domain)



T1049 / 6y4f  
93.3 GDT  
(adhesin tip)

● Experimental result  
● Computational prediction



- ❑ Classical methods fail
- ❑ Finite universe, but large combinatorial
- ❑ Clear objective, but unclear path
- ❑ Fast evaluation of trial